NUMERICAL SIMULATION OF SLAG FOAMING WITH REACTION KINETICS IN OXYGEN STEELMAKING

A Thesis Submitted for the Degree of Doctor of Philosophy

By

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Declaration

I, Anuththara Kirindigoda Hewage, declare that the work in this thesis presented for the degree of Doctor of Philosophy is entirely my work. The work is original and to the best of my knowledge, does not contain any material that has been accepted for any other academic award, or previously published or written by another person, except where due reference is made in the thesis. Further, I warrant that I have obtained, where necessary, permission from the copyright owners to use any third party copyright material reproduced in the thesis, or to use any of own published work in which the copyright is held by another party. This work was carried out during the period from March 2013 to September 2016 under the supervision of A/Prof. Jamal Naser and Prof. Geoffrey Brooks.

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Anuththara Kirindigoda Hewage

Certification

This is to certify that the above statement made by the candidate is correct to the best of our knowledge.

Associate Professor Jamal Naser

Professor Geoffrey Brooks
Research abstract

Foaming is an important phenomenon that is commonly encountered when gas is blown through a viscous liquid. Foams are a common occurrence in oxygen steelmaking which is produced by trapping the gases in the slag layer. With the progression of the blow, the quantity of slag as well as the gases generated increase, and consequently, the slag foaming also increases. Hence, slag foaming has to be properly controlled for a continuous and efficient production process. Thus, a thorough understanding of foams and the foaming process is necessary to optimize the process by minimizing the slag foaming. Traditionally, the uninterrupted operation of the steelmaking process is the sole responsibility of the operator, which is recently surpassed by models developed via experimental studies and theoretical/computational analysis.

There are several models available in the literature focusing on different aspects of the steelmaking process including refining kinetics and slag foaming using different approaches. Among those models, the CFD model developed by Sattar to predict foaming and decarburization in oxygen steelmaking was selected as the predecessor work of the present study.

This CFD model developed by Sattar was able to predict foam height, the population of the ten bubble classes, decarburization, and heat generation in the oxygen steelmaking process. Despite the better performance of this model, several inaccuracies were identified such as lack of consideration of refining kinetics and incomplete criteria for formation, drainage, and collapse of foam, which established the background for the present study. The primary goal of the present study was to improve and extend the model developed by Sattar with a semi-empirical kinetics model to calculate and predict the refining behavior of steel and more enhanced criteria for formation, drainage, and collapse of foam. In the present study, the CFD model was improved and extended in three main stages.

In the first stage, a semi-empirical kinetics model was developed and incorporated into the CFD foaming model to predict the refining behavior of main impurity elements (i.e. C, Si, Mn, and P). The kinetics model was based on first order diffusion kinetics, and the
performance of this model was analyzed using the data reported in the IMPHOS study\cite{2} before incorporating into the CFD model. The kinetics model was then incorporated into the main CFD model, and the model predictions on the removal behavior of C, Si, Mn, and P were compared with the observed data reported in IMPHOS\cite{2}. The removal behavior of all the four elements was captured reasonably well by the kinetic model incorporated in the CFD foaming model.

In the second stage, the CFD model was further enhanced by improving the criteria for formation and collapse of foam and incorporating continuous foam drainage. At this stage of the CFD model, it consisted of three phases: liquid phase (slag and metal components), gas phase (gas bubbles, O\textsubscript{2} and CO) and foam phase (foam bubbles and gas and liquid in foam). The foam phase was produced from liquid and gas phases using the same formation criteria developed by Sattar\cite{1}. The predicted foam height at this stage of the model was representative of the average foam height measured in the IMPHOS study\cite{2}.

In the third stage, the three phases CFD model was further enhanced to a four phases model by introducing slag as a separate phase. The aim of this stage of the CFD model was to produce foam from slag, upgrading the foaming model to replicate slag foaming in oxygen steelmaking. The four phases included in the CFD model were the gas phase (gas bubbles, O\textsubscript{2} and CO), the liquid phase (hot metal components), the slag phase (oxides and fluxes) and the slag foam phase (foam bubbles, liquid, slag and gas in foam). Once the slag phase was formed, it produced the foam phase in combination with the gas phase, and the same foaming model used in the three phases model was employed in this stage replacing the liquid phase with the slag phase. The slag foam height predictions of the four phases CFD model were in good agreement with the observed foam height data measured in the IMPHOS study\cite{2}.

The scope of the present study was limited to improving the CFD model developed by Sattar\cite{1} in terms of its predictions on the removal behavior of C, Si, Mn and P and the evolution of slag foam height by incorporating sub-models for removal kinetics and foam drainage, and improving the existing sub-models for formation and collapse of foam. Introducing the slag as a separate phase and producing foam from slag and gas was
carried out as part of improving the model predictions on foam height evolution. The other sub-models such as bubble break-up and coalescence which were in the initial CFD model were not modified in the present study.

Even though the predictions of the present CFD model were in reasonably good agreement with the observations reported in IMPHOS pilot plant trials\cite{2}, further improvements to the present CFD model are possible. Suggestions for such improvements include incorporating a more rigorous kinetics model instead of the semi-empirical kinetics model, use of more sophisticated criteria for creating the slag phase and calculating the evolution of physical properties of slag and slag foam via more rigorous relationships.

In conclusion, the results obtained from the CFD model are a strong step towards developing a general CFD model for oxygen steelmaking process, and therefore, the present study represents a significant contribution to knowledge in that regards. A general CFD model of oxygen steelmaking process as such will be able to predict every aspect of the process facilitating the operators to pre-define the optimal process conditions and optimum required raw material quantities and energy requirements.
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A life episode in a foreign country entirely dedicated to obtaining the doctoral qualification is always a significant, challenging and interesting experience in one’s career. At this point of submission of my thesis, I would like to recall the empowering and comforting help I received from all parties those took part in my personal life and my academic life. So I extend my sincere gratitude to all of them on behalf of their encouragement and support for completing my doctoral degree with success.

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<th>Description</th>
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<tbody>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>IMPHOS</td>
<td>IMproving PHOSphorus refining</td>
</tr>
<tr>
<td>BOS</td>
<td>Basic Oxygen Steelmaking</td>
</tr>
<tr>
<td>EAF</td>
<td>Electric Arc Furnace</td>
</tr>
<tr>
<td>BOF</td>
<td>Basic Oxygen Furnace</td>
</tr>
<tr>
<td>BOP</td>
<td>Basic Oxygen Process</td>
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<tr>
<td>Q-BOP</td>
<td>Quick-quiet BOP</td>
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<tr>
<td>DRI</td>
<td>Direct Reduced Iron</td>
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<tr>
<td>AC</td>
<td>Alternating Current</td>
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<tr>
<td>DC</td>
<td>Direct Current</td>
</tr>
<tr>
<td>LD</td>
<td>Linz Donawitz</td>
</tr>
<tr>
<td>OBM</td>
<td>Oxygen Bodenblasen Maxhuette (oxygen bottom-blowing furnace)</td>
</tr>
<tr>
<td>emf</td>
<td>Electromotive force</td>
</tr>
<tr>
<td>MO</td>
<td>Metal Oxide</td>
</tr>
<tr>
<td>Σ</td>
<td>Foaming index</td>
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<tr>
<td>PBM</td>
<td>Population Balance Modelling</td>
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<tr>
<td>FD</td>
<td>Finite Difference</td>
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<tr>
<td>FE</td>
<td>Finite Element</td>
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<tr>
<td>FV</td>
<td>Finite Volume</td>
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<tr>
<td>VOF</td>
<td>Volume of Fluid</td>
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<tr>
<td>RCS</td>
<td>Recycled Converter Slag</td>
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<tr>
<td>PCR</td>
<td>Post-Combustion Ratio</td>
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Chapter 1
Chapter 1: Introduction

1.1 Steel and steelmaking

Steel is one of the most commonly consumed raw materials globally, which is used in almost every major industry including energy, construction, automotive and transportation, infrastructure, packaging, and machinery. The increasing trend towards the use of steel as a raw material despite other lightweight metals with more promising properties such as aluminum and magnesium is mainly due to the lower costs involved in producing steel compared to the production of those other metals.\[3\] The advantages of steel also include high strength, design flexibility and fire resistance, and more importantly, there is the possibility to optimize these properties of steel by varying its composition and microstructure.\[4\] Furthermore, steel is a sustainable raw material which is entirely recyclable and reusable, and consequently, contributes to saving natural resources and energy. The steel industry is currently the second biggest industry in the world and has a growth rate of 2.5% per annum in the years 2010-2015\[5\] as illustrated in Figure 1.1.

![Figure 1.1: World crude steel production (1950 – 2015)](image)

*Source: World Steel Association (worldsteel)
Steel has been used by humans since about 3000 BC\cite{4}. At this time, the product obtained from smelting iron ore was known as wrought iron. The wrought iron was produced in a bloomery where the air was forced into a furnace containing a mixture of iron ore and charcoal, and the mixture was burnt using bellows\cite{4} or by natural means of air flow as shown in Figure 1.2.

However, iron required for producing steel is primarily obtained by smelting iron ore in a blast furnace. This iron is then refined to steel by removing the impurity elements such as Si, C, Mn, P and Al to the required level and adding alloying elements such as Cr, Mo, Nb and V to obtain the required properties in the end steel product. The method used for refining iron to produce steel has evolved through centuries starting from the bloomery to BOS and EAF in the present.

![Furnace diagram](image)

Figure 1.2: Furnace used in smelting trials reconstructed from archaeological data in southern Sri Lanka\cite{6}

Mass production of steel commenced with the acid Bessemer process, which was introduced in 1855 by Sir Henry Bessemer.\cite{7} This process needed high-quality pig iron, and the converter was lined with acidic refractories. In the next two decades, the basic Bessemer process and the open hearth process were introduced for steelmaking. However, the use of processes mentioned above declined with the invention of oxygen steelmaking. Oxygen steelmaking is the current dominant steel production method producing about 75\% of global crude steel production as reported by the World Steel Association.\cite{5} EAF is the second largest steelmaking process which accounts for about 25\% of world steel production.\cite{5}
1.2 Research Background

- **Oxygen steelmaking process**
  Oxygen steelmaking process can be categorized into several subcategories based on the furnace arrangement (i.e. BOF, Q-BOP), and in the present study, the top-blown oxygen steelmaking was used for the analysis and modeling. A high purity oxygen stream is injected onto the molten metal bath contained in the converter during the top-blown oxygen steelmaking, and the refining of hot metal is achieved by selective oxidizing and removing of the impurity elements from pig iron. The top-blown process for steelmaking is autogenous and possesses the advantages such as higher oxidizing rates, use of more scrap or DRI charge, intense mixing in the bath and high-quality output steel compared to the output from pneumatic steelmaking processes.

- **Slag foaming and slopping**
  Slag is the non-metallic material produced from the products of oxidizing reactions and dissolving fluxes during the steelmaking process. Slag is generally high in viscosity and low in density, causing slag to float on the bulk metal bath. As a result of its physical properties, slag has the capability to trap the gas bubbles produced by the chemical reactions and injected oxygen, and produce slag foam. Slag foam is beneficial for the steelmaking process in terms of the large surface area formed and the protection provided against the direct contact of the melt with the atmosphere. Usually, the physical properties of slag evolve in favor of foaming during the blow, and when coincided with high gas production rates from chemical reactions, slag foaming can become uncontrollable and overflow the converter creating a slopping event. Slopping is a detrimental event, and its consequences include yield loss, health and safety costs, damage to equipment and environmental pollution.

- **Minimizing slag foaming**
  Accordingly, it is essential to minimize slag foaming for proper and uninterrupted operation of the steelmaking process. The traditional method for minimizing the occurrence of slopping is by visual observation of the converter. Once the indications of slopping appear, the corrective actions are exercised to prevent the slopping. However, by the time of visual appearance of slopping, its consequences have already been
suffered by the plant.\textsuperscript{[10]} Therefore, modeling and predicting slag foaming through a thorough understanding of slag foaming has been the research interest of steelmaking researchers for last several decades. Even though the laboratory scale studies and pilot scale studies have contributed for gaining insights of steelmaking process, modeling has become the most reliable method of predicting slag foaming in the converter.\textsuperscript{[4]} Despite the different models and pilot scale studies available on slag foaming and refining kinetics in oxygen steelmaking, the need for a dynamic model to predict the steelmaking kinetics and slag foaming is emphasized in the literature.\textsuperscript{[11-13]} Therefore, the present study was aimed at developing a dynamic model using the CFD technique for predicting slag foaming and refining kinetics in oxygen steelmaking.

- **Experimental and numerical modeling efforts on slag foaming**

The experimental studies that were carried out to investigate and understand slag foaming in oxygen steelmaking include the studies by the researchers Cooper and Kitchener\textsuperscript{[14]}, Fruehan and co-workers,\textsuperscript{[15-18]} Ghag and co-workers,\textsuperscript{[19-21]} Stadler and co-workers,\textsuperscript{[22, 23]} Irons and co-workers\textsuperscript{[24-26]} and Seetharaman and co-workers\textsuperscript{[27, 28]}. The contribution of the experimental studies by Fruehan and the co-workers\textsuperscript{[15]} is considered significant as they introduced the foaming index for slag foaming, which represents the extent of foaming. These experiments revealed that the foaming index, (i.e. the average traveling time of gas through the slag layer), increases with increasing viscosity, and decreases with increasing surface tension, density, and bubble diameter. These findings were later extended and modified by the researchers Ghag et al\textsuperscript{[19]}, Lotun and Pilon\textsuperscript{[29]} and Stadler et al\textsuperscript{[22, 23]}. Conversely, Irons et al\textsuperscript{[24]} argued that at those higher superficial gas velocities encountered in the oxygen steelmaking converter, a foam with above description (i.e. highly dependent on the physical properties of slag) cannot exist. In the present study, the effect of both slag foaming and gas hold-up were considered.

Several numerical foam modeling efforts using CFD technique also can be found in the literature including the research works carried out by Bhole et al\textsuperscript{[30]}, Bannari et al\textsuperscript{[31]}, Chen et al\textsuperscript{[32]} and Sattar et al\textsuperscript{[33-36]}. These research works were mostly on bubble columns incorporating population balance modeling with different bubble break-up and coalescence closure terms. Among them, the work carried out by Sattar\textsuperscript{[31]} using CFD
technique was aimed at modeling slag foaming in steelmaking, and this work was used as the starting point in the present study.

- **Experimental and numerical modeling efforts on steelmaking kinetics**

Oxygen steelmaking is currently the dominant method for refining blast furnace produced pig iron into steel with required end composition, and this is achieved by injecting O\(_2\) to oxidize and remove the impurity elements.\(^7\) These impurity elements in pig iron such as C, Si, Mn, P and Al oxidize in the order of their affinity for oxygen with the injection of high purity oxygen stream. Therefore, apart from slag foaming, the kinetics of these refining reactions also have been the research focus of many steelmaking researchers, despite their well-established complex and transient nature. Consequently, various experimental and mathematical studies on understanding and modeling kinetics of steelmaking reactions can be found in the literature.\(^{37-45}\) However, a kinetics model is an essential tool for the steelmaker to optimize the process via obtaining information on required quantities of raw materials and energy as well as the pattern and the extent of the chemical reactions.\(^{38, 46, 47}\) Hence a kinetics sub model was incorporated in the present CFD model for predicting the removal pattern of main impurity elements (i.e. C, Si, Mn, and P).

Among the research works carried out on the kinetics of steelmaking reactions, some studies are focussed on modeling all the refining reactions using one approach,\(^{37, 48}\) while the others are focussed on selected reactions\(^{43, 49, 50}\). Even though most of these studies have employed more complicated mathematical relationships to explain and predict the kinetics of steelmaking reactions, a first order kinetics model was used in the present study as a starting point. First order kinetics relationship was also used by several other researchers previously to model steelmaking reaction kinetics including Ishikawa\(^{43}\), Monaghan et al\(^{51}\), Kawai et al\(^{52}\) and Dogan et al\(^{40}\).

- **Use of CFD technique for modeling**

The supersonic oxygen stream injected onto the hot metal bath during the oxygen steelmaking process causes the fluids in the converter to mix intensely. Consequently, the fluid flows in the converter are multi-dimensional, multiphase, turbulent and
reacting flows.\cite{4} Therefore, the technique employed for modeling these fluid flows needs to be capable of handling such complex fluid flow conditions.

CFD or Computational Fluid Dynamics is a powerful technique used for analyzing the systems involving fluid flow, heat transfer and associated phenomena including chemical reactions with the aid of computer-based simulations. CFD technique is frequently and efficiently used in a number of different applications including lift and drag (aerodynamics) calculations of both aircraft and vehicles, combustion in internal combustion engines and gas turbines and chemical process engineering (e.g. mixing and separation).\cite{53} Therefore, CFD is a suitable and potential technique to model fluid flows in the steelmaking converter. Use of CFD techniques in steelmaking process is an active area of research, and some of such research works include the studies by Sambasivam et al\cite{54}, Singh et al\cite{55}, Pilkas et al\cite{56} and Madan et al\cite{57}.

Hence, in the present research work, the potential for further improvements to the CFD foaming model developed by Sattar\cite{1} to model the refining kinetics and slag foaming in oxygen steelmaking was identified and carried out.

- **Summary of the model developed by Sattar\cite{1}**

The CFD model developed in the present study was initiated from the CFD foaming model developed by Sattar and co-workers\cite{1}. This CFD model by Sattar\cite{1} was initially developed to predict the foaming in bath-smelting slag contained in an aluminum crucible. This model was able to reproduce the foam height measurements obtained in the experiments carried out by Jiang and Fruehan\cite{16} approximately. This model was then improved by the same authors to predict the foam height in a plant scale oxygen steelmaking converter. The results obtained from the model on foam height were compared with the experimental data published in the IMPHOS\cite{2} research work and were in rough agreement with the observations.

In this model, the Eulerian-Eulerian approach was used to simulate the multiphase flow in the converter, where gas, liquid and foam phases interact with each other in terms of mass, momentum, and energy. The foam was a separate phase produced from liquid and gas phases, and its physical properties were determined by the liquid and gas
content in the foam. A population balance equation was used to track the population densities of bubble classes in gas and foam phases and was modified by incorporating bubble coalescence and break-up. Decarburization reaction was also considered in the simulation. This model was able to predict the foam height in the converter reasonably well, simultaneously with the decarburization, heat generation and velocities of different phases.

However, several drawbacks and limitations were identified in this CFD model developed by Sattar\cite{1} when used to model the actual steelmaking process. These avenues for further enhancement of the CFD model have created the requirement for the present study, taking advantage of the comparatively better performance of the model at this initial stage.

- **Drawbacks identified in the foaming model by Sattar\cite{1}**

Even though the CFD model developed by Sattar and co-workers\cite{1} was expected to produce good predictions on the foam height in an oxygen steelmaking converter, model predictions deviated from the actual observations in several aspects. These deviations were identified in the present study and were used as the pathways for improving the model, as stated below.

- Once the oxygen injection is started in oxygen steelmaking process, several sub-processes start simultaneously such as oxidization of the elements and flux dissolution. Hence, a model developed for predicting slag foaming and refining kinetics in steelmaking process should consider at least the major refining reactions because both slag foaming and refining process are inter-connected and have an influence on each other. However, the CFD model developed by Sattar\cite{1} only included the decarburization reaction.

- A kinetics model is necessary for calculating the rates of the chemical reactions in a model for predicting the refining kinetics in oxygen steelmaking. However, the rate of the decarburization reaction considered in the model developed by Sattar\cite{1} was calculated empirically from the results reported in the IMPHOS study\cite{2} for one particular heat. Hence, this model may not be able to produce
reliable predictions on decarburisation when the process conditions are changed.

- It is well established that pure liquids do not foam. Foam in oxygen steelmaking is produced from slag and contains a certain amount of hot metal brought in by droplets. The extent of slag foaming depends on the quantity and the physical properties of slag. So, a model developed for predicting the foaming in steelmaking should produce the foam from slag. However, in the model developed by Sattar\[1\], the foam is produced from the liquid phase in their model, which is mostly valid in the case of bubble column reactors.

- Foam naturally drains under the influence of gravity in the absence of any other disturbances until a critical bubble film thickness is reached. Hence, a model designed to predict the foam height should have a proper foam drainage mechanism to continuously drain the foam until the critical bubble film thickness is reached, which was not clearly incorporated in the CFD model developed by Sattar\[1\].

- Foam collapses when the thickness of its foam bubble films reach a critical thickness, which can also be interpreted as reaching a critical liquid fraction in foam. However, the foam collapsing criterion used in the model developed by Sattar and the co-workers\[1\] was an empirical relationship obtained mainly based on a trial and error method.

The present study was aimed at improving and extending the model developed by Sattar\[1\] by addressing the above-stated weaknesses mainly in the routes of kinetics modeling and slag foam modeling.
1.3 Research objectives

Even though, the main goal of the present study was to develop a general CFD model for oxygen steelmaking process, the scope of the study was limited to improving the CFD model in terms of its predictions on the refining behavior of C, Si, Mn and P and the evolution of slag foam height. This main goal was divided into four main tasks which were identified as the objectives of the present study and are stated below.

1.3.1 Develop a semi-empirical first order kinetics model to be incorporated in the CFD model to capture the removal behaviors of C, Si, Mn and P. Compare and validate the analysis results against the observed refining kinetics reported in IMPHOS\textsuperscript{[2]} research work.

1.3.2 Incorporate the developed kinetics model in the main CFD model to simulate and predict the refining of the main impurity elements in oxygen steelmaking. Compare the model predictions with the observations reported in IMPHOS\textsuperscript{[2]} research work.

1.3.3 Enhance the foam simulation in the model by Sattar and co-workers\textsuperscript{[1]}, with a more accurate foam formation, drainage, and collapsing phenomena. Analyze the model predictions on foam height and compare them with the results of previous foaming model (i.e. the model before incorporating the improvements) and the observations reported in IMPHOS\textsuperscript{[2]} study.

1.3.4 Improve the three phases model to a four phases model by Introducing slag as a separate phase. In this four phases model, the foam is produced primarily from slag and gas phases instead of the liquid and gas phases. Analyze the predictions on slag foam height from the four phases model and compare them with the predictions of the three phases model and the observations reported in IMPHOS\textsuperscript{[2]}. 

10
1.4 Overview of the thesis

The thesis presents the present research work in 9 chapters. Following is a brief summary of the content in each chapter of the thesis.

Chapter 2
In Chapter 2, the details of oxygen steelmaking process and slag foaming in oxygen steelmaking are discussed in detail. Since the present study was aimed at modeling slag foaming and refining kinetics in oxygen steelmaking, it was essential to investigate the process in detail. The details on the oxygen steelmaking process under the subsections of its history, the process route, raw materials and process control are presented. Further, the fundamentals of refining kinetics are explained simultaneously with a brief introduction to the investigations and modeling efforts on oxygen steelmaking kinetics. Slag foaming phenomenon is then explained in detail with information on understanding and modeling slag foaming emphasizing on the requirement for more work on modeling slag foaming in oxygen steelmaking. The chapter concludes with a description of the IMPHOS research work\[^2\], which was used in the present study to extract data required for the simulations as well as for comparing and validating the results obtained from the CFD model.

Chapter 3
A thorough understanding of foams and the foaming process was essential to understand and model slag foaming in oxygen steelmaking. In Chapter 3, foams are explained in terms of their composition, structure, and stability with particular attention on foam drainage and bubble film rupture. Also, the reason for selecting the CFD technique for the present slag foam modeling, and the process of modeling the foaming using CFD technique are explained along with a description of the CFD foaming model developed by Sattar\[^1\]. Further, the model developed by Sattar\[^1\] is critically analyzed for its drawbacks and weaknesses to identify the potential routes to improve the model.
Chapter 4

It is established that further optimization of the oxygen steelmaking process relies on the effective modeling efforts of the process, even though, most sections of the steelmaking process are not yet completely investigated and understood. However, the research work carried out by Sattar was used as the starting point for the present study after identifying the possible routes of improvement. Therefore, in Chapter 4, a summary of the literature review and the research problems addressed in the present study are presented.

Chapter 5

In the present study, a semi-empirical first order kinetics model was developed to be included in the CFD foaming model, as it was one of the main objectives. Prior to the incorporation of the developed kinetics model into the CFD model, an analysis was carried out to investigate the applicability of the developed first order kinetics model to predict plant data on refining kinetics, using the data reported in IMPHOS research report. Hence, in this chapter, the semi-empirical kinetics model developed and the analysis carried out using the observed data reported in IMPHOS study to determine the applicability of the model to predict the steelmaking kinetics are explained in detail. This kinetics model was then rearranged to be included in the CFD model, and the details regarding the rearrangement and the final model is also explained in this chapter.

Chapter 6

In this chapter, a thorough explanation is provided on the improvements applied to the CFD foaming model in the second stage of the present study for simulating the refining kinetics of impurity elements and foaming in oxygen steelmaking, which was initiated from the CFD model developed by Sattar. The results obtained from the model on the removal behavior of impure elements and the foam height variations over the period of concern are presented. Further, the foam height results from the model were compared with the foam height results from the original foaming model by Sattar and the observations reported in IMPHOS study. The kinetics results obtained from the present model were also compared with the observations reported in IMPHOS report. The details on those comparisons and analysis are presented in this chapter.
Chapter 7
Even though the three phases CFD foaming model explained in the previous chapter predicted the refining kinetics and the foam height well when compared with the observations reported in IMPHOS\textsuperscript{[2]} study, the foam was produced from the liquid phase which contained both liquid metal and slag similar to aqueous foam. Hence, as explained in this chapter, a separate slag phase was introduced to the CFD model. Then, the foam phase was produced from the slag phase instead of the liquid phase. The development and performance of the CFD model with the new slag phase are presented in detail in this chapter. The results obtained from the model were compared and validated against the observations reported in IMPHOS\textsuperscript{[2]} study.

Chapter 8
The CFD model originally developed by Sattar\textsuperscript{[1]} was further improved and extended in the present study in three stages mainly by including a kinetics model, improved foaming model, and separate slag phase. The results obtained from the model on refining behavior of impurity elements and foam height at each stage are discussed and summarized in this chapter.

Chapter 9
The conclusions derived from the model results and the possible routes for improving the model further are presented in this chapter.
1.5 Publications from the present work

**Journal article:**

**Technical article:**

**Conference papers:**

**Poster presentations:**
Chapter 2
Chapter 2: Oxygen steelmaking fundamentals and the issue of slag foaming

Steel is one of the most widely consumed and recycled raw materials globally. Steel production in one year exceeds that of all other metals combined in 10 years of production\(^5\), and in 2014 oxygen steelmaking was responsible for approximately 70% of the global crude steel production\(^6\). Although oxygen steelmaking has gained popularity among steelmakers as one of the most efficient methods to produce steel, it is important to optimize the production process further to reduce the costs involved and to produce steel with precise quality to meet the increasing demand. Therefore, the present study was aimed at developing a CFD model to simulate and predict the refining kinetics and slag foaming in oxygen steelmaking, which can assist in optimizing the steel production process. In order to develop a proper model, it is essential to analyze the oxygen steelmaking process in detail. Hence, in this chapter, the fundamentals of oxygen steelmaking and slag foaming, which formed the background for the present study, are described and analyzed.

2.1 Oxygen steelmaking fundamentals

2.1.1 Background of oxygen steelmaking

Steelmaking is the process of refining pig iron produced in a blast furnace to a pre-defined chemical composition by removing its impurity elements via selective oxidation processes.\(^4\) To achieve this purification goal, which is crucial in determining the output product quantity and quality, steelmakers have developed different methods and converters over the past two centuries.

The first process developed in the steelmaking history that can produce liquid steel at large scales by refining pig iron with less consumption of time and cost was the Bessemer or Bottom Blown Acid process. This process was developed by William Kelly and Henry Bessemer independently around 1856.\(^7\) Oxidation of impurity elements in the pig iron before the major oxidation of iron was the fundamental principle of the Bessemer process. The converter was lined with acid refractories, and the process was only suitable for high-quality pig iron with low P, high Mn and required quantity of Si for thermal needs of the process. This Bessemer process was then improved to the basic
Bessemer process by G. Thomas in 1879. The improvements involved the use of basic refractory lining instead of acid refractories and use of basic fluxes. Both the Bessemer and Thomas processes are categorized under the pneumatic steelmaking processes, where, air is injected to achieve the requisite refining.

However, by 1868, K.W. Siemens introduced the basic open-hearth process simultaneously with the development of basic Bessemer process and became popular among the steelmakers. Although the fundamental principle of the open hearth process is the same oxidation principle, high temperatures could be achieved in this process to keep the produced steel molten and free of entrapped slag. Even though about 80% of the global steel production was by open hearth process around 1950, with the introduction of oxygen steelmaking, the popularity of both the Bessemer process and the open hearth process declined mainly due to the high productivity of the new process.

Electric Arc Furnace (EAF) steelmaking is used for about 25% of world steel production and showed significant growth in recent decades simultaneously with the oxygen steelmaking. Since oxygen steelmaking process melts less amount of scrap compared to the open hearth process, scrap was available at low cost. This made the EAF steelmaking processes more popular. The first successful commercial EAF was placed in operation in 1899 by Heroult, and the furnace was a direct arc furnace. A typical EAF is 150 to 180 tons, has several natural gas burners, uses a considerable quantity of oxygen (30 m$^3$/ton), has eccentric bottom tapping and often is equipped with scrap preheating. EAF consumes about 360 to 400 kW/h of electricity to melt a ton of steel scrap and operates with either AC or DC electricity.

Although the use of pure oxygen injection instead of air for refining molten pig iron and scrap mixtures was of interest of steelmakers including Bessemer, it only became feasible around the World War 2 period with the availability of tonnage oxygen. Oxygen injection was first investigated by Durrer and Hellbrugge in Zurich ETH. It was found that blowing pressurized oxygen downwards onto the molten pig iron, produce steel with high thermal and chemical efficiency.
Various steelmaking methods are employed by steelmakers based on the factors including demographical factors and cost of power and raw materials. According to the global statistics on the production of steel by the process over the years as illustrated in Figure 2.1, it is evident that the Bessemer, Thomas and open hearth processes were the initiatives and driving force for the development of better steelmaking processes such as the BOF and EAF. The steelmaking technologies that are currently in use will improve further over time as consequences of customer demands for precise quality steels, raw material shortages, environmental concerns and reduction efforts on cost and energy consumption.

Top blowing of oxygen was utilized for steelmaking since 1952-53 at Linz and Donawitz in Austria. The improvement of this process made oxygen steelmaking the dominant process in use for producing steel in the decades followed. The terms LD (Linz-Donawitz), BOS (Basic Oxygen Steelmaking), BOF (Basic Oxygen Furnace), BOP (Basic Oxygen Process) are used in different parts of the world to identify the same basic oxygen steelmaking process.

The process of top-blown oxygen steelmaking is the injection of a high purity oxygen stream onto the surface of the molten pig iron through a multi-holed, water-cooled lance. Injection of pure oxygen delivered the advantages of higher oxidizing rates, use of more DRI or scrap charge and high-quality output steel over the pneumatic
steelmaking processes. The furnace used in this process is pear shaped and lined with basic refractories. The oxygen jet is injected at supersonic velocity, and it oxidizes the impurity elements such as Si, C, Mn and P in the bath simultaneously with the intensive mixing of the metal bath. Further, these oxidizing reactions are exothermic and generate the heat requisite for driving the refining of hot metal and melting scrap during the process (i.e. autogenous process). The furnace arrangement for top-blown oxygen steelmaking is shown in Figure 2.2a.

In the early stages of oxygen steelmaking evolution, the bottom blown technique was the first to be put on trial, as it was more convenient to convert the existing Bessemer or open hearth furnaces to be used for bottom blowing oxygen steelmaking. A successful bottom blown oxygen steelmaking process was first developed in the 1970s and sometimes is named as Q-BOP or OBM. The bottom blown process has the advantages such as quiet operation, low O, S and P in steel and low Fe in slag, simultaneously with the disadvantages such as high wear rates of tuyeres and refractory and high hydrogen and nitrogen content in steel. The furnace arrangement for bottom-blown oxygen steelmaking is shown in Figure 2.2b.

In a combined blowing steelmaking process, both the top blowing and bottom blowing of gasses are involved. Currently, there are several combined blowing processes, which differ according to the type of the bottom gas used, the possible flow rates of the bottom gasses and the equipment used to introduce the bottom gas into the furnace. In a combined blowing process, about 60 to 100% of oxygen is injected through a top mounted lance similar to the top blown process. The other gasses blown through the bottom include O₂, N₂, Ar, CO₂, CO, and air. By altering the type and the flow rate of bottom blown gases, certain specific metallurgical reactions can be controlled, and thereby achieve the desired steel compositions and temperatures. Further, in the combined blowing process, the bath is effectively agitated, so that the thermal and material inhomogeneities are minimized. Example configurations of combined blowing process for both BOF and Q-BOP processes are shown in Figures 2.2 c and d respectively.
All these three oxygen steelmaking processes involve injecting pure oxygen to oxidize the impurity elements in the molten pig iron. The oxygen stream is injected at supersonic velocity to generate an emulsion of slag, metal, and gas to facilitate the reactions with increased interfacial area. However, in the present study, the top blown oxygen steelmaking process was the subject of the analysis.

### 2.1.2 Process route

The primary aim of the top blown steelmaking process is to refine the pig iron from the blast furnace to produce steel of less than 0.1% carbon. This is achieved by injecting high purity oxygen to oxidize the impurity elements, including C, Si, Mn and P. These oxidizing reactions also provide the required heat for melting the scrap and dissolving added fluxes by raising the bath temperature up to about 1635 °C. The oxides of those impurity elements and the added fluxes form a liquid slag except carbon, which, form carbon monoxide and carbon dioxide and leave the bath. The molten metal, liquid slag and the gases injected and produced form an emulsion during the blow, creating a
large interfacial area for faster reactions and mass transfer between gas, slag, and metal. The tap-to-tap time usually is about 20 minutes with a blowing time of about 10 minutes, which depends on the heat size and logistics and can vary between 30 to 50 minutes. The process steps are schematically illustrated in Figure 2.3.

![Diagram of steelmaking process steps](image)

**Figure 2.3: Steps of top-blown steelmaking process**

The operations of a typical oxygen steelmaking process begin by ordering and preparing the required scrap to be added to the furnace. Selected scrap is loaded into a scrap box and transferred to the charging aisle. Then, the liquid pig iron from the blast furnace is conveyed to the furnace in torpedos, and a hot metal transfer ladle is filled with the pig iron. The hot metal desulfurization occurs in this ladle. A stream of lime and magnesium is injected onto the hot metal to remove sulfur in the process. This process takes about 5 to 20 minutes, and sulfur is removed approximately from 0.025% to 0.002% in weight. The hot metal weight and temperature are measured and entered into the process control computer on the shop floor. Scrap is charged into the furnace first, and then liquid hot metal is poured into the furnace from the ladle. This takes about 1 to 5 minutes, depending on the design of the furnace hood and the shop fugitive emission system.

Before charging the furnace with scrap and hot metal, the charging recipe is determined by a computer calculation. The data on temperature and chemical composition of the
hot metal, and chemistry and the temperature of the scrap, are fed to the computer program together with the heat aims to calculate the charge recipe. The main heat aims are carbon and temperature, while the other specific aims are S, P and slag composition (% FeO). The results of the calculation usually involve the hot metal and scrap weights with the amounts of oxygen, coolants, and fluxes required to be fed to the furnace.

After charging the furnace with hot metal and scrap, the furnace is turned upright, and oxygen is supplied through a water-cooled lance. Oxygen blow takes about 20 minutes on average with the possibility of varying from 13 to 25 minutes. Oxygen is usually supplied in several batches, and each batch has a different lance height and a flow rate. Flux addition starts soon after the commencement of the oxygen supply and finishes with the second batch of the oxygen. Fluxes include CaO and MgO provided from burnt lime and dolomitic lime. The CaO component of the flux controls the S and P, and the MgO component saturates the slag with MgO to prevent the dissolution of the refractory lining of the furnace into the slag. Coolants are also added simultaneously with the fluxes, which is mainly iron ore in the form of lumps or pellets. The operating oxygen steelmaking converter is schematically shown in Figure 2.4.

At the end of the blow, the furnace is tilted nearly 90° to the charging side to take samples for chemical analysis and measuring the temperature of the bath. This step takes several minutes, as the foamy slag needs to be settled down for sampling. If the temperature and the chemical composition of the bath are not up to the required values, a reblow of oxygen with or without coolant needs to take place. Once the reblow is finished, the furnace is tilted to the tap side for tapping. The steel flows through the taphole to a ladle below the furnace while slag floats on the metal surface. Slag is not allowed to enter the ladle as much as possible. After the tap, the ladle is transferred for further treatments followed by transfer of steel to the caster.

The furnace is turned upright after the tapping for the furnace maintenance. The remaining slag in the furnace is either dumped into a slag pot or splashed on the furnace lining. With the completion of repairing the furnace refractory lining, the furnace is ready for the next heat.
2.1.3 Raw materials

Raw materials with a high quality and required quantity are essential for a good yield of steel. The raw materials needed for the oxygen steelmaking process are mainly the hot metal from the blast furnace, oxygen, steel scrap, fluxes (burnt lime, dolomitic lime, dolomite stone and fluorspar) and coolants.\[^{[4, 8]}\]

**Hot metal:**
Hot metal is the primary source of iron and energy for the process, typically accounting for 70% to 90% of the charge, and comes from the blast furnace.\[^{[4]}\] The chemical composition of hot metal can vary over a wide range, while a typical chemical composition is around 4.0 to 4.5% carbon, 0.3 to 1.5% Silicon, 0.25 to 2.20% Manganese, 0.04 to 0.20% phosphorus and 0.03 to 0.08% sulfur (before desulfurization).\[^{[8]}\] The C and Si content of the hot metal is important in the perspective of energy generation, which decides the amount of scrap to be charged to the furnace. Si is of specific concern as it is a significant influence on the slag volume generated, and consequently on the lime consumption. Further, it is essential to know the weight of the hot metal and its temperature accurately before charging to the furnace, for calculating the charge recipe.
**Oxygen:**
In order to achieve the target of high-quality steel, oxygen with very high purity is injected, ideally 99.7 to 99.8%. Typical composition of the oxygen stream is approximately 99.5% oxygen, 0.005 to 0.010% nitrogen and the rest is argon.[8]

**Scrap:**
Scrap is added to the furnace before the addition of hot metal as the second main iron contributor and basically consists of recycled iron or steel and small proportions of DRI, iron ore, and cold pig iron.[4] Typically, the use of scrap is about 20 to 35% of the total metallic charge.[8] The exact quantity of scrap needed is determined by the temperature and the composition of hot metal, specifically the Si content.[4]

**Fluxes:**
Fluxes added to the furnace mainly contain burnt lime for CaO and dolomitic lime for MgO. A typical chemical composition of burnt lime is 96 wt% CaO, 1 wt% MgO, 1 wt% SiO\textsubscript{2} and 0.03 to 0.1 wt% S.[8] The sizes of the burnt lime lumps are carefully selected so that they are small in size and have high porosity. Thus, the added lime reacts fast in the slag and promotes further slag formation.[4] Dolomitic lime is used for saturating the slag with MgO and thereby reducing the dissolution of furnace refractory lining into the slag. Typical composition of dolomitic lime is about 36 to 42 %wt of MgO and 55 to 59 %wt CaO.[8]

**Coolants:**
Coolants are required to cool the bath when it is at a higher temperature than the aimed temperature at the turndown. The materials usually used as coolants are limestone (CaCO\textsubscript{3}) or dolomitic stone (CaCO\textsubscript{3}.MgCO\textsubscript{3}) and iron ore.[8] Sometimes scrap is also added to the hot metal bath as a coolant.[4]

### 2.1.4 Oxygen injection

In the top-blown oxygen steelmaking process, oxygen is blown onto the surface of the hot metal bath through a water-cooled lance at supersonic velocities (Mach > 1), as illustrated in Figure 2.5. Oxygen is generally blown over a period of 13 to 25 minutes with an average of 20 minutes, which may differ from plant to plant.[4, 8] The purity of
oxygen has to be at least 99.5%, while the rest is nitrogen and argon. The tip of the lance is designed with 4 to 8 convergent-divergent nozzles, typically delivering oxygen at the rate of $640 \text{ Nm}^3/\text{min}$ to $900 \text{ Nm}^3/\text{min}$.\cite{8}

Oxygen injection is the driving force of the process by fuelling the oxidizing reactions and thereby releasing the required heat for further refining of steel. Also, the high-speed injection creates metal droplets increasing the interfacial area for refining reactions simultaneously causing rapid mixing of the bath.\cite{13} The excessive chemical reaction rates generate large amounts of gases and slag. As a consequence of this increase in volume, the emulsion may spill from the mouth of the furnace, which is detrimental for both the furnace and the shop floor and causes a yield loss too.\cite{10} In order to control the reaction rates and flow inside the furnace, oxygen injection is controlled throughout the blow by means of changing either the lance height as shown in Figure 2.6 or the oxygen flow rate.\cite{8}

Oxygen injection is carried out in batches, typically in three batches, where, the third batch is usually considered the main batch. Each batch has a unique lance height and sometimes a pre-defined oxygen flow rate. Additionally, the lance height determines the impinge intensity of the oxygen stream on the liquid metal and the extent of droplet generation.\cite{44} In the first batch, the lance height is very high to prevent the lance tip from contacting the scrap causing damage to the lance and safely establishes the refining reactions. In the second batch, the lance is further lowered about 0.5 to 0.8 m,
and it increases the reaction rates and the slag formation. Finally, in the main batch, the lance is further lowered, and rest of the blow takes place. However, the lance height is defined by the nozzle design and experience of the operator, and is a compromise between achieving the faster carbon removal rates and proper slag generation.\cite{8, 64, 68}

\subsection{2.1.5 Nozzle design}

The oxygen-injecting nozzles are built into the tip of a water-cooled lance and is made of high thermal conductive cast copper alloy.\cite{7} Three and six nozzle lances are commonly used in larger capacity BOS furnaces.\cite{4} These nozzles are equally spaced around the tip and at an angle of about 12° to the center line of the lance. At the inlet to the lance, oxygen is at about 8 to 10 atm pressure, and at the nozzle, which is a convergent-divergent nozzle, converts the pressure energy into kinetic energy.\cite{7}

The oxygen injection velocities through the nozzles are often given by Mach number, which is a dimensionless number calculated as the ratio between the actual velocity of the oxygen stream and the velocity of sound in the same fluid at the same environment. Mach number is calculated by equation 2.1\cite{68}, where, \( U_e \) is the velocity of the jet (m/s) and \( U \) is the velocity of sound (m/s).

\[ M = \frac{U_e}{U} \]  \hspace{1cm} \text{Eq 2.1}

The flow through the nozzle is shown in Figure 2.7. The flow of fluid through the nozzle is divided into three regions: core, supersonic and subsonic. When the oxygen stream enters and flows through the nozzle’s convergent side, it gains sonic velocity, and it is then expanded on the divergent side of the nozzle increasing its velocity to supersonic. In the core region, the velocity of the oxygen stream remains constant, and gradually reduces to the subsonic velocity at a certain distance downstream from the nozzle, impinging the bath surface at a subsonic velocity.\cite{4}
In the present study, the exit diameter of the nozzle was extended to be 0.268m at a distance of 0.496m from the original nozzle exit given in IMPHOS research work[2] to get a subsonic flow (Mach number = 0.0322) from the nozzle due to simulation restrictions.[1]

2.1.6 Process control

Process control is essential in oxygen steelmaking process to produce required quantity and quality of steel without wasting input materials and other resources. Basically, the process control involves calculating the amount of raw materials and energy input to the process for producing the required composition and quantity of steel, and it depends on the facilities and the requirements of the plant.[8, 64] As the refining period of oxygen steelmaking has reduced to about 30 to 50 minutes, manual intervention to control the process is almost impossible. Therefore automating the process using computers and interconnected mechanical devices such as motors and actuators has gained popularity recently. However, two types of process control schemes can be identified in a broader perspective: the static control scheme and the dynamic control scheme.[4, 8]

The static control system or the static charge model is a computer program that can calculate the amount of charge, fluxes and the oxygen input for the particular heat based on the input details fed to the program.[4, 8] These details include the weight of hot metal and scrap charge and aimed carbon and temperature. The performance of this model depends on the accuracy of the model, accuracy of the inputs to the model and consistency of the input material quality. Also, a better control of the process results in an improved control on the final carbon, sulfur, phosphorus and temperature, reducing the need for reblows and steel bath cooling. Furthermore, the enhanced performance
of the steelmaking process, by an improved process control, produce a good yield of steel with a high productivity and increased refractory lining life.\[8\]

The dynamic control scheme is used by some plants simultaneously with the static control scheme, to manage the parameters such as oxygen pressure, blowing rate and lance height more efficiently, by taking in-blow measurements.\[4, 8, 64, 70\] A more recent development in taking on-line measurements is via submerged tuyeres.\[4\] Following are some of the other dynamic control schemes used in steelmaking plants:

- **Gas monitoring schemes**

  A gas monitoring system is used to continuously analyze the amount of CO and CO\(_2\) contained in the off-gas, and calculate the amount of carbon oxidized in the particular stage of the blow.\[8, 71\] These results are then used to calculate the carbon level in the bath at that stage, and the need for further oxygen is determined. However, this method is not very successful at the commercial level due to difficulties in taking accurate measurements.

- **Optical sensors**

  Optical sensors are used to measure the intensity of light at the mouth of the vessel continuously throughout the blow, and then correlate the variations of the intensity of light to the carbon level in the bath.\[4, 8\] This method is successful in determining the carbon levels when the carbon level in the bath is 0.06\% or less.

- **Sensor or sub-lances**

  A water cooled sub-lance containing expendable carbon, oxygen, and temperature sensors is lowered into the bath about two or three minutes before the end of the blow to measure the carbon content and temperature.\[8\] These measurements are then used to determine the amount of oxygen and coolants required to be added to the bath. This method is proved to be successful as a process control tool, even though, the capital cost and maintenance required are high.
- Drop-in thermocouples for quick tap

In a quick tap heat, where there are no strict limits on end phosphorus or sulfur, drop-in thermocouples are used to measure the carbon content and temperature towards the end of the blow.\[^{[8]}\] These drop-in thermocouples generate an emf signal which is received by the computer and converted into a temperature measurement.

### 2.1.7 Kinetics fundamentals

In oxygen steelmaking, a supersonic oxygen stream is injected onto the surface of the hot metal bath. The impurity elements in the bath (i.e. C, Si, Mn, and P) are oxidized and removed from the bath in the form of CO, CO\(_2\), SiO\(_2\), MnO, P\(_2\)O\(_5\) and iron oxides by injected oxygen. The gaseous oxides, containing 90% CO and 10% CO\(_2\), escape the furnace from the top with small amounts of iron oxide and lime dust.\[^{[8]}\] The other liquid oxides dissolve with the fluxes added forming the liquid slag which further facilitates the refining of the bath.

The success of oxygen steelmaking over the other steelmaking methods is mainly due to two reasons. The first reason is the autogenic nature of the process, as the oxidizing reactions generate the heat required to melt scrap and fluxes and to raise the temperature of the bath.\[^{[4]}\] The second reason is that the production rate of steel by oxygen steelmaking is higher compared to other processes.\[^{[8]}\] Increased interfacial area produced by the droplets ejected by the impinging oxygen stream and slag foam formed by trapping gasses in the slag, help increase the refining rates in the bath.\[^{[38, 54]}\] The major regions in the steelmaking converter including the gas-metal-slag emulsion are shown in Figure 2.8.
Major reactions that occur in a steelmaking converter are listed below, where [] indicates that the compound is dissolved in iron, and () indicates that the compound is dissolved in slag.\textsuperscript{[13]}

Oxygen pick-up by the metal:

\[ O_{\text{g}} \rightarrow [O] \]
\[ CO_{\text{v}} \rightarrow CO_{\text{g}} + [O] \]
\[ (FeO) \rightarrow Fe + [O] \]
\[ (Fe_{2}O_{3}) \rightarrow 2(FeO) + [O] \]

Oxidation of elements in the metal:

\[ [C] + [O] \rightarrow CO_{\text{g}} \]
\[ Fe + [O] \rightarrow (FeO) \]
\[ [Si] + 2[O] \rightarrow (SiO_{2}) \]
\[ [Mn] + [O] \rightarrow (MnO) \]
\[ 2[P] + 5[O] \rightarrow (P_{2}O_{5}) \]

Oxidation of compounds in the slag:

\[ 2(FeO) + \frac{1}{2} O_{2(g)} \rightarrow (Fe_{2}O_{3}) \]
$2(FeO) + CO_{(g)} \rightarrow (Fe_2O_3) + CO_{(g)}$

Flux reactions:

$MgO_{(s)} \rightarrow (MgO)$

$CaO_{(s)} \rightarrow (CaO)$

Gas reactions:

$CO_{(g)} + \frac{1}{2}O_{2(a)} \rightarrow CO_{2(a)}$

The oxidizing reactions in the steelmaking bath occur in a sequential manner starting with the mass transfer of the elements from the metal phase to the slag-metal interface. Then, mass transfer of oxygen occurs either from the gas phase to the gas-metal interface or from the metal (dissolved in the metal phase) to the slag-metal interface. At the slag-metal interface, the chemical reactions occur once the mass transfer of the elements and oxygen are started. The reaction products are then transferred to the slag phase and the gas phase.[68]

The rate of these chemical reactions is generally considered to be governed by the mass transfer of elements to the slag-metal or gas-metal interface. The chemical reactions occur at higher rates once the elements are present at the interface, because of the high temperature of the bath.[68, 72] Further, the factors including the high level of bath agitation and turbulence, intense mixing of the phases and lower viscosity, encourage higher reaction rates.[4]

Hence, the rates of reactions in steelmaking are generally predicted using the Fick’s 1st law given by the equation 2.2.[4, 68]

$$\frac{dC}{dt} = k \frac{A}{V} (C_b - C_{eq})$$  

Eq 2.2

Where $k$ is the mass transfer constant, $A$ is the interfacial area, $V$ is the volume, $C_b$ is the bulk concentration of element and $C_{eq}$ is the equilibrium concentration of the element.

Although Fick’s first law of diffusion is generally used to calculate the steelmaking kinetics, few other models can also be found in the literature.
The model developed by Robertson et al\cite{73} suggested the multicomponent transport in the metal and slag phases is the governing force of the slag/metal reaction rates and was applied for desulfurization reaction rate calculation in the molten iron. Further, it was observed by Belton et al\cite{74} that the adsorption of surface-active solutes such as S and N to the slag/metal interface retards the rates of the chemical reactions. Even so, Brooks et al\cite{44} suggested that simple ordinary differential equations are unable to capture the complex and the transient nature of the steelmaking kinetics. The removal patterns of main impure elements are shown in Figure 2.9.

![Figure 2.9: Removal pattern of impure elements during the blow\cite{64}](image)

### 2.1.7.1 Carbon oxidation

Carbon is the most abundant impurity element in the hot metal (about 4.5 %wt) and usually, is reduced to about 0.1 %wt in the end steel products\cite{8}. Decarburization is the most extensive and important reaction in the steel refining, and understanding its mechanism has been the center of focus of many steelmaking researchers. Carbon oxidizes in both impact zone and the gas-metal-slag emulsion. In the impact zone, the carbon dissolved in the metal is directly oxidized by the oxygen injected from the lance. However, in the emulsion, the decarburization occurs via the reduction of FeO in the slag by carbon in the metal droplets ejected from the metal bath\cite{38, 39}.

Decarburisation produces CO and CO$_2$ gases, which enhance the bath mixing and interfacial area for refining reactions. Three distinctive regions can be broadly identified in the rate of decarburization over the blow\cite{8} as depicted in Figure 2.9. In the first stage, decarburization rate is low due to the domination of desiliconization reaction, and in the
second stage, the rate of the reaction is at a constant higher value. In the third stage, the rate of the reaction is very low, as the carbon availability for the reaction is very low.

The kinetics of decarburization reaction at each stage can be summarized as follows:

- **At higher carbon concentrations (first and second stages), the rate of the reaction is not governed by the carbon concentration, but, the rate of the reaction reduces when the carbon concentration in the metal is low.**
- **The decarburization by CO$_2$ is affected by the sulfur concentration in the bath. When the sulfur concentration is lower than 0.05 %wt, the decarburization rate is decreased, and the retarding effect is not considerably beyond that limit.**
- **The composition of the gas mixture (especially, the partial pressure of CO$_2$ and oxygen) has a considerable effect on decarburization rate.**
- **The rate of decarburization increases with the increase of the gas flow rates and the temperature of the molten metal.**

### 2.1.7.2 Silicon oxidation

The heat requirement for the oxygen steelmaking process is mostly satisfied by the oxidation of silicon content in the metal bath. Silicon’s affinity for oxygen is high compared to other impurity elements, and its oxidation is highly exothermic. Therefore, silicon is oxidized within about three to five minutes from the start of the blow as shown in Figure 2.9. Generally, the silicon content in the hot metal is about 0.25 to 1.3 %wt and is reduced to less than 0.005 %wt,$^8$ releasing the heat required to raise the temperature of the bath. In the case of a small quantity of silicon in the hot metal, the melting capacity of scrap reduces, while in the case of high silicon content, the extra heat produced damages the refractory.$^4$ The silica (SiO$_2$) produced reacts with the added lime to form the basic slag required for further refining, specifically the dephosphorization.

### 2.1.7.3 Manganese oxidation

Manganese oxidation occurs via a more complex mechanism as shown in Figure 2.9, compared to the oxidation behavior of other impure elements in the steelmaking process. Manganese oxidizes to form MnO in the first stage of the blow, but it reverts to the metal in the middle of the blow.$^4, 8$ Towards the end of the blow, manganese is
again oxidized and removed from the metal as more oxygen is available for its oxidation. The oxidation and removal of Mn from the melt are influenced by slag basicity, operating temperature, FeO content in the slag and partial pressure of CO.¹⁴, ⁷⁵

### 2.1.7.4 Phosphorus oxidation

Phosphorous oxidation also exhibits a similar complex behavior to manganese oxidation, as shown in Figure 2.9. In the first stage of the blow, phosphorus is oxidized and removed from the metal, but it reverts to the metal in the middle part of the blow, followed by removal from the metal towards the end of the blow. Removal of phosphorous is encouraged by the low temperature, high slag basicity, high slag FeO, high slag fluidity and adequate stirring.²⁸, ⁷⁶

### 2.1.7.5 Sulphur oxidation

Sulfur removal reaction is a reducing reaction, which is in contrast to the removal of the other impurity elements. Therefore, removal of sulfur in a BOF is not effective due to the presence of high basic slag and high oxygen potential, as shown in Figure 2.9. The desulphurization of the hot metal should be carried out in the blast furnace or a separate stage before the BOF.⁴, ⁸

### 2.1.7.6 Scrap dissolution

Scrap is the second main contributor of iron units to the steelmaking converter and is charged to the furnace before charging hot metal and injecting oxygen. Scrap also satisfies the requirement for a coolant to maintain an approximately constant temperature in the metal bath⁷⁷, ⁷⁸, mainly during the silicon oxidation in the first 8 to 10 minutes of the blow.⁷⁹ When cold scrap is in contact with the hot metal, a huge temperature gradient occurs between the hot metal and scrap causing the scrap to dissolve gradually into the metal.⁶⁸

The mechanism of scrap dissolution involves simultaneous heat and mass (carbon) transfer and is assumed to follow three steps, which are the solidification, fast melting, and normal melting, as explained by Sethi et al.⁷⁹ The temperature profile of the scrap dissolution in the melt is shown in Figure 2.10. In the solidification step, a solid shell is formed around the scrap particles due to the solidification of hot metal on the surface of the scrap particle which is known as the “Chill effect”. At this stage, the rate of heat
transfer into the scrap by conduction is high, in comparison to the heat transfer by convection to the hot metal. When these heat transfer by conduction and convection equal in magnitude, the thickness of the solid shell is maximum. Once the convection heat transfer exceeds the conduction heat transfer, the solid shell begins to dissolve, and the melting of scrap occurs gradually.

Further, the scrap dissolution is also influenced by the carbon concentration gradient between the scrap and the hot metal. Usually, the carbon concentration in the hot metal is high and encourages the carbon diffusion into the scrap via the natural convective mass transfer. As explained by Guthrie et al, the melting time required for a piece of scrap reduces rapidly with the increasing temperature due to the decreasing liquidus carbon composition with increasing temperature. For example, the melting time required for vertical steel plates and cylinders of about $2.54$ mm thickness at $1480 \, ^{\circ}C$ is about $18s$, $24s$ and $40s$ in baths with a carbon concentration of $5\%$, $4\%$, and $3\%$ respectively. Even though, increasing carbon concentration in the bath reduces the melting time of scrap at a given temperature, the amount by which the melting time is reduced decreases with increasing carbon concentration. Further, at low carbon concentration in the bath, the melting time of scrap vary significantly with the variations of bath temperature.

![Temperature profile of melting of solid steel to liquid steel](image)

Figure 2.10: Temperature profile of melting of solid steel to liquid steel

Thus, the scrap dissolution is affected by the degree of superheating of scrap above the liquidus temperature of the Fe-C solutions, the carbon concentration gradient between the scrap and melt, and the interfacial area between scrap and melt. Therefore, it
is important to ensure all the scrap added is dissolved, to prevent any interruptions to the process such as rebloWS.

There are different models developed for modeling scrap melting during the blow in a liquid steel bath, where melting behaviors of scrap with different geometries were investigated under natural and forced convection. However, in the present study, the model developed by Dogan et al[38] was used. The kinetics model developed by Sethi et al[79] was used by Dogan et al to develop their model, and the assumptions made were as follows[38]:

- The geometry of the scrap pieces was plate shape.
- The carbon concentration of the metal bath was equal to that of the interface.
- The temperature of the bath is relatively higher than the scrap temperature at the interface.
- The heat transfer coefficient is a constant.

The results obtained by Dogan et al[38] are given in Figure 2.11.

![Figure 2.11: Scrap thickness change with time][38]

### 2.1.7.7 Flux dissolution

Fluxes are added to the hot metal bath during the steelmaking process to ensure the removal of oxidized products mainly of P and Si via forming a basic slag, and reducing the corrosive attack on the furnace refractory lining from the slag.[41, 81] To achieve the objectives mentioned above, the added fluxes have to be utilized in full by rapid
dissolution into the melt, and hence the flux dissolution has been the research interest for steelmaking researchers.

The lime dissolution is affected by the saturation of dicalcium silicate (2CaO.SiO$_2$) in the slag, where 2CaO.SiO$_2$ forms a layer around the lime particles when the basicity of slag is less than 2.$^{[41]}$ However, this layer grows in thickness until the FeO content in the slag reaches 20 %wt. Above this limit, the layer does not grow further allowing the dissolution of the lime particle. When the FeO concentration in the slag is less than 20 %wt, it penetrates through the formed 2CaO.SiO$_2$ layer to increase its thickness.

In addition, the dissolution of dolomite is assumed to occur via forming an intermediate compound with the FeO in the slag, which has a low melting point. This intermediate compound forms a layer at the surface or a certain distance deep into the particle by penetrating through the pores in the dolomite particle. CaO and MgO diffuse out of the dolomite particles to the melt, due to the concentration gradient between dolomite and the melt. A 2CaO.SiO$_2$ layer may also be formed between the FeO-rich layer and the molten slag that interrupts the MgO diffusion to the melt, but the layer becomes porous with the increasing MgO concentration in the slag.$^{[41]}

However, the dissolution of fluxes is encouraged by increasing temperature, stirring intensity, FeO concentration, and porosity and by decreasing the size of the particles.$^{[41, 82, 83]}$ Consequently, the complete dissolution of fluxes enhances the lifetime of the refractory lining and efficiently fluxes the impurities out of the melt.

2.1.7.8 Previous kinetics models

High-temperature metal processing including oxygen steelmaking is challenging to be analyzed and controlled while the process is in operation, due to higher temperatures and intense fluid flows involved. Further, oxygen steelmaking process involves multiphase flow (gas, liquid, solid particles and slag/foam) at unsteady state, and the bath is generally inhomogeneous with the oxides produced and the dissolution of added fluxes and scrap. Hence, sampling and analyzing the process is even more difficult, while it is in operation.
The first solution to this problem suggested by steelmaking researchers was to conduct laboratory-scale experiments at room temperatures, usually using air-water systems. Most of these laboratory scale experiments’ findings were insufficient to explain the plant scale operation clearly, and could not be adequately scaled-up to represent the operation of the actual steelmaking converter.

However, the steelmakers have been using different audio and visual parameters to evaluate the progress of the process with their experience from the start of the industry, which was usually specific to the particular plant or shop. Although these empirical models were capable of improving the productivity of the process, those models could not provide any insight into the process, similar to the “Black Box” modeling techniques. But, plant or demographically specific modeling of the process is crucial for the existence of the particular plant in the competitive steelmaking industry.

Nevertheless, analyzing and understanding the process is essential for developing more efficient and productive process routes. Even though the laboratory scale experiments have contributed significantly towards gaining insights into the process, modeling (mathematical or numerical) has proved to be the most efficient mode to accomplish the task of analyzing and understanding the process simultaneously providing means for controlling and optimizing it. A complete mathematical or numerical model developed based on the fundamental physics and chemistry, should be capable of providing insights to the complicated nature of the process, important process variables, and their interconnection. In other words, modeling can make the above mentioned “Black Box” be completely transparent. And these models can often be used for predicting and controlling those key process variables. However, developing a model completely based on the basics of physics and chemistry as such has been a difficult task. Hence, each model developed is a “Grey Box” process model involving a degree of empiricism in it in the form of constants and polynomials. These empirical relationships are extracted from plant scale trials conducted in the steel plants such as the work carried out by Millman et al, Cicotti et al and Farrand et al. Among these plant scale trials, the research work “IMPHOS” by Millman et al monitored and reported the formation and development of the slag/metal emulsion simultaneously with the refining behaviors.
in both the bulk steel bath and the emulsion for 20 heats. This research work was used in the present study for extracting data for simulations and comparison of the simulation results.

The steelmaking models developed over time can be broadly classified into two groups: kinetics models and process models. Kinetics models explain the mechanism of reactions that occur in the converter and evaluate the effect of those reactions on the temperature and the properties of the fluids involved and vice versa.\[45, 68, 93\] However, the well-known complexity and the transient nature of the kinetics involved has led the kinetics modeling a challenging task, which demands more rigorous mathematical approaches as explained by Brooks et al.\[44\] The kinetics model developed by Kitamura et al.\[48\] explained the kinetics of decarburization as well as the oxidation of other elements (i.e. Si, P, Mn, etc.) based on coupled reaction model as illustrated in Figure 2.1. Lytvynyuk et al.\[94\] also developed a BOF model for simulating the kinetics of steelmaking reactions using the coupled reaction model considering both kinetics and thermodynamics of involved phases. The dynamic model developed by Shukla et al.\[37\] based on a fundamental thermodynamic approach was capable of predicting the decarburization behavior in the middle blow period. Also, the decarburization in the emulsion zone, where approximately 60% of decarburization occurs, was modeled by Dogan et al.\[39\] They concluded that the bloating behavior of the droplets in the emulsion significantly affected the decarburization rate, while the size of the droplets and their ejecting angle contributed to their residence time in the emulsion.

Furthermore, the kinetics of decarburization and desiliconization reactions was studied by Blanco and Diaz\[50\] and Taguchi et al.\[95\]. As demonstrated in Figure 2.13, the controlling mechanism of the decarburization reaction changes from the diffusional control to kinetic control with the reduction of carbon concentration. Taguchi et al.\[95\] found that the silicon oxidation occurs in preference to the decarburization, even in the competitive region, until the silicon content in the bath is reduced to about 0.1 %wt. Desiliconization was further analyzed by Ishikawa\[43\] using the coupled reaction model and found that intense agitation and low FeO content in slag encourage silicon oxidation suppressing the carbon oxidation. An experimental study was conducted by Wu et al.\[96\]
on mass transfer of silicon and manganese as an iron drop falls through the slag layer, and observed that the rate of manganese transfer is dependent on the silicon transfer rate. (i.e. when silicon transfer is fast, the transfer of manganese is also fast and vice versa) Further, the most recent work by Rout et al[97] was able to analyze the desiliconization in the top blowing converter using a multi-zone kinetic model. The zones defined were gas-metal, slag-bulk metal and slag-metal-gas, and the highest desiliconisation rate was observed in the slag-metal-gas emulsion due to the increased surface area formed by metal droplets.[97]

Manganese removal from the steel depends on several factors including oxygen potential, slag composition, slag volume and temperature, and is well-known for its removal pattern with the reversion to the bath in the middle of the blow. However, this behavior of manganese removal was further studied by Kawai et al[52] and Takaoka et al[75]. The reaction rate model proposed by Kawai et al[52] consisted of two separate rate constants for oxidation and reduction of manganese and was capable of predicting the manganese content at the end of the blow.

Removal of phosphorus has also gained a considerable attention of steelmaking researchers in the field of kinetic modeling. This is due to the increasing demand for ultra-low phosphorus steel grades and due to the undesired properties like cold shortness imparted by higher phosphorus content.[49, 98] Similar to the demanganization, dephosphorization prefers low temperature, high oxygen potential, and high slag basicity.[51] Monaghan et al[51] investigated the kinetics of dephosphorization and found

**Figure 2.12:** Schematic diagram of the BOF model developed by Kitamura et al[93]

**Figure 2.13:** Carbon oxidation mechanisms[50]
that the rate of dephosphorization is first order with respect to the phosphorus in the metal. The rate and extent of dephosphorization increased with increasing Fe$_2$O$_3$ up to 50% and a further increase in Fe$_2$O$_3$ reduced the rate and extent of dephosphorization.\cite{51} FeO concentration also observed to have a similar impact on the dephosphorization with the critical concentration being 15 to 20 %wt FeO.\cite{49, 99}

Furthermore, Manning and Fruehan\cite{100}, Kitamura et al\cite{93}, Ohguchi et al\cite{101}, Sipos and Alvez\cite{102}, Lee and Fruehan\cite{103} and Ogasawara et al\cite{98} also carried out investigations on the kinetics of dephosphorization. The ongoing research work by Rout et al\cite{104} in analysing the refining reaction kinetics in BOF using a three zone model (i.e. gas-metal, slag-bulk metal and slag-metal-gas zones) has been able to predict the refining of C, Si, and Mn, and is currently focussed on modelling dephosphorisation using the same three-zone model. However, slag composition tends to change at least slightly from heat to heat, and these unpredictable variations cause deviations in the extent of dephosphorization.\cite{99} Hence, Urban et al\cite{105} concluded that dephosphorization models should be plant specific, because, developing an entirely global model is not possible with the available knowledge. Since the steelmaking reaction kinetics are yet to be fully explained based on the basics of physics and chemistry, a degree of empiricism is used in these models as mentioned earlier.

In addition to the investigations of reaction kinetics of elements in the bath as explained before, the kinetics of scrap melting and flux dissolution also has been the focus of steelmaking researchers. Among those research works on flux dissolution, the work carried out by Satyoko and Lee\cite{81} on investigating the dissolution mechanisms of dolomite and doloma in a model basic oxygen furnace slag, experimental work by Hamano et al\cite{106} on measuring the dissolution rate of lime in several different slags at hot metal temperatures, investigation of the effect of lime particle size on the melting behaviour of lime by Yang et al\cite{83} and the research work by Li et al\cite{107} on the lime dissolution in BOS slag under varying conditions from laboratory experiments to industrial converter, can be shown as examples. On the other hand, the research works on scrap melting kinetics include the work carried out by Li et al\cite{42}, which was focussed on the effect of sizes, shapes and initial temperatures of added scrap on its melting rate,
and the work carried out by Guthrie et al\cite{80} focused on the sizes of scrap added on its melting rate.

The process models explain the steps of the process and how they are to be performed. Further, these models provide information on the behavior of important process variables such as temperature, concentration of the elements and compounds, and slag foam height, over the total blow time. Accordingly, these models allow a better understanding of the process leading to the innovation of more efficient and productive process routes. Different process models can be found in the literature, and following are some examples. The dynamic model developed by Deo et al\cite{108} for computer simulation and control of the steelmaking was based on the multicomponent mixed transport control theory with the incorporation of energy balance calculations. Kattenbelt and Roffel\cite{109} developed a dynamic model for the main blow using the step response data of decarburization rate and the accumulation rate of oxygen to the step changes in the oxygen blowing rate, lance height, and iron ore addition rate. A process model for oxygen steelmaking was also developed by Li et al\cite{110} based on the bath mixing degree. The comprehensive oxygen steelmaking model developed by Dogan et al\cite{38-40} included sub-models for the kinetics of scrap melting, flux dissolution, slag chemistry, the temperature profile of the system, formation and residence of metal droplets in the emulsion and kinetics of decarburization reaction in different reaction zones. Guo et al\cite{46} and Sarker et al\cite{111} developed BOF process models to simulate the composition and temperature changes of slag and metal, where the model developed by Guo et al\cite{46} was aimed mostly at improving the plant operation. Apart from these, several process models can be found in the literature on scrap melting and flux dissolution in oxygen steelmaking. The research work carried out by Guthrie and Stubbs\cite{80} was on developing a mass transfer model to predict the time consumption of various sized scrap additions to melt when added to the pig iron bath, while the most recent work carried out by Kruskopf\cite{77} was also focussed on calculating the melting pattern of scrap added to the hot metal bath. Also, the dissolution rate of fluxes (i.e. lime and dolomite) throughout the blow was mathematically modeled by Dogan et al\cite{68}, where the dissolution rates were predicted as a function of saturation concentration of CaO and MgO in the slag, CO gas flow rate and the physical properties of the slag.
Yet, modeling of the oxygen steelmaking process is continuous and need more work to
optimize the process regarding the quality, quantity and the variety of the output,
energy consumption, environmental concerns, and flexibility. This is because of the
increasing demand for the improved steel qualities and new steel grades for industries
such as automotive industry. Reducing the capital cost of the steelmaking process to be
competitive has also been a motivation for optimizing the process through modeling.\cite{13, 62, 63}

Even so, there is still a growing need for dynamic models that are capable of predicting
the behavior of key process variables with time over the blow. Therefore, the present
work was aimed at developing a dynamic process model to predict the behavior of the
concentration of elements in the bath and the slag foam height with time over the blow.
As mentioned earlier, semi-empirical submodels and constants were used in the present
study to reduce the complexity of the programming required in the simulations.

2.2 Slag foaming

2.2.1 Slag formation

Slag is the non-metallic material formed by the oxides of elements in the molten metal
(i.e. SiO$_2$, P$_2$O$_5$, MnO, and FeO) and the added fluxes (i.e. Lime and dolomite). Slag may
also contain the oxide compounds, dissolved gases, dissolved refractory lining and solid
particles of undissolved fluxes or precipitated oxides/oxide compounds. The evolution
of slag composition is illustrated in Figure 2.14. Even though the general output of slag
from different steel industries was traditionally between 100 to 150 kg/ton of steel
output, this quantity has been reduced to about 60 kg/ton of steel output nowadays due
to the better understanding of slag formation mechanisms.\cite{58, 112} Slag has a low density
and thus floats on the liquid metal. The main requirement of a slag in the steelmaking
converter is to operate as a pool for the oxides of the oxidized and removed impurities
to collect. Further, the composition and temperature of this slag pool assist the progress
of refining reactions in the converter. The other advantages of having a slag layer in the
operating converter comprise of shielding the metal bath from the ambient air,
retarding the dissolution of the refractory lining of the converter, and controlling the
bath temperature.\cite{8}
Although the common variation of slag composition in the oxygen steelmaking process is as shown in Figure 2.14, the composition of the slag is determined by the slag path of the process. The slag path varies from one plant to another depending on their BOF practice including nature of the blowing (i.e. top, bottom and combined) and flux addition characteristics. For example, four slag paths reported for CaO-FeO-SiO$_2$ slags are plotted in Figure 2.15. It can be observed that at the beginning of the blow, iron and other impurities in the bath are oxidized by the injected oxygen, forming the oxides. Since desiliconization dominates initially in the blow, the slag path starts with high silica content. Accordingly, the acidity of the slag is high, and the dissolution of added fluxes is encouraged. As the oxygen blowing progress, Si gets oxidized almost completely, and the decarburization accelerates reducing the FeO content in the slag. However, it is evident from Figure 2.15 that the sequence and extent of the composition change are generally specific to the plant due to the reasons mentioned previously.

The composition of the slag in a low alloy steelmaking process varies within the ranges specified in Table 2.1 based on the end carbon content required. However, the combined mass of the oxides CaO, MgO, FeO and SiO$_2$ accounts for about 88% – 92% of the total slag mass.
Table 2.1: Typical composition of the slag in a low alloy steelmaking process\textsuperscript{[64]}

<table>
<thead>
<tr>
<th>Slag component</th>
<th>Weight %</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaO</td>
<td>40 – 60</td>
</tr>
<tr>
<td>MgO</td>
<td>4 – 8</td>
</tr>
<tr>
<td>MnO</td>
<td>3 – 8</td>
</tr>
<tr>
<td>FeO (Total)</td>
<td>5 – 35</td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>10 – 28</td>
</tr>
<tr>
<td>P$_2$O$_5$</td>
<td>1 – 3</td>
</tr>
<tr>
<td>Al$_2$O$_3$</td>
<td>1 – 2</td>
</tr>
<tr>
<td>CaF$_2$</td>
<td>0 – 2</td>
</tr>
<tr>
<td>S and other oxides</td>
<td>0.1 – 0.2</td>
</tr>
</tbody>
</table>

2.2.2 Slag structure

Slags are ionic materials in nature and consist of cations and anions. The anions are the negatively charged complex ions such as silicates, aluminates, and phosphates, which are capable of forming network-like structures, and the cations are the positively charged ions provided by the metal oxides. Silica is the most abundant oxide in the steelmaking slag during first few minutes into the blow and has silicate tetrahedron (SiO$_4^{4-}$) as its fundamental building unit both in its crystal and molten states\textsuperscript{[114]} as illustrated in Figure 2.16. At this bonding status, each silicon atom is bonded to four oxygen atoms, and each oxygen atom is bonded to two silicon atoms, resulting in 4 negative charges per unit silicate tetrahedron.\textsuperscript{[4, 64, 115]} This fundamental unit polymerize together by bridging oxygen ions to form complex anions such as Si$_2$O$_7^{6-}$ and Si$_3$O$_{10}^{8-}$. Thus the degree of polymerization increases with the increasing silica content in the slag, which increases the viscosity consequently.\textsuperscript{[116]} This structural information on slag is more available recently with the use of techniques such as X-ray and neutron diffraction, vibrational spectroscopy (e.g. FT-IR (Fourier transformed infra-red), Raman) and nuclear magnetic resonance.\textsuperscript{[115, 117]}
With the progress of the blow, the metal oxides (i.e. FeO, CaO, and MgO), which are basic in nature, accumulate in the acidic silica slag. This addition of basic metal oxides has the potential to break down the silica network, and the resulting depolymerized silica network in the slag is schematically represented in Figure 2.17. In this resultant structure, the amount of free oxygen increases with the increasing atom ratio O/Si, and when the slag becomes highly basic, (i.e. MO/SiO$_2$ > 2), the network completely breaks down to individual SiO$_4$ tetrahedrons intermixed with cations M$^{2+}$ and some oxygen ions O$^{2-}$. Therefore, the degree of depolymerization increases with the addition of cations, and the slag viscosity reduces accordingly. Amphoteric oxides such as Al$_2$O$_3$ and Fe$_2$O$_3$ may operate as network modifiers/formers or breakers depending on their composition in the slag. This structure of slag and its evolution affects the physical properties of slag during the blow and is discussed in the following section.

### 2.2.3 Slag physicochemical properties

#### 2.2.3.1 Density

The density of slag plays a vital role in producing the slag metal emulsion and slag foam. Slag floats on the liquid metal due to its less density compared to the density of the hot metal. This assists the separation of steel from the slag at the tapping stage of the process. Silica, which is the major component in the slag during the first few minutes into the blow, has a very low density compared to the other metal oxides encountered in steelmaking. So the density of a slag decreases with the increase of its silica content, as illustrated in Figure 2.18. Further, it can be observed from Figure 2.18 that with the
addition of other oxides such as FeO, MgO, CaO and MnO, the density of the slag tends to increase. Further, the density is generally considered to be decreasing with the increasing temperature.

**Figure 2.18: Densities of binary silicate melts**

### 2.2.3.2 Viscosity

The viscosity of a slag is an important physical property, and it is an indication of its internal friction or the extent to which the relative motion of adjacent liquid layers is retarded.\(^{114}\) Stability of the slag foam by retarding the bubble film drainage and reducing the slag attack on the refractory lining is encouraged by increasing viscosity\(^{113}\), even though the formation of metal droplets and their escape to the emulsion are discouraged by increasing viscosity.\(^{118}\) Viscosity is directly and strongly related to the structure of the slag.

**Figure 2.19: Viscosity (Ns/m\(^2\)) of CaO-FeO-SiO\(_2\) melts at 1400 °C**\(^{64}\)

Figure 2.19 illustrates the viscosity of CaO-FeO-SiO\(_2\) slag at 1400 °C. It is evident that the viscosity of the slag increases with increasing SiO\(_2\) and reduces with increasing FeO. The other major factors affecting the slag viscosity are the temperature and the presence of solid particles in the slag. The presence of solid particles such as undissolved fluxes and
precipitated slag particles tends to increase the viscosity of the slag, while, the increase in temperature decreases the viscosity of slag exponentially.\textsuperscript{[119]} Information on the viscosity of slags is essential in optimizing the metallurgical processes, which can be either empirical measurements or theoretical estimations. Some of the widely used models are Urbain model, Riboud model, Iida model and KTH model.\textsuperscript{[120]}

### 2.2.3.3 Surface tension

![Surface tension change with the addition of different elements to liquid iron\textsuperscript{[121]}](image1)

Figure 2.20: Surface tension change with the addition of different elements to liquid iron\textsuperscript{[121]}

![Surface tensions of binary iron oxide melts at 1400 °C\textsuperscript{[64]}](image2)

Figure 2.21: Surface tensions of binary iron oxide melts at 1400 °C\textsuperscript{[64]}

The surface tension of a liquid exists because of the cohesive forces exerted on the molecules on the liquid surface by other molecules in the liquid. Consequently, surface tension is responsible for the formation of droplets and for retarding the liquid molecules from escaping the liquid. In the case of BOS process, the formation of slag/metal emulsion and foam is affected by the slag surface tension. Furthermore, the mass transfer between slag and metal is also affected by the slag surface tension to a significant extent.\textsuperscript{[113]} The surface tension of pure liquid iron is about 1.8 N/m at 1823 K, which is about 25 times larger than that of water. Conversely, the surface tension of pure liquid oxides and slags are very low, ranging between 0.20 N/m and 0.70 N/m.\textsuperscript{[121]}

The surface tension of slags tends to vary with the temperature and the composition of the slag. Effect of additions of different non-metals on the surface tension of liquid iron
is illustrated in Figure 2.20, and it is evident from the figure that the non-metals such as S, O, N and P, are surface active with different strengths in liquid iron.\textsuperscript{[121]} On the other hand, the effect of the accumulation of different oxides on the surface tension of liquid FeO is shown in Figure 2.21. It is evident that the oxides including SiO\textsubscript{2}, P\textsubscript{2}O\textsubscript{5}, and MnO, decrease the surface tension of the slag, while Al\textsubscript{2}O\textsubscript{3} slightly increases the surface tension.\textsuperscript{[64]}

### 2.2.3.4 Interfacial tension

![Interfacial tension between metal and slag](image)

Interfacial tension between metal and slag is also an important factor in the steelmaking process, similar to the surface tension. Therefore, the interfacial tension affects the formation of metal/slag emulsion and mass transfer between metal and slag similar to the behavior of surface tension.\textsuperscript{[121, 122]} When the interfacial tension at the slag/metal interface is low, the refining process is encouraged via assisting the interfacial mass transfer and foam/emulsion formation, which is advantageous. However, low interfacial tension may also encourage the entrapment of slag droplets by the liquid metal, and the strong adhesion between the slag and the metal, which makes the physical separation of slag from metal more difficult at the tapping stage.\textsuperscript{[113]}

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**Figure 2.22:** Effect of added elements to liquid iron on its interfacial tension\textsuperscript{[121]}

**Figure 2.23:** Effect of added oxides on the interfacial tension of CaO-SiO\textsubscript{2}-Al\textsubscript{2}O\textsubscript{3} slag\textsuperscript{[121]}
As illustrated in Figure 2.22, various elements added to the liquid iron exert different levels of influence on the interfacial tension between the liquid metal and slag. In general, almost all of the added elements decrease the interfacial tension of liquid iron. In steelmaking processes, O and S are considered to be the strongest surface active elements in metal, which decreases the interfacial tension remarkably.\textsuperscript{[121]} Moreover, FeO and MnO are considered to be the surface active oxide components in slag which reduces the interfacial tension between the metal and slag\textsuperscript{[121]} as shown in Figure 2.23.

### 2.2.3.5 Basicity

According to the general concept of acids and bases, the electron acceptors are the acids, while the electron donors are the bases. In the case of oxide melts, the same concept is applied to categorize oxides, and can be expressed as; the donors of $O^{2-}$ ions are basic oxides, and the acceptors of those ions are acidic oxides.\textsuperscript{[123]} For example, when the basic oxide CaO and the acidic oxide SiO\textsubscript{2} are mixed, the neutralization occurs as given below:\textsuperscript{[123]}

\[
\text{Base} \quad \text{CaO} = \text{Ca}^{2+} + O^{2-} \\
\text{Acid} \quad \text{SiO}_2 + O^{2-} = \text{SiO}_3^{2-} \\
\text{CaO} + \text{SiO}_2 = \text{Ca}^{2+} + \text{SiO}_3^{2-}
\]

The traditional method of representing the basicity of a steelmaking slag is by calculating the mass concentration ratio of CaO and SiO\textsubscript{2} and is given by the equation 2.3.\textsuperscript{[64]}

\[
\text{Basicity}(V) = \frac{\% \text{CaO}}{\% \text{SiO}_2} \quad \text{Eq 2.3}
\]

Since the basicity measures the relative basicity or acidity of a slag mixture, it can also be expressed as the difference between the sum of concentrations of basic oxides and acidic oxides as expressed below.\textsuperscript{[64]}

\[
\text{Basicity}(V) = \left( \% \text{CaO} + \% \text{MgO} + \% \text{MnO} \right) - \left( \% \text{SiO}_2 + \% \text{P}_2\text{O}_5 + \% \text{TiO}_2 \right) \quad \text{Eq 2.4}
\]

This expression for basicity can vary according to the composition of the slag under investigation. Moreover, when there are undissolved CaO and MgO particles present in the slag, which is common for steelmaking slags, the basicity calculation needs to be carried out with extra caution.\textsuperscript{[64]}
As explained previously, the calculation of the basicity of a slag considers the presence of only a few major oxides. This limitation was overcome by considering the optical basicity of the slag, which was first proposed by Duffy and Ingram.\textsuperscript{[123]} Although optical basicity was first introduced for normal metal oxides, this parameter is now extensively used for predicting other parameters of interest of oxide melts/slags. In the calculation of optical basicity of a slag, calcium oxide is defined as the anchor point with an optical basicity value of 1.0, and the other oxides are assigned a numerical value for their optical basicity based on that.\textsuperscript{[124]} Accordingly, the optical basicity of the slag is calculated as a function of its composition as given by equation 2.5.\textsuperscript{[124]}

$$\Lambda = \Lambda_1 X_1 + \Lambda_2 X_2 + \ldots$$ \hspace{1cm} \text{Eq 2.5}

Where the $\Lambda_i$ is the optical basicity of the pure oxide $i$, and $X_i$ is the equivalent fraction of oxide $i$.

Another method for measuring basicity is the NBO/T or Non-Bridged Oxygen per tetrahedrally coordinated atom which is calculated using the slag structure revealed via techniques such as FT-IR (Fourier Transformed Infra-Red) and Raman spectroscopy.\textsuperscript{[115, 119]}, which is given by the following equation 2.6\textsuperscript{[125]}:

$$\frac{NBO}{T} = \sum 2\left( X_{MO} + X_{M_2O} - X_{Al_2O_3} \right) / \left( X_{SiO_2} + 2X_{Al_2O_3} \right)$$ \hspace{1cm} \text{Eq 2.6}

Where $X_{MO}$ and $X_{M_2O}$ are the metal oxides (e.g. CaO and Na$_2$O).

A higher value of NBO/T indicates that the slag consists of higher free oxygen (O$^{2-}$) count, which means that the slag is higher in basicity. Further, NBO/T is an indication of the extent of depolymerization of the slag structure, because, an increase in free oxygen (O$^{2-}$) at higher NBO/T will interact with bridged oxygen to form more NBOs, breaking down the network structures in the slag.\textsuperscript{[117]}


## 2.2.3.6 Other properties

Other properties of steelmaking slags that are of significant importance are mass diffusivity, electrical conductivity, and thermal conductivity.

In the molten slags, mass diffusion occurs via ions, and hence mass diffusivity is a function of the ionic diffusivities, which are measured by dissolved radioactive tracer elements in an oxidized form in the melt. In order to maintain the electroneutrality, diffusion of a cation is accompanied by the diffusion of an oxygen ion.\[^{64}\]

The electrical conductivity of slags is also an important property, as it is closely related to the structure of the slag. Electrical conduction in a slag is dominated by the movement of ions, and increase with the increasing temperature. The electrical conduction mechanism changes from ionic conduction to electronic conduction when the concentration of FeO or MnO is greater than 70%. Cations in the slag are the major contributors to the electrical conduction, while the anion complexes form obstructions to the movement of cations. Hence, it is observed that the electrical conductivity is dependent upon the network breaking capacity of the cations for silicate slags.\[^{113}\]

Thermal conductivity is also an important physical property of slags. The thermal conductivity of slags and mould fluxes are in the range of 0.5 W/mK to 1.2 W/mK.\[^{64}\]

## 2.2.4 Slag foaming literature

Slag foam is formed when the gases injected and generated by the refining reactions are trapped by the slag during the process. This phenomenon of slag foaming is also observed in other ferrous pyro-metallurgical processes such as open hearth process, hot metal pre-treatment practices (i.e. desiliconization, dephosphorization) and some non-ferrous smelting processes such as copper making as well.\[^{126}\]

For slag foams, the amount of gas trapped by the slag is measured by the void fraction or the gas fraction, and the void fraction generally varies between 0.7 to 0.9.\[^{26}\]

Figure 2.24 illustrates a typical foam column with different foam layers according to the void fraction. The combined effect of evolving physical properties of slag during the blow is in favor of foam stabilization, and when coincided with the high rate of decarburization in the first half of the blow, the volume of the slag foam increases rapidly.\[^{126}\]
Slag foaming is beneficial as it assists the refining process in different means, for example, by providing an increased surface area for refining reactions, protecting the molten metal bath from the direct contact of the atmosphere, protecting the refractory lining from extreme combustion effects and forming the medium for post-combustion and heat transfer. On the other hand, slag foaming can become disadvantageous and hazardous when formed in massive quantities, and overflow from the mouth of the vessel, which is termed slopping of the bath. The consequences of these slopping events include loss of yield, interruptions to the continuous production, environmental pollution, health and safety costs and damage to fume hoods and vessel mouths. Conversely, if slag foaming is prevented or limited to subtle amounts, the dust generation and heat loss from the vessel via radiation tend to increase.

Traditionally, it is the responsibility of the operator to visually monitor the converter, and exercise necessary corrective actions to prevent any hazardous slopping events. Since it is of great importance to drive the process without any interruptions for a yield with requisite quality and quantity, the need to suppress slag foam is significant. Therefore, understanding and modeling slag foaming have been the research interest of steelmaking researchers, resulting in different empirical studies, and modeling and predicting efforts. This section discusses the available literature on slag foaming briefly.

Fruehan and his colleagues carried out a significant work on investigating slag foaming using laboratory experiments and expressed the findings in terms of the foaming index. However, a considerable level of understanding was available on foaming of...
slags at the time of these works by Fruehan et al. Kitchener and Cooper had explained the foaming and factors of influence on the stability of foam including the viscosity and surface elasticity in their review.\cite{14} Further, it was understood by that time that the slopping occurs due to two main factors: 1. The evolution of slag with the characteristics such as low basicity, high viscosity and low surface tension, 2. Decarburization encouraged by high bath temperature and increased iron content in slag.\cite{127, 128}

However, in the present review, the work carried out by Fruehan et al\cite{15-18} is used to summarize the effect of physical properties on slag foaming.

The effect of slag composition on its foaming was experimentally studied by Ito and Fruehan\cite{15}, using a CaO-SiO$_2$-FeO slag in the temperature range of 1250 °C to 1400 °C. The slag was contained in an alumina crucible, and Ar gas was injected to foam the slag. The observed results on the effect of different parameters on the slag foaming were expressed using foaming index (Σ), which was first used by Bikerman for aqueous systems.\cite{17} The foaming index has the meaning of average traveling time of gas through the foam layer\cite{15} and can be expressed by equation 2.7. The foaming index was observed to change between 0.3s to 56s for metallurgical slags with different compositions.\cite{23}

\[
\Sigma = \frac{\Delta h}{\Delta V_g^s} \quad \text{Eq 2.7}
\]

\[
V_g^s = \frac{Q_g}{A} \quad \text{Eq 2.8}
\]

Where $Q_g$ is the gas flow rate, $A$ is the cross-sectional area of the container, $\Delta h$ is the change of slag height, and $V_g^s$ is the superficial gas velocity. The above relationship was considered to be valid when the void fraction of the foam is independent of foam height. The extent of slag foaming has since been defined frequently by using the foaming index.

Another method of calculating the foaming index was proposed by Lahiri and Seetharaman\cite{27} which can be expressed as follows.

Rate of change of foam volume = Rate of gas generation or injection – Rate of volume change due to bubble rupture
Therefore, the foaming index given by equation 2.7 can also be expressed in the following form.

\[
\Sigma = \frac{1}{k\epsilon}
\]  
Eq 2.9

Where, \(k\) is the rate constant for bubble decay, and \(\epsilon\) is the average void fraction.

However, the foaming index as defined by Fruehan and co-workers and Lahiri and Seetharaman is for a steady state system, which has an almost constant gas flow rate and chemical composition. However, in order to explain the foaminess of oxygen steelmaking slag, a dynamic foaming index which takes into account the dynamic nature of the gas generation and the slag composition, was proposed as follows.\[^{[11]}\]

\[
\Sigma_d = f_r \Sigma
\]  
Eq 2.10

\[
f_r = \frac{\text{Rate of gas generation} + \text{Rate of change of slag volume}}{\text{Rate of change of slag volume}}
\]  
Eq 2.11

The foaming index is a property of the slag that changes with time throughout the blow (goes through a maximum) as illustrated in Figure 2.25.\[^{[65]}\]

Figure 2.25: Foaming index estimation over blow time for a completely liquid slag and a slag with free lime particles\[^{[65]}\]

The foaming index was then related to the physical properties of slag through dimensional analysis by Jiang and Fruehan.\[^{[16]}\] At the start of the analysis, the foaming index was assumed to be a function of all the variables and dimensional constants which may affect it.
\[ \Sigma = f(\rho, \mu, \sigma, g) \]  

\text{Eq 2.12}

Where \( \Sigma \) is the foaming index (s), \( \rho \) is the liquid slag density (kg/m\(^3\)), \( \mu \) is the slag viscosity (kg/ms), \( \sigma \) is the slag surface tension (kg/m\(^2\)), and \( g \) is the gravity (m/s\(^2\)).

Then two dimensionless groups were formed, and the dimensional analysis was carried out on them. The results of the analysis were the following two dimensionless numbers.

\[ \Pi_1 = \frac{\Sigma g \mu}{\sigma} \]  

\text{Eq 2.13}

\[ \Pi_2 = \frac{\rho \sigma^3}{\mu^4 g} \]  

\text{Eq 2.14}

The final relationship obtained between the foaming index and the physical properties of the slag was as below.

\[ \Sigma = 108 \frac{\mu}{\sqrt{\rho \sigma}} \]  

\text{Eq 2.15}

According to the above relationship, it is evident that the foaming index increased with the increase of slag viscosity, while it is decreased with the increase of density and the surface tension of the slag. This relationship between the foaming index and the physical properties was modified later by different researchers, and Table 2.4 summarizes some of those relationships. A further discussion on the effect of different factors including the chemical composition, interfacial characteristics, rheology and the temperature of slag on the extent of slag foaming is presented in the following subsections.
Table 2.2: Different expressions on the relationship of foaming index with the slag physical properties

<table>
<thead>
<tr>
<th>Authors</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Zhang and Fruehan[18]</td>
<td>$\Sigma = 115 \frac{\mu^{1.2}}{\sigma^{0.2} \rho D_b^{0.9}}$, where $D_b$ is the bubble diameter.</td>
</tr>
<tr>
<td>2. Ghag et al[20]</td>
<td>$\Sigma = 1 \times 10^6 \left( \frac{\mu E_{eff}}{(\rho g)^2 d^4} \right)$, where $E_{eff}$ is the effective elasticity.</td>
</tr>
<tr>
<td>3. Lotun and Pilon[29]</td>
<td>$\frac{H}{r} = 2617 \frac{\mu^{0.73}}{\rho^{1.74}} \frac{L^{0.79}}{g^{1.77}} r^{3.51}$</td>
</tr>
<tr>
<td></td>
<td>Where $r$ is the average bubble radius, and $j_r$ is the reduced superficial gas velocity.</td>
</tr>
<tr>
<td>4. Stadler et al[22]</td>
<td>$\Sigma = K \frac{\mu^{0.704}}{g^{0.574}} \frac{L^{0.250}}{\rho^{0.278}} \frac{D^{0.426}}{U^{0.603}} \frac{U^{0.353}}}$</td>
</tr>
<tr>
<td></td>
<td>Where $L$ is the liquid depth, $D$ is the column diameter, and $U$ is the gas velocity.</td>
</tr>
</tbody>
</table>

2.2.4.1 Effect of superficial gas velocity on slag foaming

Jiang and Fruehan[16] measured the effect of superficial gas velocity on the foaming of CaO-SiO₂-FeO slag, where the foam was produced by injecting Ar gas. They observed that the foam height increased linearly with the increasing superficial gas velocity as illustrated in Figure 2.26. This observation was also captured by the dimensional analysis carried out by Lotun and Pilon as mentioned in Table 2.4.
In the smelting reduction processes, the converters operate around 0.3 to 3.0 m/s of superficial gas velocities. As explained by Zhu et al\cite{26}, the foam observed at low superficial gas velocities is different to that observed at high gas velocities. The foam at high superficial gas velocity (i.e. >1 m/s) is the expanded slag as shown in Figure 2.27, where the entire volume of liquid is expanded uniformly in a turbulent and churning method. The mixture height and the void fraction of this expanded slag increase with increasing superficial gas velocity, and it collapses immediately with the stopping of the gas flow. Conversely, the foam produced at low superficial gas velocities (i.e. 0.01 m/s to 0.1 m/s) is like beer or soap foam, and this foam collapses gradually with the stopping of the gas flow. Although the experimental studies carried out by Fruehan and co-workers were at low superficial gas velocities, it was found that those predictions were valid for higher superficial gas velocities typical for smelting reduction processes, when there are no undissolved oxides which alter the viscosity of the slag\cite{26}.

On the other hand, Gou et al\cite{24} suggested that the foaming at such higher superficial gas velocities as encountered in oxygen steelmaking (i.e. >1 m/s), the liquid is held up by the gas flow. It is argued that in this situation the void fraction strongly depends on the superficial gas velocity, while weakly dependent on the physical properties of slag and liquid. Further, formation and existence of this gas hold up are governed by the gravity and the drag forces on the liquid exerted by the gas\cite{24}.
2.2.4.2 Effect of slag composition on slag foaming

The composition of slag is one of the most important factors that affect its foaming\textsuperscript{[124]}, which evolves throughout the blow, generally, in favor of foaming. This owes to the fact that the physicochemical properties of slag such as the density, viscosity, surface tension, and basicity, vary with the composition of the slag. Thus, in this section, the observations on the effect of slag composition on the extent of foaming are presented briefly, and a detailed discussion is provided in the following sections.

As illustrated in Figure 2.28, the addition of $P_2O_5$ slightly decreased the foaming index, while the addition of $S$ marginally decreased the foaming index. The foaming index was found to decrease with the addition of $CaF_2$ significantly, while it has increased notably with the addition of $MgO$. These observations were made for a $CaO-SiO_2-FeO$ slag at 1673 K, where the Ar gas injection produced the foam.\textsuperscript{[15]} In this experiment, $\Sigma_0$ is the foaming index with no additives. In the same series of experiments, the authors observed that the foaming index increased with the increasing particle concentration as shown in Figure 2.29. In this experiment, $2CaO.SiO_2$ or $CaO$ particles were added to the slag for measuring its effect, and the $\Sigma_0$ was the foaming index with no second-phase particles.\textsuperscript{[15]}

The effect of the addition of $FeO$ and $MgO$ on the foaming index of $CaO-SiO_2-FeO-MgO$ slag was studied by Jung and Fruehan,\textsuperscript{[17]} and are illustrated in Figures 2.30 and 2.31.
The foaming index was observed to decrease with increasing FeO content up to about 20% of FeO mass in the slag and then stayed constant up to a mass concentration of about 32% FeO in the slag.\cite{17, 129} MgO addition also exhibited a similar trend to that of FeO by decreasing the foaming index with its addition to a 35%CaO-35%SiO\textsubscript{2}-30%FeO slag.\cite{17}

When analyzing the foaming index evolution with the composition of slag, the effect of the addition of MnO and P\textsubscript{2}O\textsubscript{5} on the foaming index is also worth considering. Figures 2.32 and 2.33 show the effect of MnO and P\textsubscript{2}O\textsubscript{5} addition to the CaO-SiO\textsubscript{2}-30FeO-MgO\textsubscript{satd} slag respectively. It was observed by Kim et al\cite{130} that the foaming index slightly decreased with increasing MnO in the slag, while it increased with the addition of P\textsubscript{2}O\textsubscript{5} up to 3% and then decreased with the further addition of P\textsubscript{2}O\textsubscript{5}.
2.2.4.3 Effect of temperature on slag foaming

Increasing the temperature of slag was observed to decrease the foam index of 35%CaO-35%SiO$_2$-30%FeO-10%MgO slag during the experiments carried out by Jung and Fruehan\cite{17} in the temperature range of 1673 K – 1823 K.

This observation can be attributed to the positive temperature coefficient of surface tension and the negative temperature coefficient of viscosity. The effect of surface tension and the viscosity on the foaming of the slag is such that increase in surface tension destabilizes the foam while the increase in viscosity stabilizes the foam. Therefore, the combined effect of the above two properties reduces the foaming index with the increase of temperature.\cite{17,65}
2.2.4.4 Effect of bubble size on slag foaming

The common observation was that the slag foaming is inversely proportional to the size of the bubbles. In other words, a foam consisting of larger bubbles collapses earlier compared to that consists of smaller bubbles.\[9, 20\] This observation was put under investigation by Zhang and Fruehan\[18\] by injecting Ar gas through a multi-orifice nozzle into a bath smelting type slag. They also studied the foaming of the same slag by the bubbles generated from interfacial reactions. The average bubble diameter of bubbles produced from the single orifice nozzle was 13.5 mm, while that from the multi-orifice nozzle was about 7.5 mm, and the measured foam height when the gas injection was through the multi-orifice nozzle was about 70% greater than that measured when the gas injection was through a single orifice nozzle. The bigger bubbles produced from injecting Ar gas through the single orifice nozzle were of polyhedral shape. However, when the bubbles were produced from the CO generated by the interfacial reactions, the bubbles were observed to be fine spherical gas bubbles, and the foam produced was comparatively more stable.\[9\] However, in both cases, the size of bubbles was inversely proportional to the foaming index\[18\] as illustrated in Figure 2.35.

![Figure 2.35: Effect of bubble diameter on the foaming index\[18\]](image1)

![Figure 2.36: Example of approximated transfer area of plateau border\[131\]](image2)

This observation was explained by the fact that increasing bubble size increases the drainage.\[18\] According to the expression on drainage velocity given by equation 2.16\[131\], it is evident that the transversal area of the plateau borders as shown in Figure 2.36 affects the drainage velocity. In other words, the transversal area is larger for larger
bubbles increasing the drainage compared to that for smaller bubbles as indicated by the equation 2.17.\[131\]

\[
\dot{x}_g = \frac{g \rho A_{plateau}}{\eta} \left[ 1 - \exp \left( -\frac{\eta}{\rho A_{plateau}} t \right) \right] 
\]

Eq 2.16

Where \( g \) is the gravity, \( \rho \) is the slag density, \( A_{plateau} \) is the transverse area of the plateau border, \( \eta \) is the kinematic viscosity and \( t \) is the time.

\[
A_{plateau} = r^2 \left( \frac{1}{3} \frac{\pi}{2} \right), \text{ where } r \text{ is the bubble radius.} 
\]

Eq 2.17

This influence of bubble diameter on the foaming index was addressed in the dimensional analysis carried out by all the authors mentioned in Table 2.4. All those expressions show the inverse proportionality between the bubble size and the foaming index, despite the different degree of influence. However, in oxygen steelmaking, the slag foam is primarily produced by trapping CO gas in the slag layer, and in this case, the rate and quantity of CO production, turbulent fluid flow, and surface tension are the primary effects on the size of the bubbles.

### 2.2.4.5 Effect of slag basicity on slag foaming

The experiments carried out by Ito and Fruehan\[^{15}\] on CaO-SiO\(_2\)-FeO slags to investigate the factors that affect foaming, also focused on the effect of basicity of the slag on its foaming. The basicity of slag was calculated using the equation 2.3. The observations are presented in Figure 2.37, and it is clear that the foaming index goes through a minimum with increasing basicity.\[^{23, 130}\] Initial decrease of the foaming index with the increasing basicity is due to the decreasing viscosity and increasing surface tension, which have a negative effect on the foaming index. The CaO composition at the minimum foaming index refers to that of the liquidus composition, which will precipitate if exceeded. Therefore, after the liquidus composition, further addition of CaO precipitate as solid 2CaO.SiO\(_2\) particles, increasing the viscosity and thereby stabilizing the foam.\[^{15}\]
2.2.4.6  Effect of slag density on slag foaming

Density is another important physical property, which has a considerable effect on the foaming of slags. As illustrated in Figure 2.38 and Figure 2.18, the density of slags increases with the accumulation of slag components like FeO, MnO, and MgO, and decreases with the increasing SiO$_2$ and temperature.$^{[21, 22]}$ Consequently, the foaming index decreases with the accumulation of FeO, MnO, and MgO, and increases with increasing silica content in the slag. Further, FeO is also considered capable of lowering the viscosity with its increasing content in the slag. This inverse proportionality between the foaming index and the slag density is better explained by the dimensional analysis carried out by the authors given in Table 2.4. It is evident from these expressions that foaming index reduces with increasing slag density, despite the different degree of influence found by the authors.$^{[18, 20, 22, 29]}$

Figure 2.38: Estimated densities of CaO-SiO$_2$-FeO slags at 1823 K$^{[21]}$
2.2.4.7 Effect of slag viscosity on slag foaming

Slag viscosity and its evolution during the blow also play a significant role in slag foaming. As discussed in Section 2.2.3.2, the viscosity of a slag is primarily governed by the network formers like $\text{SiO}_2$, and the addition of metal oxides, such as $\text{FeO}$, $\text{MgO}$, $\text{MnO}$, and $\text{CaO}$, breaks the network structures and reduces the slag viscosity.

![Estimated viscosities of CaO-SiO$_2$-FeO slags at 1823 K](image)

Figure 2.39: Estimated viscosities of CaO-SiO$_2$-FeO slags at 1823 K$^{[21]}$

It is the common observation that the slopping occurs in the first few minutes of the blow during the oxygen steelmaking process. This is because of the increasing slag viscosity due to lower temperature and the presence of undissolved lime particles at the beginning of the process, simultaneously with the high rate of decarburization.$^{[65]}$

Further, if the slag path (as explained in Section 2.2.1), goes below the liquidus temperature of the slag, second phase particles precipitate. These second phase particles, which are smaller in size compared to the foam bubbles, increase the viscosity of the liquid slag stabilizing the foam.$^{[17]}$ However, the foam volume increases with the increase of viscosity only until a critical viscosity value, after which the gas starts to channel through the slag without foaming.$^{[22]}$ The dimensional analysis carried out by the authors given in Table 2.4 also proves that the foaming index increases with the increasing slag viscosity.

Basically, the effect of viscosity is on the drainage and rupture of bubble films in the foam. The increase in viscosity stabilizes the foam by increasing the thickness of bubble films to retard the bubble coalescence and by reducing the downward flow of the liquid (i.e. liquid drainage) from the films through the plateau borders.$^{[132]}$
2.2.4.8 Effect of slag surface tension on slag foaming

In order for a bath smelting slag to foam, the presence of a surface active component such as Fe$_2$O$_3$, V$_2$O$_5$, CaF$_2$, Na$_2$O, and P$_2$O$_5$ is essential. Surface active compounds as such have the capability to reduce the viscosity, and most importantly can reduce the surface tension of the slag, allowing the slag to trap the gases and produce foam. The effect of surface tension on the foaminess of the slag is illustrated in Figure 2.40, and slag surface/interfacial tension was further explained in the Sections 2.2.3.3 and 2.2.3.4.

One aspect of the influence of surface/interfacial tension is its capability to determine the size of the bubbles generated at the slag/metal interface, as shown in Figure 2.41. Therefore, increasing slag surface tension and slag/metal interfacial tension increases the diameter of the bubbles, which destabilize the foam. Conversely, the foam is stabilized by small bubbles produced when the surface tension of the metal is increased.\cite{18,132} Further, the bubbles of an already produced foam experience increased drainage of their films with the increase of surface tension. This is due to the increased suction of the liquid in the films towards the plateau borders as the curvature of the bubble films increases with the increasing surface tension.\cite{133}

According to the dimensional analysis results given in Table 2.4, the relationship between the foaming index and the surface tension of slag is under debate. While Zhang and Fruehan\cite{18} and Stadler et al\cite{22} suggest an inverse proportionality between the two properties with a degree of influence less than 1.0, Lotun and Pilon\cite{29} propose that it be
a proportionality with the degree of influence of almost 1.0. Further, Ghag et al\textsuperscript{[20]} argue that the level of surface tension depression or the effective elasticity be the property that affects the foaming index instead of the actual surface tension.

### 2.2.5 Prevention of slopping

Slopping in a converter during the oxygen steelmaking process is considered to be costly, dangerous and unpredictable as explained earlier. Although the slopping is an expected event when extreme foaming of slag occurs during the process, the exact moment of the event can be hardly predicted, while the process is in operation.

The traditional method of preventing a slopping event is by observing the converter, once the signs of slopping are visible, take corrective actions manually. However, this approach of controlling and minimizing the occurrence of slopping events has been proven to be less effective. The reason is that, once the slopping signs are visible, the slopping has already begun and the damage has been already sustained by the vessel and other equipment, simultaneously with a yield lost. Further, if the operator is not experienced and less aware of corrective actions, the damage and the loss will be extensive.\textsuperscript{[10]} Therefore, the level of experience of the operator is a crucial factor, even when a computerized control system is in use.

The next stage of identifying the dawn of slopping was the experience of acoustics and light intensity behavior of the converter at the situation, and different models have been developed depending on the acoustic and light intensity signals to predict any slopping events. Iso et al\textsuperscript{[128]} were able to predict the slopping in a steelmaking converter by image processing of the in-furnace environment obtained via an image fiberscope. Birk et al\textsuperscript{[12]} used the sound signals from the converter to study the dynamic foaming, and the suggested corrective action was changing the lance height. Sound signals captured from a microphone in the off-gas funnel were used by Evestedt and Medvedev\textsuperscript{[71]} to estimate the slag level in the converter. In addition to sound and image analysis, intelligent computational techniques such as fuzzy logic, genetic algorithms and neural networks, lance vibration analysis, and microwave method were also used to control the slopping events.\textsuperscript{[128, 134]}
The slag foam suppression techniques have been in use to control the excessive foaming during the process. One common technique is to sprinkle carbonaceous materials like coke on the foaming slag. It is revealed from the X-ray fluoroscopy that these coke particles promote the coalescence of foam bubbles which then destabilize the foam. However, the size of the particles should be larger than the foam bubbles, as the foam is stabilized when the particles are smaller than the foam bubbles as explained in the earlier sections.\cite{9} Other methods in use include injection of aluminum powder, changing the lance height and manipulating the gas flow rates.\cite{71, 128}

However, as explained by Evestedt and Medvedev\cite{71}, even though, the prevention, prediction, and mitigation of slopping is a long-standing issue in steelmaking, it is essential for cost-efficient steel production with high quality, optimal furnace design, and minimum environmental impact. Further, the techniques mentioned above, which depend on the on-line physical measurements from the operating converter, are indirect, low in accuracy and reliability, especially at high temperatures.\cite{128} Therefore, predictive models for preventing slopping events are needed and have been the center of research interest for steelmaking researchers last few decades. Different studies have been carried out to understand the slag foaming and slopping as discussed previously in this chapter. However, still, there is a need for a dynamic predictive model that can simulate the process with time, and predict any slopping events before occurrence. Hence, the present research work was aimed at developing a dynamic process model for oxygen steelmaking to predict the slag foaming behavior and the progress of refining reactions in the converter.

### 2.2.6 Summary review of slag foaming

The foaming of slag in oxygen steelmaking is considered to be a phenomenon which should be controlled to a limited volume to get the benefits as explained in Section 2.2.4. In the case of true foam, the rate and extent of foaming depend on the gas evolution rates and the physical properties of slag such as viscosity, density, surface tension and interfacial tension as explained in Sections 2.2.4.1 to 2.2.4.8. Further, the size of the gas bubbles also has an inverse effect on the foaming extent of slag. Therefore, according to the studies on slag foaming,\cite{15-21, 29} it is evident that the small gas bubbles produced from decarburization in the BOF are trapped by the high viscous slag to produce true
foam. This foam is further stabilized and increased in volume by increasing slag volume and its evolving properties.

Conversely, due to the high gas flow rates involved in oxygen steelmaking, the formation of the gas hold-up is also a possibility. A gas hold-up is formed when the liquid metal and slag are lifted by the gas flow at higher superficial gas velocities. During the first few minutes into the blow, the gas hold-up phenomenon may be responsible for the increase in the bath height, because, during this period, the volume of slag available for trapping the gas bubbles is less, and the rate of gas evolution is high. In this situation, the physical properties of slag have very less influence on the foam height and the increased height of the bath should reduce instantly with the termination of the gas flow.

However, the common observation of steelmakers is that the slag foam they encounter in BOF does not collapse immediately after the blow and very similar to true foam produced at low superficial velocities. Hence, in the present study, the slag foaming in the BOF was assumed to be the combined effect of true foaming produced from trapping gas bubbles by the slag layer and the gas hold-up caused by high gas flow rates.

2.3 IMPHOS research work \(^{[2, 135, 136]}\)

The CFD model developed in the present study was aimed at predicting slag foaming and the refining kinetics of the impure elements in BOF. Therefore, there is a need for observations from the actual oxygen steelmaking process obtained in pilot plant trials to compare and validate the predictions made by the CFD model.

Several such pilot plant trials can be found in the literature including the work carried out by Cicutti et al, Van Hoorn et al, Holloppa et al, and Meyer et al.\(^ {68, 91, 137}\) These studies provided observations on metal and slag chemistry, slag volume and other important factors in BOF operation. However, in the present study, the plant trial data reported in IMPHOS research work was used for the comparison, analysis and validation requirements of the CFD model. The data reported in IMPHOS are complete and are presented more clearly compared to other data sets.
2.3.1 Introduction to IMPHOS research report\textsuperscript{[2]}

The data set published in IMPHOS research report\textsuperscript{[2]} is the most recent and reliable set of data available on top blown oxygen steelmaking under plant conditions, which were on plant trials conducted in a 6-tonne MEFOS converter. In this research work, the issues of intermittent nature and the imprecise positioning when sampling with the methods such as stopping the blow and turning down the vessel to retrieve the samples, stopping the blow and immersing a sampling device to obtain samples and dropping bomb samplers into a blowing converter several times during a blow to get samples, were overcome to a considerable extent during its trials. In the present study, the requirement for the experimental data obtained from a BOS converter for initialising the simulations and validating the simulation results was fulfilled using the data extracted from this IMPHOS research work.

The main aim of this IMPHOS research work was to examine the processing events during the oxygen steelmaking process in a systematic and comprehensive way with a special emphasis on the phosphorus refining\textsuperscript{[2]}. Therefore, the formation and development of the slag/metal emulsion and its refining throughout the blow relative to the bulk steel bath were directly monitored using an integrated fully automatic sampling system. This sampling system consisted of single use samplers which were built to take samples simultaneously at seven different locations inside the converter and eight times during the blow. Samples were taken from 20 heats and were reported in five different groups, which were categorized based on the phosphorus removal pattern of the heats. The five phosphorus removal profiles identified are listed as follows:\textsuperscript{[2]}

1. Near constant phosphorus removal profile
2. Phosphorus reversion profile
3. High phosphorus removal profile
4. Phosphorus reversion and slow down profile
5. Reversion with rapid phosphorus removal profile

The data set reported in this research work comprise of steel bath composition changes, slag composition changes, metal/slag profiles, the size distribution of steel droplets and bubbles in the slag/metal emulsion and lime dissolution characteristics. The data on steel bath and slag composition were used in the present study. Further discussion on
the geometry of the converter used in IMPHOS and the results reported are presented in the following sections.

2.3.2 Geometry and process details of IMPHOS pilot plant trials \cite{2}

The geometry of the 6-tonne universal converter used in the IMPHOS research is schematically shown in Figure 2.42. The converter volume was about 3.9 m$^3$, and the internal height to diameter ratio was 2.15 approximately. The initial liquid steel height in the converter was 660 mm from the vessel bottom, and the vessel was lined with Mg-C bricks. Scrap and hot metal were added to the converter via overhead cranes, and oxygen was blown at a rate of 17 Nm$^3$/min through a single De-Laval nozzle lance. Bath agitation was obtained by injecting N$_2$ at a rate of 0.5 Nm$^3$/min. Lime was continuously fed within the first two minutes into the blow, and readings for off-gas analysis, temperature and the volume were continuously recorded. The aimed tapping conditions were 1680 °C and 0.05% carbon. Samples were retrieved using the automated sampling system, and seven sampling pots were attached to the sampling lance as illustrated in Figure 2.43, such that the sampling pot at the level 1 was in the bulk liquid metal bath.
2.3.3 Removal patterns of impure elements

The main impure elements in the bath are C, Si, Mn, P and S, and IMPHOS reported the refining behavior of those elements for twenty heats under the five categories mentioned earlier. Figure 2.44 shows the removal patterns of those elements for the heats in the first two categories (i.e. near constant phosphorus removal profile and phosphorus reversion profile). In the present study, these removal patterns were used to compare the results obtained from the simulations on removal behavior of C, Si, Mn and P.

(a) Carbon removal pattern

(b) Silicon removal pattern

(c) Manganese removal pattern
2.3.4 Slag composition details

Composition changes in the slag component of the slag/metal emulsion for seventeen heats were reported in IMPHOS. The composition change of slag with respect to the evolution of its components CaO, SiO$_2$, MnO, P$_2$O$_5$, MgO, and FeO are given below in Figure 2.45 for heats categorized under near constant phosphorus removal profile and phosphorus reversion profile.

(d) Phosphorus removal pattern

Figure 2.44: Steel bath analysis results for heats in near-constant phosphorus removal group and phosphorus reversion group\cite{2}

(a) Change in wt % dissolved CaO

(b) Change in wt % SiO$_2$
Figure 2.45: Composition change of slag for heats in the first two categories\(^2\)

### 2.3.5 Slag foam height variation

The slag height is also one of the main observations reported in IMPHOS for the heats under investigation, where, the measurements were obtained from the sampling pots.
placed inside the converter as shown in Figure 2.43. As illustrated in the figure the observed slag heights were reported on a scale of 0 to 8 (i.e. slag height index), determined by observing the extent of hot metal adhering to the sampling lance. The slag height index 7 was the controlled maximum height in the converter and index beyond 7 indicated a slopping event.

Figure 2.46: Slag height indices for heats categorized into the five categories

(a) Near constant phosphorus removal profile
(b) Phosphorus reversion profile
(c) High phosphorus removal profile
(d) Phosphorus reversion and slow down profile
(e) Reversion with rapid phosphorus removal profile

Figure 2.46: Slag height indices for heats categorized into the five categories[^2]
2.4 Positioning present work

Therefore, the necessity for a more general model for simulating and predicting the slag foaming and refining reaction kinetics during the oxygen steelmaking process is considerable for a more efficient and productive process. This requirement was emphasized in the literature by several researchers and is established to be a difficult task, as the process is not yet fully understood due to high temperatures and intense fluid flow conditions involved. However, steelmaking researchers have been working on modeling the process since the invention of the Bessemer process gradually overcoming the challenges, and the most recent research work carried out by Sattar\cite{1} on modeling the foam height, and the decarburization in an oxygen steelmaking converter was able to produce some approximate predictions. Thus, this research work by Sattar\cite{1} was used in the present research work as the starting point, with the intention to further improve this model in terms of slag foaming phenomena and the reaction kinetics simulation. The fundamentals of foam and the background of foam modeling using the CFD technique are discussed in detail in the first two sections of the following chapter (Chapter 3). The next section of Chapter 3 consists of a detailed description of the model developed by Sattar\cite{1} together with a brief discussion on the drawbacks identified in it and the solutions suggested. A semi-empirical kinetics model was formulated in the present study to predict the refining reactions by incorporating it into the CFD model and is presented in Chapter 5. The CFD models developed in the present research work incorporating the kinetics model and the suggested improvements are explained in detail in Chapters 6 and 7.
Chapter 3
Chapter 3: Fundamentals of foam and review of previous CFD modeling and simulation of foam

3.1. Foam fundamentals

Foam has attracted the attention of many researchers in various fields comprising of food processing, detergency, and mineral and metal processing, due to its favorable physical properties. In the case of steelmaking, foam is advantageous on the one hand, as it increases the interface area for refining reactions, and it protects the hot metal bath from the direct contact with the atmosphere. Conversely, if the foam is formed extensively, it may overflow the steelmaking converter (a slopping event), creating a hazardous environment for both the equipment and people involved. Hence, a thorough understanding of foams and foaming process are essential to optimize the process by minimizing the slag foaming. In this chapter, foams are explained in terms of their composition, structure, and stability. Also, the process of modeling the foaming on a CFD basis is explained based on the model developed by Sattar et al[31, 36]. Further, the drawbacks and weaknesses of that model were identified, and the suggested improvements which were incorporated in the present study are discussed as well.

3.1.1. Overview of foam

Foams are either a mixture of a gas and a liquid, or a gas and a solid. Foams are formed by mixing or agitation, the evolution of dissolved gases, or physically blowing gas through the liquid. Foam consists of a continuous phase (liquid or solid), in which the gas is dispersed in the form of bubbles. These dispersed gas bubbles evolve in size with time due to different processes, including coalescence, Ostwald ripening, break-up, and drainage, causing the foam to be meta-stable. These metastable systems rearrange and coarsen with time, where the coarsening time span may range from a few seconds to few months.\[138\] Hence the foams are widely recognized as complex polydispersed systems.

The variations in the stability of foams have generated various useful applications as well as destructible and undesirable events. For example, in the events of fire extinguishing, detergency, food processing and mineral processing, stable foams are of extreme importance, while in the BOF steelmaking, engine oils and boilers, stable foams reduce
the process efficiency and can become destructive. In the case of slag foaming in the oxygen steelmaking process, the foam formation in excessive amounts can be detrimental, while if controlled and limited to smaller quantities, it assists better performance of the process, which is the focus of the present study.

3.1.2. Examples of foam
The liquid foams, where the gas is dispersed in a liquid, are used for various applications including food products such as whipped cream and chocolate mousse, toiletries such as shaving foam and hair mousse, and household cleaning products. On the other hand, solid foams, where the gas is dispersed in a solid, most commonly polymer or metal (aluminum), are used for insulation purposes, packaging, construction applications in vehicles and vibration and sound absorption. In general, foams possess a high specific surface area, a low interphase slip velocity, a large expansion ratio and a finite yield stress.\cite{139} In the case of solid foams, properties such as ultra-light weight, high porosity, high compression strength and good energy absorption have made it further suitable for the applications mentioned above. These useful properties of both liquid and solid foams are produced by the combined effect of its complex structure and the desirable properties of parent materials which formed the foam.\cite{140}

3.1.3. Foaming of a liquid
Although foams have attracted a considerable research interest among different fields as mentioned above, the conclusions and insights of those different studies are often specific to the system under investigation, and can hardly be used globally for any foam system. However, it is generally accepted that a pure liquid does not foam. A liquid has to have surface-active solutes to produce foam, and the level of foaming of the liquid differs according to the quality and the quantity of the solutes dissolved.

A general classification of foams can be derived from their order of stability. The stability of foams depends on the strength of the opposing force generated by the fluid films in the foam retarding the local thinning and eventual rupture of the thin films. The magnitude of this opposing force is the combined effect of the physical properties of the liquid such as viscosity, density, and surface tension. Therefore, unstable foams, in which, this opposing force is not adequately strong, collapse due to liquid drainage, and
their lifetime is limited to around 20 seconds. In contrast, the lifetime of metastable foams can be indefinite, because the liquid drainage from the foam is eventually stopped by the counterbalancing force: film elasticity. However, an unstable foam can be stabilized by adding a chemical to increase the viscosity of the liquid, so that the drainage of liquid is slowed down.[14]

3.1.4. Foams and emulsions

Foams and emulsions are subcategories of a wider category of substances called “colloidal dispersions”, which also consist of the subcategories: aerosols and suspensions. A colloidal dispersion comprises of a collection of small particles, droplets, or bubbles of one phase dispersed in the second phase.[14] When, in a colloidal dispersion, the dispersed phase is a liquid and the continuous phase is also a liquid with a different composition, the colloidal dispersion is known as an “emulsion” as shown in Figure 3.2. Moreover, when the dispersed phase is a gas and the continuous phase is a liquid, that colloidal dispersion is known as “foam” as shown in Figure 3.1. Foam can also have an emulsion as its continuous liquid phase, which is known as an “aerated emulsion”. Thus, the foam encountered in steelmaking can be identified as an aerated emulsion, because the continuous phase of the foam is the slag-metal emulsion. Emulsification is of considerable importance in many metal processing operations as in the case of steelmaking.[118, 127] However, in the present work, the foam was assumed to be generated from a continuous liquid phase.

Figure 3.1: A typical soap foam
Figure 3.2: An emulsified crude oil droplet in an aqueous solution[141]
3.1.5. Structures of foam

Foam is formed by bubbles, and as the bubbles flocculate they form different structures. These structures change and evolve with time due to deformations and drainage. The foams are generally polydisperse with different sized bubbles, creating disordered structures. However, in the case of monodisperse foams, ordered structures can be found. Foams can be broadly classified into two groups termed wet foam and dry foam based on the liquid volume fraction of the foam, which can change from about 1% to 30%. The structure of the foam is a division of space into cells when its liquid content reaches the dry limit, while, it becomes a close packing of spheres when its liquid content reaches the wet limit. The structure of the foam can be properly determined by its average bubble diameter and the capillary length ($l_0$), calculated using equation 3.1 below. When the capillary length is larger than the average bubble diameter, a wet foam is formed which consists of small bubbles. The foam in which the average bubble diameter is larger than the capillary length consists of larger bubbles and is known as a dry foam. [142]

\[
\frac{l^2}{\Delta \rho g} = \frac{\gamma}{\Delta \rho g}
\]

Eq 3.1

Where $\gamma$ is the surface tension of the liquid, $g$ is the acceleration due to gravity, and $\Delta \rho$ is the density difference between the gas and the liquid.

At the dry limit (i.e. when the liquid content of the foam is minimum), the interface between the bubbles is assumed to be thin curved surfaces, which are not spherical but takes the shape of faces of polyhedral cells. When forming a polyhedral shape, there are important geometrical and topological restrictions to be adhered to, which were first stated by the foam morphologist: Plateau. His rules were as follows: [143]

1. Faces and films of bubbles always meet three at a time creating an angle of $120^0$, so that, at a cell edge, three cells symmetrically join.

2. Edges meet four at a time forming an angle of around $109.43^0$ and at each edge, six cells meet symmetrically.
Further, the dry foam bubbles forming a cellular structure should adhere to the Laplace-Young law given by equation 3.2. This calculates the balance of forces on a small element of bubble film in terms of the pressure difference and can be used to determine the equilibrium shape of the fluid film.

$$\Delta p = \frac{4\gamma}{r}$$

Eq 3.2

Where $\gamma$ is surface tension, and $r$ is the mean radius of curvature. The mean radius of curvature is calculated by the following equation 3.3 using the two principle radii of curvature, $R_1$ and $R_2$.

$$\frac{1}{r} = \frac{1}{2} \left[ \frac{1}{R_1} + \frac{1}{R_2} \right]$$

Eq 3.3

Generally, $R_1$ and $R_2$ are different values forming different forms of bubble structures, but in the case of spheres: $R_1 = R_2$.\textsuperscript{[142]} Although different structures of bubbles are possible, in reality, these possibilities are limited under stress or during evolution.\textsuperscript{[140]}

Conversely, at the wet limit (i.e. when the liquid content of the foam is at maximum), foam bubbles are spherical. These spheres should be in contact with at least three other spheres according to Plateau’s rules. However, real foams are in between these two idealized extremes of liquid volume fraction. As explained earlier, at the dry limit, the foam bubbles form polyhedral shapes as shown in Figure 3.4. The addition of liquid occupy the interstitial spaces at the cell edges, and those spaces fill from liquid and grow
to form plateau borders, as shown in Figure 3.5. Towards the wet limit, the bubbles become slightly deformed spheres, and the Plateau’s rules are progressively violated.\[142\]

In the three-dimensional space, the structure to which the foam bubbles arrange in a dry foam is bcc or the body-centered cubic arrangement of cell centers, and this was first proposed by Lord Kelvin in 1887.\[142\] The Kelvin cell or the tetrakaidecahedron is made of six flat quadrilateral faces and eight hexagonal faces which have a subtle curvature and can fill the space when packed. This structure is shown in Figure 3.6 and was derived by considering the equilibrium of surface tension forces and gas pressures.\[144\]

In a three-dimensional wet foam, the foam bubble structure with the lowest energy is supposed to be the fcc (face centered cubic) arrangement. As shown in Figure 3.7, both the fcc and bcc structures become mechanically unstable at a certain liquid volume fraction between the two idealized liquid fraction extremes in the foam. The possible
bubble structures that are stable in this intermediate zone are termed “Clathrate” structures, and these structures are generally close to the shape of pentagonal dodecahedra. Although these polyhedral structures are of lower surface energy, they do not fill the space by packing closely as the Kelvin cell.\[^{140}\]

![Figure 3.7: Schematic diagram of relationship between the relative energies for fcc, bcc, and clathrate structures, with full lines indicating regions of stability\[^{140}\]](image)

Although, the Kelvin structure of foam bubbles was considered to be the best possible structure with the lowest surface energy for dry foam for about a century, Weaire and Phelan proposed a new structure with further low surface energy (with 0.3% less surface area compared to Kelvin structure) for a monodisperse dry foam as shown in Figure 3.8.\[^{144}\] This structure consists of two different bubble types and eight bubbles per periodic unit cell. The bubble types are an irregular dodecahedron with pentagonal faces and a tetrakaidecahedron with two hexagonal faces and twelve pentagonal faces, where all the pentagonal faces of the structure are slightly curved.\[^{142}\]

**3.1.6. Foam stability**

Stability of foam determines its life span, and several factors are affecting the stability of foams. The structure of the bubbles in the foam is one of such main factors, which was briefly described in the previous section. The other factors include the drainage of foam, rupture of bubble films and coarsening of foam either by Ostwald ripening or...
coalescence. Knowledge of the extent of influence of these factors on the stability of foam can help in controlling the foam to be within the necessary quality and quantity boundaries.

3.1.6.1. Drainage of foam

Foam is produced from a continuous phase (liquid or solid) and a dispersed phase (gas). The gas bubbles in the foam can be considered as a porous skeleton through which the continuous phase (i.e. liquid) flows. Since this dispersed bubble matrix is not rigid, it is prone to deformations. These deformations lead to various consequences, among which, the flow of liquid under gravity out of foam is an important process, and this process of flow of liquid is known as foam drainage.\[146\]

Most of the foam drainage models developed have considered the process of liquid drainage in the foam to be similar to the fluid flow through porous solid media. Fluid flow through a porous media is well-described by Darcy’s law as given by equation 3.4, \[147, 148\] and it expresses the foam drainage as the balance between the gravity and the bulk shear dissipation in the fluid network (plateau borders) as in typical porous material. Further, in porous materials, the permeability is generally characterized by the liquid fraction (ε) and has been recently proved to be accurate for aqueous foams also. Hence, the permeability of the foam can be calculated from the equation 3.5, which is specific for foam in which the surfactants flow with the liquid phase.\[146\]

\[ Q = k \frac{Dg}{\mu} \]  \hspace{2cm} \text{Eq 3.4}

\[ k = 6.7 \times 10^{-4} \varepsilon^{3/2} D_b^2 \]  \hspace{2cm} \text{Eq 3.5}

Where, \( Q \) is the flow rate through the plateau border (m\(^3\)/s), \( k \) is the permeability of the foam (m\(^2\)), \( S \) is the cross sectional area of the plateau border (m\(^2\)), \( \mu \) is the viscosity of the fluid (kg/ms), \( \rho \) is the density of the fluid (kg/m\(^3\)), \( g \) is the acceleration due to gravity (m/s\(^2\)), \( \varepsilon \) is the liquid volume fraction of the foam, and \( D_b \) is the bubble diameter (m).
The liquid fraction of foam defines the structure most of the times. The dry foams with a liquid fraction less than 0.02 have a unique geometry and have straight and slender channels. At this stage, the bubbles are tetrakaidecahedra or kelvin bubbles with bcc packing. According to Figure 3.9, at the liquid fraction of $\varepsilon^*$, the structural arrangement of the foam bubbles start to change from tetrakaidecahedra to dodecahedra (i.e. pentagonal dodecahedra and rhombic dodecahedra). However, in reality, this structural change from bcc to fcc is expected to occur over the range of 0.05 to 0.12 of liquid fraction in the foam. With the further increase of liquid volume fraction, the channels swell and the bubbles become more spherical. When the volume fraction of foam surpasses the limit of 0.26, the foam becomes an fcc hexagonal close pack of spheres. Therefore, the liquid fraction of the foam and the drainage of liquid in the foam play an important role in the structure of the foam and thereby on its stability.

![Figure 3.9: Relationship between the liquid fraction and the edge length of foam](image)

### 3.1.6.2. Film rupture in foam

Foam bubble films rupture due to thinning of the film when external disturbances are absent. One of the leading causes of this thinning of foam film is the drainage of liquid under gravity. In addition, the growth of transverse waves by the nucleation of dissolved gas or vapor is also responsible for localized thinning of foam films. In order to counterbalance this thinning of the film, the fluid should possess film-elasticity, so that the initial displacement of material is restored before rupture.

Several theories that explain the film elasticity of a foam film can be found in the literature including the theories proposed by Gibbs, Marangoni, Plateau and Derjaguin. Gibbs’s surface elasticity theory explained that, if a thin foam film of a
solution with dissolved surface active solute is subjected to local thinning, the surface tension of that thinning area of the film is increased. This surface tension gradient then drives the liquid to flow from surrounding low surface tension surface area towards the thinning location and restores the film. Marangoni explained that the surface tension gradient explained by Gibbs’s theory is greater under dynamic conditions such as for a rapidly expanding surface. Further, this gradient of surface tension operates on any expanding surface carrying an adsorbed layer to restore local thinning, irrespective of the thickness of the underlying liquid. The surface transport theory further added to the Marangoni’s explanation that, this surface tension gradient first creates a surface flow towards the thinned location of the film, and this flow then moves the adjacent liquid layers with it. Hence the process of restoration is more efficient compared to a single surface flow. Plateau suggested the effect of surface viscosity as a factor of film stability because the increased surface viscosity and the bulk viscosity retards drainage of the foam and stabilize it. Derjaguin’s suggestion on the stability of very thin films was that the restoration of thinning of these films is due to the electrical repulsions between the ionic double layers formed by adsorption on two sides of the lamellae. However, in the case of external disturbances and weak restoration of local thinning of films, foam films rupture.

3.1.6.3. Coarsening of foam

Meta-stable systems like foams rearrange and coarsen with time and this time span for coarsening can range from few seconds to few months. Two primary mechanisms can be identified as causes of foam coarsening: Ostwald ripening and the coalescence.

Ostwald ripening occurs due to the diffusion of the gas from the smallest bubbles to biggest ones. The major driving force of Ostwald ripening is the pressure difference across the bubbles, and its relaxation proceeds over a time scale of 10 hours. In contrast, the coalescence occurs due to the rupture of film shared by two bubbles and is a rapid process compared to the Ostwald ripening.

In the present study, only the effect of coalescence on foam coarsening was taken into consideration. Coalescence between two bubbles occurs in three steps. Bubbles collide with each other trapping a small amount of liquid between them in a thin film, which is
the first step. This thin film drains gradually under gravity until a critical film thickness is met and eventually ruptures creating a single bubble. Hence, the coalescence of bubbles is affected by both the collision efficiency, which is the number of collisions that results in coalescence and the period they remain intact, as this time span should be sufficient for the thin film separating them to drain and reach the critical thickness. The bubble coalescence occurs due to various mechanisms, including turbulence, buoyancy and laminar shear as shown in Figure 3.10.

![Figure 3.10: Bubble coalescence due to: (a) Turbulent eddy, (b) Buoyancy, (c) Laminar shear][149]

In the present study, coalescence was assumed to occur only due to the turbulence, and the coalescence model developed by Prince and Blanch[150] was used in the simulations, which was also employed by the foaming model developed by Sattar[1]. A brief summary of the used bubble coalescence model follows.

The coalescence rate resulting from a collision between two bubbles with diameters $d_i$ and $d_j$ was calculated by the equation 3.6[1]:

$$\Omega_c = \theta_{ij} \times P_c(d_i,d_j)$$  \hspace{1cm} \text{Eq 3.6}$$

Where $\theta_{ij}$ is the collision rate due to turbulence and $P_c$ is the coalescence efficiency.

The rate of collision of the bubbles was calculated by equation 3.7[150]:

$$\theta_{ij}^T = 0.089 n_i n_j \left( d_i + d_j \right)^2 e^{\frac{3}{2}} \left( d_i^{\frac{3}{2}} + d_j^{\frac{3}{2}} \right)^\frac{1}{2}$$  \hspace{1cm} \text{Eq 3.7}$$

Where, $n_i$ and $n_j$ are the concentrations of bubbles with diameters $d_i$ and $d_j$ respectively, and $\varepsilon$ is the energy dissipation per unit mass.
Coalescence efficiency is the number of collisions that lead to coalescence, which can be determined by the equation 3.8:\[150]\:

\[ P_c (r_i, r_j) = \exp \left( -\frac{t_{ij}}{\tau_{ij}} \right) = \exp \left( -\frac{r_i^3 \rho_l}{16 \sigma} \frac{\frac{1}{2} \ln \frac{h_0}{h_{ij}}}{r_i^{2/3}} \right) \tag{Eq 3.8} \]

Where \( t_{ij} \) is the coalescence time, \( \tau_{ij} \) is the contact time between the bubbles and \( r_{ij} \) is the equivalent radius of the bubbles. The coalescence time, the equivalent radius of the bubbles and the bubble contact time can be calculated from equations 3.9\[150]\], 3.10\[150]\] and 3.11\[150]\] respectively as given below.

\[ t_{ij} = \left( \frac{r_i^3 \rho_l}{16 \sigma} \right)^{\frac{1}{2}} \ln \frac{h_0}{h_{ij}} \tag{Eq 3.9} \]

Where \( h_0 \) is the initial film thickness, \( h_{ij} \) is the critical film thickness, \( \sigma \) is the surface tension, and \( \rho_l \) is the density of the liquid.

\[ r_{ij} = \frac{1}{2} \left( \frac{1}{r_{bi}} + \frac{1}{r_{bj}} \right)^{-1} \tag{Eq 3.10} \]

Where \( r_{ij} \) is the equivalent radius of the bubbles with radii \( r_{bi} \) and \( r_{bj} \).

\[ \tau_{ij} = \frac{r_{ij}^{2/3}}{\epsilon^{1/3}} \tag{Eq 3.11} \]

### 3.1.6.4. Other factors

There are several other factors which influence the foam stability. The concentration of the surface-active solutes in the liquid is one important factor in developing a sufficient surface tension for restoring the local thinning of a film. Generally, the effectiveness of the solutes is accepted to be at maximum at an intermediate concentration of the solute. The presence of two or more surface-active solutes in the liquid will further stabilize the foam in comparison to the effect caused when either solute is present separately.\[14]\] Temperature is also another important factor in the foam stability because the increase of temperature reduces the bulk viscosity of the liquid increasing the rate of foam drainage. Moreover, this effect of temperature on the viscosity is greater compared to its effect on the surface tension.
Particles in the foam are also considered as foam stabilizers either with or without the presence of a surfactant. Particles with a relatively small size compared to the foam bubbles in the foam, retard the drainage and the coalescence, by operating as a physical barrier for coalescence as well as by increasing the bulk viscosity of the liquid.\textsuperscript{[153]} Particles, those are bigger than the foam bubbles, destroy foam when added, which is used in the steelmaking process to collapse the slag foam at the turn-down. Similarly, the evaporation and other external disturbances also can cause foam collapse.

Foam life is generally determined by the balance between bubble coalescence rate and the bubble break-up rate. Bubble coalescence occurs by the rupture of the film separating two bubbles, producing a new bigger bubble. Conversely, due to various reasons, foam bubbles which are relatively big, break-up to form new smaller bubbles as shown in Figure 3.11.

![Figure 3.11: Bubble breakup due to (a) Turbulent eddy collision, (b) Instability of large bubbles\textsuperscript{[149]}](image)

In the present study, the bubble break-up was taken into account in the population calculation of foam bubbles. Bubbles were assumed to break-up when they are met with eddies with the required size and energy. The binary break-up model, where the parent bubble break-up only to form two daughter bubbles was used in the present study. This model was developed by Luo and Svendson\textsuperscript{[152]} and was also used by the foaming model developed by Sattar\textsuperscript{[1]}.

The break-up rate of a bubble of volume $v_i$ into daughter bubbles of $v_k$ and $v_{i-k}$ was calculated by the product of bubble collision frequency of bubble class $i$ with the eddy $\lambda_i (\omega_b)$ and the probability of bubble break-up ($P_B$).\textsuperscript{[1]}
\[ \Omega_{B}(d_i, d_k) = \omega_B(d_i, \lambda_j, d_k) \times P_B(d_i, \lambda_j, d_k) \]  \hspace{1cm} \text{Eq 3.12}

Where, \( d_i \) and \( d_k \) are the diameter of the bubbles that collide and the \( \lambda_j \) is the size of the eddy. The collision frequency of the bubbles of class \( i \) with the eddy \( \lambda_j \) was calculated by the following equation 3.13.\[\text{[1]}\]

\[ \omega_B(d_i, \lambda_j, d_k) = \frac{\pi}{4} \left( d_i + \lambda_j \right)^2 \frac{u_\lambda}{\lambda_j} \times n_{\lambda_j} \times n_{d_i} \]  \hspace{1cm} \text{Eq 3.13}

The average turbulent velocity of the eddy \( \lambda_j \) (\( u_\lambda \)), the number of eddies (\( n_{\lambda_j} \)) and the number of bubbles with the diameter \( d_i \) was calculated as follows:\[\text{[1]}\]

\[ \bar{u}_\lambda = \beta^{\frac{3}{2}} (c\lambda)^{\frac{1}{3}} \]  \hspace{1cm} \text{Eq 3.14}

Where \( \beta \) is a constant.

\[ n_{\lambda_j} = \frac{0.822 \left( 1 - \alpha_d \right)}{\lambda_j^4} \]  \hspace{1cm} \text{Eq 3.15}

Where \( \alpha_d \) is the local fraction of the dispersed phase.

\[ n_{d_i} = \frac{\alpha_j}{v_i} \]  \hspace{1cm} \text{Eq 3.16}

The probability of bubble break-up was calculated by the following relationship:\[\text{[152]}\]

\[ P_B(d_i, \lambda_j, d_k) = \exp(-x_c) \]  \hspace{1cm} \text{Eq 3.17}

Where \( x_c \) is the critical dimensionless energy and can be calculated as shown below:\[\text{[152]}\]

\[ x_c = \frac{12c_f \sigma}{\beta \rho_c \varepsilon^{2/3} d_i^{4/3} \xi^{1/3}} \]  \hspace{1cm} \text{Eq 3.18}

Where, \( c_f \) is the increase coefficient of surface area calculated by equation 3.19, \( \sigma \) is the surface tension, \( \xi \) is the ratio between an eddy and a bubble as given by equation 3.20 and \( \rho_c \) is the density of the continuous phase.

\[ C_f = f_{BV}^{2/3} + \left( 1 - f_{BV} \right)^{2/3} - 1 \]  \hspace{1cm} \text{Eq 3.19}

\[ \xi = \frac{\lambda_j}{d_i} \]  \hspace{1cm} \text{Eq 3.20}

\[ f_{BV} = \frac{v_k}{v_i} \]  \hspace{1cm} \text{Eq 3.21}

Where \( f_{BV} \) is the breakage volume fraction.
3.2. CFD modeling and simulation of foam

One of the major objectives of the present research work was modeling slag foaming in oxygen steelmaking. The characteristics of slag foam in steelmaking, as well as, foam in general, were explained in the previous chapter and the previous sections of this chapter. In this chapter, this section onwards, the CFD model developed for the simulation, is described in detail.

3.2.1. CFD technique for modeling and simulation

CFD or Computational Fluid Dynamics is a method of analyzing the systems involving fluid flow, heat transfer and associated phenomena including chemical reactions with the aid of computer-based simulations. CFD technique is frequently and efficiently used in a number of different applications including the following examples:[53]

- Lift and drag (aerodynamics) calculations of both aircraft and vehicles.
- Analysis of hydrodynamics of ships.
- Combustion in internal combustion engines and gas turbines.
- Chemical process engineering. (e.g. Mixing and separation)
- Biomedical engineering applications. (e.g. Blood flow through veins and arteries)

CFD is a powerful technique and is spreading over various fields, both industrial and non-industrial since the 1990s. This is due to the unique advantages of CFD simulations over experimental approaches for analyzing systems involving fluids. Some of those advantages include the capability to be used in situations where analysis through experiments is impossible (e.g. hazardous fluids and conditions, large and complicated systems), less time and cost consumption compared to those incur when experimental set up has to be built for the first time, and the ability to produce unlimited level of detail of results.[53]

Therefore, CFD is a suitable and potential technique to be used in the analysis of oxygen steelmaking. Oxygen steelmaking involves fluids at extremely high temperatures and velocities, and experimental analysis of the process is difficult and hazardous at the plant level. Although the experiments carried out in the laboratory help gain insights into the process, when scaled up to the plant scale, most of those findings do not produce the expected improvements. Hence, in the present research work, CFD technique was used
to develop a model for analyzing and predicting the refining kinetics and slag foaming in oxygen steelmaking.

3.2.2. Examples of CFD modeling and simulations

CFD is a viable technique to be used in simulating and analyzing flows under different extreme conditions. Therefore, researchers have tried analyzing different fluid flow systems using CFD, and several such researches can be found in the literature on flows involving bubbles similar to foam. In the work carried out by Buwa et al\textsuperscript{[153]} investigating the effect of various parameters on the gas-liquid flow in a rectangular bubble column, the Eulerian-Eulerian approach was used with a population balance framework including the bubble coalescence and break-up. A similar approach was followed by the Chen et al\textsuperscript{[32]} in their study to evaluate the effect of different closure terms for bubble coalescence and break-up terms. A CFD-PBM (Computational Fluid Dynamics – Population Balance Model) coupled model with a gas-liquid mass transfer model was used by Wang et al\textsuperscript{[149]} in their work on bubble columns, and bubble coalescence and break-up due to various causes were considered in the population balance model. Bannari et al\textsuperscript{[31]} and Bhole et al\textsuperscript{[30]} also studied the flow in bubble columns using the population balance framework.

Use of CFD techniques in iron and steelmaking process is an active area of research for last three decades, and its usage can be observed throughout the process, beginning from the basic oxygen furnace or electric arc furnace, up to the tundish and moulds.\textsuperscript{[154]} Models have been developed using CFD techniques for predicting the mixing behavior, gas-liquid interactions, multiphase flows and heat and mass transfer for each of those steps in the steelmaking process. Some of those studies include lance design for BOF steelmaking\textsuperscript{[54]}, optimising the bottom tuyere configurations for the BOF steelmaking vessel\textsuperscript{[55]}, flow field and surface deformation caused by an impinging jet in a top blown converter\textsuperscript{[155]}, designing fume control systems for steelmaking vessels\textsuperscript{[56]}, mixing behaviour in ladles fitted with two porous plugs\textsuperscript{[57]} and inclusion behaviour in a gas-agitated ladle\textsuperscript{[156]}.

However, still, there is no general CFD model developed for BOF operations, even though it is not an unachievable target.\textsuperscript{[154]} However, the study carried out by Sattar\textsuperscript{[1]}
on modeling the slag foaming in oxygen steelmaking using CFD technique could produce results which were in good agreement with the IMPHOS pilot plant trials\textsuperscript{[2]}. The present work was an extension of the model developed by Sattar\textsuperscript{[1]} incorporating a kinetics model and a more rigorous slag foaming phenomenon.

3.2.3. Summary of the model by Sattar\textsuperscript{[1]}

Sattar et al developed a CFD model to predict the foam height, the number densities of bubble classes in gas and foam phases, decarburization, heat generation and the velocities of the phases.\textsuperscript{[1]} The model geometry was designed according to the geometry of the steelmaking converter used in the IMPHOS pilot plant trials. The multiphase flow simulation was carried out with a Eulerian-Eulerian approach. The population balance equation was used to calculate the population densities of the components of each phase, and in the case of population calculations of the bubble classes, the bubble coalescence and breakup were taken into consideration. Only the decarburization reaction was considered in their work, and the heat generation due to carbon oxidation was incorporated in the simulation. The results obtained from the simulation were compared with the observed data published in IMPHOS\textsuperscript{[2]} and were in good agreement. Hence this work was used as the basis for the present work and a detailed summary of the work carried out by Sattar\textsuperscript{[1]} on foaming in oxygen steelmaking in relation to the present work, is given in the following sections of this chapter.
3.3. Slag foaming model developed by Sattar and co-workers\textsuperscript{[1]}

In this section, the model developed by Sattar and his co-workers\textsuperscript{[1]} for predicting the foam height and other parameters in oxygen steelmaking, is described in detail.

Figure 3.12: (a) Schematic diagram of the BOF used in IMPHOS\textsuperscript{[2]} (b) Mesh developed for simulation\textsuperscript{[1]}

Figure 3.12 (a) and (b) show the geometry of the 6-tonne Basic oxygen steelmaking (BOS) converter used in the simulation and the mesh developed for the simulation respectively. The eulerian-eulerian approach was used to simulate the multiphase flow in the converter, where gas, liquid and foam phases interacted with each other in terms of mass, momentum, and energy. Population balance equation was used to track the population densities of bubble classes in gas and foam phases and was modified by incorporating bubble coalescence and break-up. Decarburization reaction was also considered in the simulation. The results of the model on foam height and rate of decarburization were in good agreement with the observed data published in IMPHOS research work\textsuperscript{[1]}. Therefore, in the present study, the mesh shown in Figure 3.12b was used for simulations.

3.3.1. Navier-Stokes equations

Navier-Stokes equations are the governing equations for a flow of a Newtonian fluid and consist of a set of non-linear second order equations in four independent variables. These equations represent the mathematical statements of the conservation laws of
physics, which are, the mass of a fluid is conserved, the rate of change of momentum equals to the sum of the forces on a fluid particle (Newton’s second law), the rate of change of energy is equal to the sum of the rate of heat addition to and the rate of work done on a fluid particle (first law of thermodynamics). The fluids are considered to be continuums, disregarding the molecular structure and the molecular motions in it.[53]

3.3.1.1 Equation for mass conservation

\[
\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \alpha_k \rho_k \mathbf{V}_k = \sum_{l=1, l \neq k}^{N} \Gamma_{kl} \quad \text{Eq 3.22}
\]

Where \( \alpha_k \) is the volume fraction of phase \( k \), \( \mathbf{V}_k \) is the velocity of the phase \( k \), and \( \Gamma_{kl} \) is the mass exchange between the phases \( k \) and \( l \).

The mass exchange between the phases was captured with the following equations, where “\( f \)”, “\( l \)” and “\( g \)” are foam, liquid, and gas phases respectively. The mass in a cell containing gas and liquid phases was transferred to the foam phase when the volume fraction of the gas phase and the liquid phase in the cell were equal to or more than 75% and 5% respectively. Moreover, when the foam volume fraction and the liquid volume fraction in a “foam” cell were more than or equal to 15% and the predetermined minimum volume fraction respectively, the total mass in that cell was transferred to liquid and gas phases.

\[
\Gamma_f = \frac{\frac{\pi}{6} d_b^3}{dt} \left( \rho_g \sum N_g - \rho_f \sum N_f \right) = -\Gamma g N_g \leq N_{g_{max}} \quad \text{Eq 3.23}
\]

\[
\Gamma_f = \frac{n_p a_p}{dt} \left( \rho_f \sum N_f - \rho_g \sum N_g \right) = -\Gamma f N_f \leq N_{f_{max}} \quad \text{Eq 3.24}
\]

Here, \( N_g \) is the number of gas bubbles transformed into foam bubbles, \( N_f \) is the number of foam bubbles transformed into gas bubbles, \( dt \) is the time step and \( N_{g_{max}} \) is the gas bubbles available in the cell.
The number of gas bubbles transformed into foam bubbles \((N_g)\) and the number of foam bubbles transformed into gas bubbles \((N_f)\) were calculated from the equations 3.25 and 3.26 respectively, where \(\alpha_i\) is the liquid volume fraction of the cell and \(v_i\) is the cell volume.

\[
N_g = \frac{\alpha_i v_i}{n_p a^l_i} \alpha_g \geq 0.75 \quad \text{Eq 3.25}
\]

\[
N_f = \frac{q_{f0}}{n_p a^l_i} \alpha_f \geq 0 \quad \text{Eq 3.26}
\]

### 3.3.1.2 Equation for momentum conservation

\[
\frac{d(\alpha_k \rho_k v_k)}{dt} + \nabla \cdot \alpha_k \rho_k v_k v_k = -\alpha_k \nabla p + \nabla \cdot \alpha_k \left( \tau_k + T^l_k \right) + \alpha_k \rho_k f + M_k, k = 1...N \quad \text{Eq 3.27}
\]

Where \(f\) is the body force vector including the gravity, \(M_k\) is the interfacial momentum exchange between phases and \(p\) is the pressure.

The shear stress and the Reynolds stress were calculated using equations 3.28 and 3.29 respectively, where \(I\) is a unit tensor.

\[
\tau_k = \mu_k \left( \nabla v_k + \nabla v_k^T \right) - \frac{\tau}{3} \nabla v_k \quad \text{Eq 3.28}
\]

\[
T^l_k = \mu^l_k \left( \nabla v_k + \nabla v_k^T \right) - \frac{\tau}{3} \nabla v_k I - \frac{2}{3} \rho_k K_k \quad \text{Eq 3.29}
\]

The turbulent viscosity was calculated using equation 3.30, where, \(K\) is the turbulent kinetic energy and \(\epsilon\) is the turbulent dissipation rate.

\[
\mu^t_k = C_{\mu} \rho_k \frac{K_k^2}{\epsilon_k} \quad \text{Eq 3.30}
\]

The interfacial momentum exchange was calculated considering the bubble induced drag force. The source term in the momentum conservation equation accounts for momentum exchange between bubbles (gas phase) and liquid due to bubble coalescence and bubble break-up.

\[
M_i = C_{\alpha} \frac{1}{8} \rho_i A_i |V_r| V_r = -M_g \quad \text{Eq 3.31}
\]

The relative velocity of phases was calculated using the equation 3.32.
\[ V_r = V_g - V_l \]  

Eq 3.32

The interfacial area density was calculated using equation 3.33.

\[ A_i = \frac{6\alpha_g}{D_{SMD}} \]  

Eq 3.33

Mean bubble size of the distribution is usually given by the Sauter diameter, and the mean Sauter diameter was calculated using the equation 3.34\(^{[31]}\).

\[ D_{SMD} = \frac{1}{n} \sum_{i=1}^{n} \frac{\phi_i}{d_i} \]  

Eq 3.34

The Reynolds number and the drag coefficient are calculated by equations 3.35 and 3.36 respectively.

\[ \text{Re}_b = \frac{V_b D_{SMD}}{\nu_l} \]  

Eq 3.35

\[ C_D = \begin{cases} 24 \left( 1 + 0.15 \text{Re}_b^{0.687} \right) & \text{Re}_b \leq 1000 \\ 0.438 & \text{Re}_b \geq 1000 \end{cases} \]  

Eq 3.36

### 3.3.1.3 Equation for enthalpy conservation

The enthalpy conservation equation was used to calculate the enthalpy transfer between the phases.

\[ \frac{\partial (\alpha_k \rho_k h_k)}{\partial t} + \nabla \cdot \alpha_k \rho_k \nu_k h_k = \nabla \cdot \alpha_k \left( q_k + q_k' \right) + \alpha_k \rho_k q_k'' + \alpha_k \rho_k f \cdot \nu_k + \nabla \cdot \alpha_k \left( \tau_k + \tau_k' \right) \cdot \nu_k \]  

Eq 3.37

\[ + \alpha_k \frac{\partial p}{\partial t} + \sum_{i=1,j=k}^{N} H_{ki} + h_{ki} \sum_{i=1,j=k}^{N} \Gamma_{ki}, k = 1...N \]

Where \( q_k'' \) is the enthalpy volumetric source and \( H_{ki} \) is the energy interfacial exchange between the phases \( k \) and \( l \). The volumetric enthalpy source was calculated from the decarburization reaction rate and the heat generated by the reaction in the model developed by Sattar\(^{[3]}\), but in the present study, the heat generation by the chemical reactions was not calculated.
The heat flux $q_k$ and the turbulent heat flux $q^T_k$ were calculated using equations 3.38 and 3.39.

$$q_k = \frac{K_k}{C_{p,k}} \nabla h_k$$  \hspace{1cm} \text{Eq 3.38}

$$q^T_k = \frac{\mu_T}{\sigma} \nabla h_k$$  \hspace{1cm} \text{Eq 3.39}

Where, $K_k$ is the thermal conductivity of the phase $k$.

The interfacial energy exchange was calculated using the Ranz-Marshall enthalpy exchange model, which is as follows:

$$H_c = \frac{k_c}{D_b} \text{Nu} \frac{A_i''}{A''} (T_d - T_c) = -H_d$$  \hspace{1cm} \text{Eq 3.40}

Where $k_c$ is the thermal conductivity of the continuous phase, and $D_b$ is the bubble diameter.

$$\text{Nu} = 2.0 + 0.6 \text{Re}_b^{\frac{7}{6}} \text{Pr}^{\frac{1}{3}}$$  \hspace{1cm} \text{Eq 3.41}

The Nusselt number $\text{Nu}$ was calculated by using the equation 3.41, where, $\text{Re}_b$ is the local bubble Reynolds number, $\text{Pr}$ is the Prandtl number and $\frac{A''}{A''}$ is the interfacial area density.

### 3.3.2 Finite volume discretization

The purpose of simulating a flow model is to predict the flow variables with time by solving the above-explained system of Navier-stokes equations. These equations for complex flow systems such as the fluid flows in the steelmaking converter are almost impossible to be solved analytically. Therefore, computers are used to solve these equation sets. The solving process starts with the grid generation, where the physical space is divided into grid cells. Next step is the spatial discretization of the Navier-Stokes equations, where, the numerical approximation is carried out for the convective and viscous fluxes and the source term. There are three main discretization schemes: Finite Difference (FD), Finite Volume (FV) and Finite Element (FE). [157]

Finite difference (FD) method was first used by Euler in around 1768 for numerically solving the differential equations. [157] This approach is directly applied to the differential form of the governing equations, and a Taylor series expansion is used for the
discretization. The advantages of FD include its simplicity and the possibility to obtain high-order approximations. But, the need for a structured grid for the solving process limits the FD method to simple geometries.

In addition, Finite element method requires an unstructured grid. For a certain number of pre-specified points inside and/or at the boundaries, the set of governing equations is solved. This method was introduced by Turner and his co-workers and was first used only for structural analysis. The governing equations have to be transformed to their integral form to be solved by FE method. FE method of discretization has gained attention due to its integral formulation and use of unstructured grids and has a very rigorous mathematical foundation.

Sometimes, the solution method of FE discretization is similar to the Finite volume method. However, in the sense of numerical effort required, FV method is preferred over the FE method. FV method was first used by McDonald P.W. for 2-D inviscid flows. The solving process starts by dividing the physical space into a number of arbitrary polyhedral control volumes. This is carried out either by a cell-centred scheme where the flow quantities are stored at the centroids of the grid cells or by a cell-vertex scheme where the flow quantities are stored at the grid points. Advantages of the FV method of discretization include its flexibility to be adapted to simulate flows in or around complex geometries. Therefore, the AVL-FIRE software which uses the FV method for discretization of the governing equations was used by Sattar as well as in the present study for simulating the flow in the steelmaking converter.

3.3.3 Multiphase flow simulation – Euler-Euler approach
Multiphase flow is when two or more phases are present in the fluid flow, similar to steelmaking converter, where, gas, liquid, and foam phases coexist and interact with each other. Moreover, the capability to predict the behavior of these multiphase flows can enhance the efficiency and the effectiveness of the process. Multiphase flows can be explored and analyzed either experimentally by laboratory and plant scale experiments, or theoretically by mathematical modeling and using computer simulations. Clearly, mathematical modeling and computer simulations are preferred over the experiments due to many reasons including the less time and cost
consumption. However, the results obtained from the simulations are sometimes questionable when the flow system is large and complex.\textsuperscript{[158]}

Figure 3.13: Difference between observing the fluid properties inside a control volume (Eulerian method) and observing the position, pressure and other properties of material volumes (Lagrangian method).\textsuperscript{[159]}

The main two methods used to observe and analyze multiphase flows are Lagrangian method and Eulerian method, which are shown in Figure 3.13. The Lagrangian method involves tracking specific and identifiable fluid material volumes that are carried about with the flow, while the Eulerian method involves tracking the velocity at locations that are fixed in space. The Lagrangian method is the most efficient method of analyzing multiphase flows and is natural for the statement of the fundamental conservation theorems. However, its application to three-dimensional fluid flows is complex. Eulerian method, in contrast, observes the fluid properties at fixed sites, which generally is the requirement of most of the engineering applications.\textsuperscript{[159]} The Eulerian approach has been used by many researchers in modeling systems with bubbles and foams.\textsuperscript{[30-32, 153, 160]} Hence, the AVL FIRE 2009.2 simulation software, which is based on the Eulerian method, was used for modeling the multiphase flow in the steelmaking converter.

3.3.4 Multifluid-model

Multifluid-model is the Eulerian method based multiphase model used in the AVL FIRE software, which is used in the present study. It is one of the three models that can be used in the multiphase module of FIRE, and it requires the calculation of the complete set of conservation equations for each phase. The other two models are the homogeneous/ equilibrium model and volume-of-fluid (VOF)/free-surface model. In the
homogeneous model, a volume fraction equation is calculated for each phase, although, only one momentum equation is calculated for all the phases in momentum equilibrium. Moreover, it is assumed to be the least accurate model among the three models under consideration. VOF model is similar to the homogeneous model in the numerical perspective but has a more accurate calculation of the volume fraction equation, which sometimes leads to very high-resolution requirements. Hence, the multifluid model is the best model to be used when considering both the computational requirements and accuracy.\[161]\]

3.3.5 Population balance modeling (PBM)

Many multiphase flow systems, which gain the interest of engineers, usually contain entities such as solid particles, drops, bubbles and cells, and these entities influence the behavior of the system as a whole. Therefore, it is of great importance to consider the population density of those entities when predicting the behavior of the entire system. Population balance modeling is required for this population density calculation of those entities in terms of their number, mass or volume. These entities of interest can be distinguished from each other by a number of variables that can be either external coordinates (physical location) or internal coordinates (size, temperature, and composition), and these variables collectively define the state of the entity.\[162]\]

Population balance can be one-dimensional or multi-dimensional, depending on the modeling requirement of the system under study. One-dimensional population balance is when the population calculation is carried out only using one coordinate of the entities in the system. For example, analysis of the distribution of crystals in a reactor with respect to the diameter of the spherical crystals\[163]\] and calculation of the population of particles in a granulating batch fluid bed system.\[162]\] The one-dimensional population balance is preferred in occasions where the single coordinate chosen is the most influential coordinate on the behavior of the system. Conversely, in the case of more complex systems, more than one coordinate has to be used for modeling the population balance, leading to the multi-dimensional population balance modeling. For example, in the case of crystal distribution calculation in the reactor, more than one length coordinate was considered by the authors to take into account the shape evolution of the crystals, which is more influential on the population of the crystals compared to one
length coordinate.\textsuperscript{163} Also, in the case of fluid bed system, several researchers have tried using a different number of coordinates including, particle total volume and liquid binder volume, and volume of solid, volume of liquid and volume of gas.\textsuperscript{162} Although it is clear that multi-dimensional population balance is the most accurate method for calculating the population balance, it demands expensive computational resources. Hence, researchers have been using sets of one-dimensional population balance equations occasionally to meet the required accuracy.\textsuperscript{162} However, in the present study, one-dimensional population balance was used, as only the volume of the bubbles was of concern in foam simulation and only the mass of each element was of concern in kinetics simulation.

The population density of the entities in a system under study is influenced by birth and death processes which create new entities and destroy existing entities respectively. Examples of such processes are nucleation of particles and break-up and aggregation of entities. When solving population balance equation with these mass changes, finite volume scheme can be used, because, the finite volume scheme is frequently used for solving mass conservation law. The other numerical methods for solving the population balance equation include the method of successive approximations, the method of Laplace transforms, the method of moments, weighted residuals, sectional methods and Monte Carlo simulation methods.\textsuperscript{164, 165} Sattar\textsuperscript{1} used the population balance to calculate the number densities of the bubble classes. In the present study, the birth and death of bubbles and birth and death of chemical species due to chemical reactions were considered, and the population balance used for the calculation was based on the finite volume scheme.

The population balance equation used in the present simulation is shown below.

\[
\frac{\partial}{\partial t} \left( \alpha_g \rho_g \phi_i \right) + \nabla \cdot \alpha_g \rho_g \nu_g \phi_i = \nabla \cdot \alpha_g \rho_g D_g \nabla \phi_i + S_i \tag{3.42}
\]

The source term ($S_i$) of the scalar transport equation is calculated from the balance of break-up and coalescence of the bubbles in both gas and foam phases and is given below. Where, $B_B$, $B_C$, $D_B$ and $D_C$ are birth and death of the bubbles due to break-up and coalescence respectively.
\[ S_i = \rho_g \left( B_B - D_B + B_C - D_C \right) \]  
Eq 3.43

\[ B_B = \sum_{k=1, j \in N}^{N} \Omega_g \left( \vartheta_k^i, \vartheta_j^i \right) + \sum_{k=1, j \in N}^{i} X_{i, k} \Omega_g \left( \vartheta_{i+1}^i, \vartheta_k^i \right), \quad i = 1, \ldots, N \]  
Eq 3.44

\[ D_B = \sum_{k=1}^{i-1} \Omega_g \left( \vartheta_k^i, \vartheta_j^i \right) + \sum_{k=1, j \in N}^{i} X_{i, k} \Omega_g \left( \vartheta_{i+1}^i, \vartheta_j^i \right), \quad i = 2, \ldots, N \]  
Eq 3.45

\[ B_C = \sum_{j=1}^{i-1} X_{i, j} \Omega_c \left( \vartheta_i^j, \vartheta_j^i \right) + \sum_{j=1}^{i-1} \left( 1 - X_{i-1, j} \right) \Omega_c \left( \vartheta_{i-1}^j, \vartheta_j^j \right), \quad i = 2, \ldots, N \]  
Eq 3.46

\[ D_C = \sum_{j=1}^{N-1} \Omega_c \left( \vartheta_{i-1}^j, \vartheta_j^i \right) - \sum_{j=1}^{i-1} X_{i, j} \Omega_c \left( \vartheta_i^j, \vartheta_j^j \right), \quad i = 1, \ldots, N - 1 \]  
Eq 3.47

As mentioned earlier, bubble break-up and bubble coalescence were taken into account when calculating the population balance of gas and liquid phases. Bubbles break-up when they meet with eddies with sufficient energy and size, and produce two daughter bubbles (binary break-up model). The bubble break-up model developed by Luo and Svendsen\textsuperscript{152} was used in the present study similar to Sattar’s work\textsuperscript{1} and was explained in Section 3.1.6.4. Bubbles coalescence occurs in the gas-liquid dispersion due to various reasons including the collision of bubbles carried around by the turbulence, buoyancy, and viscous shear. In the present study, bubbles were assumed to coalescence only due to turbulence. The coalescence model used was the model developed by Prince and Blanch\textsuperscript{150} and was explained in Section 3.1.6.3.

### 3.3.6 Foaming criteria developed by Sattar\textsuperscript{1}

The model developed by Sattar\textsuperscript{1} has foam as a separate phase, which was produced from liquid and gas phases. In reality, the foam is a substance produced by trapping gas bubbles in a liquid. Foam volume at a particular instance is the balance between the foam produced by the formation of bubbles, and the destruction of foam due to various reasons including bubble break-up, coalescence and foam drainage. These characteristics of foam are difficult to be integrated into an ordinary gas-liquid two-phase simulation. Therefore, a separate phase was introduced, which was produced when the presence of gas phase and the liquid phase exceeded 75% and 5% respectively in terms of volume fraction in the gas-liquid mixture. The foam bubbles were considered
to be closely packed pentagonal dodecahedrons which are typical for foam in the transition region between dry and wet liquid volume fraction extremes. In this model, Sattar[1] considered ten bubble classes in the foam and change of the bubble population via the bubble coalescence at the top of the foam and bubble bursting due to drainage. The density and the viscosity of the foam were calculated at each time step according to the fraction of gas and liquid present in the foam as expressed by equations 3.48 and 3.49.

\[ \rho_f = \alpha_g \rho_g + \alpha_l \rho_l \]  
Eq 3.48

\[ \mu_f = \alpha_g \mu_g + \alpha_l \mu_l \]  
Eq 3.49

In foam, the liquid is trapped in the bubble films and plateau borders, which is reduced by drainage and bursting of foam bubbles. In this model, the liquid in the foam was considered to drain only when the foam collapses. Once the foam collapses, the liquid and gas that were in the foam add back to the relevant phases. The total amount of liquid in the foam was calculated by equation 3.50.

\[ \phi_i = N_i n_p a_p l_i + N_f n_f a_f x_f \]  
Eq 3.50

Where \( N_i \) is the number of bubbles in the \( i \)th bubble class, \( n_p \) is the number of plateau border channels per bubble, \( a_p \) is the cross-sectional area of the plateau border, \( l_i \) is the length of plateau border, \( n_f \) is the number of films per bubble, \( a_f \) is the cross-sectional area of the foam bubble film and the \( x_f \) is the thickness of the film.

Since the liquid entrapped in the bubble films is negligible compared to that in the plateau border channels, equation 3.50 was modified to equation 3.51, and the total liquid amount in the foam was calculated using equation 3.52.

\[ \phi_i = N_i n_p a_p l_i \]  
Eq 3.51

\[ \phi = \sum_i N_i \phi_i \]  
Eq 3.52
In the foaming model developed by Sattar\cite{1}, the coalescence of bubbles in the foam was considered and was calculated using the model developed by Tong et al\cite{166} as given by equation 3.53.

\[ \Omega_{i,j}^f = n_{pi} P_{i,j} f_{i,j} \]  
\text{Eq 3.53}

Where, \( n_{pi} \) is the number of films per bubble in the \( i \)th group, \( P_{i,j} \) is the failure rate of films separating the bubbles of the \( i \)th and \( j \)th groups, \( f_{i,j} \) is the probability of a bubble of the \( i \)th group sharing the same film with a bubble of the \( j \)th group in the foam.

Since the bubbles in the foam were considered to be of pentagonal dodecahedron shape, \( n_{pi} \) was assumed to be 6. Then the probability of sharing the same film by the bubbles of the \( i \)th and \( j \)th groups was calculated using equation 3.54 below, where, \( n_i \) and \( n_j \) are the number of bubbles in the \( i \)th and \( j \)th groups respectively.

\[ f_{i,j} = \frac{n_{pi} n_j}{\sum_{k=1}^{M} n_{pi} n_k} \]  
\text{Eq 3.54}

The failure rate of films separating two bubbles was calculated using the following equation 3.55, which shows an inverse proportionality between the failure rate and the film lifetime (\( \tau \)), where \( k \) is the proportionality coefficient.

\[ P_{i,j} = k \frac{1}{\tau} \]  
\text{Eq 3.55}

The film lifetime was calculated using the equation 3.56 below, where, \( \phi / d_i \) is the amount of liquid in the bubble and \( q_{PB} \) is the drainage flow through the plateau borders.

\[ \tau = \frac{\phi / d_i}{q_{PB}} \]  
\text{Eq 3.56}

The required condition for the foam to collapse was considered as the foam becoming dry enough with very less amount of liquid in the foam. Moreover, when this condition is met, the foam collapses and the gas and liquid masses add to the relevant phase. The foaming model developed by Sattar and his co-workers\cite{1} was used as the basis and was
improved in the present study. The details of the improved foaming phenomenon are discussed in Chapter 6.

### 3.3.7 Results of the model developed by Sattar[1]

The main aim of the study by Sattar[1] was to predict the foam height in oxygen steelmaking using the developed CFD model. The results obtained from simulating the model for 10 minutes in real time are shown in Figure 3.14. The foam height was assumed to be the average height of three height measurements taken between the gas and foam interface (top surface of the foam) and the liquid and foam interface (bottom surface of the foam). As shown from the figure, the foam height prediction during the first 5 minutes of the blow is over-predicted and shows an increasing trend. After that, during the rest of the blow, the average foam height prediction is lower compared to the observed values. The simulation results show an oscillating nature in the first 9 minutes and apparently reach a quasi-steady state after that.

![Figure 3.14: Foam height variation over the blowing time[1]](image)

As explained by the authors, the over-prediction of foam height during the first 4 minutes was due to higher decarburisation, as the injected oxygen was consumed by the carbon in the hot metal. Only the decarburization at the liquid-gas interface was considered in this model, and the under-prediction of foam height during the middle part of the blow was considered due to the decreasing amount of carbon availability for the decarburization reaction. Moreover, the quasi-steady foam height towards the end of simulation time was explained as because of only the injected gas and birth and death
of bubbles in the foam without being affected by the CO generated from
decarburization, as carbon availability is very less in the melt at the moment of
consideration.

As mentioned above, in this study by Sattar\textsuperscript{[1]}, only the decarburization reaction was
considered as a chemical reaction in the melt, where, the carbon dissolved in the hot
metal reacts with the injected oxygen at the gas-liquid interface and produces only the
CO gas. The kinetics of the decarburization reaction was assumed to be first order, and
an empirical rate constant was used in the simulation. The simulation results on the
decarburization pattern are shown in Figure 3.15.

According to the simulation results, the decarburization reaction is started from the
beginning of the blow and occurs at a constant rate until the end of the simulation time.
This was explained by the authors to be due to the sole consumption of oxygen by the
decarburization reaction from the start of the blow and also due to the consideration of
the multi-step decarburization reaction as a single step reaction.

The heat generation due to the decarburization reaction was also predicted by the
model developed by Sattar\textsuperscript{[1]}. The temperature prediction of the bulk metal bath by the
model is shown in Figure 3.16.
Although the simulation results exhibit the increasing trend of temperature as those observed, a temperature surge can be noted in the predicted values during the first part of the blow, which was explained to be due to the excessive decarburization during the first part of the blow.

3.4 Drawbacks identified in the model developed by Sattar\cite{1}

The model, developed by Sattar and his co-workers\cite{1} produced reasonably agreeable predictions on foam height and the removal behavior of carbon in an oxygen steelmaking converter, as shown in Figures 3.14 and 3.15. This model for oxygen steelmaking converter was an extension to the model they developed previously for simulating and predicting the bubble number density and foam height in the bubble column reactor, and slag foaming in a crucible containing slag following the experiments carried out by Fruehan et al.\cite{16} Same foaming model was applied in modeling the steelmaking converter with added decarburization reaction and heat generation by the decarburization reaction. Even though, the model produced agreeable results when compared to the plant trial observations reported in the IMPHOS report\cite{2}, the extent of consideration and incorporation of the actual oxygen steelmaking operations in the model was not adequate. Hence, following is a summary of the drawbacks identified in the model developed by Sattar and the co-workers\cite{1}, some of which were also their recommendations for improving the model.

- Oxygen steelmaking process involves the refining of steel by removing the impure elements, mainly C, Si, Mn, and P, via direct oxidation and metal-slag
reactions, to produce steel with the required quality. Also, these chemical reactions cause the slag composition to evolve and, as a result, the physical properties of the slag also evolve, most of the times, in favor of foaming. Hence, a model developed for predicting steelpmaking process has to incorporate these refining reactions, to predict the refining behavior and the foaming with a good accuracy. However, the model developed by Sattar\cite{1} only considered the decarburization reaction in the converter.

- Modeling of steel refining during the steelpmaking process via incorporating the chemical reactions requires developing and incorporating a kinetics model which calculates the rates of the reactions. The rate of the decarburization reaction considered in the model developed by Sattar\cite{1} was calculated empirically from the results reported in the IMPHOS report\cite{2} on the carbon removal behavior of heat S1830. Due to this reason, the model may not be able to produce reliable predictions on decarburization in the steelpmaking converter when the process conditions are changed.

- In oxygen steelpmaking, the foam is produced when the gases injected and produced are trapped in the slag layer. Hence, the extent of slag foaming depends on the slag quantity and the physical properties of the slag. So, a model developed for predicting the foam height in steelpmaking should produce the foam from the slag. However, in the model developed by Sattar\cite{1}, the foam is produced from the pure liquid (i.e. liquid metal), which was only valid in the case of bubble column reactors. According to the available slag foaming literature, pure liquids do not foam, as explained in Section 3.1.3. The presence of surface-active solutes in the liquid is essential for the foaming of the liquid by reducing the surface tension and the density of the liquid. Hence, use of liquid metal to produce foam in this model is not reasonable.

- Once the foam is formed, the bubble films and the plateau borders in the foam continuously drain due to several factors including the gravity and physical properties of the liquid. Once the bubble films drain and reach a critical thickness, foam bubbles rupture, reducing the foam volume. Therefore, a model to predict the foam height should have a foam drainage mechanism to
continuously drain the foam until the bubble film thickness reach the critical thickness and rupture, which was not clearly incorporated in the foaming model developed by Sattar\cite{1}.

- Bubble films in the foam rupture when they reach a critical thickness due to drainage. Foam collapses due to different reasons such as the turbulence in the liquid, drainage of bubble films and external disturbances. So, the foam collapsing criteria in the foaming model should be developed in relation to the effect of these factors. However, the foam collapsing criterion used in the model developed by Sattar and the co-workers\cite{1} was an empirical relationship obtained from a trial and error method.

Although these drawbacks were identified in the model developed by Sattar and his co-workers\cite{1}, the results produced by their model were acceptable when compared with the plant trial observations. Therefore, their model was used as the starting point for the present study, and an effort to overcome the drawbacks mentioned above was assumed to improve the model to be more representative of the actual oxygen steelmaking process.

3.5 **Answers from the present study**

The model developed by Sattar and the co-workers\cite{1} on foaming in oxygen steelmaking converter produced reasonably acceptable foam height predictions despite the drawbacks mentioned above. Therefore, in the present study, that model was improved by providing rectifications to the identified drawbacks as listed below.

- In the present study, the major oxidizing reactions and other slag-metal reactions were included in the model as explained in Section 2.1.7.
- A semi-empirical kinetics model was developed and used in the model to determine the reaction rates of oxidizing reactions as explained in Chapter 5.
- Slag was defined as a separate phase, and the foam was produced by both slag and liquid phases as explained in Chapter 7.
- A foam drainage phenomenon was introduced into the model which calculates the drainage until the liquid fraction in the foam reaches a critical limit as explained in Chapter 6.
Foam collapsing was defined as the reduction of liquid fraction in the foam beyond a critical liquid fraction as explained in Chapter 6. These suggestions were incorporated in the already developed model by Sattar\cite{1} in two stages. In the first stage, the same three phases model (i.e. the model with liquid, gas and foam phases) was used to model the refining reactions. The improved foaming phenomena with continuous drainage and new foam collapse criteria were also first incorporated in the three phases model. The detailed description of these improvements in the three phases model is given in Chapter 6. The next stage was to introduce the separate slag phase to the three phases model which was already improved with the refining kinetics and the new foaming criteria. And, in this four phases model, the foam was produced from the slag and liquid phases simultaneously. The details of this model are presented in Chapter 7.

Yet, the results obtained from the new models do exhibit a certain level of deviation from the observed data as reported in the IMPHOS trials\cite{2}. This can be attributed to the reasons such as CFD modeling limitations and lack of data available on certain parameters of the process. These research issues are addressed in detail in the discussion.
Chapter 4
Chapter 4: Research questions

Slag foaming is an important phenomenon encountered in oxygen steelmaking which is advantageous when controlled to a limited quantity and can be detrimental when produced in excessive amounts creating a slopping event. Hence, it is essential to properly control slag foaming in oxygen steelmaking for a continuous and efficient production process.

Based on the literature review presented in previous two chapters, it is clear that steelmaking researchers have been conducting studies to investigate and model slag foaming and reaction kinetics in oxygen steelmaking since several decades. Some of those leading research works carried out on slag foaming include the studies by Cooper and Kitchener\cite{14}, Fruehan and co-workers\cite{15-18}, Ghag and co-workers\cite{19-21}, Stadler and co-workers\cite{22, 23}, Irons and co-workers\cite{25, 26} and Seetharaman and co-workers\cite{11, 27}. The slag foaming was found to be dependent on the physical properties of slag and the gas production rates, but, an argument exists that true foam cannot be produced at the higher superficial gas velocities encountered in oxygen steelmaking.\cite{24} However, the need for a more accurate and dynamic slag foaming model is emphasized in the literature\cite{11-13}. Hence, in the present study, a slag foaming model was developed using the CFD technique starting from the foaming model developed by Sattar\cite{1}.

The CFD model developed by Sattar\cite{1} was able to predict the foam height, the number densities of bubble classes in gas and foam phases, decarburization, heat generation and the velocities of the phases as explained in Section 3.3. The multiphase flow simulation was carried out with a Eulerian-Eulerian approach. The population balance equation was used to calculate the population densities of the components of each phase, and in the case of population calculations of the bubble classes, the bubble coalescence and breakup were taken into consideration. Only the decarburization reaction was considered in their work, and the heat generation due to carbon oxidation was incorporated in the simulation. The results obtained from the simulation were compared with the observed data published in IMPHOS\cite{2} and were in reasonable agreement.
Nonetheless, several drawbacks were identified in this model developed by Sattar\cite{1} including the less number of chemical reactions considered, empirical decarburization rate calculation, the formation of aqueous foam instead of a slag foam and insufficient accuracy in the foam simulation. These drawbacks were recognized as potential pathways to improve the existing CFD foaming model to become more representative of the actual steelmaking process.

The primary goal of the present study was to improve the CFD model to predict slag foaming in oxygen steelmaking converter, and this goal was divided into four main tasks as given in Section 1.3 which were identified as the objectives of the present study. These four tasks were achieved in three main stages of the CFD model.

In the first stage, a semi-empirical first order kinetics model was developed using the pilot plant data reported in IMPHOS\cite{2} report and was incorporated in the CFD foaming model. The kinetics model calculates the removal pattern of the impurity elements C, Si, Mn, and P assuming the rate of the oxidizing reactions of those elements to be first order. An analysis was carried out on the kinetics model prior to being incorporated in the CFD model in order to check its performance in terms of calculating the removal pattern of C, Si, Mn and P. The details of the analysis, the methodology and the results obtained after incorporating the kinetics model as a submodel in the CFD foaming model are presented in Chapters 5, 6 and 7.

In the second stage, the foaming model developed by Sattar\cite{1} was further enhanced in terms of foam formation and collapse and continuous foam drainage as explained in Chapter 6. The model geometry and the sub-models for bubble coalescence and breakup in gas and foam developed by Sattar\cite{1} were not changed in the present work. The foam formation criteria used by Sattar\cite{1} was used in the present study with improved mass exchange between the phases. The collapsing criterion of foam used in the present study was defined based on the minimum liquid volume fraction carried by dry foam. The pilot plant data reported in the IMPHOS\cite{2} research report was used in the present study for comparing and validating the model results.

The foam produced in the three phases CFD model was more related to aqueous foam than slag foam. Therefore, this three phases CFD model was further improved to a four
phases model by incorporating slag as a separate phase and producing foam from the slag phase in the third stage. These improvements are expected to upgrade the CFD foaming model to be able to predict slag foaming similar to the slag foaming in actual oxygen steelmaking. The IMPHOS\cite{2} research report was used to extract data on slag foaming observed during a blow for comparing the model results. The details of the four phases model and its performance are presented in Chapter 7.
Chapter 5
Chapter 5: The kinetics model*

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One of the primary objectives of the present research work was to model and predict the refining kinetics of main impure elements during the blow in oxygen steelmaking. Employing a kinetics model based on the first order kinetics was recognized appropriate as a starting point, and therefore a semi-empirical first order kinetics model was developed to be included in the present CFD model. Prior to the incorporation of the developed kinetics model into the CFD model, an analysis was carried out to investigate the applicability of the developed first order kinetics model to predict plant data on refining kinetics, using the data reported in IMPHOS research report [2]. Further, the relevant values of constants required for the model were also determined during this analysis, so that, the CFD model predictions on the refining kinetics are more consistent and can be compared with those observations reported in IMPHOS [2]. Hence, in this chapter, the semi-empirical kinetics model developed, the analysis carried out on the observed data published in IMPHOS [2], and the rearranged form of the kinetics model that was included the CFD model, are explained in detail.

5.1. Introduction

5.1.1. Requirement for a kinetics model

The fundamental principle of refining steel from the blast furnace produced pig iron is oxidizing and removing the impure elements in the form of oxides until the required composition is obtained. [4, 7, 167] In oxygen steelmaking, a pure oxygen stream is utilized for this purpose, and with the injection of oxygen, the elements in the metal bath oxidize according to their affinity for oxygen. The amount of oxygen required to be injected and the extents of oxidation achieved with the injection of that quantity of oxygen have to be predetermined to produce a particular grade of steel. [49, 168] Hence, a proper kinetics model, which is capable of explaining the extent and pattern of oxidizing of impure elements and the dissolution of added fluxes and scrap into the hot metal, is essential. Further, this model can be utilized to optimize the process in terms of steel yield and the resources consumed, which is a necessary tool for a steelmaking plant as emphasized in the literature. [38, 46, 47, 64, 109] Even though the model developed in the present study was
aimed primarily at predicting the slag foaming, it was also expected to predict the refining behavior of the impure elements. This is mainly because of the effect of reaction kinetics on the slag composition and gas generation, which has a direct influence on foaming in the converter. Therefore, a kinetics model was developed and incorporated into the CFD slag foaming model as explained in the following sections.

5.1.2. First order reaction kinetics

Modeling the refining kinetics of oxygen steelmaking process has been the interest of steelmaking researchers; because of the process optimizing opportunities arose by such models. Refining kinetics in a steelmaking converter is well-recognized for its transient nature and complexity, due to both the intense mixing conditions involved and dynamic composition of the bath throughout the process with flux addition and refractory dissolution. Among those modeling efforts available in the literature, some studies have focussed on investigating and modeling all the major refining reactions based on a single approach, while, the other studies have focussed only on selected refining reactions. However, most of those research were based on industrial plant trial data and were capable of predicting end blow parameters with certain accuracy. However, these industrial data sets are often specific to the particular plant and are usually difficult to be employed on a general basis.

Even though most of those models have suggested and incorporated more complicated mathematical relationships compared to the first order kinetics, some modeling efforts have used the first order kinetics successfully for predicting the kinetics of refining reactions in steelmaking. For example, in the analysis carried out by Ishikawa on desiliconization, the refining rates of Si, Mn and P were calculated using the first order kinetics relationship. The rate of dephosphorisation was assumed to follow a first order relationship by Monaghan et al and Nasu et al, while Kawai et al used a first order relationship to calculate the demanganization rate in their analysis. First order rate equations were also used by Dogan et al and Shukla et al in their models to calculate the rate of decarburization. Hence, the use of first order kinetics for modeling and predicting the steelmaking reactions is not a novel effort and was the approach selected in the present study to model the major refining reactions as an initiation.
However, as mentioned earlier, before integrating the first order kinetics model into the CFD model, an analysis was carried out to validate its applicability to calculate the rates of refining reactions, using the plant data published in IMPHOS\[^2\]. The details of the analysis are presented in Section 5.2.

### 5.1.3. IMPHOS\[^2\] summary

Present analysis on the applicability of first order kinetics to predict the steelmaking reaction rates was performed on the data published in the IMPHOS research report\[^2\]. IMPHOS is the research work published on the information obtained from plant trials conducted in a 6-tonne MEFOS converter and is the most recent reliable set of data on oxygen steelmaking process under plant conditions. The main aim of this IMPHOS research was to provide an improved explanation of the dynamics of phosphorus refining as a function of slag formation, and development and dispersal of metal droplets.\[^2, 135\] This study provides results on different process variables such as steel bath composition, slag composition, the temperature during the blow and lance height.\[^2, 136\] The data set comprises of data for 20 heats, and in each heat, samples were collected at seven different locations inside the converter every two minutes from the start to the end of the oxygen blow. These samples were then magnetically separated to slag and metal components and were analyzed using different methods such as spark emission spectroscopy, inductively coupled plasma, optical microscopy, and SEM analysis.\[^2\] A detailed description of the IMPHOS research work was given in Section 2.3, Chapter 2. However, the data extracted from the IMPHOS report for the present analysis were the composition of slag and metal over the blow and the initial and turndown analysis of each heat.

### 5.2. First order kinetics model

The rates of refining reactions in oxygen steelmaking are expected to be governed mostly by the mass transfer of the reactants to the interface. Once the reactants are available at the interface, the reactions occur at the maximum rate encouraged by the higher temperatures available in the bath.\[^4, 68\] Fick’s first law of diffusion can be employed to calculate the rates of the refining reactions under these conditions, as it assumes that reaction rates are limited by the diffusion of reactants to the interface.\[^72\] The Fick’s first law of diffusion states that the rate of diffusion of the reactant is
proportional to the concentration gradient of the reactant, and can be expressed as following equation 5.1.[68]

$$\frac{dC}{dt} = kA \frac{\rho_m}{W_M} (C_b - C_{eq})$$

Eq 5.1

Where, C is the concentration of the reactant (%wt), k is the mass transfer coefficient (m/s), A is the interfacial area (m²), $\rho_m$ is the density of the metal (kg/m³), $W_M$ is the weight of the metal (kg), $C_b$ and $C_{eq}$ are the bulk and equilibrium concentration of the reactant in the metal bath (%wt).

The analysis was carried out in two stages based on the calculation method of $C_{eq}$ in the first order kinetics equation 5.1. In the first stage, the reaction rates were calculated for all the four elements (i.e. C, Si, Mn, and P), assuming the equilibrium concentration ($C_{eq}$) of each element is static and is equal to their composition in the turndown steel as reported in IMPHOS report[2]. Since the results of the analysis at this stage for Mn and P were not satisfactory, the analysis was extended to the second stage. The second stage of the analysis was dedicated to investigate the applicability of first order kinetics to calculate the reaction rates of Mn and P using dynamically calculated equilibrium values.

The calculation procedures for both stages of the analysis are given in Sections 5.2.1 and 5.2.2 respectively. Further, the data required for the variables in the first order kinetics equation 5.1 were extracted from the IMPHOS report[2], and are tabulated below.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_0$</td>
<td>The concentration of the element at the start of the blow extracted from the hot metal analysis.</td>
<td>Table A2-1, Appendix 2[2]</td>
</tr>
<tr>
<td>$C_t$</td>
<td>The concentration of the element at a particular instance extracted from reported steel bath compositions.</td>
<td>Steel bath analysis, Section 2.2.2.1[2]</td>
</tr>
<tr>
<td>$W_M$</td>
<td>Total mass of hot metal input and the scrap added as reported in input materials to the converter</td>
<td>Table A2-2, Appendix 2[2]</td>
</tr>
<tr>
<td>$C_{eq}$</td>
<td>The equilibrium concentration of the element given in the turndown steel analysis</td>
<td>Table A2-3, Appendix 2[2]</td>
</tr>
</tbody>
</table>

*Used in the static equilibrium method
5.2.1. Static equilibrium method

The first stage of the analysis was the static equilibrium method, where, the equilibrium concentration ($C_{eq}$) of the element was assumed to be constant throughout the blow, and the value of $C_{eq}$ was extracted from the turndown steel analysis reported in the IMPHOS report[2].

5.2.1.1. Calculation method

The analysis was started by integrating and rearranging equation 5.1 into equation 5.2. Since the variable $C_{eq}$ in this stage is a constant value, and the value of the multiplication $kA$ was assumed to be constant, equation 5.2 should generate a straight line when

$$-\ln \left( \frac{C_t - C_{eq}}{C_0 - C_{eq}} \right)$$

was plotted against time $t$. Then, the value of the constant

$$kA \frac{\rho_m}{W_M} \left( \frac{C_0}{C_0 - C_{eq}} \right)$$

can be estimated from the slope of the graph.

$$-\ln \left( \frac{C_t - C_{eq}}{C_0 - C_{eq}} \right) = kA \frac{\rho_m}{W_M} t \left( \frac{C_0}{C_0 - C_{eq}} \right)$$

Eq 5.2

Where $C_t$ and $C_0$ are the concentration of the reactant at time $t$ and $t=0$ respectively.

Therefore, the above relationship given by equation 5.2 was plotted for each of the four elements (i.e. Si, C, Mn, and P) for each heat, and the deviation of the data points from the straight regression line for each case was determined using the coefficient of determination ($R^2$). By analyzing the $R^2$ values for each graph plotted for 20 heats, the applicability of the first order kinetics to calculate the refining rate of those elements was decided. As mentioned previously, the constant $kA \frac{\rho_m}{W_M} \left( \frac{C_0}{C_0 - C_{eq}} \right)$ is equal to the slope of the graph, and by using the values of $\rho_m$, $W_M$, and $\left( \frac{C_0}{C_0 - C_{eq}} \right)$ extracted from IMPHOS[2] report; the value of the multiplication $kA$ was calculated for each heat. The results of this calculation are given in Table A1 in Appendix A1, and the values of this constant $kA$ used in the kinetics model incorporated in the CFD foaming model are explained in Section 5.3.
5.2.1.2. Results

The plots of \(-\ln\left(\frac{C_t - C_{eq}}{C_0 - C_{eq}}\right)\) against time were generated for each of the four elements for all the 20 heats according to the above-explained procedure. Following Figures 5.1 to 5.4 show selected two plots for each element, where the left-hand side figure in each row shows the best fit of the data points to the regression line, while the right-hand side figure shows the least fit of the data points to the regression line for the element under investigation.

Figure 5.1: Carbon removal kinetics (a) Heat S1839 (b) Heat S1841

Figure 5.2: Silicon removal kinetics (a) Heat S1838 (b) Heat S1839
By observing the generated graphs, a conclusion was drawn that the refining kinetics of C and Si can be calculated with a considerable accuracy by the first order kinetics using the static equilibrium values. The reason is that almost all the plots generated for C and Si showed a good fit to the linear regression line. In summary, the coefficient of determinations ($R^2$) of the twenty graphs generated for C varied between 0.99 and 0.58 as illustrated in Figure 5.1, where, in about 60% of all the twenty heats analyzed, the $R^2$ values were more than 0.90. The graphs generated for Si were showing $R^2$ variation between 0.99 and 0.89 as shown in Figure 5.2, where, about 95% of the analyzed heats were displaying $R^2$ values more than 0.9.

Conversely, the plots generated for Mn and P were not in compliance to the first order kinetics using static equilibrium values. The variation of the $R^2$ values over the twenty heats for P was between 0.95 and 0.55 as shown in Figure 5.4, where, about 75% of the heats among the 20 heats analyzed were demonstrating $R^2$ values more than 0.7. With
respect to Mn, plots were generated only for 12 heats, due to restrictions arose in calculating the logarithmic values of the data available. However, the results of the analysis carried out on those 12 heats were such that, the $R^2$ varied between 0.92 and 0.0001 as illustrated in Figure 5.3, where, only 25% of the heats showed $R^2$ values more than 0.7.

Hence, it is evident from the results at this stage that the first order reaction kinetics using the static equilibrium values can be used for predicting the refining behavior of Si with a significant accuracy. Similarly, the refining of C can also be predicted by employing the first order kinetics using the static equilibrium values with a considerable precision. However, the refining of Mn and P cannot be predicted by the first order kinetics using static equilibrium values. These observations on Mn and P are in agreement with the common experience of steelmaking researchers, as the general refining behavior of Mn and P is complex involving interchanging oxidation and deoxidation during the blow. However, there is evidence of using the first order kinetics for predicting the kinetics of Mn and P refining, as explained in Section 5.1.2. Therefore, the present analysis was extended to investigate the applicability of the first order kinetics to predict the refining kinetics of Mn and P using dynamically calculated equilibrium values.

### 5.2.2. Dynamic equilibrium method

The refining kinetics of Mn and P are recognized for their complex nature and are generally explained by their dependence on the composition of the slag and temperature, as discussed in Section 2.1.7. Since the composition of the slag evolves with time during the blow with the oxidized elements and added fluxes, a model assigned to calculate the kinetics of Mn and P has to consider the effect of the evolving slag composition as well as the temperature. Therefore, at this stage of the analysis, the refining kinetics of Mn and P were calculated using a dynamic equilibrium value based on the temperature and slag composition as explained in the following sections.
5.2.2.1. Recycled Converter Slag (RCS)

Slag produced in the converter during the steelmaking process is a source of calcium oxide (CaO), iron (Fe), iron oxide (FeO), silicon dioxide (SiO$_2$), magnesium oxide (MgO) and manganese oxide (MnO), and is generally produced in amounts of 100 to 150 kg/tonne of steel.$^{[112]}$ The traditional method of disposing of this slag was dumping, which required a large area of land and caused environmental pollution. Hence, the slag recycling opportunities such as cement production, road construction, fertilizer production and land filling were identified,$^{[58, 112, 173]}$ among which, some methods were developed to reuse the slag in iron and steelmaking processes creating a sustainable system loop. These latter applications of slag include its use as a fluxing material mixed with limestone and dolomite encouraged by its rich CaO composition, and as a consumable refractory coating splashed onto the refractory lining.$^{[8, 58, 112, 173, 174]}$ Further, recycled slag is easy to melt due to the presence of pre-melted compounds, and provides additional Fe units to the bath.$^{[112]}$ Figure 5.5 schematically illustrates the use of recycled converter slag in the steelmaking process. However, the quantities of elements such as P and S brought forward by the recycled slag may cause troubles in achieving the required extent of refining during the process.$^{[112]}$

![Figure 5.5: Schematic of RCS use in the steelmaking process$^{[112]}$](image)

In the plant trials reported in IMPHOS$^{[2]}$, 30kg of recycled converter slag was added to the bath at the start of the blow in each heat. Therefore, in the present analysis, the addition of RCS was considered in the slag composition calculation, as it increases the volume of the slag in the converter. The composition of the added RCS (given in Table
5.1), was assumed to be similar to the average composition of turndown slag reported in the IMPHOS report[2], and the added RCS was assumed to be completely liquid at the start of the blow.

Table 5.2: Composition of typical RCS

<table>
<thead>
<tr>
<th>Compound in RCS</th>
<th>Wt% in RCS</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaO</td>
<td>42.4</td>
</tr>
<tr>
<td>FeO</td>
<td>17.3</td>
</tr>
<tr>
<td>SiO₂</td>
<td>12.3</td>
</tr>
<tr>
<td>MnO</td>
<td>3.6</td>
</tr>
<tr>
<td>P₂O₅</td>
<td>1.2</td>
</tr>
<tr>
<td>MgO</td>
<td>10.3</td>
</tr>
<tr>
<td>S</td>
<td>0.2</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>1.2</td>
</tr>
</tbody>
</table>

5.2.2.2. Flux dissolution

Fluxes are one of the main raw materials added to the bath during the first few minutes in the steelmaking process.[8] The main ingredients of fluxes are lime and dolomite, and fluxes fulfill two main requirements when added to the bath. Firstly, the fluxes are added to the bath to flux the impurities in the molten metal. The lime (CaO) in the fluxes added increases the basicity of the slag, and accelerates the refining of acidic oxide formers such as P and S. Secondly, fluxes are expected to protect the refractory lining of the converter from the corrosive attack of acidic slag, and the MgO contained in the added fluxes fulfils this requirement by saturating the slag with MgO.[41, 81, 83]

In order to utilize the added fluxes in full, the total quantity of fluxes added should properly and quickly dissolve into the bath.[41, 81] The factors affecting the dissolution of fluxes are the bath temperature, stirring intensity, the composition of slag, and porosity and size of flux particles, [41, 83, 107] as explained in Section 2.1.7.6. Therefore, investigating and understanding the flux dissolution mechanism, and its effect on the refining process have been the research interest of steelmaking researchers, and several studies on flux dissolution are available in the literature. A brief discussion on the studies carried out on investigating flux dissolution was presented in Section 2.1.7.7.
In the present analysis, flux addition and its dissolution were taken into consideration, because lime and dolomite were added to the bath during the plant trials reported in IMPHOS\textsuperscript{[2]}. The dissolution of lime was assumed to be linear at a rate of 11.2 kg/min in the present analysis. Even though the dissolution of fluxes are complex in nature, this simple assumption was made as an initiation for the analysis, and the value of the dissolution rate was obtained from the data provided in IMPHOS report\textsuperscript{[2]} on lime addition. Dolomite addition was neglected in the present analysis, because, dolomite was only added to two heats from the 20 heats reported. However, the quantity of MgO added to the bath via the dissolution of lime according to the composition given in Table 5.2 was considered simultaneously with the CaO and MgO brought in by the added RCS according to Table 5.1.

Table 5.3: Composition of lime added to the bath in IMPHOS plant trials (Table A4-1, Appendix 4)\textsuperscript{[2]}

<table>
<thead>
<tr>
<th>Compound in Lime</th>
<th>Wt% in Lime</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaO</td>
<td>92.20</td>
</tr>
<tr>
<td>SiO\textsubscript{2}</td>
<td>1.80</td>
</tr>
<tr>
<td>MnO</td>
<td>0.03</td>
</tr>
<tr>
<td>MgO</td>
<td>1.60</td>
</tr>
</tbody>
</table>

The evolution of both CaO and MgO in the slag was calculated according to the assumptions mentioned above. Then the calculated flux compositions were plotted in graphs with the observed CaO and MgO mass evolutions reported in the IMPHOS report\textsuperscript{[2]} for the relevant heat for the purpose of comparison. Figures 5.6 and 5.7 illustrate the graphs of CaO and MgO evolution for two selected heats, and as it is evident from the graphs, the assumption of linear dissolution of fluxes made during the present analysis was confirmed valid.
Scrap is basically recycled iron or steel and is the second main iron contributor to the steelmaking converter.\cite{8} Even though EAF is the primary consumer of scrap, a certain quantity of scrap is recycled in BOS converters. Since the melting of scrap is endothermic, it absorbs the excessive heat generated by the desiliconization during the first 8 to 10 minutes into the blow, operating as a coolant.\cite{8,77} Hence, the amount of scrap added to the converter is determined by the heat generation capacity of the process via oxidizing reactions and should be calculated precisely to ensure the complete melting of the added scrap quantity to prevent the need for any re-blows.\cite{68}
Therefore, it is essential to understand the mechanism of scrap melting and its consequences on the refining process. Due to that reason, melting of scrap has been investigated by researchers as explained in Section 2.1.7.5. Researchers have carried out studies under different process conditions and on various shapes of scrap pieces.\textsuperscript{38, 42, 77, 79, 80} However, in the present study, a simplified relationship derived from the results obtained by Dogan et al\textsuperscript{38}, as illustrated in Figure 2.11, was used to calculate the scrap melting rate.

Rate of change of scrap thickness \[= 1.8 \times 10^{-4} \text{ m/s}\]

According to the data used by Dogan et al\textsuperscript{38};

Area of scrap/liquid interface \[= 5.4 \text{ m}^2\]
Density of scrap \[= 7200 \text{ kg/m}^3\]
Scrap weight change \[= 7200 \times 1.8 \times 10^{-4} \times 60 \times 5.4 \text{ kg/min} \]
\[\approx 420.0 \text{ kg/min}\]

Area of scrap/liquid interface in IMPHOS converter \[= 1.41 \text{ m}^2\]
Therefore;

Scrap weight change \[= 7200 \times 1.8 \times 10^{-4} \times 60 \times 1.41 \text{ kg/min} \]
\[\approx 110.0 \text{ kg/min}\]

The composition of scrap used in the calculation was assumed to be the composition of the average turndown steel reported in the IMPHOS research report\textsuperscript{[2]}, and is given in Table 5.3.

<table>
<thead>
<tr>
<th>Compound in Scrap</th>
<th>Wt% in scrap</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>4.03</td>
</tr>
<tr>
<td>Si</td>
<td>0.57</td>
</tr>
<tr>
<td>Mn</td>
<td>0.44</td>
</tr>
<tr>
<td>P</td>
<td>0.08</td>
</tr>
<tr>
<td>S</td>
<td>0.05</td>
</tr>
<tr>
<td>Fe</td>
<td>94.83</td>
</tr>
</tbody>
</table>

Table 5.4: Composition of scrap used in the calculation (Table A2-3, Appendix 2)\textsuperscript{[2]}
5.2.2.4. Iron oxide (FeO) calculation with oxygen balance

Post-combustion ratio:
The oxidation of C to CO is generally considered as the principle reaction to occur in the steelmaking converter. Most of the CO gas produced by this reaction exits the converter and oxidizes to CO$_2$ when mixed with ambient air. When the heat generation by these primary and post combustion of carbon are compared as given by equations 5.3 and 5.4, it is evident that the post-combustion releases about three times more heat.$^{[4, 175]}$

$$C(s) + \frac{1}{2}O_{2(g)} \rightarrow CO_{(g)}; \Delta H = -112.2 \text{kJ} / m$$  \hspace{1cm} \text{Eq 5.3}

$$CO_{(g)} + \frac{1}{2}O_{2(g)} \rightarrow CO_{2(g)}; \Delta H = -282.3 \text{kJ} / m$$  \hspace{1cm} \text{Eq 5.4}

The extent of post-combustion is measured via an off-gas analysis and is expressed using the post combustion ratio or PCR, as given below by equation 5.5$^{[92, 175]}$. The typical range of post combustion ratio for a top blown BOF converter is 10% to 15%, and usually, the heat generated from this amount of post-combustion is capable of processing 75% hot metal and 25% scrap charge.$^{[175]}$ More efficient post-combustion during the oxygen steelmaking process creates the advantages of increasing the bath temperature for enhanced scrap melting and reduced Green House Gases (GHG) emission. For example, if 100% of the heat generated by the post-combustion is recovered, liquid steel temperature will rise by 10 $^\circ$C for every 1% increase in PCR, increasing the scrap ratio from 25% to 50%.$^{[8, 175]}$ Even though, the necessity for post-combustion optimization is not significant in BOF compared to the EAF, it is beneficial to recover the heat generated by post combustion to optimize the BOF process in terms of energy consumption.

$$PCR = \frac{\%CO_2}{\%CO + \%CO_2} \times 100\%$$  \hspace{1cm} \text{Eq 5.5}

However, in the present analysis, the post-combustion values were assumed for each time step in each heat due to lack of data available in the IMPHOS research report$^{[2]}$ on PCR. Final PCR value for each time step was determined by varying it in a way such that the FeO amount calculated in the analysis is equal to the FeO amount observed in that time step. In other words, the O$_2$ consumed by Fe to produce FeO was limited by varying the O$_2$ consumed by the post-combustion.
Oxygen balance:
The kinetics of Fe during the oxygen steelmaking process is difficult to be calculated using the first order kinetics, due to its low affinity for oxygen compared with that of other elements in the bath such as C, Si, Mn, P, Al, and V. According to the oxygen potential diagram given in Figure 5.8, it is understood that the oxygen potential line for Fe lies noticeably above those lines of C, Si, Mn, Al and V. In the case of P, the oxygen potential line of Fe lies above that of P at low temperatures, and exceeds P at high temperatures. In other words, the oxygen injected onto the bath is consumed by Al, Si, Mn and C in the order of their affinity for oxygen prior to P and Fe. P consumes oxygen before Fe at lower temperatures and vice versa. Consequently, the oxidation of Fe is difficult to be calculated solely by using the first order kinetics relationship. However, it is essential to calculate the FeO quantity in the slag accurately for calculating the kinetics of Mn, P, and dissolution of lime. Hence, in the present study, the method of oxygen balance was used, which was used by several researchers for the purpose of calculating the FeO composition in the slag.

The basis of oxygen balance method is that the total mass of oxygen injected is equal to the mass of oxygen output, in the form of either oxides or excess oxygen. In the present analysis, the oxygen balance was used with the assumption of complete consumption of oxygen injected and calculated the amount of O\textsubscript{2} consumed by Fe as the total remaining O\textsubscript{2} amount after oxidizing other impurity elements. The weight of slag was calculated by taking the sum of the weight of the slag components considered, and the PCR was calculated according to the method explained earlier. The values of the variables required for the calculation were extracted from the IMPHOS report, and the calculation method is described below.

Calculation of mass of FeO produced:
Oxygen flow rate \hspace{1cm} = 24.3 kg/min
O\textsubscript{2} used by Fe (O\textsubscript{2, Fe}) \hspace{1cm} = (24.3 kg/min \times t \text{ min}) kg – (O\textsubscript{2} used by Carbon + O\textsubscript{2} used by Si + O\textsubscript{2} used by Mn + O\textsubscript{2} used by P + O\textsubscript{2} used by CO) kg

Where t is the magnitude of the time step (min).
Oxidised Fe mass ($m_{Fe}$) = \((O_{2,Fe}) \times \frac{56 \times 2}{16 \times 2} \) kg

Amount of FeO produced ($m_{FeO}$) = $m_{Fe} \times \frac{72}{56}$ kg  \hspace{1cm} \text{Eq 5.6}

Figure 5.8: Oxygen potential diagram[72]
5.2.2.5. Dynamic slag composition calculation

As explained in previous Sections 5.2.2.1 to 5.2.2.4, the generation and accumulation of slag by flux dissolution, RCS addition, and Fe oxidation were considered in the present analysis. The other main contributors to the slag volume are the oxidised products from the impure elements such as Si, Mn, and P. Since these oxides are produced gradually over the blow, the slag composition is required to be calculated for each time step in order to account for its influence on the refining of Mn and P at the particular time step.

Therefore, the slag composition at each time step was calculated in terms of SiO$_2$, MnO, P$_2$O$_5$, FeO, CaO and MgO masses, in the present analysis. Following equations 5.7–5.10 show the calculation of the mass of SiO$_2$, MnO, P$_2$O$_5$ and FeO for one time step.

\[
\text{Mass of SiO}_2 \text{ produced} = \frac{60}{28} \left[ S_i - S_t \right] + \Delta S_{\text{scrap}} + \Delta S_{\text{RCS}} + \Delta S_{\text{Ox}} \quad \text{Eq 5.7}
\]

\[
\text{Mass of MnO produced} = \frac{71}{55} \left[ Mn_i - Mn_t \right] + \Delta Mn_{\text{scrap}} + \Delta Mn_{\text{RCS}} \quad \text{Eq 5.8}
\]

\[
\text{Mass of P}_2\text{O}_5 \text{ produced} = \frac{142}{32} \left[ P_i - P_t \right] + \Delta P_{\text{scrap}} + \Delta P_{\text{RCS}} \quad \text{Eq 5.9}
\]

\[
\text{Mass of FeO produced} = m_{FeO} + \Delta FeO_{\text{RCS}} \quad \text{Eq 5.10}
\]

Where subscripts $i$ and $t$ represent the initial state and the state at time $t$ respectively, and $m_{FeO}$ was obtained from equation 5.6.

The required observations on the slag composition for each time step were only available for 13 heats in the IMPHOS research report\textsuperscript{[2]}. Hence, the calculation was limited to those 13 heats, and the graphs generated from the calculation for the evolution of the slag components; SiO$_2$, MnO, P$_2$O$_5$ and FeO for selected two heats are given in Figures 5.9 to 5.12.

According to the figures, it is evident that calculated quantities of slag components with time are in reasonable agreement with the observed data. In this calculation, the oxygen consumption by Fe in the bath was calculated by assuming values for PCR for each time step as explained previously in Section 5.2.2.4, and the calculated mass evolution for FeO is shown in Figure 5.12. In summary, the calculated SiO$_2$ amount in the slag was
underpredicted by about 5 kg in total as shown in Figure 5.9. The calculated MnO quantity in the slag illustrated in Figure 5.10 was approximately similar to that observed, but is under predicted towards the end of the blow by about 5 kg. The mass calculated for P$_2$O$_5$ was almost double the mass observed in IMPHOS\textsuperscript{[2]}, even though the pattern of evolution is similar, as shown in Figure 5.11. It is evident from the graphs that the results generated from the present calculation are reasonably representative of the observed data. Therefore, the dynamic equilibrium values calculation was continued with the calculation mentioned above for dynamic slag composition.

![Figure 5.9: SiO$_2$ mass in the slag (a) Heat S1838 (b) Heat S1841](image)

![Figure 5.10: MnO mass in the slag (a) Heat S1838 (b) Heat S1841](image)
5.2.2.6. Calculation of dynamic equilibrium values

The main aim of this stage of the analysis was to calculate the kinetics of Mn and P by first order kinetics using dynamic equilibrium values. This was because the predictions made on the kinetics of Mn and P by the first order kinetics using static equilibrium values were not sufficiently accurate compared to those predictions made on the kinetics of C and Si. Hence, in this stage of the calculation, the equilibrium values (C_{eq}) required for the calculation was determined for each time step based on the slag composition and bath temperature.
The dynamic equilibrium composition for Mn was calculated using the relationship proposed by Morales and Fruehan\textsuperscript{[171]} and is given by equations 5.11 and 5.12. This relationship was developed for a slag system; CaO-MgO-SiO$_2$-Al$_2$O$_3$-P$_2$O$_5$-Fe, O-MnO (<4 wt %), which is a similar composition to the slag reported in IMPHOS\textsuperscript{[2]}.

\[
\log k'_{Mn} = \frac{7406}{T} - 3.436 \quad \text{Eq 5.11}
\]

\[
k'_{Mn} = \frac{MnO(\text{wt})}{FeO(\text{wt}) \times Mn(\text{wt})} \quad \text{Eq 5.12}
\]

Where \(k'_{Mn}\) is the apparent equilibrium constant for Mn, and T is the temperature (K).

The relationship proposed by Manning and Fruehan\textsuperscript{[100]} on the phosphorus equilibrium between slag and metal was used in the present analysis to calculate the dynamic equilibrium values for phosphorus. This relationship, as expressed in equation 5.13, includes the effect of most of the slag components encountered in steelmaking. However, in the present analysis, the effect of CaF$_2$ and higher oxidation of Fe were not considered.

\[
\log \frac{P_{\text{slag}}(\text{wt})}{P_{\text{metal}}(\text{wt})} = \frac{10730}{T} + 4.11\log[CaO(\text{wt})] + 0.15MgO(\text{wt}) + CaF_2(\text{wt})
\]

\[-0.05Fe,O(\text{wt}) + 2.5\log FeO(\text{wt}) + 0.5\log P,O_5(\text{wt}) - 13.8718 \quad \text{Eq 5.13}
\]

Where T is the temperature (K).

Then, the above calculated dynamic equilibrium values were used in equation 5.1 to calculate the kinetics of Mn and P. In order to compare the observed data on the removal kinetics of Mn and P with the results of the calculation, and to determine the applicability of first order kinetics using the dynamic equilibrium values to predict the Mn and P removal pattern, graphs were generated rearranging the equation 5.1 into the following form.

\[
-ln\left(\frac{C_t - C_{eq}}{C_0 - C_{eq}}\right) = kA \frac{\rho_m}{WM} t \quad \text{Eq 5.14}
\]
In this equation 5.14, the $C_{eq}$ was calculated for each time step. Then, graphs were generated by plotting the $-\ln\left(\frac{C_t - C_{eq}}{C_0 - C_{eq}}\right)\left(\frac{C_0}{C_0 - C_{eq}}\right)$ against time $t$. The applicability of first order kinetics using the dynamic equilibrium values for predicting the kinetics of Mn and P was determined by examining the coefficient of determination ($R^2$) of the graphs, similar to the procedure explained in Section 5.2.1.1. Further, the slopes of the graphs generated were used in calculating the value of the multiplication: $kA$, and the calculation results are given in Table A2 of Appendix A2.

5.2.2.7. Results

Figures 5.13 and 5.14 show the graphs generated for Mn and P calculated using the first order kinetics equation with the dynamically calculated equilibrium values for selected two heats.

![Figure 5.13: Manganese removal kinetics (a) Heat S1840 (b) Heat S1832](image-url)
As illustrated in Figure 5.13, the removal kinetics calculated for Mn with the first order kinetics using the dynamic equilibrium values, showed the coefficient of determination ($R^2$) values in the range between 0.95 and 0.0002. Similar to the previous stage of the analysis, the calculation was limited to 9 heats due to restrictions in calculating the logarithmic values. However, among the nine heats analyzed, 44% of heats showed $R^2$ values more than 0.80, while, the rest of the heats had $R^2$ values less than 0.5. A similar calculation restriction limited the analysis of P to only 12 minutes into the blow for 11 heats. Yet, the analysis was carried out for those 11 heats, and the $R^2$ values were observed to be within 0.92 and 0.08, among which, about 90% of the heats had $R^2$ values more than 0.6.

Therefore, the conclusions derived from the analysis can be listed as follows;

- The removal kinetics of Si and C can be predicted using the first order kinetics when the equilibrium concentration of the element ($C_{eq}$) was assumed static and equals to the elements’ composition in turndown steel.
- The removal kinetics of Mn and P can be predicted using the first order kinetics when the equilibrium concentration of each element ($C_{eq}$) was calculated dynamically.

Accordingly, the first order kinetics model used in the analysis was rearranged and incorporated in the user subroutines of the CFD model as explained in the next section.
5.3. The kinetics model incorporated in the CFD model

The first order kinetics model given in equation 5.1 was rearranged to equation 5.15 to be used in the present CFD model. According to the conclusions of the above analysis, the equilibrium compositions \(C_{eq}\) of C and Si were assumed to be constants throughout the blow, and equal to their average composition (in terms of the mass fraction) in the turndown steel as reported in IMPHOS\(^2\), which were 0.00070 and 0.00001 respectively. The equilibrium compositions \(C_{eq}\) for Mn and P were calculated using the relationships given by equations 5.11, 5.12 and 5.13.

\[
\frac{dc}{dt} = K \left( m_{j,b} - m_{j,eq} \right) \alpha_i \rho_i \nu_c
\]

Eq 5.15

Where \(K\) is constant \((k \times A \text{ in equation 5.1})\), \(m_{j,b}\) is bulk mass fraction of the element in the cell, \(m_{j,eq}\) is the equilibrium mass fraction of the element in the cell, \(\alpha_i\) is the liquid volume fraction, \(\rho_i\) is the density of the liquid and \(\nu_c\) is the volume of the cell.

The value of the constant \(K\) was calculated for C, Si, Mn and P separately for each heat under two stages during the analysis, and the results are given in Tables A1 and A2 in Appendix. These \(K\) values were calculated assuming the weight and the density of the metal in the converter were constant throughout the blow. Further, it was assumed that the oxidation reaction occurs at the interface between the metal-oxygen interface where the reaction area remains approximately constant. These assumptions were used in order to simplify the kinetics model and may have under-predicted the \(K\) values as in the actual steelmaking process the weight of the metal and the interfacial area where the reactions occur are varying with time during the blow. The \(K\) values used in the CFD model for C and Si were 0.00164 and 0.00407 respectively and were the average of the \(K\) values calculated for those elements in the first stage of the analysis, as given in Table A1 of Appendix A1. The values of \(K\) used for Mn and P in the CFD model were 0.02136 and 0.04710 respectively, which were the average of \(K\) calculated for those elements in the second stage of the analysis, as given in Table A2 of Appendix A2.
Further, the oxidation products of C, Si, Mn, P and Fe were limited to CO, CO\textsubscript{2}, SiO\textsubscript{2}, MnO, P\textsubscript{2}O\textsubscript{5}, and FeO respectively. The amount of Fe reacting was calculated by the oxygen balance method as explained in Section 5.2.2.4, and its use in the CFD model user subroutine is as follows.

\[
\text{Amount of O}_2 \text{ used by Fe} = (\text{Oxygen available} - \text{Oxygen used by Si, C, Mn, and P respectively})
\]

\[
\text{Amount of Fe reacted} = (\text{Amount of O}_2 \text{ used by Fe}) \times (112/32)
\]

The post combustion of CO to CO\textsubscript{2} was assumed to follow a linear relationship up to 5 minutes, as a starting point. Post-combustion ratio as given by equation 5.5 was assumed to change from 100% at time=0 s to 0.15% at time=300 s and was assumed negligible after that.

The first order kinetics relationship was used in the present CFD model to calculate the refining kinetics in a steelmaking converter assuming that the diffusion of the reactants to the slag-metal interface is the rate limiting step. The above calculation was used to determine the diffusion of the elements C, Si, Mn and P, and their reaction rates. However, the oxygen is also a reactant in the reactions considered, and its availability imposes limitations on the reaction rates. Hence, the availability of oxygen was also included in the model as a variable in determining the reaction rates.

When the rate-limiting factor of the chemical reaction was the supply of O\textsubscript{2}, the mass of the reactant (O\textsubscript{2}) was calculated by the stoichiometry of the chemical reaction according to equation 5.16.

\[
\frac{d\text{O}_2}{dt} = r_f \text{O}_2,\text{available}
\]

Eq 5.16

Where \(r_f\) is the stoichiometric constant of the oxidizing reaction under consideration.

Therefore, the reaction rates are determined by the minimum available reactant for the reaction under consideration according to the following rearranged equation 5.17.

\[
\frac{dC_i}{dt} = \min\left(\frac{dC}{dt}, \frac{d\text{O}_2}{dt} \alpha_f \rho \nu_e\right)
\]

Eq 5.17
Equation 5.17 was the kinetics equation used in the user subroutine of the CFD model developed in the present study to calculate the reaction rates of the oxidation of C, Si, Mn, and P. The results obtained from the CFD model are presented in the next chapter (Chapter 6) combined with the details and results of the foaming model developed in the present study.
Chapter 6
Chapter 6: Three Phases CFD Foaming Model

Modelling slag foaming and the refining kinetics in oxygen steelmaking has been the centre of focus of research among steelmaking researchers, due to the process optimizing opportunities arose by such models\cite{[13, 17, 35, 44, 64, 68, 93, 133, 151, 169]}, as explained previously in Chapters 2, 3 and 5. Amidst these modeling efforts reported in the literature, several numerical analysis and simulations on general foaming as well as on slag foaming can be found including research works by Wang et al\cite{149}, Buwa et al\cite{153}, Chen et al\cite{32} and Bhole et al\cite{30}. The most recent study carried out by Sattar and his co-workers\cite{1} on modeling foaming in oxygen steelmaking produced some reasonable predictions of foam height and the decarburization in oxygen steelmaking, as explained in Section 3.3.7. Despite the reasonable foam height and decarburization predictions, several drawbacks were identified in this model developed by Sattar\cite{1} as discussed in Section 3.4. Hence, in the present study, their model was further improved and extended via the suggested enhancements explained in Section 3.5.

In this chapter, a thorough explanation is provided on the CFD model developed in the present study for simulating the refining kinetics and foaming in oxygen steelmaking, which is initiated from the CFD model developed by Sattar\cite{1}. Further, the results obtained from the model on removal behavior of impure elements and foam height variations over the period of concern are also included and analyzed.

6.1 Summary of the foaming model developed by Sattar\cite{1}

The model developed by Sattar\cite{1} was able to predict foam height in oxygen steelmaking converter reasonably well, simultaneously with decarburization, number densities of bubble classes in gas and foam phases, heat generation and velocity of different phases. This model was an extension to the previous CFD model Sattar et al developed\cite{35} for reproducing the experimental results obtained by Jiang and Fruehan for slag foaming\cite{16}, where the experiments were carried out using bath smelting slag (CaO-SiO_2-Al_2O_3-FeO) in a crucible and injecting Ar gas. The geometry of the oxygen steelmaking model was that of the steelmaking converter used in the IMPHOS pilot plant trials\cite{2}, which is shown in Figure 3.12.
The model consisted of three phases; gas, liquid, and foam, which interacted with each other by means of mass, momentum, and energy. The foam phase was produced from gas and liquid phases in the case when the volume fraction of gas phase was more than 75% and that of the liquid phase was more than 5% in the cell under investigation. In this model, the multiphase flow simulation was carried out with a Eulerian-Eulerian approach, and the population balance equation was used to calculate the population densities of the components of each phase as explained in Sections 3.3.1 to 3.3.5. The gas phase contained ten bubble classes, and in the case of population calculations of the bubble classes, the bubble coalescence and breakup were taken into consideration. The physical properties of the foam were calculated according to the gas and liquid content in foam as explained in Section 3.3.6. The decarburization reaction was the only chemical reaction considered in their work, and the heat generation due to carbon oxidation was incorporated in the simulation. The results obtained from the model were compared with the observed data published in IMPHOS research report\(^2\) as shown in Figures 3.14 to 3.16 in Section 3.3.7 and were in reasonably good agreement with the reported observations.

However, several drawbacks were identified in this foaming model developed by Sattar\(^1\) when used to model the actual oxygen steelmaking process. The only chemical reaction considered in the model was the decarburization reaction, and its rate of removal was obtained from the observations reported in IMPHOS research\(^2\). Continuous drainage of foam was not considered in the model, and the criterion used for the collapse of foam was not clearly explained. Further, no liquid oxides were considered in the model, as the oxide produced from the decarburization was the gas CO. These drawbacks identified in the model developed by Sattar\(^1\) were explained in detail in Section 3.4.

Nonetheless, the model developed by Sattar\(^1\) was used as the initiating point in this study, and the drawbacks mentioned above were addressed in the present work using the methods discussed in Section 3.5. The improvements to the model include the incorporation of the semi-empirical kinetics model developed by the author and the continuous drainage and improved foam formation and collapsing criteria, as explained in Sections 6.8 and 6.9.
6.2 Geometry and simulation details

The geometry of the model used in the present simulation was the geometry developed by Sattar\[1\] using the dimensions of the pilot plant converter as shown in Figure 3.12. This was the geometry of the converter used in pilot plant trials in IMPHOS\[2\] research work. Figure 6.1 shows the complete volume mesh and the 3D thin slice of that mesh used for simulations in the present work.

Initially, the converter contained liquid phase up to a height of 0.66 m from its bottom, and the rest of the volume was filled with the gas phase. In the middle of the geometry, the vertical lance was placed. Its inner diameter is 0.0155 m, and the extended lance tip forms the inlet of the model at a distance of 0.496 m below the original lance exit of the actual converter.

![Figure 6.1: The mesh generated for the simulation\[1\]](image)

Three different phases were considered at this stage of the model; gas phase, liquid phase, and the foam phase. The scalars of each phase used in the present study are given in Table 6.1. The liquid phase in this stage of the study contains the components of both hot metal and slag. This was because the introduction of slag as a separate phase increases the complexity and the time consumption at the present stage of the model. Hence one liquid phase was considered containing the combined slag and liquid metal.

The next stage of the model investigated the possibility of introducing slag as a separate
phase. Further, at this stage of the study, the fluxes, other impurity elements in steel and other oxidation levels of the impure elements were not taken into consideration.

Table 6.1: Scalars list of the three phases considered in the CFD model

<table>
<thead>
<tr>
<th>Phase</th>
<th>Scalars</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas phase</td>
<td>Ten gas bubble classes, CO and O₂</td>
</tr>
<tr>
<td>Liquid phase</td>
<td>Fe, C, Si, Mn, P, S, FeO, SiO₂, MnO, and P₂O₅</td>
</tr>
<tr>
<td>Foam phase</td>
<td>Ten foam bubble classes, Gas in foam and liquid in foam</td>
</tr>
</tbody>
</table>

Ten bubble classes were included in the gas phase and foam phase similar to the initial model by Sattar[1]. The diameters of the bubbles were chosen to be between 2.5 mm and 20.0 mm as given in Table 6.2. Under the influence of flow conditions, these bubbles collide with each other resulting in bubble coalescence and break-up and change in size and number. Liquid drainage also affects the bubble break-up and coalescence. Hence, in the present CFD model, coalescence and break-up in gas bubbles and coalescence of foam bubbles were included as explained in Section 3.1.6.

Table 6.2: Details of the bubble classes used in the CFD model[1]

<table>
<thead>
<tr>
<th>Bubble class</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of</td>
<td>2.50</td>
<td>3.15</td>
<td>3.97</td>
<td>5.00</td>
<td>6.30</td>
<td>7.94</td>
<td>10.00</td>
<td>12.60</td>
<td>15.87</td>
<td>20.00</td>
</tr>
<tr>
<td>bubbles (mm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The simulation was carried out using the commercial CFD package AVL FIRE 2009.2. The software uses the finite volume method for discretization of the governing equations. The resulting discretized governing equations were then solved iteratively using a segregated approach. Since the model includes three different phases, multiphase flow simulation was carried out using the Eulerian-Eulerian reference frame. The phases interact with each other in terms of mass and momentum, and the fluids were considered incompressible. For momentum and continuity, an unsteady state multiphase solution was used, while for the turbulence, a standard k-ε model was used. The differencing scheme used for momentum and turbulence was the first order upwind
differencing scheme, while that used for continuity equation was the central differencing scheme.

The simulation was run in an unsteady state with a time step of 0.001s for 600s, on an Intel(R) Xenon(R) CPU E5-1620 0 machine, where the RAM and the speed of the processor were 16GB and 3.60GHz respectively.

6.3 Boundary conditions imposed on the model
The boundary conditions imposed on the inlet, outlet and the walls of the modeled BOF were as follows:

Velocity boundary conditions were applied to the inlet of the model, which is the tip of the extended lance (Section 2.1.5), and pure oxygen was injected into the converter through the lance. Further, the inlet gas stream was at 1648 K at the inlet to the converter.

The outlet was defined as the top surface of the model excluding the lance, and static pressure boundary conditions were applied to the outlet. The gases exiting the outlet were assumed to be at atmospheric pressure and 293.15 K temperature and mostly contained the CO gas.

The walls of the converter were specified solid, even and non-slip, and were at the same temperature as the bath (i.e. 1648 K).

6.4 Initial conditions used in the simulation
Prior to the start of the simulation, the converter contained about 5.5 tons of liquid metal at the temperature of 1648 K as shown in Figure 6.1, and the rest of the volume inside the converter was filled with the gas phase at 1648 K. In the present simulation, the total molten metal bath was assumed to be one liquid phase, and the initial composition of the liquid phase considered is given in Table 6.3. Since the introduction of a separate slag phase increases the complexity of the model at this stage of the model, one liquid phase consisting of both liquid metal and slag components was used. The composition of this single liquid phase in terms of the mass fraction of each component was decided assuming the total mass of the phase to be the combined mass of liquid metal and slag.
Table 6.3: Initial composition of the liquid phase in the model

<table>
<thead>
<tr>
<th>Component</th>
<th>Wt % in the liquid phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>95.096</td>
</tr>
<tr>
<td>C</td>
<td>3.588</td>
</tr>
<tr>
<td>Si</td>
<td>0.515</td>
</tr>
<tr>
<td>P</td>
<td>0.075</td>
</tr>
<tr>
<td>Mn</td>
<td>0.424</td>
</tr>
<tr>
<td>S</td>
<td>0.048</td>
</tr>
<tr>
<td>FeO</td>
<td>0.110</td>
</tr>
<tr>
<td>SiO₂</td>
<td>0.110</td>
</tr>
<tr>
<td>P₂O₅</td>
<td>0.008</td>
</tr>
<tr>
<td>MnO</td>
<td>0.023</td>
</tr>
</tbody>
</table>

The gas phase considered in the present model consisted of ten bubble classes and oxygen (O₂) and carbon monoxide (CO) gases. The foam phase also consisted of twelve components, which included ten bubble classes and liquid and gas in foam, as given in Table 6.1.

6.5 Properties of the fluids included in the model

The gas phase considered in the present model was assumed to possess the properties of air, while the properties of the liquid phase were assumed to be similar to the properties of molten iron. Even though the assumption of properties of the present liquid phase to be similar to those of molten iron is not accurate, the simulation was run with this assumption as an initiation and as a method to reduce the complexity of the model of this stage. The simulation was run under isothermal conditions at 1648 K, and the properties of both gas and liquid phases were assumed to be constant throughout the simulation period. Table 6.4 summarizes the main properties of the three phases considered in the present model.
Table 6.4: Properties of the fluids involved in the model

<table>
<thead>
<tr>
<th>Properties</th>
<th>Gas phase</th>
<th>Liquid phase</th>
<th>Foam phase</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Density (kg/m$^3$)</strong></td>
<td>0.233</td>
<td>6980.0</td>
<td>703.2</td>
</tr>
<tr>
<td><strong>Dynamic viscosity (Ns/m$^2$)</strong></td>
<td>1.82e-11</td>
<td>1.01e-06</td>
<td>1.37e-07</td>
</tr>
</tbody>
</table>

The properties of the foam were calculated using the equations 3.48 and 3.49 given in Section 3.3.6 and were determined depending on the gas and liquid content in the foam. The properties of the foam phase included in Table 6.4 were used for initiating the simulation.

6.6 Governing equations solved in the simulation

In the present study, three different phases (i.e. gas, liquid, and foam) were considered as explained before. Gas and liquid phases were in the converter from the start of the simulation, while, the foam phase was produced from the gas and liquid phases after the initiation of the simulation. In the actual oxygen steelmaking process, the high velocity oxygen stream injected onto the molten metal bath agitates the bath extensively, accelerating the chemical reactions and foam formation. In other words, the interactions between the fluids in terms of mass, momentum, and energy are encouraged by the intense mixing conditions. Similarly, in the present CFD model, the interactions between the phases were considered using the governing equations for mass and momentum. The governing equations used in the present study were explained in Section 3.3.1. The mass, momentum, and enthalpy conservation equations were incorporated in the present simulation together with the mass and momentum interfacial exchanges. Heat generation by the chemical reactions was not considered in the present study, and isothermal conditions were assumed throughout the blow. The author is aware that this assumption of isothermal operation of the steelmaking process is not true, and causes errors in the model results by not considering the effect of increasing temperature on the physical properties of the phases and rate of chemical reactions. However, this assumption was made to reduce the complexity of the programming required in the present stage of the model.
6.6.1 Mass conservation equation
A Eulerian-Eulerian approach based mass conservation equation was used in the present study to account for the interactions between the three phases considered (i.e. gas, liquid, and foam) in terms of mass. The mass conservation equation explained in Section 3.3.1.1 (equation 3.22) was used in the present simulation.

6.6.2 Mass interfacial exchange
The formation and the collapse of the foam phase considered in the present study are related to the mass of the gas and liquid phases. The mass in a cell containing gas and liquid phases was transferred to the foam phase when the volume fraction of the gas phase and the liquid phase in the cell are equal to or more than 75% and 5% respectively. And, when the foam volume fraction in a “foam” cell was more than or equal to 15% and the volume fraction of the ‘liquid in foam’ component in a “foam” cell was less than or equal to 10%, the total mass in that cell was transferred to liquid and gas phases. This mass exchange was addressed by the mass interfacial exchange term in equation 3.22 as explained in Section 3.3.1.1 and is further explained in Section 6.9. In addition, the mass exchange between the gas and liquid phases via the chemical reactions were also incorporated using the mass interfacial exchange term.

6.6.3 Momentum conservation equation
Momentum exchange between the phases in oxygen steelmaking converter is significant, and in the present model, this was included in the CFD model using the momentum conservation equation. The momentum conservation equation given by equation 3.27 is a mathematical representation of the Newton’s second law, which states that the rate of change of momentum is equal to the sum of forces on a fluid particle. In the present simulation, the momentum conservation equation in the finite volume method in Eulerian – Eulerian approach was solved for each phase.

6.6.4 Momentum interfacial exchange
Interfacial exchange of momentum occurs via different processes including the bubble break-up and coalescence and bubble-induced drag forces. The effects of these processes were considered in the present simulation and were incorporated in the momentum conservation equation using the momentum interfacial exchange source
term. This momentum interfacial exchange source term was calculated using the equations 3.31 to 3.36 in Section 3.3.1.2.

**6.6.5 Population balance modeling**

Population balance modeling involves the use of population balance equation given by equation 3.42 in Section 3.3.5 to calculate the population density of the entities included in the model. In the present model, different entities were included in the three phases considered. For example, ten bubble classes were included in the gas and foam phases, while, six elements and four oxides were included in the liquid phase. Therefore, the density of the population of such entities was calculated using the scalar transport equation (equation 3.42), which is the population balance equation in AVL FIRE software.

The population of the entities mentioned above is influenced by the birth and death of those entities. For example, the coalescence and break-up of bubbles modify the population density of bubble classes, while the chemical reactions modify the population of the elements and oxides in the liquid phase. This effect is incorporated into the population balance equation using the source term in equation 3.42 as explained in Section 3.3.5.

**6.6.6 Chemical species population calculations**

As explained in previous Section 6.6.5, the population balance equation (equation 3.42) was used to calculate the concentration of each element in the liquid and gas phases, similar to the population of the bubble classes. The concentration of the elements and oxides in the liquid and gas phases change due to the chemical reactions, which occur within and between liquid and gas phases. These changes in concentration were captured by the kinetics model incorporated in the CFD model. The kinetics model was developed assuming that the reaction rates are governed by the mass diffusion and are first order, as explained in chapter 5. The mass changes calculated by the kinetics model (i.e. \( \frac{dC_i}{dt} \)) were included as the source term \( (S_i) \) in the population balance equation.

**6.6.7 Bubble break-up and coalescence**

In the present study, the population density of bubble classes in gas and foam phases were calculated using the population balance equation, and the changes caused by birth
and death of bubbles on their population were included in the calculation as the source term given by equation 3.43, as explained before.

The population of bubbles changes due to the break-up of bubbles. In the present study, the binary break-up model was used to calculate the rate of bubble break-up, where, bubbles were assumed to break-up due to collision with turbulent eddies smaller than or similar in size to the bubbles, and produce two daughter bubbles. The mathematical model used for calculating the rate of bubble break-up was given in Section 3.1.6.4.

The number of bubbles also changes due to coalescence of bubbles which initiates by collision with each other. Even though, collisions between bubbles are induced by different factors like turbulence in the liquid, laminar shear, buoyancy and the wake entrainment, only the bubble coalescence that occurs under the influence of turbulence in the liquid was considered in the present study. The bubble coalescence rate was calculated using the equations 3.6 to 3.11 explained in Section 3.1.6.3. Further, the coalescence of bubbles in the foam phase was also considered in the present study. The coalescence of bubbles in the foam was assumed to occur due to drainage of liquid in the films separating the bubbles causing those films reach a critical thickness and burst, resulting in one bigger bubble. The rate of coalescence of foam bubbles was calculated as explained in Section 3.3.6.

6.7 Graphical results on evolving volume fraction of three phases (i.e. gas, liquid, and foam) with time

The CFD model at this stage of simulation consisted of three phases, which were gas, liquid and foam phases with the composition given in Table 6.1. The foaming model in this stage of simulation was similar to the foaming model developed by Sattar[1], while the liquid phase and gas phase involved in the chemical reactions specified in Section 6.8.1. Figure 6.2 illustrates the evolving volume fraction of the three phases at five different instances from the total simulation time of 10 minutes. The complete set of illustrations is given in Figure A5, Appendix A5.
Time | Gas phase | Liquid phase | Foam phase
--- | --- | --- | ---
60s
180s
300s
6.8 Semi-empirical first order kinetics model

In oxygen steelmaking, the impure elements in the bath (i.e. C, Si, Mn, and P) and a certain amount of Fe are oxidized by the injected oxygen stream, to obtain the requisite end composition of the steel. During this steelmaking process, the oxides of the impure elements and Fe combined with the added fluxes (i.e. CaO and MgO) form the slag; while the gases formed (i.e. CO and CO₂) escape from the converter. These oxides assist in further refining of the steel bath. Hence, a dynamic model is essential to analyze and optimize the dynamic steelmaking process further by taking into account the kinetics of the reactions mentioned above as well as the fluid flow characteristics.

Therefore, in the present study, major chemical reactions were included in the model using a semi-empirical kinetics model. Even though it is established that kinetics of the
chemical reactions in steelmaking converter are complex, and understanding and predicting the refining behavior of the elements are complicated tasks, in the present study, the first order diffusion kinetics equation was used to develop a semi-empirical kinetics model as a start.

### 6.8.1 The kinetics model used in the CFD model

The chemical reactions that occur in an oxygen steelmaking converter include oxidation of elements in the metal, slag-metal reactions, flux reactions and gas reactions, as explained in Section 2.1.7. However, in the present CFD model, only several major chemical reactions were considered, and those reactions are stated below.

1) \[ 2C + O_2 = 2CO \]
2) \[ 2CO + O_2 = 2CO_2 \]
3) \[ 2Fe + O_2 = 2FeO \]
4) \[ Si + O_2 = SiO_2 \]
5) \[ 2Mn + O_2 = 2MnO \]
6) \[ 4P + 5O_2 = 2P_2O_5 \]
7) \[ 5Si + 2P_2O_5 = 4P + 5SiO_2 \]
8) \[ 5C + P_2O_5 = 2P + 5CO \]
9) \[ 5Mn + P_2O_5 = 2P + 5MnO \]
10) \[ Si + 2FeO = 2Fe + SiO_2 \]
11) \[ 5Fe + P_2O_5 = 2P + 5FeO \]
12) \[ C + FeO = Fe + CO \]
13) \[ Si + 2MnO = 2Mn + SiO_2 \]
14) \[ C + MnO = Mn + CO \]
15) \[ Mn + FeO = Fe + MnO \]

The chemical reactions 1 to 6 are oxidizing reactions, while the rest of the chemical reactions occur between the elements in the hot metal and slag components.
The rates of the oxidizing reactions were calculated by the semi-empirical kinetics model developed in the present study, which was explained in detail in Chapter 5. Available quantity of the slag component was assumed to be the rate limiting factor in calculating the composition changes caused by the reactions between elements and slag components (i.e. reactions 7 to 15).

The first order diffusion kinetics equation (equation 5.1), which is also known as Fick’s first law of diffusion, was used to calculate the mass of the reactant element (i.e. C, Si, Mn, P or Fe) available in the cell for the reaction, in the case of unlimited O\(_2\) supply. The equation 5.1 was then rearranged to equation 5.15 and was used in this case as explained in Section 5.3. When the reaction rate was governed by the oxygen availability, the mass of the reactant spent for the reaction was calculated by using equation 5.16. The kinetics equation used in the CFD model is equation 5.17, which calculates reactant mass using both equation 5.15 and 5.16, and takes the minimum as the final mass change of the particular element. The sequence of oxidizing of the impurity elements in the model was determined by their relative affinity for oxygen, and the order of oxidizing was Si, C, Mn and P. Fe was assumed to consume all the remaining oxygen after oxidizing the impurity elements at the time step of concern.

According to the conclusions of the analysis presented in Chapter 5, the equilibrium compositions (C\(_{eq}\)) of C and Si were assumed to be constants throughout the blow, and equal to their average composition (in terms of mass fraction) in the turndown steel as reported in IMPHOS report\(^2\), which were 0.00070 and 0.00001 respectively. The equilibrium compositions (C\(_{eq}\)) for Mn and P were calculated using the relationships given by equations 6.1 and 6.2, which were derived from equations 5.11, 5.12 and 5.13 explained in Section 5.2.2.6. The temperature was assumed to be 1648 K.

\[
Mn_{eq} = \frac{MnO (wt\%) \times 11.427}{FeO (wt\%)} \\
P_{eq} = \frac{P_{slag} (wt\%)}{antilog(2.5logFeO (wt\%) + 0.5logP_2O_5 (wt\%) - 7.3608)}
\]

Eq 6.1

Eq 6.2

The value of constant K in equation 5.15 was determined by the analysis explained in Chapter 5. The values used for K in the present model for C, Si, Mn, and P, are 0.1636,
0.4070, 0.042 and 0.0700 respectively. Further, the oxidization products of C, Si, Mn, P and Fe were limited to CO, CO$_2$, SiO$_2$, MnO, P$_2$O$_5$, and FeO respectively. The amount of Fe reacted was calculated by the oxygen balance, as explained in Section 5.2.2.4. Post-combustion ratio was assumed to change from 100% at time=0 s to 0.15% at time=300 s, and stay negligible after that. The calculated change in mass due to the reactions was included in the source term of the population balance equation for calculating the population concentration of the element for the next time step.

Before the incorporation of the kinetics model mentioned above into the CFD model, the concentration evolution of the impure elements was directly extracted from the IMPHOS research report[2] as polynomials and was incorporated into the CFD model as a trial step of the simulation. This step was carried out as an initial test on the performance of the CFD model and polynomials used in the model are given below.

\[
\frac{dC}{dt} = (4.0e-13)t^3 - (9.0e-10)t^2 + (2.0e-07)t - (8.0e-06) \quad \text{Eq 6.3}
\]

\[
\frac{dSi}{dt} = -(4.0e-14)t^3 - (3.0e-11)t^2 + (8.0e-08)t - (3.0e-05) \quad \text{Eq 6.4}
\]

\[
\frac{dMn}{dt} = -(2.4e-13)t^3 - (3.0e-10)t^2 + (1.4e-07)t - (2.0e-05) \quad \text{Eq 6.5}
\]

\[
\frac{dP}{dt} = -(3.2e-14)t^3 + (6.0e-11)t^2 - (1.8e-08)t + (4.0e-07) \quad \text{Eq 6.6}
\]

### 6.8.2 Kinetics results of the CFD model

Even though the principle objective of the present study was developing a CFD model for predicting foaming in oxygen steelmaking converter, a semi-empirical kinetics model was incorporated in the present CFD model to include the effect of evolving composition of the metal bath and slag on foaming. Therefore, a semi-empirical first order kinetics model with oxygen balance was developed and included in the CFD model for calculating the removal behaviors of the elements in the converter, as explained in the previous section (Section 6.8.1). In this section, the results obtained from the CFD model on the kinetics of the refining of impure elements (i.e. Si, C, Mn, and P) are presented in terms of the mass fraction of the particular element from the total mass of the bath (i.e. the Total mass of the liquid phase). As explained in the previous sections, in the present
simulation, the liquid phase consists of the molten metal components and slag components as given in Table 6.1. The results obtained from the model were compared with the experimental data extracted from the IMPHOS research report\textsuperscript{[2]} for heat S1843, and are presented in Figures 6.3 to 6.5.

The results plotted as “Polynomial results” are the results obtained when the rate of removal of each impure element over time was calculated from the polynomial extracted from the IMPHOS research report.\textsuperscript{[2]} The polynomials used in the model for C, Si, Mn and P were given by equations 6.3 to 6.6. The results plotted as the “Diffusion model results” are those obtained when equation 5.17 (i.e. the first order kinetics model developed in the present study) was used in the CFD model.

![Figure 6.3: Carbon removal behavior](image-url)
Figure 6.4: Silicon Removal behavior

Figure 6.5: Manganese removal behavior
The kinetics model included in the CFD model was a semi-empirical first order kinetics model developed using several assumptions as explained in Chapter 5. Even though, the refining kinetics encountered in oxygen steelmaking are established to be more complex in nature, the present simplifications were used as a starting point, as well as, to reduce the complexity of the subroutines used in the CFD model. Similarly, the order of the polynomials extracted from the IMPHOS report\(^2\) was limited to 3 for reducing the complexity of the subroutines. Yet, the results obtained from the CFD model on the kinetics are approximately representative of the observed removal behavior of the impure elements as shown in Figures 6.3 to 6.6.

It is evident from Figure 6.3 that the observed removal behavior of carbon is approximately captured by the kinetics model developed in the present study, with a slight over-prediction of the decarburization rate during the middle part of the blow time considered. The rate of desiliconization is under-predicted by the kinetics model as shown in Figure 6.4. This under-predicted rate of desiliconization can be mostly due to the effect of the under-estimated K value in equation 5.15 and partly due to the over-prediction of the decarburization.
Figure 6.5 exhibits the predictions of the present kinetics model on the Mn removal pattern, and it is evident that the kinetics model has captured the demanganization rate and pattern comparatively well. The common observation of steelmaking researchers on Mn removal is that Mn reverses to the metal from the slag in the middle section of the blow as explained in Sections 2.1.7.3 and 2.1.7.8. The behavior of Mn removal as calculated by the present model shows a similar pattern with an approximate constant removal of Mn up to 4 minutes, followed by a very slow reversion of Mn to metal for the next 2 to 3 minutes. During the final 3 to 4 minutes considered, Mn removes from the metal to slag again at a slightly low rate compared to the first four minutes’ demanganization rate. Although the illustrated observations for heat S1843 does not show any reversion within the considered period, some of the other heats reported in IMPHOS\(^2\) exhibits the reversion behavior of Mn within the first ten minutes. (e.g. The heats S1830, S1837, S1839, and S1841 of which some are shown in Figure 2.44 c)

Conversely, the model predictions on the rate of dephosphorization are over-predicted, while, the pattern of dephosphorization was approximately captured, compared to the observation for heat S1843, as shown in Figure 6.6. However, it is evident from Figure 6.6 that the model predicts the reversion of P from slag to metal during the blow. P reversion to the metal from slag during the blow is a common observation and has been investigated by steelmaking researchers as explained in Sections 2.1.7.4 and 2.1.7.8. Even though reversion of P during the middle section of the blow is common to almost all the heats reported in IMPHOS report\(^2\), a P removal pattern similar to the present model predictions can be observed in the heats S1830 (Figure 2.44 d), S1837, and S1841.

The model predictions on the concentration of slag components in the bath were not representative of the observed values, because, the concentration of slag components were not properly modeled in the kinetics model incorporated in the CFD model. However, the model predicted the evolution of SiO\(_2\) approximately but in accordance with the evolution pattern of the observed values as shown in Figure 6.7. This is because SiO\(_2\) was not involved in any slag-metal reaction considered, as mentioned in section 6.8.1. The approximate under-prediction of the de-siliconisation rate as shown in Figure 6.4 also may have contributed to the observed under-prediction in the SiO\(_2\) generation rates. Further, it should be noted that this under-prediction of the slag components
caused a level of error in the calculation of the equilibrium values of Mn and P (i.e. equations 6.1 and 6.2), causing those equilibrium values to stay almost constant throughout the blow time considered.

As illustrated in Figures 6.3 to 6.6, the predictions of the present CFD model on the removal behavior of the impure elements were approximately reproducing those observed during the IMPHOS\cite{2} plant trials. The main reason for the deviations of the model results from those observed is the simplified relationships used in developing the kinetics model as explained in Chapter 5, while the simplifications and assumptions used during the programming may also have contributed, which are explained in detail in Section 8.2.

### 6.9 Foam simulation

Foams are created either by a mixture of gas and liquid, or by a mixture of gas and solid, and consist of a continuous phase (i.e. liquid or solid) and a dispersed phase (i.e. gas). Foams are usually meta-stable systems. They rearrange and coarsen with time under the influence of different processes such as coalescence, drainage, break-up, and Ostwald ripening of the bubbles in the foam.\cite{138} The nature of foams is such that, they
become desirable in situations like fire extinguishing and detergency while being
detrimental in situations like engine oils and boilers, as explained in Chapter 3. However,
in oxygen steelmaking, the foams produced are desirable as they create an expanded
surface area for refining reactions while protecting the bath from the direct contact of
the atmosphere. However, such foams in oxygen steelmaking can become detrimental
when formed in extensive amounts and overflow from the converter mouth (i.e.
slopping event).

A layer of foam is formed over the steelmaking bath when the gas bubbles generated
from the chemical reactions and the injected oxygen stream are trapped by the slag
layer. Slag foaming similar to that in oxygen steelmaking is experienced in many ferrous
and non-ferrous smelting processes, and the typical void fraction of slag foam is
between 0.7 and 0.9.\cite{26, 126} As explained in Section 2.2.4, the physical properties of slag
evolve in favor of foam stabilization with time, increasing the volume of slag foam.
However, in the case of excessive foaming, a slopping event may occur, causing
interruptions to the continuous process and damaging the surroundings. Hence, it is vital
to have a model, which is capable of predicting the extent of foaming under the relevant
process conditions, prior to the start of the blow.

Therefore, the primary aim of the present study was to model and predict the foaming
in oxygen steelmaking. The foaming model developed by Sattar\cite{1} was used as the
initiation for the present study, and a brief explanation of the model developed by
Sattar\cite{1} was provided in Section 6.1. As explained in Section 3.5, several drawbacks were
identified in this foaming model by Sattar\cite{1} including the absence of proper foam
collapse criteria and continuous drainage of foam. The suggested solutions for these
problems were discussed in Section 3.5. The improvements incorporated into the CFD
model in terms of foaming model at this stage of the simulation are the continuous
drainage of foam, improved mass exchange between the foam and liquid phases and
the new foam collapsing criteria, which are explained in Section 6.9.2.

6.9.1 Foam height results (stage 1)
The results presented in this section on foam height prediction are obtained from the
CFD model before the suggested improvements to the foaming model were
incorporated. Therefore the foaming model at this stage is similar to that developed by Sattar\cite{sattar}, but, the CFD model includes the chemical reactions within its liquid phase and between liquid and gas phases.

The foam was produced from a mixture of gas phase and liquid phase when the composition of a cell was such that gas phase volume fraction is equal to or more than 75\% and liquid phase volume fraction is equal to or more than 5\%. When this condition was met, the gas and liquid mass in the cell was transferred to foam phase, which consists of 10 bubble classes and gas and liquid as scalars. The requirement for collapsing the foam was such that; the liquid phase volume fraction in the cell is equal to or less than the predefined minimum volume fraction of a phase (i.e. $1.0 \times 10^{-6}$) and foam phase volume fraction in the cell is equal to or more than 15\%. At the completion of this requirement, the mass in the cell was transferred back to gas and liquid phases. The properties of the foam were calculated by the following equations 6.7 and 6.8 depending on the volume fraction of each phase present in the foam cell.

\[
\rho_f = \alpha_g \rho_g + \alpha_l \rho_l \quad \text{Eq 6.7}
\]

\[
\mu_f = \alpha_g \mu_g + \alpha_l \mu_l \quad \text{Eq 6.8}
\]
Figure 6.8 illustrates the results obtained from the simulation on the foam height and the total bath height measured from the initial upper surface of the bath, as shown in Figure 6.9. The data points representing the observed data in Figure 6.8 are the data extracted from IMPHOS research report\cite{2} for the slag height profile of heat S1830. The slag height profile for heat S1830 was converted to foam height according to the explanation given in Appendix A3. In the present study, the simulations were run for 10 minutes.

It is evident from Figure 6.8 that the model predictions on the foam height (i.e. the height of phase 3 in the CFD model as shown in Figure 6.9) are in agreement with the observed results to a considerable extent. In the first 4 minutes, the foam height is over-predicted, but, towards the end of the time considered, the average foam height prediction is representative of the observed measurements. According to the foam formation criteria used in the present simulation, in the event of high availability of gas and liquid phases (i.e. more than 75% and 5% respectively), the foam production can increase and can exhibit an over-prediction of foam height similar to the present model results. In other words, the higher rate of foam formation predicted by the model at the start of the blow within the first two minutes may have caused by the high availability of gas and liquid phases.
In actual foam, the liquid content of the foam can vary between 0.01 and 0.26 before becoming a close pack of spheres as explained in Section 3.1.6.1 in Chapter 3. Accordingly, the gas content of the foam can vary from 99% to 74%. This variation of the gas fraction of foaming slag was experimentally studied by Kapilashrami et al.[11] using slag samples with different initial compositions. The observations made during the experiments are illustrated in Figure 6.10. According to the figure, it is evident that the gas fraction in the foaming slag varied between 85% and 60% for the two slags considered within the first 10 minutes.
The small amount of slag foam observed in the first few minutes in the heat S1830 can be related mainly to the less quantity of slag formed. Therefore, the foam formed at this stage can be assumed to be dry and contain about 1% liquid and 99% gas. However, in the present study, the foam was produced with a minimum gas content of 75% and may have caused the over-prediction of foam height within the first few minutes. As the blow progresses, the amount of available liquid for foaming increases and the liquid content of the foam is increased gradually. In this case, the gas content in the foam can reach 75% and hence the model predictions towards the end of the considered time are more agreeable with the observations.

Furthermore, at this stage of the CFD foaming model, the controlling phenomena of foam volume such as the liquid drainage and slag physical properties evolution were not considered. Once the foam was produced, the formed volume exists until the collapse criterion was met, without the influence of any other phenomenon. Real foam undergoes the effect of liquid drainage and varying physical properties of the liquid before collapsing. Since these effects were not addressed in the model at this stage, the model predictions tend to show an oscillatory pattern as illustrated in Figure 6.8.

The total bath height is the increase of bath height compared to the initial bath height before the oxygen injection as shown in Figure 6.9, and is higher than the foam height. The combined effect of gas hold-up and the increase of liquid phase in the CFD model due to the production of oxides are assumed to contribute to the bath height increase in addition to the foam height. As illustrated in Figure 6.8, the change between the foam
height and the total bath height is at maximum within the first three minutes of the blow. This observation can be interpreted mainly as the effect of high oxide production rates which increase the volume of the liquid phase. After about five minutes into the blow, the formation of slag components reduces with the reducing reaction rates. Hence, the difference between foam height and the total bath stays almost constant for the rest of the time.

6.9.2 The improvements introduced to the foaming model

Even though the foam height predictions from the model as shown in Figure 6.8 are approximately representative of the observed results from IMPHOS research work\cite{2}, the foaming model still has some deviations when compared with the actual foaming phenomenon. Therefore, at this stage of the simulation, the following improvements were incorporated in the foaming model.

- Continuous drainage of the foam until a critical volume fraction of liquid in the foam is reached.
- Foam collapses when the liquid content in the foam is less than the critical liquid volume fraction.
- Improved mass exchange between foam phase and the gas and liquid phases.
- Improved calculation of the scalars: gas and liquid fractions in foam.

Although, the foaming model at this stage (with the above improvements) mostly represents a general aqueous foam instead of a slag foam, this type of model can be used to understand the nature of slag foam as explained by Nexhip et al\cite{133}. They explained that slag foam could be approximated to well-drained soap foam as the structure of both foams under the well-drained condition was similar.

It is commonly observed that in the absence of other disturbances, the thickness of the bubble films in foam reduces gradually due to drainage until a critical thickness is reached, and once this thickness is exceeded, the film ruptures. Slag foams also exhibit a similar behavior as observed by Nexhip et al\cite{133}. They observed that the rate of thinning of the slag foam film retards with time and reaches a constant critical thickness before rupture. The critical thickness of the foam bubble films was observed to be about 0.1 to 0.4 μm as illustrated in Figure 6.11\cite{133}, which is approximately similar to that of
aqueous films (i.e. 0.1 to 0.2 μm\textsuperscript{176}). These observations were made during experiments on slag bubble films withdrawn from CaO-SiO\textsubscript{2}-Al\textsubscript{2}O\textsubscript{3} slags using platinum wire frames.

At the critical film thickness of foam bubbles, the foam is well-drained, and the liquid content in foam has reached the minimum or the dry limit as explained in Section 3.1.5. In foam, the liquid is contained in the bubble films and plateau border channels. At the dry limit (i.e. when the liquid fraction in foam is usually less than 0.02); the foam consists of Kelvin bubbles with bcc packing. Conversely, at the wet limit (i.e. Liquid fraction in foam is usually more than 0.26); the foam is an fcc hexagonal close pack of spheres.\textsuperscript{148}

The intermediate region between the above two extremes is the transition region from dry foam to wet foam, in which the foam bubbles take the shape of pentagonal dodecahedra or rhombic dodecahedra. Dodecahedrons are the clathrate structures that are stable in the transition region. This transition usually occurs over the range of 0.05 to 0.12 of liquid fraction in foam.\textsuperscript{148} Therefore, in the present study, the foam bubbles were assumed to take the shape of pentagonal dodecahedrons, and the critical liquid fraction, at which the foam transforms to dry foam completely, was assumed to be 0.10. Once the foam reaches this liquid content, the foam was assumed dry enough to collapse.

When the liquid content in foam is more than that of dry foam, the liquid in the foam flows downwards under the influence of gravity. This process is known as drainage and continuously occurs in foam causing rupture of bubble films leading to bubble

![Figure 6.11: Thinning pattern of a slag foam film\textsuperscript{176}](image)
coalescence or collapse. As explained in Section 3.1.6.1, this drainage in the foam can be approximated to flow of liquid through a porous solid media. Therefore, the drainage in the foam can be calculated using equations 3.4 and 3.5 in Section 3.1.6.1, and following is the drainage model incorporated in the present CFD foaming model by rearranging and simplifying equations 3.4 and 3.5.

\[ k = 6.7 \times 10^{-4} \varepsilon^{3/2} D_{avg}^2 \]  
Eq 6.9

\[ Q = k a_p \rho g \frac{\rho g}{\mu} \]  
Eq 6.10

\[ a_p = 0.161 r_b^2 \]  
Eq 6.11

Where: \( k \): permeability of the foam (m\(^2\)), \( \varepsilon \): liquid volume fraction of the foam, \( D_{avg} \): average bubble diameter (m), \( Q \): Flow rate through the Plateau border (m\(^3\)/s), \( a_p \): Cross-sectional area of the Plateau border (m\(^2\)), \( \rho \): density of the draining liquid (kg/m\(^3\)), \( \mu \): viscosity of the draining liquid (Ns/m\(^2\)), \( g \): acceleration due to gravity (m/s\(^2\)) and \( r_b \): radius of the Plateau border (m).

The values used for the variables were as follows:

\[ D_{avg} = 0.0087 \text{mm}; r_{avg} = 0.0048 \text{mm}; \rho = 6980 \text{kg/m}^3; g = 9.81 \text{m/s}; \mu = 6.1 \times 10^{-3} \text{Ns/m}^2 \]

Therefore, in the present stage of the foaming model, the foam was produced when the volume fraction of the liquid phase and gas phase in the cell exceeded 75% and 5% respectively, similar to the previous stage. The total amount of gas which was present in the newly formed foam cell was transferred to produce foam bubbles, and the liquid quantity was first transferred to produce the films of the foam bubbles, and the rest was considered to contain in the plateau border channels. Once the volume fraction of foam in the cell under consideration was more than the predefined minimum volume fraction (i.e. \( 1.0 \times 10^{-6} \)), the liquid content in foam was allowed to drain until the liquid fraction is 10%. The above-explained drainage model was incorporated in the CFD foaming model to determine the mass of the liquid transferred to liquid phase before foam collapse. When the liquid fraction in foam was less than 10% in a cell where the volume fraction of foam was more than 15%, the foam was collapsed, and the liquid and gas contained in the foam was transferred to the relevant phases.
6.9.3 Graphical results on the evolution of foam phase with time after improvements

Figure 6.12 illustrates the evolution of volume fraction of the foam phase at five different instances during the total simulation time of 10 minutes. The foam simulation at this stage was enhanced with the improvements explained in Section 6.9.2. The simulation results are presented and explained in detail in following sections. The complete set of graphical illustrations on foam phase evolution over time is included in Figure A6, Appendix A5.

Figure 6.12: Evolving foam phase volume fraction in the model with time
6.9.4 Foam height results (stage 2)

The foam height predictions obtained from the CFD model after incorporating the suggested improvements are shown in Figure 6.13. The improvements included were the continuous liquid drainage from the foam, foam collapse when the critical liquid fraction in foam is reached and improved interfacial mass exchange between the three phases and scalar volume fraction calculation in foam as explained in Section 6.9.2. The results obtained were compared against the slag height observations reported in IMPHOS\cite{2} for heat S1830 similar to Section 6.3.1.

As it is evident from Figure 6.13, the foam height prediction is almost constant throughout the time considered, which is over-predicted in the first 5 minutes and almost reaches the observed foam height for the rest of the period considered. Nonetheless, the oscillatory behavior observed in the previous stage results is minimized in the present foam height predictions and total bath height predictions. In other words, the present results show the average behavior of foam height and total bath height results of the previous stage shown in Figure 6.8.

![Figure 6.13: Model results on foam height and total bath height (Stage 2)](image-url)
The foam at this stage of simulation was improved and extended by incorporating the foam drainage and collapse phenomena as explained in Section 6.9.2. Therefore, the cause of the over-prediction of foam height shown in Figure 6.13 can be related to the fact of increased availability of gas and liquid volumes to produce foam. The model contains more gas volume due to the under-predicted rate of desiliconization and over-predicted rate of decarburization as shown in Figures 6.3 and 6.4 encouraging a high rate of foam production during the first few minutes. However, in the actual steelmaking process, the foam production during the first few minutes is less due to less volume of slag available and less gas production rates.

However, the effect of changing the minimum requisite gas fraction to produce foam on the foam height during the first part of the blow time considered was investigated under the same simulation conditions. The minimum requisite gas volume fraction to produce foam was changed from 0.75 to 0.90 at intervals of 0.05 gas volume fraction. The results obtained from the CFD model on foam height for various gas volume fractions are shown in Figure 6.14.

Figure 6.14: Variation of foam height with changing minimum requisite gas volume fraction to produce foam
It is evident from Figure 6.14 that the minimum gas volume fraction required to produce foam under the present conditions starts with very high value (i.e. ≈ 90%) and reduces to about 75% within the first 6 minutes of the time considered. However, this investigation on the behavior of foam height with changing minimum requisite gas volume fraction was carried out in the absence of the other major factors such as changes in slag volume and physical properties of slag which influence the foam height considerably and requires more investigation.

### 6.9.5 Foaming index

The foaming index is the ratio between the foam height and the superficial gas velocity and is an indication of the extent of foaming. As explained in Section 2.2.4 in Chapter 2, foaming index was initially used for aqueous systems by Bikerman\[17]\ and was later used for slag foaming in steelmaking by Fruehan et al\[15]\. However, this foaming index for slag foaming was first derived using data obtained during steady state experiments involving slag and Ar gas by Fruehan et al\[15]\. However, slag foaming in steelmaking is not at steady state due to the evolving chemical composition, slag physical properties and changing rates of chemical reactions. In this situation, the foaming index also changes with time. Therefore, steelmaking researchers have been using the dynamic foaming index,\[11, 12]\ which is calculated at each time step as explained in Section 2.2.4. Further, it is observed that this dynamic foaming index goes through a maximum. Nonetheless, the steady state foaming index explained by Fruehan et al\[15]\ is argued to be useful in the event of no change in slag viscosity by undissolved oxides\[26]\.

In the present study, the foaming index was calculated at intervals of 60 s and is shown in Figure 6.15. The foam height was obtained according to the procedure explained in Section 6.9.4, and the superficial gas velocity was calculated using the average of three gas phase velocity readings at three different locations at which foaming was clearly initiated. At this stage of simulation, the foam was produced from the gas phase and the liquid phase with the respective minimum required volume fractions of 75% and 5%.
According to Figure 6.15, the foaming index in the present stage of the model is oscillating between 0.70s and 1.25s with a slightly reducing average. The foaming index calculated by Cicuttì et al\cite{65} over a total blow time as shown in Figure 2.25 was approximately between 0.60s and 0.30s and exhibited a reducing trend within the initial 10 minutes. Further, this foaming index was at maximum around 4 to 6 minutes. Even though the present simulation results are not in the range of those observations reported by Cicuttì et al\cite{65} for liquid slag, present results are possible in the presence of solid particles in the slag according to Figure 2.25. Further, a clear maximum foaming index can be observed, which is typical for both the reported values for both liquid slag and the slag with solid particles. Therefore, the model predictions on the foaming in the converter approximately follows the pattern observed in the actual process even with the errors involved in obtaining the superficial gas velocities and the foam height values from the model results.
6.10 Summary analysis of the three phases model

The foaming model developed by Sattar et al\cite{36} was further improved and extended by incorporating the semi-empirical kinetics model explained in Section 6.8.1, and the foam simulation improvements explained in Section 6.9.2. The results obtained on the removal behavior of the impure elements and the foam height evolutions are summarized below.

The removal behavior of impure elements (C, Si, Mn and P) was incorporated in the CFD model using the semi-empirical first order kinetics model developed in the present study as explained in detail in Chapter 5. According to the results obtained from the CFD model shown in Section 6.8.2, the kinetics model has captured the removal pattern of all the elements despite some deviations in determining the refining rates. The decarburization predictions from the present CFD model given in Figure 6.3 are slightly over-predicted, while the desiliconization predictions shown in Figure 6.4 are under-predicted. However, in both cases, the observed removal behavior is captured by the model predictions reasonably well. The model predictions on demanganization and dephosphorization also have captured the observed refining pattern including the reversion of element from slag to metal reasonably well as illustrated in Figures 6.5 and 6.6. However, the rate of dephosphorization is slightly over-predicted, while the rate of demanganization is almost equal to the observed rate of Mn removal in heat S1843. The deviations observed in the kinetics predictions are mainly because the kinetics model used in the present study was a simple and semi-empirical developed using several simplifications and assumptions as explained in Chapter 5. This model was assumed sufficiently accurate for the present study as the primary target was developing a model for slag foaming.

The foaming model used in the present stage of simulations was an extension of the model developed by Sattar\cite{1}. The results obtained from the CFD model before any improvements to the foam simulation are shown in Figure 6.8. These results shown in Figure 6.8 were produced when the foaming model was identical to that developed by Sattar\cite{1}, but, the kinetics model was included in the CFD model. According to Figure 6.8, the foam height predictions were over-predicted in the first 5 minutes, and towards the
end of the 10 minutes, the foam height predictions were agreeable with the observed data. Despite the considerable oscillatory behavior observed, the model predictions have improved by the kinetics model included as evident from comparing with Figure 3.14. However, the deviations of the model predictions were attributed to several reasons which were addressed in the subsequent stage of the model.

Figure 6.13 illustrates the foam height predictions by the CFD model after incorporating the improvements to the foaming model. The improvements included were explained in detail in Section 6.9.2 and can be stated as follows:

- Continuous drainage of the foam until a critical volume fraction of liquid in the foam is reached.
- Foam collapses when the liquid content in the foam is less than the critical liquid volume fraction.
- Improved mass exchange between foam phase and the gas and liquid phases.
- Improved calculation of the scalars: gas and liquid fractions in foam.

It is evident from Figure 6.13 that the improvements have damped the oscillatory behavior of the predictions, while the over-prediction of foam height in the first 5 minutes was not improved as explained in Section 6.9.4 indicating that this over-prediction of foam height was not due to the issues addressed by the improvements mentioned above.

Hence, the effect of minimum requisite gas volume fraction on the foam height during the first 5 minutes was investigated and the results obtained from the model are shown in Figure 6.14. By comparing the foam height results for varying minimum requisite gas volume fractions with the observed data, it was concluded that the foam produced during first few minutes into the blow was dry foam produced with less liquid quantity and more gas quantity, and the gas fraction in foam gradually reduced to about 75% in around 6 minutes.

The CFD model at this stage was developed for predicting foaming in oxygen steelmaking in combination with a simple first order kinetics model, as there is no similar model in the open literature. According to the predictions of the present CFD model in this stage
of the study, which were reasonably agreeable results on foam height and refining kinetics of impure elements, it is evident that this model has been an original contribution to the knowledge of modeling foaming and kinetics in oxygen steelmaking. However, the deviations observed in the model predictions can be mainly because the slag foam is partly aqueous or liquid phase hold-up by the gas phase. The other drawbacks identified in the present stage of CFD model are listed below.

- The kinetics model incorporated in the CFD model was a simplified one compared to the currently available knowledge on the kinetics of actual oxygen steelmaking process. For example, the flux dissolution, scrap melting, post combustion and equilibrium relationships for Mn and P were simplified in developing this kinetics model as explained in Section 5.2.2 in Chapter 5.

- In the present CFD model, the foam was generated from the liquid phase and gas phase. Hence, the foam simulation was more related to aqueous foams instead of slag foam. Slag foam is produced from slag and gas and is affected by the evolving composition and physical properties of slag.

- Fluxes and scrap addition and other stirring gases were not considered in the present CFD model, and the composition of each phase was limited as explained in Table 6.1.

- Present simulations were run under isothermal conditions, which is not valid when actual steelmaking operations are considered because the rising temperature influences the chemical reaction rates and the physical properties of the fluids.

- The simulations were run only for 10 minutes, which is almost half the actual blow time of about 20 minutes for oxygen steelmaking.

Most of these drawbacks were simplifications made intentionally to reduce the time consumption and complexity of the programming required. Nonetheless, the following two methods were broadly identified as possible improvements to the CFD model.
• Use of a more rigorous kinetics model that includes more accurate and detailed relationships for determining the equilibrium values and sub-processes such as flux dissolution and scrap melting.
• Define slag as a separate phase and produce foam from slag.

In the next stage of the present CFD model, the second suggestion of separate slag phase was incorporated and investigated the results of the model’s foam height predictions. This improvement was expected to predict the foam height more accurately. The details and the results obtained from the four phases model are presented in Chapter 7.
Chapter 7: Four Phases Model

Oxygen steelmaking is well-established for its complex, transient and intense nature of both the fluid flows involved and the kinetics of refining reactions in the converter. As explained in the previous chapters, despite these complications, researchers have investigated the process in detail and have developed different models to predict different variables such as refining patterns of impure elements, slag foaming, scrap dissolution and flux dissolution. Among these modeling efforts, the foaming model developed by Sattar was used as the starting point in the present study. Even though this original model consisted of only three phases (i.e. gas, liquid, and foam), it produced reasonable predictions mainly on the foam height and decarburization. In the previous stage of simulations of the present study, that model was improved and extended by incorporating more chemical reactions, a kinetics model for calculating the reaction rates and more rigorous foaming phenomenon. As explained in Chapter 6, the model predictions were improved and were more representative of the actual oxygen steelmaking observations as reported in IMPHOS research work, despite the consideration of one liquid phase instead of two separate liquid metal and slag phases.

Nonetheless, in the actual oxygen steelmaking process, the slag is a separate phase and involve in refining reactions and foaming as a separate major component in the bath. Hence, in the final stage of the present CFD model, the slag was introduced as a separate phase. In this chapter, this four phases model is explained in detail, simultaneously with the results obtained from the model on slag foam height.

7.1. Limitations of three phases model and requirement for a separate slag phase

Limitations of the three phases model:
The CFD model in the previous stage consisted of only three phases: liquid, gas, and foam with the composition given in Table 6.1. The liquid phase was considered consisting of both elements in the hot metal and slag components. The limitations imposed by these considerations on the model and its predictions on foam height and refining kinetics of impure elements can be expressed as follows.
The liquid phase contributed to the formation of the foam phase instead of the slag phase in the three phases model similar to aqueous foam as explained in Section 6.3, which was the main drawback of the three phases model.

The mass fractions of elements and slag components in this three phases model were calculated by considering both slag and the hot metal as a single phase. Hence, the mass fractions were underestimated and may have caused deviations in the kinetics model calculations.

The physical properties of foam such as density and viscosity were calculated by assuming the gas and liquid content in the foam. Since, in the three phases model, the liquid phase contributed in producing the foam instead of slag, the physical properties calculations of foam may have deviated from the actual values.

**Improvements expected from introducing a separate slag phase:**

In oxygen steelmaking process, a part of the gases injected and produced from chemical reactions are trapped by the slag layer producing slag foam. The physical properties such as density, viscosity and surface tension as well as other factors including bubble diameter and gravity affect the foaming capacity of the slag. Further, most of these factors evolve in favor of foaming with time into the blow as explained in Section 2.2.4. Even though, the three phases model explained in the previous chapter produced reasonable predictions on foaming and refining kinetics in oxygen steelmaking, incorporation of the separate slag phase was expected to improve the model further due to following reasons.

- The foam phase in the four phases model is slag foam formed by slag phase and gas phase instead of aqueous foam produced from the liquid phase (mostly liquid metal) and gas phase.

- The physical properties of the foam are determined from the slag and gas content in foam, which is more accurate than previously calculated physical properties when foam was formed by liquid and gas phases.
In the four phases model, the mass fraction of elements and slag components are calculated separately as fractions from the liquid phase and slag phase respectively.

Therefore, the slag was introduced as a separate phase during this stage of the study, and the details of the process are explained in the following sections.

7.2. Slag phase forming criteria in the four phases model

Slag is the third phase in the present four phases CFD model. The first two phases are the liquid phase containing the hot metal components and the gas phase containing the $\text{O}_2$, $\text{CO}$, $\text{CO}_2$ and the gas bubbles. The slag phase, which is the third phase, is produced from the gas and liquid phases. Then, the foam phase is produced from slag and the gas phases as the fourth phase which is termed as slag foam phase in the CFD model.

A precise definition to produce the ‘slag phase’ in the CFD model was difficult to be found from the literature as this ‘slag phase’ in the CFD model was more related to the emulsion observed in the actual oxygen steelmaking instead of the real slag produced from the oxides and dissolving fluxes. In the emulsion formed in the actual steelmaking converter as shown in Figure 2.8 consist of slag, gas and liquid metal due to the intense mixing caused by the supersonic oxygen jet. Accordingly, the ‘slag phase’ in this four phases model was produced from gas, liquid and slag phases instead of only the oxides and fluxes. The criteria used for producing this slag phase was finalized via trial and error method.

Therefore, the slag phase formation criteria were defined considering both the metal components and the oxides. This four phases CFD model contained a very small quantity of slag (i.e., fluxes: $\text{CaO}$ and $\text{MgO}$) which was assumed to be evenly mixed in the bath at the start of the simulation. The author is aware that this assumption of mixed hot metal and slag is not accurate, but, it was used for initiating the simulations. Once the simulations were initiated, the phases separated according to their density.

Slag phase was formed when the cell under consideration contained more than 90% volume fraction of combined slag phase and liquid phase, and the combined mass fraction of liquid metal components was less than or equal to 75%. The slag phase
collapse criterion was such that, the cell under consideration contained more than 10% slag phase but the liquid components contained in this slag quantity was greater than 90%. Accordingly, a cell nominated to be ‘slag phase’ in the four phases CFD model contained more than 90% of combined hot metal and slag volume fraction, and more than 25% of that volume was slag components. In this case, a cell nominated to be liquid phase may contain up to 25% mass of slag components.

In the plant trials reported in IMPHOS\textsuperscript{[2]}, the average change of slag in the emulsion measured as the “Slag / (Slag + Metal) ratio” was in the range of approximately 18% to 40%. Therefore the criteria used for forming the ‘slag phase’ in this four phases CFD model was defined as the requirement to contain combined mass fraction of slag components in the cell to be equal to or more than 25%. According to the measurements reported in IMPHOS\textsuperscript{[2]}, this criterion was considered reasonable as a starting point.

### 7.3. Slag foam simulation in the four phases model

Slag foaming occurs in the oxygen steelmaking converter when the gases produced from the chemical reactions and a part of the gases injected (i.e. O\textsubscript{2} and stirring gases) are trapped by the slag layer in the form of bubbles. This process of trapping the bubbles is encouraged by the physical properties of the slag such as the viscosity and the surface tension and the increasing gas evolution rates and slag volume. This process of slag foaming can become extensive and uncontrollable, and may produce a slopping event by overflowing the converter. Hence, it is vital to develop a model to replicate the slag foaming process sufficiently accurately to predict the slopping events.

The foaming model in the three phases CFD model was explained in detail in Section 6.9. That model consisted only of three phases; gas, liquid, and foam, where, the foam phase was produced from the liquid phase and the gas phase. Hence, the foam was similar to aqueous foam produced in a bubble column reactor. In this three phases model, the liquid phase consisted of both the hot metal components and the slag components and contained the improved criteria for formation, drainage, and collapse of the foam. However, the foam height results as illustrated in Figure 6.13, were over-predicted at the beginning of the blow and approximately reached the observed foam height in the
second part of the blow. Therefore, in this four phases CFD model, a separate slag phase was introduced and the ‘slag phase’ mainly contributed in producing the slag foam.

The four phases CFD model consisted of slag foam produced from the slag phase and the gas phase. The slag phase was produced from the criteria explained in Section 7.2. The slag foam was created once the cell under investigation contained more than 75% volume fraction of gas phase and 5% of slag phase. This quantity of slag was assumed to form the foam bubble films, and the rest of the slag and any liquid quantity that was in the cell when the slag foam was produced were assumed to be the fluid in the plateau borders in the slag foam. The slag foam was collapsed when the foam is dry enough indicated by the quantity of combined slag and liquid scalars lesser than 10% in the foam. The slag foam phase consisted of ten bubble classes similar to the initial model. The foam bubbles were assumed to take the shape of pentagonal dodecahedrons, and the coalescence of foam bubbles due to film rupture was considered in the slag foam using the coalescence model developed by Tong et al.\(^\text{[166]}\) similar to the previous stage of the model.

The drainage of slag foam was also considered in the four phases model using the model developed by Bhakta and Ruckenstein\(^\text{[178]}\) similar to that in the foaming model developed by Sattar\(^\text{[1]}\) as given by equations 7.1 to 7.3.

\[
q_{pb} = \frac{3}{15} NRn_p a_p u \\
Eq 7.1
\]

\[
u = \frac{c_v a_p \rho g}{20\sqrt{3} \mu} \\
Eq 7.2
\]

\[
a_p = 0.161r_p^2 \\
Eq 7.3
\]

Where \(q_{pb}\): liquid drainage through plateau border channels, \(N\): number of bubbles, \(R\): radius of the foam bubble, \(n_p\): number of plateau border channels, \(a_p\): cross sectional area of the plateau border channel, \(u\): average drainage velocity, \(c_v=1\), \(\rho\): density of slag, \(g\): acceleration due to gravity, \(\mu\): viscosity of slag, \(r_p\): Radius of curvature of plateau border.
The density and the viscosity of the slag foam were calculated from the relevant volume fraction of slag and gas phases in the foam using equations 7.4 and 7.5.

\[
\rho_f = \alpha_g \rho_g + \alpha_s \rho_s \quad \text{Eq 7.4}
\]

\[
\mu_f = \alpha_g \mu_g + \alpha_s \mu_s \quad \text{Eq 7.5}
\]

Where \( \alpha_g \): gas volume fraction, \( \alpha_s \): slag volume fraction, \( \rho_f \): density of the foam, \( \rho_g \): density of gas, \( \rho_s \): density of slag, \( \mu_f \): viscosity of foam, \( \mu_g \): viscosity of the gas, \( \mu_s \): viscosity of slag.

### 7.4. Model geometry and details

The geometry used in the four phases CFD model was the same geometry as that of the previous stage as shown in Figure 7.1. The figure illustrates the complete volume mesh and the 3D thin slice of that mesh used for the present simulation. As explained in Section 6.2, this geometry was initially developed by Sattar[1] according to the geometry of the pilot plant converter used for IMPHOS trials[2].

![Figure 7.1: The mesh used in the present stage of the CFD model[1]](image)

The initial bath height was 0.66 m similar to the previous stage of the model. The volume above the hot metal bath in the converter was filled with the gas phase. The vertical lance for oxygen injection was located in the middle of the converter. The inner diameter of the lance is 0.0155 m, and the exit of the lance was extended by 0.496 m from its original location reported in IMPHOS[2].
As explained in Section 7.1, the present stage of the model consists of four phases; gas phase, liquid phase, slag phase, and the slag foam phase. The list of the scalars contained in each phase is given in Table 7.1.

Table 7.1: Scalars list of the four phases considered in the CFD model

<table>
<thead>
<tr>
<th>Phase</th>
<th>Scalars</th>
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<tbody>
<tr>
<td>Gas phase</td>
<td>Ten gas bubble classes, CO, CO₂ and O₂</td>
</tr>
<tr>
<td>Liquid phase</td>
<td>Fe, C, Si, P, Mn, S, FeO, SiO₂, P₂O₅, MnO, CaO, MgO</td>
</tr>
<tr>
<td>Slag phase</td>
<td>CaO, MgO, FeO, SiO₂, P₂O₅, MnO, Fe, C, Si, P, Mn, liquid and gas in slag</td>
</tr>
<tr>
<td>Foam phase</td>
<td>Ten foam bubble classes, gas, slag and liquid in foam</td>
</tr>
</tbody>
</table>

The same ten bubble classes used in the previous stage of the model were used in the four phases model. The diameters of the bubble classes were between 2.5 mm and 20 mm and are given in Table 6.2. Bubble coalescence and break-up in the gas phase, as well as the bubble coalescence in the slag foam phase, were considered in the model using the relevant sub-models used in the previous stage of the model as explained in Section 7.8.7.

The commercial CFD package AVL FIRE 2009.2 was used for simulations in the present study. The software uses the finite volume method for discretization of the governing equations. The resulting discretized governing equations were then solved iteratively using a segregated approach. Since the model includes four different phases, multiphase flow simulation was carried out using the Eulerian-Eulerian reference frame. The phases interact with each other in terms of mass and momentum, and the fluids were considered incompressible. For momentum and continuity, an unsteady state multiphase solution was used, while for the turbulence, a standard k-ε model was used. The differencing scheme used for momentum and turbulence was the first order upwind differencing scheme, while that used for continuity equation was the central differencing scheme. The fluids involved were assumed to be incompressible. The simulation was run in an unsteady state with a time step of 0.001s for 600s, on an Intel(R) Xenon(R) CPU E5-1620 0 machine, where the RAM and the speed of the processor were 16GB and 3.60GHz respectively.
7.5. **Boundary conditions imposed on the model**

Boundary conditions were imposed on the model in order to define the operation of the model boundaries according to that of the pilot plant converter in IMPHOS\(^2\).

The inlet of the model was the tip of the extended lance, and velocity boundary condition was applied to the inlet. Pure oxygen was injected onto the bath via the lance, and the temperature of the oxygen stream was assumed to be 1648 K. Further, the inlet gas stream contained bubbles of the smallest diameter.

The outlet of the model was defined as the top surface of the model excluding the area of the lance and pressure boundary condition was applied to the outlet of the model. The gas stream that exits from the outlet was assumed to be mainly CO\(_2\) and CO and was assumed to be at atmospheric pressure.

The surrounding walls of the model were assumed to be solid, even and non-slip walls. The temperature of the walls was assumed to be 1648 K similar to the hot metal bath.

7.6. **Initial conditions**

The converter contained about 5.5 tons of hot metal before the start of the simulations. Both the slag and slag foam phases were initiated from the minimum volume fraction (i.e. \(1.0e\text{-}06\)), and a small mass fraction of the liquid phase was defined to be slag components at the start of the simulation. The rest of the volume of the converter above the hot metal was the gas phase. All the hot metal, slag, and gas were at the temperature of 1648 K. The initial composition of the liquid phase and the slag phase are given in Tables 7.2 and 7.3.
### Table 7.2: Initial composition of the liquid phase in the model

<table>
<thead>
<tr>
<th>Component</th>
<th>Wt% in the liquid phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>88.77</td>
</tr>
<tr>
<td>C</td>
<td>4.03</td>
</tr>
<tr>
<td>Si</td>
<td>0.57</td>
</tr>
<tr>
<td>P</td>
<td>0.44</td>
</tr>
<tr>
<td>Mn</td>
<td>0.08</td>
</tr>
<tr>
<td>S</td>
<td>0.01</td>
</tr>
<tr>
<td>FeO</td>
<td>0.01</td>
</tr>
<tr>
<td>SiO₂</td>
<td>0.01</td>
</tr>
<tr>
<td>P₂O₅</td>
<td>0.01</td>
</tr>
<tr>
<td>MnO</td>
<td>0.01</td>
</tr>
<tr>
<td>CaO</td>
<td>4.75</td>
</tr>
<tr>
<td>MgO</td>
<td>1.31</td>
</tr>
</tbody>
</table>

### Table 7.3: Initial composition of the slag phase in the model

<table>
<thead>
<tr>
<th>Component</th>
<th>Wt% in the slag phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>FeO</td>
<td>5.00</td>
</tr>
<tr>
<td>SiO₂</td>
<td>5.00</td>
</tr>
<tr>
<td>MnO</td>
<td>5.00</td>
</tr>
<tr>
<td>P₂O₅</td>
<td>5.00</td>
</tr>
<tr>
<td>CaO</td>
<td>50.00</td>
</tr>
<tr>
<td>MgO</td>
<td>10.00</td>
</tr>
<tr>
<td>Fe</td>
<td>1.00</td>
</tr>
<tr>
<td>C</td>
<td>1.00</td>
</tr>
<tr>
<td>Si</td>
<td>1.00</td>
</tr>
<tr>
<td>Mn</td>
<td>1.00</td>
</tr>
<tr>
<td>P</td>
<td>1.00</td>
</tr>
<tr>
<td>Liquid</td>
<td>10.00</td>
</tr>
<tr>
<td>Gas</td>
<td>5.00</td>
</tr>
</tbody>
</table>
The gas phase in the four phases CFD model contained 13 scalars which were the gases \( \text{O}_2 \), \( \text{CO} \) and \( \text{CO}_2 \) and the ten gas bubble classes. The slag foam phase also contained 13 scalars which were the ten bubble classes, gas in foam, liquid in foam and slag in foam.

### 7.7. Fluid properties and components

Main properties of the four fluids considered in the present stage of the model are given in Table 7.4. Properties of the gas phase were assumed to be similar to the properties of the air at 1648 K, while those of the liquid phase were assumed to be similar to the properties of liquid iron at 1648 K. For the slag phase, the properties of average BOF slag at 1648 K were used. Since the simulation was run with the isothermal condition, the properties of the gas, liquid, and slag phases were considered to be constant throughout the simulation time.

<table>
<thead>
<tr>
<th></th>
<th>Density (Kg/m(^3))</th>
<th>Dynamic viscosity (Ns/m(^2))</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Gas phase</strong></td>
<td>0.233</td>
<td>1.82e-11</td>
</tr>
<tr>
<td><strong>Liquid phase</strong></td>
<td>6980.0</td>
<td>1.01e-06</td>
</tr>
<tr>
<td><strong>Slag phase</strong></td>
<td>3600.0</td>
<td>1.01e-06</td>
</tr>
<tr>
<td><strong>Slag foam phase</strong></td>
<td>703.2</td>
<td>1.37e-07</td>
</tr>
</tbody>
</table>

The density and viscosity of the slag foam phase were calculated according to the amount of gas and slag phases in the foam cell at the time step using equations 7.4 and 7.5 while the other properties were assumed to be constant throughout the simulation time. The properties of slag foam given in Table 7.4 were used for initiating the simulations.

### 7.8. Governing equations

Four phases were considered in the present CFD model which were gas, liquid, slag and the slag foam as explained previously. These four phases interact with each other in terms of mass, momentum, and energy in the actual oxygen steelmaking due to the intense mixing. In the present CFD model, the interaction between these four phases in terms of mass and momentum were considered via the governing equations for mass and momentum. Therefore mass, momentum, and enthalpy conservation equations
were incorporated into the simulation together with the mass and momentum interfacial exchanges. Heat generation by the chemical reactions was not considered in the present study, and isothermal conditions were assumed throughout the blow. The author is aware that this assumption of isothermal operation of the steelmaking process is not true in the actual operation, and causes errors in the model results by not considering the effect of increasing temperature on the physical properties of the phases and rate of chemical reactions. However, this assumption was made as a starting point and to reduce the complexity of the programming required in the simulations.

7.8.1. Mass conservation equation
The mass conservation equation used in the present study was Eulerian-Eulerian approach based and was used to calculate the mass interaction between the four phases. The mass conservation equation employed in the present stage of the simulation was equation 3.22 which was explained in Section 3.3.1.1.

7.8.2. Mass interfacial exchange
The mass interfacial exchange occurred in the present stage of the simulation in the event of chemical reactions and formation of slag and slag foam phases. The slag phase was created from the liquid and gas phases based on the composition of the liquid phase contained in the control volume under consideration as explained in Section 7.2. Slag foam is formed from slag phase and the gas phase according to the respective volume present in the cell under consideration as described in Section 7.3. Mass interfacial exchange term was used to account for these mass interactions between phases in the present stage of the simulation. Equation 3.22 explained in Section 3.3.1.1 is the mass interfacial exchange term employed in the present simulation.

7.8.3. Momentum conservation equation
According to the Newton’s second law, the rate of change of momentum equals to the sum of the forces on the fluid particles. This conservation law of physics was included in the CFD model using the momentum conservation equation, because the particles of the four fluids considered in the present model were under the influence of several forces including the gravity. The momentum conservation equation for the finite volume
method in Eulerian-Eulerian approach was used in the simulation as explained in Section 3.3.1.2 and was given by equation 3.27.

7.8.4. Momentum interfacial exchange
Momentum exchange between the phases is significant in the oxygen steelmaking converter due to the activities such as coalescence and break-up of bubbles and bubble-induced drag forces. In the present CFD model, the effect of these activities on the momentum conservation of each phase was calculated using the momentum interfacial exchange term. The momentum interfacial exchange term utilized in the present simulation was explained in Section 3.3.1.2 and was given by equations 3.31 to 3.36.

7.8.5. Population balance modeling
Four different phases were considered in the present CFD model, which were the gas, liquid, slag and slag foam. Each of these phases consisted of scalars that change in its numbers due to factors such as reacting with other scalars or coalescence and break-up in the case of bubbles. In order to keep track of such scalars in each phase, the population balance modeling is required. The population balance equation in the AVL FIRE software is the scalar transport equation as explained in Section 3.3.5 by the equation 3.42. The influence of activities that change the numbers of the scalars was included in the population balance equation using a source term as explained in the following sections.

7.8.6. Chemical species population calculations
Chemical species were considered in all the four phases, but the kinetics model included in the model involved the scalars in gas and liquid phases only. The concentration of the chemical species in these two phases change with the progression of the chemical reactions, and these changes were tracked by the semi-empirical kinetics model as the \( \frac{dC}{dt} \). Moreover, the changes calculated by the kinetics model were then included in the population balance equation as a source term \((S_i)\) as was explained in Section 6.6.6.

7.8.7. Bubble break-up and coalescence
Ten bubble classes were considered in both gas and slag foam phases in the present stage of the model similar to the previous stage. The population of these bubble classes was tracked using the population balance equation as explained previously. The number
densities of the bubbles change due to coalescence and break-up caused by different factors such as colliding with turbulent eddies and rupture of films of the bubbles due to drainage. In the present study, these changes caused by the break-up and coalescence were included in the model using the source terms given by equations 3.43 to 3.47.

7.9. Graphical results for the evolution of four phases

The CFD model in the present stage consisted of four phases: the gas phase, liquid phase, slag phase and the slag foam phase. The CFD model was simulated for 10 minutes, and the evolution of the four phases in terms of the volume fraction is shown in Figure 7.2. The complete set of illustrations is given in Appendix A9.

It is evident from the figures that at this stage of the model, the quantity of slag phase formed increased by a small quantity over time and floats over the liquid phase concentrated towards the periphery of the converter. The semi-empirical kinetics model developed in the previous stage of the model was included in the present stage of the model. In the four phases CFD model, the impurity elements were observed to be oxidized very quickly producing the oxides, which may be due to the higher mass fractions of those elements calculated during the simulations, because the total mass of the liquid phase in the four phases model is lower than that of the three phases model. These oxides were then used for producing the slag phase. Therefore, the quantity of slag reached near the maximum slag quantity within the first 2 to 3 minutes. The slag foaming is increasing over time in the first 180 s with slopping at the 180 s as shown in Figure 7.2.
Figure 7.2: Graphical representation of the evolution of volume fraction of the four phases in CFD model with time.

7.10 Slag foam height results

The main aim of the present research work was to improve and extend the foaming model developed by Sattar[1] to predict the slag foaming in oxygen steelmaking. The model developed by Sattar[1] consisted of only three phases which were gas, liquid, and foam. In this initial model, slag components were not considered, and therefore the foam was produced from the liquid phase containing Fe and C similar to an aqueous foam produced in bubble column reactors.

In the four phases CFD model, the foam was produced from the slag phase and the gas phase. As explained in Section 7.2, the slag phase was produced when the cell under consideration contained more than 90% volume fraction of combined slag phase and liquid phase, and the combined mass fraction of liquid metal components was less than
or equal to 75%. The slag phase collapse criterion was such that, once the cell under consideration contained more than 10% volume fraction of slag phase but the liquid components contained in this slag quantity was greater than 90%. The slag phase produced according to the criterion mentioned above then involved in producing the slag foam phase. Slag foam was produced when the cell under consideration contained more than 75% gas volume fraction and 5% slag volume fraction. This slag foam was collapsed when a slag foam cell was dry enough so that the liquid and slag content in foam was less than 10%. The slag foam phase consisted of ten bubble classes and the coalescence of foam bubbles due to film rupture was considered similar to the previous stages of the present CFD model.

At the present stage, the CFD model was simulated for 10 minutes with a time step of 0.001s and the results obtained for the evolution of slag foam height are illustrated in Figure 7.3.

It is evident from the figure that the foam height prediction at the start of the blow is over-predicted similar to the previous stages of the present CFD model. The main reason

![Figure 7.3: Slag foam height evolution with time](image)

At the present stage, the CFD model was simulated for 10 minutes with a time step of 0.001s and the results obtained for the evolution of slag foam height are illustrated in Figure 7.3.
for this over-prediction may be due to the high gas availability during this period in the model. As shown in Figure 6.14 in Section 6.9.4, the minimum requisite gas phase volume fraction at the start of the blow is around 80% to 90%. Therefore, the use of the condition to produce foam when the gas phase volume fraction in the foam is 75% or more may have caused this over-prediction of the foam height. Further, in the period between 120 s and 240 s, a slopping event is predicted by the model as shown in Figure 7.2 as well as was shown graphically in Figure 7.2. It is well-established in literature that slopping events occur in the first part of the blow mainly due to high gas generation rates and high slag viscosity due to undissolved lime particles. Even though slopping was not observed in the heat S1830 shown in Figure 7.2 as the observed data, some of the other heats reported in IMPHOS including S1841 and S1843 experienced slopping events around 4 to 5 minutes into the blow (Figures 2.46 c and d).

The foam height prediction of the four phases CFD model during the period from 360s to 540s is in good agreement with the observed foam height as shown in Figure 7.2, even though the model grossly over-predicts the foam height in the first part of the blow. The average under-prediction of the foam height during this period observed in the previous stage of the model (Figure 6.13) is rectified in the present stage with the introduction of the separate slag phase. Hence, producing the foam from slag and gas phases similar to the actual oxygen steelmaking process has improved the model predictions compared to its predictions when the foam was produced from the liquid metal and gas phases. However, the reducing trend observed in the foam height predictions from the model at this stage has to be investigated further by increasing the simulation time beyond 10 minutes.

However, it is evident from Figure 7.2 that the slag phase volume fraction was not evolving considerably with time. The simplified condition used for slag phase simulation has caused this level of error. In the actual oxygen steelmaking process, the slag quantity increase with time due to flux addition and oxidation of the impurity elements and iron as well as the dissolution of the refractory lining. However, in the present study, the flux addition was not considered. Instead, flux components were included in the initial composition of the bath as given in Table 7.2, and assumed that the fluxes were in the liquid state at the start of the simulations. The same kinetics model used in the three
phases CFD model was used in the four phases CFD model, but, its performance was not exactly similar due to variations created by introducing the new slag phase such as changed mass fractions as explained in Section 7.9. Hence, improving the performance of the kinetics model as well as the criteria for producing and collapsing the slag phase in the model are the routes of improving the present four phases CFD model.

7.11 Summary analysis of the four phases model
The predecessor research work of the present study was the study by Sattar[1]. Their model consisted mainly of a foaming model and a decarburization model and was able to predict the foam height with reasonable approximation compared to the data published in IMPHOS[2]. However, several drawbacks were identified in this model as explained in Section 3.4. Hence, in the previous stages of the present work a kinetics model was developed and the foaming model in the three phases CFD model was improved. In the present stage of the model, slag was introduced to the CFD model as a separate phase and the foam produced was slag foam as it was produced from slag and gas phases. The model was simulated for 10 minutes, and its predictions on the slag foam height were compared with the slag height profile for the heat S1830 reported in IMPHOS[2] as illustrated in Figure 7.2.

In the four phases model, the slag phase was formed when the cell under consideration contained more than 90% volume fraction of combined slag phase and liquid phase, and the combined mass fraction of liquid metal components was less than or equal to 75%. The slag phase collapse criterion was such that, once the cell under consideration contained more than 10% slag phase but the liquid components contained in this slag quantity was greater than 90%. It is notable that this ‘slag phase’ produced in the four phases model was more related to the emulsion observed in the steelmaking converter than to the actual slag made of oxides and dissolving fluxes as explained in Section 7.2. The slag phase evolution with time was graphically illustrated in Figure 7.2, and the change of the quantity of slag was not significant with time. In the four phases CFD model, the impurity elements were observed to be oxidized very quickly producing the oxides, which may be due to the higher mass fractions of those elements calculated during the simulations, because the total mass of the liquid phase in the four phases model is lower than that of the three phases model. These oxides were then used for
producing the slag phase. Therefore, the quantity of slag reached near the maximum slag quantity within the first few minutes. However, the slag phase produced was involved in producing slag foam.

The slag foam was produced when the cell under investigation contained more than 75% volume fraction of gas phase and 5% of slag phase. The slag foam was collapsed when the foam is dry enough indicated by the quantity of combined volume fraction of slag and liquid phases being less than 10% in the foam. The foam bubbles were pentagonal dodecahedrons, and the slag foam consisted of ten bubble classes. The drainage of the foam was included in the simulation using equations 7.1 to 7.3. The density and the viscosity of the slag foam phase were calculated using equations 7.4 and 7.5 based on the respective volume fraction of slag and gas phases in foam.

The slag foam height predictions of the present CFD model are illustrated in Figure 7.3. It is evident from the figure that the present model predictions have improved compared to the previous stage of the CFD model. Even though the foam height is over-predicted in the first part of the blow, the model predicts the foam height in the latter part of the considered period with a good agreement to the observed foam height. As explained in Section 7.10, the over-prediction of foam height in the first part of the considered blow time was assumed mainly due to the high availability of the gas phase, while the improved foam height predictions during the latter part were mainly encouraged by the new slag phase. Hence, it is evident that slag foam produced from a slag phase has improved the predictions of the model on foam height compared to that when the foam was produced from liquid metal phase, despite the over-predicted foam height at the start of the blow and the oscillatory behavior of foam height which were commonly observed in each stage of the model.

Nonetheless, the present four phases model can be further improved in several routes to enhance its predictions on slag foam height further. Considering the flux addition and dissolution and improving the performance of the kinetics model will improve the CFD model in terms of slag phase simulation. The slag foam simulation can be further improved by incorporating more accurate foam production, drainage, and collapse criteria.
Chapter 8
Chapter 8: Discussion

Slag foaming is an important phenomenon encountered in both ferrous pyrometallurgical processes and non-ferrous smelting processes due to its characteristic advantages including the large surface area formed and protection against the direct contact of the melt with the atmosphere. Slag foam is produced when the slag layer traps the gas bubbles produced by the chemical reactions. With the progression of the blow, the quantity of slag increases and the physical properties of slag evolve in favor of foaming. Then, with high rates of gas production, the slag foaming may become uncontrollable creating a slopping event. Slopping is an adverse event, and its unfavorable consequences include yield loss, health and safety costs, damage to equipment and environmental pollution. Hence, it is essential to properly control slag foaming in oxygen steelmaking for a continuous and efficient production process.

Understanding and modeling slag foaming and reaction kinetics in oxygen steelmaking have been the focus of steelmaking researchers, and therefore, several different models and experimental/pilot plant studies on slag foaming and reaction kinetics can be found in the literature. However, the need for a more accurate and reliable dynamic model is still emphasized.\cite{11-13} The experimental studies on investigating and understanding slag foaming in oxygen steelmaking include the studies by Cooper and Kitchener\cite{14}, Fruehan and co-workers\cite{15-18}, Ghag and co-workers\cite{19-21}, Stadler and co-workers\cite{22, 23}, Irons and co-workers\cite{24-26} and Seetharaman and co-workers\cite{11, 27}. Gou et al argued that it is a gas holdup instead of true foam that occurs at such high superficial gas velocities experienced in the oxygen steelmaking converter.\cite{24} Several numerical foam modeling efforts using CFD technique also can be found in the literature including research works by Bhole et al\cite{30}, Bannari et al\cite{31}, Chen et al\cite{32} and Sattar\cite{1}. These studies were mostly on bubble columns using population balance modeling with different bubble break-up and coalescence closure terms. Among them, the foaming model developed by Sattar\cite{1} using CFD technique was able to produce promising results on slag foaming in oxygen steelmaking. Hence, this work was used as the starting point of the present study.
The CFD model developed by Sattar\cite{1} was able to predict the foam height, the number densities of bubble classes in gas and foam phases, decarburization, heat generation and the velocities of the phases as explained in Section 3.3. The multiphase flow simulation was carried out with a Eulerian-Eulerian approach. The population balance equation was used to calculate the population densities of the components of each phase, and in the case of population calculations of the bubble classes, the bubble coalescence and breakup were taken into consideration. Only the decarburization reaction was considered in their work, and the heat generation due to carbon oxidation was incorporated in the simulation. The results obtained from the simulation were compared with the observed data published in IMPHOS\cite{2} and were in reasonable agreement.

The present study was aimed at further improving and extending the CFD model developed by Sattar\cite{1} by addressing the drawbacks identified in that model as explained in Section 3.4. The main goal of the present study was to develop the existing CFD model to predict slag foaming in oxygen steelmaking converter, and this goal was divided into four main tasks as given in Section 1.3 which were identified as the objectives of the present study. These four tasks were achieved in three main stages of the CFD model. In the first and second stages, a semi-empirical first order kinetics model was developed using the pilot plant data reported in IMPHOS\cite{2} study and was incorporated in the CFD foaming model. In the third stage, the foaming model developed by Sattar\cite{1} was further enhanced in terms of foam formation and collapse and continuous foam drainage. Then, in the fourth stage, the CFD model was further improved by incorporating slag as a separate phase and producing foam from the slag phase. The methodology of improvement and the results of the CFD model at each of these three stages were presented in Chapters 5, 6 and 7 respectively.

In summary, the foam height predictions made by the CFD model showed different levels of agreement with the foam height data reported in IMPHOS\cite{2} report. However, the major improvements incorporated into the model at each stage of the model caused the model predictions to be more agreeable and reliable progressively. In the following section, an analysis of the main results is provided at each stage of the model.
Even though it is established that modeling the actual oxygen steelmaking process is a very tough and challenging task, the present work has improved the initial CFD model\textsuperscript{[1]} to be more representative of the actual steelmaking process. Hence, the present research work has made an original contribution to knowledge in regards to developing a CFD slag foaming model for oxygen steelmaking process. However, the deviations of the model predictions on foam height were apparent at each stage of the model, and the limitations and simplifications occurred during the model development which were identified as the causes, are discussed in detail in Section 8.2.

8.1. Results of the present study

8.1.1. Semi-empirical kinetics model

Slag foaming in oxygen steelmaking is directly related to the physical properties of slag, the quantity of slag and the rate of gas generation. A kinetics model in the main CFD foaming model is essential to calculate the rates of the chemical reactions that produce gases and slag. Therefore, in the present study, a semi-empirical first order kinetics model was developed and incorporated into the CFD foaming model as explained in Chapter 5.

An analysis was carried out on the semi-empirical first order kinetics model developed in the present study using the data reported in the IMPHOS\textsuperscript{[2]} study to verify its performance before incorporating into the CFD model. The conclusions of the analysis were such that; the removal rate of C and Si can be predicted using the first order kinetics when the equilibrium concentration of the element was assumed static, and equals to the elements’ composition in turndown steel, while, the removal kinetics of Mn and P can be predicted using the first order kinetics when the equilibrium concentration of each element was calculated dynamically. Accordingly, the first order kinetics model used in the analysis was rearranged and incorporated in the CFD model as explained in Section 5.3. The CFD model predictions on the removal behavior of C, Si, Mn, and P are presented in Section 6.8.2.

According to the model predictions, the kinetics model has captured the removal pattern of all four impurity elements despite some deviations in determining the refining rates. The decarburization predictions from the present CFD model are slightly over-
predicted, while the desiliconization predictions are under-predicted. However, in both cases, the observed removal pattern is captured by the model predictions reasonably well. The model predictions on demanganization and dephosphorization also have captured the observed refining pattern including the reversion of element from slag to metal reasonably well. However, the rate of dephosphorization predicted by the CFD model is slightly over-predicted, while the predictions on the rate of demanganization are almost equal to the observed rates for Mn removal in heat S1843 of IMPHOS trials\(^2\).

Accordingly, the kinetics model incorporated in the present CFD model can be considered reasonably accurate, because, there is no completely rigorous kinetics model in the open literature using the CFD technique to predict the refining kinetics of the impure elements to this extent.

8.1.2. Three phases CFD foaming model

The CFD foaming model in the second stage of the present study consisted of three phases: gas, liquid, and foam, similar to the foaming model developed by Sattar\(^1\). The foam phase was produced from gas and liquid phases as explained in Section 6.9. The foam height predictions of the model after incorporating the kinetics model are presented in Section 6.9.1, and it is evident that the model over-predicted the foam height in the first part of the blow time considered and reaches the observed data in the latter part. Also, the predicted foam height shows a considerable oscillatory behavior.

Therefore, the foaming model was further improved in several aspects, which were: continuous drainage of foam until a critical volume fraction of liquid in the foam is reached, foam collapses when the liquid content in the foam is less than the critical liquid volume fraction, improved mass exchange between foam phase and the gas and liquid phases, improved calculation of the scalars: gas and liquid fractions in foam. After incorporating these improvements, the model predictions on the foam height were improved by dampening the oscillatory behavior observed in the second part of the blow time considered (i.e. from 4 to 10 minutes) compared to the foam height predictions before including the above improvements, as explained in Section 6.9.4. However, the over-prediction of the foam height in the first part of the period considered (i.e. from start to 4 minutes) was not affected by the improvements mentioned above.
Hence, the effect of minimum requisite gas volume fraction on the foam height during the first 5 minutes was investigated, because, it was suspected that the high availability of gas phase during this period may have caused the over-prediction of foam height. It was concluded by analyzing the model results given in Section 6.9.4 that the foam produced during first few minutes into the blow is dry foam produced with less liquid quantity and more gas quantity, and the gas fraction in foam gradually reduces from about 90% to about 75% in around 6 minutes. These results compare well with the observations reported in the literature that the liquid content of the foam can vary between 1% and 26% and the gas content of the foam can vary between about 60% and 85%.[11, 148]

The variation of the foaming index over time was also investigated in this stage of the study as explained in Section 6.9.5, and it was observed that the foaming index oscillated between 0.70s and 1.25s with slightly reducing average over the 10 minutes period with an apparent maximum of 1.25s at 2 minutes. Even though the range of foaming index variation predicted by the CFD model is higher to the observations reported by Cicutti et al[65], the model has captured the pattern of foaming index variation with a clear maximum in the foaming index in the first few minutes into the blow.

It is notable that the CFD model in this third stage of the study generated reasonably agreeable results on foam height and refining kinetics of impure elements even though the foam generated was more related to aqueous foam than slag foam. This can be because the actual slag foam formed in oxygen steelmaking is partly liquid hold-up by gases (i.e. aqueous foam). The existing debate on the gas hold up instead of true foaming by Irons et al[24] is partially proved in the present study, because the foaming model predictions further improve with the use of slag phase to produce foam as explained in the next section.

8.1.3. Four phases slag foaming model

The foam height predictions in the previous stage of the model were in reasonable agreement with the observed data reported in IMPHOS[2] study although the foam produced was more related to aqueous foam than slag foam observed in oxygen steelmaking. In order to improve this three phases model to predict slag foaming, the
slag was introduced as a separate phase. Hence, in the final stage of the present study, the CFD model was improved to a four phases model where the foam phase was produced from the slag and gas phases.

As explained in Section 7.2, in this four phases model, the slag phase was formed when the cell under consideration contained more than 90% volume fraction of combined slag phase and liquid phase, and the combined mass fraction of liquid metal components was less than or equal to 75%. The slag phase was collapsed once the cell under consideration contained more than 10% slag phase but the liquid components contained in this slag quantity was greater than 90%. This ‘slag phase’ included in the four phases CFD model was more related to the emulsion in the actual oxygen steelmaking converter instead of the actual slag that is produced from the oxides and the fluxes as explained in Section 7.2. It is evident from the figures given in Section 7.9 that the change in slag volume fraction was not significant with time during the blow time considered. The main reason for this was assumed to be the higher rate of oxidation of the impurity elements calculated by the kinetics model in the four phases model compared to the previous stage of the model. Even though the same kinetics model was used in both stages of the CFD model, the mass fractions of the elements calculated by the four phases model were higher due to the reduced volume of liquid phase compared to the three phases model. Hence the slag quantity reached the maximum during the first few minutes and did not vary significantly after that.

The slag foam was then produced from slag and gas phases when the cell under investigation contained more than 75% volume fraction of gas phase and 5% volume fraction of slag phase. The slag foam was collapsed when the foam is dry enough indicated by the quantity of combined volume fraction of slag and liquid phases reduced to less than 10% in the foam. The slag foam height predictions of the four phases CFD model are explained in Section 7.10. It is evident from the results that the present model predictions have improved significantly compared to the previous stages of the model. Even though the foam height is over-predicted in the first part of the blow with a maximum of about 1.3 m at 3 minutes into the blow, which is not usually observed in real steelmaking blow, the model predicts the foam height in the latter part of the considered period with a good agreement to the observed foam height. As explained in
Section 7.10, the over-prediction of foam height in the first part of the considered blow time was mainly due to the high availability of the gas phase similar to the previous stage model predictions, while the improved foam height predictions during the latter part were mainly encouraged by the new slag phase.

According to the model predictions illustrated in Figure 7.2, it is evident that the new slag phase has improved the model predictions during the 6 to 10 minutes period. It is notable that the slag phase produced in the four phases model was not exactly similar to the real slag. Instead, it was defined as a combined phase containing slag, gas and liquid metal similar to the slag-gas-metal emulsion in the actual oxygen steelmaking converter. Hence, the slag foam produced in the present CFD model is a combination of aqueous foam and slag foam and indicates that the slag foam produced during actual oxygen steelmaking is partially true foam and partially liquid hold up by gases.

8.2. Limitations of the present CFD model

Even though the present CFD model predicted slag foaming and removal behavior of the impurity elements with a good agreement when compared with the observed data reported in IMPHOS\textsuperscript{[2]}, there are several limitations that restricted the performance of the present CFD model as explained below.

8.2.1. Use of simplified relationships

The capacity of the two computers used for simulations in the present study was 3.60GHz and 2.66 GHz in terms of speed of the processor and 16 GB and 8 GB in terms of RAM respectively. Therefore, the submodels developed required to deliver a simple but reasonable relationship that could be incorporated in the subroutines without over-complicating them.

Hence, the kinetics model developed in the present work was based on the Fick’s first law of diffusion, even though, it is argued that the complex and transient reaction kinetics involved in the oxygen steelmaking process cannot be well-explained with first-order relationships. Despite that the literature consists of more complex methods to determine the equilibrium values, simplified semi-empirical relationships were used to develop the kinetics model in the present study. Further, the sub-processes such as flux dissolution and scrap melting were considered in developing the kinetics model, but
those subprocesses were not separately included in the CFD model developed, in order to reduce the complexity of the model. The fluxes were assumed to be dissolved in the bath at the start of the oxygen injection in the four phases model. Furthermore, several relationships used in the bubble population calculations were also simplified via assigning pre-calculated values for variables such as the amount of liquid in the bubble films to reduce the calculation time.

These simplifications have caused a certain level of error in the model results. However, in the present study, these simplifications were used because the primary aim was to develop a general and functional model as a starting point.

**8.2.2. Insufficient availability of plant data**

IMPHOS\[^2\] is the research work used in the present study to extract data required for developing the kinetics model, initiating the simulations and validating the simulation results. IMPHOS\[^2\] research provides the most recent and reliable set of data on top blown oxygen steelmaking under plant conditions, and it reports data for 20 heats, and for each heat, data were obtained at each 2 minutes for 18 minutes.

Even though, the IMPHOS\[^2\] reports a large set of data on those 20 heats, some deficiency in data were found regarding post-combustion and slag foam height, which were of main concern in the present study. Post-combustion data were required for calculating the extent of oxidation of iron for developing the kinetics model. As a consequence of this data deficiency, some assumptions were made in developing the kinetics model such as values for the post combustion ratio (PCR). Further, the slag foam height data were reported in IMPHOS\[^2\] in terms of the uppermost sampling pot number in which slag was collected. However, transforming this scale into a height measurement was a difficult and doubtful task for validating the results from the present simulations.

The effect of these assumptions on the model results was negligible compared to the effect caused by the use of simplified and semi-empirical relationships in the subroutines for calculating the refining kinetics and foam height.
8.2.3. Comparison of model results only with plant trials reported in IMPHOS\textsuperscript{2}

In the present study, the model results were compared only with the data reported in IMPHOS\textsuperscript{2} research report as explained previously. IMPHOS\textsuperscript{2} was selected for the present work due to its content which can be used to describe the oxygen steelmaking process almost completely despite the issues mentioned above in Section 8.2.2. In other words, IMPHOS\textsuperscript{2} reports information on the raw materials and the initial conditions before the start of the process, details on the refining of the bath during the process, and information on the output product and by-products once the process is finished. These data were essential to initiate the simulations and for comparing and validating the model results.

The other data sets that report observations on oxygen steelmaking such as data reported by Cicutti et al\textsuperscript{91} and Van Hoorn et al\textsuperscript{137} do not provide a comparable quantity of information. Therefore, comparison of the model results with these data sets will not provide useful insights.

The author is aware that by using only one plant data set for comparing and validating the results of the model can lead to over-estimating the performance of the model. However, the model developed in the present study was estimated approximately representative of the oxygen steelmaking process because the IMPHOS\textsuperscript{2} was established to be a complete set of data representing the process.

8.2.4. Use of already developed models

Since the model developed by Sattar\textsuperscript{1} was capable of predicting the foam height and decarburization to a reasonable extent, several sub-models in the original model were not modified in the present study. The reasons for this negligence were due to their sufficient accuracy and was considered as out of the scope of the present study. Following are the main submodels which were not modified:

- Foam formation

The criterion used by Sattar\textsuperscript{1} for producing foam was defined as the requirement of 75\% volume fraction of gas phase and 5\% volume fraction of the liquid phase in a cell. It is observed that 70\% to 99\% of total volume of foam can be gas in bubbles.\textsuperscript{142} Hence,
the criteria used for foam formation was assumed sufficiently accurate and was not modified in the three phases model, even though the mass exchange between the phases in the event of foam formation was modified. In the four phases model, this criterion was modified to the requirement of 75% volume fraction of gas phase and 5% volume fraction of slag phase to produce the foam.

- Bubble coalescence
In the CFD model developed by Sattar\cite{1} the coalescence of bubbles was assumed to occur only due to turbulence. The coalescence model developed by Prince and Blanch\cite{150} was used for modeling coalescence of gas bubbles, and the coalescence model developed by Tong et al\cite{166} was used for modeling coalescence of foam bubbles in the model developed by Sattar\cite{1}. In the present study, these coalescence models were not modified assuming those were sufficiently accurate.

- Bubble break-up
The break-up of bubbles was assumed to occur due to colliding with eddies of required size and energy in the model developed by Sattar\cite{1}. Bubble break-up was considered only for gas bubbles, and the model developed by Luo and Svendson\cite{152} was used to incorporate it in the CFD model. In the present study, the same model was used assuming it was reasonable and sufficiently accurate for this stage of the model.

- Ten bubble classes
There are ten bubble classes used in the model with diameters between 2.50 mm to 20.00 mm defined in the model developed by Sattar\cite{1}. Hence, in the present study, the number of bubble classes and the defined size of those bubbles were not modified.

Even though the sub-models mentioned above were simplified via different assumptions, those were performing well in the model developed by Sattar\cite{1}. Hence, in the present study, same sub-models were used assuming similar performance despite the improvements incorporated into the model in the present work.

8.2.5. Introducing the separate slag phase
In the oxygen steelmaking process, foam is produced from slag which is formed from the oxides produced from the oxidation of the elements in the bath and dissolving fluxes
and refractories. The physical properties of this slag such as viscosity, density, and surface tension evolve in favor of trapping gas bubbles in the slag layer producing slag foam.

However, in the model developed by Sattar[1], the foam was produced from the liquid phase which contained only iron and carbon as scalars. This foam was more like aqueous foam instead of slag foam. Even though same foaming model was used in the three phases model, slag was introduced as a separate phase with the aim of producing foam from slag in the four phases model. It is well established that the slag mainly consists of oxides of the elements in the bath and the added fluxes. However, the ‘slag phase’ produced in the four phases model was a mixture of slag, gas and liquid components similar to the slag-gas-metal emulsion observed in the actual steelmaking process.

Hence, an assumption was made to distinct the ‘slag phase’ in the CFD model from its liquid phase using the measurements reported in the IMPHOS[2] study. A cell was defined to be slag phase if the cell contained more than 90% volume of combined slag phase and liquid phase, and the combined mass fraction of liquid metal components was less than or equal to 75%. The slag phase was collapsed once the cell under consideration contained more than 10% slag phase but the liquid components contained in this slag quantity was greater than 90%. Even though this criterion for slag phase formation was derived partly via trial and error method, the model predictions on foam height were reasonable. However, the author is aware that this condition is not sufficiently strong to distinct the slag phase from the liquid phase, but was successful as the model could produce a separate slag phase and then produce foam from slag upgrading the CFD model to the position to predict slag foaming. Further enhancing this slag forming criteria is identified as a possible future improvement to the present CFD model.

8.2.6. Isothermal conditions

In each stage of the present CFD model, isothermal conditions were assumed during the simulations. The author is aware that this assumption of isothermal operation of the steelmaking process is not true, and causes errors in the model results by not considering the effect of increasing temperature on the physical properties of the
phases and rate of chemical reactions. At the start of the blow in the actual steelmaking process, the low temperatures and undissolved flux particles increase the viscosity of the slag. However, the lower slag foam height observed in this part of the blow is mainly due to the less quantity of slag and comparatively high density of the slag. Accordingly, the present model was expected to over-predict the foam height encouraged by the large amount of slag phase formed at the beginning of the blow. This over-prediction was further fuelled by the constant requirement of gas phase and liquid/slag phase defined to produce the foam phase. (i.e. the requirement to contain 75% gas and 5% slag/liquid volume fraction in a cell to produce foam throughout the simulation, instead of a reducing gas volume fraction from about 90% to 75% over first few minutes). However, this assumption was made to reduce the complexity and the time consumption of programming required in the present model.

8.2.7. Simulation time was limited to 10 minutes
The total simulation time was 10 minutes for each stage of the present study. The actual steelmaking process runs for about 20 minutes on average, and the period considered in the present simulations was half of that actual duration.

The reason for limiting the simulation time was to reduce the actual time consumption of the simulations. The author is aware that the results obtained in the present study may vary if extended beyond 10 minutes of simulation time as it was not investigated in the present work.

8.2.8. Trial and error troubleshooting
Most of the criteria used in the present study needed modifications before being confirmed the final. For example, the criteria used for foam collapse in the three phases model needed a variable for checking the volume of foam phase present in the cell to determine whether to collapse the foam mass in the cell. Since this type of variable is not available in the literature and is difficult to determine theoretically, a trial and error method had to be employed. Another example is the criteria used for the slag formation as explained in Section 8.2.5. For many of the criteria used in the present subroutines, the method to finalize the best performing situation was by trial and error method.
The effects of using trial and error method include the excessive time consumption and the model performance becoming specific to certain conditions. Time consumption was a big issue in the present study, as the three phases model consumed about 20 days for one complete simulation, while the four phases model consumed about 30 days for one complete simulation. Further, the solutions obtained via trial and error method force the model to perform accurately only under the specified conditions. In other words, the model deviates from a general model for oxygen steelmaking process.

Nonetheless, the foam height predictions of the present CFD model can be concluded as in good agreement with the reported observed foam height data at each stage despite the limitations and simplifications mentioned in the sections earlier in the chapter. In the present research work, the difficult task of modeling the kinetics and the slag foaming in oxygen steelmaking was achieved to a reasonably good extent when the difficulties involved in literature available on the steelmaking process as well as in using the CFD technique for the modeling work are taken into account.
Chapter 9
Chapter 9: Conclusions and recommendations

The foaming model developed by Sattar[1] was enhanced and extended in the present study by improving the foaming model in terms of formation, drainage, and collapse of foam, incorporating a semi-empirical kinetics model and introducing slag as a separate phase to produce slag foam. The results of the CFD model were promising when compared with the pilot plant data reported in the IMPHOS[2] research report and indicated the possibility of improving and extending the present model further into a more general CFD model for oxygen steelmaking process.

Following conclusions were drawn based on the performance of the present CFD model over the three stages explained in the previous Chapters 5, 6 and 7.

1. A semi-empirical first order kinetics model was developed in the present study, and the performance of this model was analyzed using the pilot plant data reported in IMPHOS[2]. The analysis showed that this first order semi-empirical model can be used to predict the removal pattern of the impurity elements: C, Si, Mn and P as a starting point.

2. The first order semi-empirical kinetics model was incorporated in the CFD model, and the CFD model was able to predict the removal behavior of the impurity elements by capturing the removal pattern with a good agreement when compared with the data reported in IMPHOS[2] study. This indicates that the present CFD model can predict the refining of the bath in terms of the removal of C, Si, Mn and P.

3. The three phases foaming model was further enhanced by improving the foam formation and collapse criteria, and incorporating the continuous foam drainage. The foam height prediction of the model was improved, and the unstable, oscillating behavior observed in the model predictions previously was damped as a result of the improvements in the latter part of the blow time considered.
4. The three phases CFD model was upgraded to a four phases model by introducing slag as a separate phase, and the foam was produced from slag and gas phases. The slag foam height predictions of the four phases model were in reasonable agreement with the observations. It is indicative from the model predictions that the present CFD model can be used to predict slag foaming in oxygen steelmaking reliably.

In summary, the difficult task of modeling the kinetics and the slag foaming in oxygen steelmaking was achieved to a reasonably good extent in the present research work, when the difficulties involved in literature available on the steelmaking process as well as in using the CFD technique for the modeling work are taken into account. However, the deviations of the model predictions on foam height and the removal pattern of the impurity elements considered were apparent at each stage of the model which were acknowledged and discussed respectively. The other simplifications and limitations that contributed to restrictions on the performance of the current modeling work were also identified and discussed. Hence, it can be concluded that the present work is an original contribution to the field, because, no other study in the open literature has successfully combined the reaction kinetics and foaming in oxygen steelmaking using the CFD technique.

However, there are several aspects of the present CFD model which require further improvements for perfecting the model predictions, which are recommended by the author as the possible future research pathways.

1. The relationships used in developing the first order semi-empirical kinetics model such as equilibrium concentrations of Mn and P and flux dissolution were simplified relationships. Use of more rigorous and accurate relationships in the kinetics model may improve the performance of the CFD model.

2. In the present CFD model, the kinetics model involves only the components in liquid and gas phases. Extending the kinetics model to slag and slag foam phases will improve the performance of the model in terms of predicting the kinetics in oxygen steelmaking.
3. The criteria used for producing and collapsing the slag phase were derived by trial and error method in the present study. Improved criteria may enhance the slag phase simulation and the slag foaming of the CFD model.

4. The physical properties, such as the density and viscosity of the foam, were calculated according to the gas, liquid and slag content in foam in the present CFD model. Similarly, the physical properties of slag can be calculated according to the composition of the slag. This will improve the slag foam simulation of the CFD model.

5. In the present study, the flux dissolution and the scrap melting were not included in the CFD model. The fluxes and the scrap added to the converter cause changes to the composition of the bath as well as to the physical properties of slag when dissolved in the hot metal bath. Incorporation of fluxes and scrap will improve the slag and the slag foam simulation of the present CFD model.

6. The CFD model was simulated only for 10 minutes in the present study. The average blow time of the oxygen steelmaking process is about 20 minutes. Extending the model simulation time to about 20 minutes will provide more insights into the process.

7. Isothermal conditions were assumed in the present simulations despite the errors that can occur due to the negligence of the changes caused by increasing temperature such as increasing reaction rates and reducing viscosity. Incorporation of heat exchange between phases and heat generation due to chemical reactions will improve the model further.
8. IMPHOS$^2$ was the set of plant data used in the present study to compare and validate the predictions of the CFD model. Comparison of the present model results with other experimental data available in literature may assist in further improving the model.

These suggestions will further advance the present CFD model further to a more reliable and sophisticated model.

In conclusion, the results obtained from the CFD model developed in the present study are a strong step towards developing a general model for oxygen steelmaking process, and therefore, the present study represents a significant contribution to knowledge in that regards.
References


[67] S. DEMAG, "Prozesslinien ".


Appendix

A1. Calculation results for carbon, silicon, manganese, and phosphorus with static equilibrium values

Table A1: Calculation results for C, Si, Mn and P with static equilibrium values

<table>
<thead>
<tr>
<th>Heat No.</th>
<th>Carbon</th>
<th>Silicon</th>
<th>Manganese</th>
<th>Phosphorus</th>
</tr>
</thead>
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<td>R²</td>
<td>kmA (m³/min⁻¹)</td>
<td>R²</td>
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<tr>
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**A2. Calculation results for manganese and phosphorus with dynamic equilibrium values**

Table A 2: Calculation results for manganese and phosphorus with dynamic equilibrium values

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<th>Heat No.</th>
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<th>Phosphorus</th>
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<td>kmA (m³min⁻¹)</td>
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<td>S1831</td>
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<td>S1832</td>
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<td>0.0002</td>
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<tr>
<td>S1833</td>
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</tr>
<tr>
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**NC:** Not calculated due to restrictions in calculating the logarithmic of negative values.
A3. Slag height index

The position of the sampling lance carrying the sampling pots inside the converter is shown in Figure A1, and the sampling lance is schematically illustrated in Figure A2. The slag height measurement was obtained by direct observation of the extent of the hot slag adhering to each sampling lance following its withdrawal from the converter. Hence, the measurement at each time step was the maximum height of slag foam in the converter. Slag foam height measurements were reported for 16 minutes for each heat, and the heat S1830 was used in the present study for comparing the foam height results. As reported in IMPHOS, the slag foam height for this heat reached index 7 at 6 minutes, remained at this height for 4 minutes, and then started to slop heavily for heat S1830 as shown in Figure A3. According to the given dimensions of the sampling lance and its position inside the converter in Figures A1 and A2, the slag height profile given by indices in Figure A3 was converted to slag height profile in meters as shown in Figure A4 to be used in the present study.
A4. CFD model results used to generate the result graphs in Chapter 6

- The CFD model results when polynomials were used in the kinetics model

The mass fractions for each impure element was obtained for each 60s time slot, and the removal profile for each element was generated using those data. The data obtained are tabulated below.

Table A3: The readings from the CFD model simulation when the polynomials were used in the kinetics model

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Carbon</th>
<th>Silicon</th>
<th>Manganese</th>
<th>Phosphorus</th>
<th>Silicon Dioxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.035880</td>
<td>0.005150</td>
<td>0.004240</td>
<td>0.000750</td>
<td>0.001100</td>
</tr>
<tr>
<td>60</td>
<td>0.033574</td>
<td>0.003107</td>
<td>0.002178</td>
<td>0.000386</td>
<td>0.005466</td>
</tr>
<tr>
<td>120</td>
<td>0.028976</td>
<td>0.001629</td>
<td>0.001185</td>
<td>0.000210</td>
<td>0.008777</td>
</tr>
<tr>
<td>180</td>
<td>0.023883</td>
<td>0.000848</td>
<td>0.000653</td>
<td>0.000116</td>
<td>0.010476</td>
</tr>
<tr>
<td>240</td>
<td>0.018969</td>
<td>0.000425</td>
<td>0.000361</td>
<td>0.000064</td>
<td>0.011346</td>
</tr>
<tr>
<td>300</td>
<td>0.015026</td>
<td>0.000202</td>
<td>0.000203</td>
<td>0.000037</td>
<td>0.011761</td>
</tr>
<tr>
<td>360</td>
<td>0.012119</td>
<td>0.000085</td>
<td>0.000118</td>
<td>0.000021</td>
<td>0.011939</td>
</tr>
<tr>
<td>420</td>
<td>0.010375</td>
<td>0.000022</td>
<td>0.000071</td>
<td>0.000013</td>
<td>0.012000</td>
</tr>
<tr>
<td>480</td>
<td>0.009516</td>
<td>0.000000</td>
<td>0.000044</td>
<td>0.000008</td>
<td>0.012009</td>
</tr>
<tr>
<td>540</td>
<td>0.009336</td>
<td>0.000000</td>
<td>0.000029</td>
<td>0.000006</td>
<td>0.012012</td>
</tr>
<tr>
<td>600</td>
<td>0.009150</td>
<td>0.000000</td>
<td>0.000019</td>
<td>0.000004</td>
<td>0.012014</td>
</tr>
</tbody>
</table>

- The CFD model results when the first order diffusion kinetics model was used

The mass fractions for each impure element was obtained for each 60s time slot, and the removal profile for each element was generated using those data. The data obtained are tabulated below.

Table A4: The readings from the CFD model simulation when the first order diffusion kinetics model was used

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Carbon</th>
<th>Silicon</th>
<th>Manganese</th>
<th>Phosphorus</th>
<th>Silicon Dioxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.035880</td>
<td>0.005150</td>
<td>0.004240</td>
<td>0.000750</td>
<td>0.001100</td>
</tr>
<tr>
<td>60</td>
<td>0.035022</td>
<td>0.004458</td>
<td>0.003509</td>
<td>0.000607</td>
<td>0.002377</td>
</tr>
<tr>
<td>120</td>
<td>0.034254</td>
<td>0.003891</td>
<td>0.002990</td>
<td>0.000510</td>
<td>0.003634</td>
</tr>
<tr>
<td>180</td>
<td>0.033640</td>
<td>0.003329</td>
<td>0.002467</td>
<td>0.000413</td>
<td>0.004921</td>
</tr>
<tr>
<td>240</td>
<td>0.033119</td>
<td>0.002866</td>
<td>0.001872</td>
<td>0.000271</td>
<td>0.006010</td>
</tr>
<tr>
<td>300</td>
<td>0.032511</td>
<td>0.002530</td>
<td>0.001764</td>
<td>0.000254</td>
<td>0.006854</td>
</tr>
<tr>
<td>360</td>
<td>0.031923</td>
<td>0.002243</td>
<td>0.001781</td>
<td>0.000259</td>
<td>0.007565</td>
</tr>
<tr>
<td>420</td>
<td>0.031349</td>
<td>0.001901</td>
<td>0.001590</td>
<td>0.000230</td>
<td>0.008364</td>
</tr>
<tr>
<td>480</td>
<td>0.030635</td>
<td>0.001649</td>
<td>0.001430</td>
<td>0.000204</td>
<td>0.008886</td>
</tr>
<tr>
<td>540</td>
<td>0.030069</td>
<td>0.001406</td>
<td>0.001128</td>
<td>0.000155</td>
<td>0.009378</td>
</tr>
<tr>
<td>600</td>
<td>0.029537</td>
<td>0.001249</td>
<td>0.001009</td>
<td>0.000136</td>
<td>0.009690</td>
</tr>
</tbody>
</table>
The CFD model results on foam height and total bath height (Section 6.9.1)

Foam height measurement was obtained at three different positions as the foam height was not same in the radial direction from the center of the model. The average of the three height measurements was taken as the final foam height, which was used in the analysis and is tabulated below.

Table A 5: Foam height and total bath height measurements obtained from the simulations (Section 6.9.1)

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Foam height (m)</th>
<th>Total bath height (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>0.827107</td>
<td>1.178993</td>
</tr>
<tr>
<td>120</td>
<td>1.104135</td>
<td>1.840693</td>
</tr>
<tr>
<td>180</td>
<td>0.711075</td>
<td>1.240783</td>
</tr>
<tr>
<td>240</td>
<td>0.933284</td>
<td>1.578473</td>
</tr>
<tr>
<td>300</td>
<td>0.829529</td>
<td>1.237987</td>
</tr>
<tr>
<td>360</td>
<td>0.942292</td>
<td>1.382860</td>
</tr>
<tr>
<td>420</td>
<td>1.220697</td>
<td>1.456473</td>
</tr>
<tr>
<td>480</td>
<td>0.986612</td>
<td>1.578473</td>
</tr>
<tr>
<td>540</td>
<td>0.942165</td>
<td>1.471833</td>
</tr>
<tr>
<td>600</td>
<td>0.857014</td>
<td>1.150532</td>
</tr>
</tbody>
</table>

The CFD model results on foam height and total bath height (Section 6.9.4)

Foam height measurement was obtained at three different positions as the foam height was not same in the radial direction from the center of the model. The average of the three height measurements was taken as the final foam height, which was used in the analysis and is tabulated below.

Table A 6: Foam height and total bath height measurements obtained from the simulations (Section 6.9.4)

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Foam height (m)</th>
<th>Total bath height (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>1.03688</td>
<td>1.23929</td>
</tr>
<tr>
<td>120</td>
<td>1.03102</td>
<td>1.41543</td>
</tr>
<tr>
<td>180</td>
<td>1.00729</td>
<td>1.44210</td>
</tr>
<tr>
<td>240</td>
<td>0.97472</td>
<td>1.41851</td>
</tr>
<tr>
<td>300</td>
<td>1.00435</td>
<td>1.41544</td>
</tr>
<tr>
<td>360</td>
<td>0.97767</td>
<td>1.41543</td>
</tr>
<tr>
<td>420</td>
<td>0.97473</td>
<td>1.41854</td>
</tr>
<tr>
<td>480</td>
<td>0.97473</td>
<td>1.41854</td>
</tr>
<tr>
<td>540</td>
<td>0.97770</td>
<td>1.38891</td>
</tr>
<tr>
<td>600</td>
<td>0.97767</td>
<td>1.41850</td>
</tr>
</tbody>
</table>
• The CFD model results on the variation of foam height with changing gas volume fraction (Section 6.9.4)

Table A 7: Foam height measurements obtained from the simulation when the minimum requisite gas volume fraction was varied

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Foam height (m)</th>
<th>Gas fraction 0.65</th>
<th>Gas fraction 0.70</th>
<th>Gas fraction 0.80</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>1.44216</td>
<td>0.91256</td>
<td>0.47386</td>
<td></td>
</tr>
<tr>
<td>120</td>
<td>1.05477</td>
<td>0.82362</td>
<td>0.41471</td>
<td></td>
</tr>
<tr>
<td>180</td>
<td>0.87403</td>
<td>0.77030</td>
<td>0.41471</td>
<td></td>
</tr>
<tr>
<td>240</td>
<td>0.84792</td>
<td>0.76732</td>
<td>0.47383</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>0.75903</td>
<td>0.85324</td>
<td>0.44432</td>
<td></td>
</tr>
<tr>
<td>360</td>
<td>1.33650</td>
<td>0.76733</td>
<td>0.47385</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Foam height (m)</th>
<th>Gas fraction 0.85</th>
<th>Gas fraction 0.90</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>0.29627</td>
<td>0.32559</td>
<td></td>
</tr>
<tr>
<td>120</td>
<td>0.41460</td>
<td>0.35484</td>
<td></td>
</tr>
<tr>
<td>180</td>
<td>0.44422</td>
<td>0.11804</td>
<td></td>
</tr>
<tr>
<td>240</td>
<td>0.32573</td>
<td>0.14763</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>0.58941</td>
<td>0.23621</td>
<td></td>
</tr>
<tr>
<td>360</td>
<td></td>
<td>0.11840</td>
<td></td>
</tr>
</tbody>
</table>

• The CFD model results on the variation of foaming index

Table A 8: Calculated foaming index values with time

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Foaming index (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>1.044</td>
</tr>
<tr>
<td>120</td>
<td>1.250</td>
</tr>
<tr>
<td>180</td>
<td>1.055</td>
</tr>
<tr>
<td>240</td>
<td>0.740</td>
</tr>
<tr>
<td>300</td>
<td>0.865</td>
</tr>
<tr>
<td>360</td>
<td>1.031</td>
</tr>
<tr>
<td>420</td>
<td>0.699</td>
</tr>
<tr>
<td>480</td>
<td>0.855</td>
</tr>
<tr>
<td>540</td>
<td>1.047</td>
</tr>
<tr>
<td>600</td>
<td>0.847</td>
</tr>
</tbody>
</table>
A5. Graphical results of evolving three phases in three phases model (Chapter 6)

- The graphical results for evolving three phases in three phases model (Section 6.9.1)
Figure A 5: Evolving volume fraction of three phases with time
The graphical results for foam phase in three phases model (Section 6.9.4)

Figure A 6: Foam phase evolution with time
A6. Subroutines used in CFD three phases model

- User subroutine to calculate sources in scalar equation

**SUBROUTINE** usesc_mscal(mat,isc,mph)

---

*author: Anuththara Kirindigoda Hewage (2070065)*

*date: 30/08/2016*

*project: Kinetics Model(Diffusion Model)*

---

**USE** comm1

**USE** comm2

**USE** comm0

**INCLUDE** 'comdp.inc'

**INCLUDE** 'com90.inc'

**INCLUDE** 'SwiftIO_FortranFunctions.inc'

**INTEGER**, **INTENT**(in):: mat,isc,mph

---

**INTEGER**:: I_i,I_j,I_k,I_m,nc,ip,ip1,ip2,ip3

**REAL**, **DIMENSION**(1:24,NCELL)::R_S

**REAL**, **DIMENSION**(NCELL)::R_lqt,R_tDgbt,R_tdgf,R_lq_f,R_tffl,R_foam

**REAL**, **DIMENSION**(1:10)::R_tv,R_tvf,R_BCF,R_DCF,R_BC,R_DC,R_d,R_v

**REAL**, **DIMENSION**(1:10,1:10)::R_ccarea,R_TCR,R_colef,R_tij

**REAL**, **DIMENSION**(NCELL)::R_fm_g_com,R_g_fm_com,R_gfr_com,R_L_av_Si

**REAL**, **DIMENSION**(NCELL)::R_P_final,R_L_av_Fe,R_L_av_C,R_Mn_ch,R_P_ch

**REAL**, **DIMENSION**(NCELL)::R_O2_av_g,R_Si_Fickrate,R_Si_av_l,R_G_Gen

**REAL**, **DIMENSION**(NCELL)::R_C_P1,R_Si_P1,R_Mn_P1,R_P_P1,R_CO_used_O2

**REAL**, **DIMENSION**(NCELL)::R_C_P2,R_Si_P2,R_Mn_P2,R_P_P2,R_SiO2_b2

---

*REAL*, **DIMENSION**(NCELL)::R_O2_av_g,R_CO_av,R_CO_r,R_O2_r,R_O_CO_t,R_O2_a,R_bubble,R_Id

*REAL*, **DIMENSION**(NCELL)::R_CRate,R_FeRate,R_Si_RATE,R_Mn_RATE,R_Mn_eq,R_C_req_FeO

*REAL*, **DIMENSION**(NCELL)::R_P_Rate,R_P_eq,R_C_req_O2,R_C_req_P2O5,R_C_req_MnO

*REAL*, **DIMENSION**(NCELL)::R_Si_req_O2,R_Si_req_P2O5,R_Si_req_MnO,R_Si_req_FeO

*REAL*, **DIMENSION**(NCELL)::R_Fe_req_O2,R_Fe_req_P2O5,R_P_req_O2,R_Mn_req_O2

*REAL*, **DIMENSION**(NCELL)::R_Preq_P2O5,R_Mnreq_FeO,R_Mn_final_3,R_t

*REAL*, **DIMENSION**(NCELL)::R_C_final_1,R_C_final_2,R_C_final_3,R_C_final_4

*REAL*, **DIMENSION**(NCELL)::R_Fe_final_1,R_Fe_final_2,R_Mn_final_1,R_Mn_final_2

*REAL*, **DIMENSION**(NCELL)::R_Si_final_1,R_Si_final_2,R_Si_final_3,R_Si_final_4

*REAL*, **DIMENSION**(NCELL)::R_Fe_final_1,R_Fe_final_2,R_Mn_final_1,R_Mn_final_2

---

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REAL, DIMENSION(NCELL):: R_Fe_used_P2O5, R_C_used_FeO, R_MnO_av_l
REAL, DIMENSION(NCELL):: R_Si_used_MnO, R_C_used_MnO, R_Mn_used_FeO
REAL, DIMENSION(NCELL):: R_Si_O2, R_Fe_O2, R_Mn_O2, R_C_O2, R_P_O2
REAL, DIMENSION(NCELL):: R_C_P2O5, R_C_MnO, R_C_FeO, R_C_used_P2O5
REAL, DIMENSION(NCELL):: R_Si_P2O5, R_Si_MnO, R_Si_FeO, R_Fe_P2O5
REAL, DIMENSION(NCELL):: R_Mn_P2O5, R_Mn_FeO, R_Fe_b, R_C_b, R_P_b
REAL, DIMENSION(NCELL):: R_C_P2O5, R_C_MnO, R_C_FeO, R_C_used_P2O5
REAL, DIMENSION(NCELL):: R_Si_P2O5, R_Si_MnO, R_Si_FeO, R_Fe_P2O5
REAL, DIMENSION(NCELL):: R_P2O5_b, R_P2O5_b1, R_P2O5_b2, R_P2O5_b3
REAL, DIMENSION(NCELL):: R_SiO2_b, R_SiO2_b, R_SiO2_b, R_SiO2_b
REAL, DIMENSION(NCELL):: R_C_b, R_C_b, R_C_b, R_C_b, R_C_b
REAL, DIMENSION(NCELL):: R_Si_b, R_Si_b, R_Si_b, R_Si_b, R_Si_b
REAL, DIMENSION(NCELL):: R_P_b, R_P_b, R_P_b, R_P_b, R_P_b
REAL, DIMENSION(NCELL):: R_CO2_b, R_CO2_b, R_CO2_b, R_CO2_b
REAL, DIMENSION(NCELL):: R_P2O5_b, R_MnO_b, R_MnO_b, R_MnO_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_FeO_b, R_FeO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_FeO_b, R_FeO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_C_b, R_C_b, R_C_b, R_C_b, R_C_b
REAL, DIMENSION(NCELL):: R_P_b, R_P_b, R_P_b, R_P_b, R_P_b
REAL, DIMENSION(NCELL):: R_SiO2_b, R_SiO2_b, R_SiO2_b, R_SiO2_b
REAL, DIMENSION(NCELL):: R_Si_b, R_Si_b, R_Si_b, R_Si_b, R_Si_b
REAL, DIMENSION(NCELL):: R_P_b, R_P_b, R_P_b, R_P_b, R_P_b
REAL, DIMENSION(NCELL):: R_CO2_b, R_CO2_b, R_CO2_b, R_CO2_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_FeO_b, R_FeO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_FeO_b, R_FeO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_C_b, R_C_b, R_C_b, R_C_b, R_C_b
REAL, DIMENSION(NCELL):: R_P_b, R_P_b, R_P_b, R_P_b, R_P_b
REAL, DIMENSION(NCELL):: R_SiO2_b, R_SiO2_b, R_SiO2_b, R_SiO2_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_FeO_b, R_FeO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_FeO_b, R_FeO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_C_b, R_C_b, R_C_b, R_C_b, R_C_b
REAL, DIMENSION(NCELL):: R_P_b, R_P_b, R_P_b, R_P_b, R_P_b
REAL, DIMENSION(NCELL):: R_SiO2_b, R_SiO2_b, R_SiO2_b, R_SiO2_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_FeO_b, R_FeO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_C_b, R_C_b, R_C_b, R_C_b, R_C_b
REAL, DIMENSION(NCELL):: R_P_b, R_P_b, R_P_b, R_P_b, R_P_b
REAL, DIMENSION(NCELL):: R_SiO2_b, R_SiO2_b, R_SiO2_b, R_SiO2_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_FeO_b, R_FeO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_C_b, R_C_b, R_C_b, R_C_b, R_C_b
REAL, DIMENSION(NCELL):: R_P_b, R_P_b, R_P_b, R_P_b, R_P_b
REAL, DIMENSION(NCELL):: R_SiO2_b, R_SiO2_b, R_SiO2_b, R_SiO2_b

--- Bubble volume, diameter and length of plateau border ---

--- Bubble volume ---
R_v(1)=65.416E-09
R_v(2)=130.833E-09
R_v(3)=261.667E-09
R_v(4)=523.333E-09
R_v(5)=1046.667E-09
R_v(6)=209.333E-08
R_v(7)=418.667E-08
R_v(8)=837.333E-08
R_v(9)=167.467E-07
R_v(10)=334.933E-07

--- Bubble diameter ---
R_d(1)=2.500E-03
R_d(2)=3.149E-03
R_d(3)=3.968E-03
R_d(4)=5.000E-03
R_d(5)=6.299E-03
R_d(6)=7.937E-03
R_d(7)=10.000E-03
R_d(8)=12.599E-03
R_d(9)=15.874E-03
R_d(10)=20.000E-03

--- Bubble break up, Coalescence model and population balance ---

DO nc=nsp(mat), nep(mat)
ip1=nc
ip2=nc+ncell
ip3=nc+ncell+ncell
IF(edm(ip2).LT.1.0e-06) THEN
edm(ip2)=1.0e-06
END IF
R_ld=(8.42e-05)/(edm(ip2)**0.25)
c---volume of each scalar in each cell

c---Scalar in gas phase

c---gas bubble
\[ R_{tv}(1) = \Phi_m\text{mscal}(1-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(2) = \Phi_m\text{mscal}(2-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(3) = \Phi_m\text{mscal}(3-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(4) = \Phi_m\text{mscal}(4-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(5) = \Phi_m\text{mscal}(5-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(6) = \Phi_m\text{mscal}(6-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(7) = \Phi_m\text{mscal}(7-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(8) = \Phi_m\text{mscal}(8-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(9) = \Phi_m\text{mscal}(9-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]
\[ R_{tv}(10) = \Phi_m\text{mscal}(10-1)\times ncell+nc)\times vfm(ip1)\times vol(nc) \]

c-----Scalar in foam phase

c-----bubble
\[ R_{tvf}(1) = \Phi_m\text{mscal}(24-1)\times ncell+nc) \]
\[ R_{tvf}(2) = \Phi_m\text{mscal}(25-1)\times ncell+nc) \]
\[ R_{tvf}(3) = \Phi_m\text{mscal}(26-1)\times ncell+nc) \]
\[ R_{tvf}(4) = \Phi_m\text{mscal}(27-1)\times ncell+nc) \]
\[ R_{tvf}(5) = \Phi_m\text{mscal}(28-1)\times ncell+nc) \]
\[ R_{tvf}(6) = \Phi_m\text{mscal}(29-1)\times ncell+nc) \]
\[ R_{tvf}(7) = \Phi_m\text{mscal}(30-1)\times ncell+nc) \]
\[ R_{tvf}(8) = \Phi_m\text{mscal}(31-1)\times ncell+nc) \]
\[ R_{tvf}(9) = \Phi_m\text{mscal}(32-1)\times ncell+nc) \]
\[ R_{tvf}(10) = \Phi_m\text{mscal}(33-1)\times ncell+nc) \]

c-----liquid in foam

c-----Number of gas bubble in each cell in gas phase
\[ R_{nb}(1) = R_{tv}(1)/R_v(1) \]
\[ R_{nb}(2) = R_{tv}(2)/R_v(2) \]
\[ R_{nb}(3) = R_{tv}(3)/R_v(3) \]
\[ R_{nb}(4) = R_{tv}(4)/R_v(4) \]
\[ R_{nb}(5) = R_{tv}(5)/R_v(5) \]
\[ R_{nb}(6) = R_{tv}(6)/R_v(6) \]
\[ R_{nb}(7) = R_{tv}(7)/R_v(7) \]
\[ R_{nb}(8) = R_{tv}(8)/R_v(8) \]
\[ R_{nb}(9) = R_{tv}(9)/R_v(9) \]
\[ R_{nb}(10) = R_{tv}(10)/R_v(10) \]

c-----Number of foam bubble in each cell in foam phase
\[ R_{nbf}(1) = R_{tvf}(1)/R_v(1) \]
\[ R_{nbf}(2) = R_{tvf}(2)/R_v(2) \]
\[ R_{nbf}(3) = R_{tvf}(3)/R_v(3) \]
\[ R_{nbf}(4) = R_{tvf}(4)/R_v(4) \]
\[ R_{nbf}(5) = R_{tvf}(5)/R_v(5) \]
\[ R_{nbf}(6) = R_{tvf}(6)/R_v(6) \]
\[ R_{nbf}(7) = R_{tvf}(7)/R_v(7) \]
\[ R_{nbf}(8) = R_{tvf}(8)/R_v(8) \]
\[ R_{nbf}(9) = R_{tvf}(9)/R_v(9) \]
\[ R_{nbf}(10) = R_{tvf}(10)/R_v(10) \]

c-----Initialization for Birth and death term for break up
\[ R_{DB}(1) = 0.0 \]
\[ R_{DB}(2) = 0.0 \]
\[ R_{DB}(3) = 0.0 \]
\[ R_{DB}(4) = 0.0 \]
\[ R_{DB}(5) = 0.0 \]
\[ R_{DB}(6) = 0.0 \]
\[ R_{DB}(7) = 0.0 \]
R_DB(8)=0.0
R_DB(9)=0.0
R_DB(10)=0.0
R_BB(1)=0.0
R_BB(2)=0.0
R_BB(3)=0.0
R_BB(4)=0.0
R_BB(5)=0.0
R_BB(6)=0.0
R_BB(7)=0.0
R_BB(8)=0.0
R_BB(9)=0.0
R_BB(10)=0.0

C-----Initialization for Birth and Death term for Coalescence in gas phase
R_DC(1)=0.0
R_DC(2)=0.0
R_DC(3)=0.0
R_DC(4)=0.0
R_DC(5)=0.0
R_DC(6)=0.0
R_DC(7)=0.0
R_DC(8)=0.0
R_DC(9)=0.0
R_DC(10)=0.0
R_BC(1)=0.0
R_BC(2)=0.0
R_BC(3)=0.0
R_BC(4)=0.0
R_BC(5)=0.0
R_BC(6)=0.0
R_BC(7)=0.0
R_BC(8)=0.0
R_BC(9)=0.0
R_BC(10)=0.0

C-----Initialization for Birth and Death term for Coalescence in foam phase
R_DCF(1)=0.0
R_DCF(2)=0.0
R_DCF(3)=0.0
R_DCF(4)=0.0
R_DCF(5)=0.0
R_DCF(6)=0.0
R_DCF(7)=0.0
R_DCF(8)=0.0
R_DCF(9)=0.0
R_DCF(10)=0.0
R_BCF(1)=0.0
R_BCF(2)=0.0
R_BCF(3)=0.0
R_BCF(4)=0.0
R_BCF(5)=0.0
R_BCF(6)=0.0
R_BCF(7)=0.0
R_BCF(8)=0.0
R_BCF(9)=0.0
R_BCF(10)=0.0

C----------------------------------------------------------------------------------------------------------------
c-----Bubble coalescence
  c-----Bubble Coalescence model by Prince and Blanch
  c-----Birth of bubble class i+1 due to coalescence of bubble class i to N-1

IF(vfm(ip1).LT.0.75) THEN
  DO i_i=1,9
    DO i_j=1,i_i
      R_ccarea(i_i,i_j)=((R_d(i_i)+R_d(i_j))**2.0)
      c-----Turbulent collision rate R_TCR
      R_TCR(i_i,i_j)=0.089*R_nb(i_i)*R_nb(i_j)*R_ccarea(i_i,i_j)*
                      ((edm(ip2))**0.333)*((R_d(i_i)**0.666+R_d(i_j)**0.666)**0.5)
      c-----Min number of bubble calculation
      R_min_nb(i_i,i_j)=min(R_nb(i_i),R_nb(i_j))
      c-----Total coalescence
      IF(R_TCR(i_i,i_j).GT.R_min_nb(i_i,i_j)) THEN
        R_TCR(i_i,i_j)=R_min_nb(i_i,i_j)
      END IF
      c-----Coalescence efficnecy,log(ho/hf=4)
      R_rbij(i_i,i_j)=(0.5)*(((1.0/R_d(i_i))+(1.0/R_d(i_j)))**(-1.0))
      R_tauij(i_i,i_j)=((1.0/edm(ip2))**0.333)*((R_rbij(i_i,i_j))**0.33)
      R_tij(i_i,i_j)=26151.6*(R_rbij(i_i,i_j)**3.0)
      R_colef(i_i,i_j)=EXP(-R_tij(i_i,i_j)/R_tauij(i_i,i_j))
      c-----Total coalescence rate due to turbulence, Buoyancy and laminar shear collision
      R_CR(i_i,i_j)=R_TCR(i_i,i_j)*R_colef(i_i,i_j)
      R_Xij(i_i,i_j)=(1.0)-((2.0)**(i_j-i_i))
    END DO
  END DO
END IF

R_vbc1(1)=0.0
R_vbc2(1)=0.0
R_vbc3(1)=0.0
R_vbc4(1)=0.0
R_vbc1(2)=0.0
R_vbc2(2)=0.0
R_vbc3(2)=0.0
R_vbc4(2)=0.0
R_vbc1(3)=0.0
R_vbc2(3)=0.0
R_vbc3(3)=0.0
R_vbc4(3)=0.0
R_vbc1(4)=0.0
R_vbc2(4)=0.0
R_vbc3(4)=0.0
R_vbc4(4)=0.0
R_vbc1(5)=0.0
R_vbc2(5)=0.0
R_vbc3(5)=0.0
R_vbc4(5)=0.0
R_vbc1(6)=0.0
R_vbc2(6)=0.0
c-----Seventh Scalar value update
R_vbc1(7)=0.0
R_vbc2(7)=0.0
R_vbc3(7)=0.0
R_vbc4(7)=0.0

c-----Eighth Scalar value update
R_vbc1(8)=0.0
R_vbc2(8)=0.0
R_vbc3(8)=0.0
R_vbc4(8)=0.0

c-----Ninth Scalar value update
R_vbc1(9)=0.0
R_vbc2(9)=0.0
R_vbc3(9)=0.0
R_vbc4(9)=0.0

c-----Tenth Scalar value update
R_vbc1(10)=0.0
R_vbc2(10)=0.0
R_vbc3(10)=0.0
R_vbc4(10)=0.0

c-----Death of I_j for the birth of I_i
R_vbc1(I_i)=R_Xij(I_i,I_j)*R_CR(I_i,I_j)*R_v(I_j)

c-----Death of I_i that goes to I_i+1
IF(I_i==I_j)
R_vbc2(I_i)=0.0
ELSE
R_vbc2(I_i)=(1.0-R_Xij(I_i,I_j))*R_CR(I_i,I_j)*R_v(I_i)
ENDIF

R_vbc3(I_i)=(1.0-R_Xij(I_i,I_j))*R_CR(I_i,I_j)*R_v(I_j)

c-----Total death of I_j
R_vbc4(I_j)=R_vbc1(I_i)+ R_vbc3(I_i)

c-----Number of bubble update
R_tv(1)=R_tv(1)-(R_vbc2(1)+R_vbc4(1))
R_tv(2)=R_tv(2)-(R_vbc2(2)+R_vbc4(2))
R_tv(3)=R_tv(3)-(R_vbc2(3)+R_vbc4(3))
R_tv(4)=R_tv(4)-(R_vbc2(4)+R_vbc4(4))
R_tv(5)=R_tv(5)-(R_vbc2(5)+R_vbc4(5))
R_tv(6)=R_tv(6)-(R_vbc2(6)+R_vbc4(6))
R_tv(7)=R_tv(7)-(R_vbc2(7)+R_vbc4(7))
R_tv(8)=R_tv(8)-(R_vbc2(8)+R_vbc4(8))
R_tv(9)=R_tv(9)-(R_vbc2(9)+R_vbc4(9))
R_tv(10)=R_tv(10)-(R_vbc2(10)+R_vbc4(10))

c-----Number of bubble update
R_nb(1)=R_tv(1)/R_v(1)
R_nb(2)=R_tv(2)/R_v(2)
R_nb(3)=R_tv(3)/R_v(3)
R_nb(4)=R_tv(4)/R_v(4)
R_nb(5)=R_tv(5)/R_v(5)
R_nb(6)=R_tv(6)/R_v(6)
R_nb(7)=R_tv(7)/R_v(7)
R_nb(8)=R_tv(8)/R_v(8)
R_nb(9)=R_tv(9)/R_v(9)
R_nb(10)=R_tv(10)/R_v(10)
R_DC(1) = R_DC(1) + R_vbc2(1) + R_vbc4(1)
R_DC(2) = R_DC(2) + R_vbc2(2) + R_vbc4(2)
R_DC(3) = R_DC(3) + R_vbc2(3) + R_vbc4(3)
R_DC(4) = R_DC(4) + R_vbc2(4) + R_vbc4(4)
R_DC(5) = R_DC(5) + R_vbc2(5) + R_vbc4(5)
R_DC(6) = R_DC(6) + R_vbc2(6) + R_vbc4(6)
R_DC(7) = R_DC(7) + R_vbc2(7) + R_vbc4(7)
R_DC(8) = R_DC(8) + R_vbc2(8) + R_vbc4(8)
R_DC(9) = R_DC(9) + R_vbc2(9) + R_vbc4(9)
R_DC(10) = R_DC(10) + R_vbc2(10) + R_vbc4(10)

R_BC(1) = R_BC(1) + R_vbc1(1)
R_BC(2) = R_BC(2) + R_vbc1(2) + R_vbc2(1) + R_vbc3(1)
R_BC(3) = R_BC(3) + R_vbc1(3) + R_vbc2(2) + R_vbc3(2)
R_BC(4) = R_BC(4) + R_vbc1(4) + R_vbc2(3) + R_vbc3(3)
R_BC(6) = R_BC(6) + R_vbc1(6) + R_vbc2(5) + R_vbc3(5)
R_BC(7) = R_BC(7) + R_vbc1(7) + R_vbc2(6) + R_vbc3(6)
R_BC(8) = R_BC(8) + R_vbc1(8) + R_vbc2(7) + R_vbc3(7)
R_BC(9) = R_BC(9) + R_vbc1(9) + R_vbc2(8) + R_vbc3(8)
R_BC(10) = R_BC(10) + R_vbc2(9) + R_vbc3(9)

END DO

END DO

R_BC(1) + R_vbc1(1)
R_BC(2) + R_vbc1(2) + R_vbc2(1) + R_vbc3(1)
R_BC(3) + R_vbc1(3) + R_vbc2(2) + R_vbc3(2)
R_BC(4) + R_vbc1(4) + R_vbc2(3) + R_vbc3(3)
R_BC(5) + R_vbc1(5) + R_vbc2(4) + R_vbc3(4)
R_BC(6) + R_vbc1(6) + R_vbc2(5) + R_vbc3(5)
R_BC(7) + R_vbc1(7) + R_vbc2(6) + R_vbc3(6)
R_BC(8) + R_vbc1(8) + R_vbc2(7) + R_vbc3(7)
R_BC(9) + R_vbc1(9) + R_vbc2(8) + R_vbc3(8)
R_BC(10) + R_vbc2(9) + R_vbc3(9)

DO I_i=1,9
   DO I_k=I_i+1,10
      c-----Coefficient of surface area increase
      R_dr(I_k) = R_d(l_i)/R_d(l_k)
      R_Cf(I_k) = ((R_dr(l_i) ** 2.0) - 1.0) + ((1.0 - (R_dr(l_i)) ** 3.0) ** 0.666)
      c-----Dimensionless size of eddy
      R_zita(I_k) = (11.4 / R_d(l_k)) * ((edm(ip2) * vimm(ip2)) ** (-0.25))
      c-----Critical dimensionless energy for break up
      R_chaiC(I_k) = (6.21e-05 * R_Cf(I_k)) / ((edm(ip2) ** 0.666) * (R_d(l_k) ** 1.66) * (R_zita(l_k) ** 3.66))
      c-----Probability of bubble size k colliding with eddy lamda breaking up into size i
      R_pb(I_k,l_i) = EXP(-R_chaiC(l_i))
      c-----Collision frequency of bubble class k with pi=3.14 eddy size lamda
      c----R_nde*R_ald=8.22e14**vfm(ip2)*(edm(ip2)**2)
      R_cfq(I_k) = 8.22e14 * ((R_d(l_i) + R_id) ** 2.0) * vfm(ip2) * (edm(ip2) ** 2) * R_nb(l_i)
      IF(R_cfq(l_i).GT.R_nb(l_i)) THEN
         R_cfq(l_i) = R_nb(l_i)
      END IF
      c-----Break up rate of bubble class k into class i
      IF (R_pb(l_k,l_i).GT.1.0) THEN
         R_pb(l_k,l_i) = 1.0
      END IF
      R_BR(l_k,l_i) = R_cfq(l_i) * R_pb(l_k,l_i)
      IF (R_id.GE.R_d(l_k)) THEN
         R_BR(l_k,l_i) = 0.0
      END IF
   END DO
END DO

C-----Scalar Value update for the birth of each bubble class due to death of other class
C----------------------------------------------------------------------------------------------------------------
R_vbb(1)=0.0
R_vbb(2)=0.0
R_vbb(3)=0.0
R_vbb(4)=0.0
R_vbb(5)=0.0
R_vbb(6)=0.0
R_vbb(7)=0.0
R_vbb(8)=0.0
R_vbb(9)=0.0
R_vbb(10)=0.0
R_vbb(l,i)=R_BR(l,k,l,i)*R_v(l,i)

--- Scalar Value update for the birth of each bubble class due to death of other class

R_Xik(l_k,l,i)=(2.0)**(1.0+l_i-l_k)

--- First Scalar value update
R_vbd1(1)=0.0
R_vbd(1)=0.0

--- Second Scalar value update
R_vbd1(2)=0.0
R_vbd(2)=0.0

--- Third Scalar value update
R_vbd1(3)=0.0
R_vbd(3)=0.0

--- Fourth Scalar value update
R_vbd1(4)=0.0
R_vbd(4)=0.0

--- Fifth Scalar value update
R_vbd1(5)=0.0
R_vbd(5)=0.0

--- Sixth Scalar value update
R_vbd1(6)=0.0
R_vbd(6)=0.0

--- Seventh Scalar value update
R_vbd1(7)=0.0
R_vbd(7)=0.0

--- Eighth Scalar value update
R_vbd1(8)=0.0
R_vbd(8)=0.0

--- Ninth Scalar value update
R_vbd1(9)=0.0
R_vbd(9)=0.0

--- Tenth Scalar value update
R_vbd1(10)=0.0
R_vbd(10)=0.0

--- Scalar of birth
R_vbd1(l_k)=R_BR(l_k,l,i)*R_v(l_i)
R_vbd(l_k)=R_Xik(l_k,l,i)*R_BR(l_k,l,i)*((R_v(l_k)-R_v(l_i))

--- Scalar Value update for the birth of each bubble class due to death of other class

R_tv(1)=R_tv(1)-(R_vbd1(1)+R_vbd(1))
R_tv(2)=R_tv(2)-(R_vbd1(2)+R_vbd(2))
R_tv(3)=R_tv(3)-(R_vbd1(3)+R_vbd(3))
R_tv(4)=R_tv(4)-(R_vbd1(4)+R_vbd(4))
R_tv(5)=R_tv(5)-(R_vbd1(5)+R_vbd(5))
R_tv(6)=R_tv(6)-(R_vbd1(6)+R_vbd(6))
R_tv(7)=R_tv(7)-(R_vbd1(7)+R_vbd(7))
R_tv(8) = R_tv(8) - (R_vbd1(8) + R_vbd(8))
R_tv(9) = R_tv(9) - (R_vbd1(9) + R_vbd(9))
R_tv(10) = R_tv(10) - (R_vbd1(10) + R_vbd(10))

--- Number of bubble update
R_nb(1) = R_tv(1)/R_v(1)
R_nb(2) = R_tv(2)/R_v(2)
R_nb(3) = R_tv(3)/R_v(3)
R_nb(4) = R_tv(4)/R_v(4)
R_nb(5) = R_tv(5)/R_v(5)
R_nb(6) = R_tv(6)/R_v(6)
R_nb(7) = R_tv(7)/R_v(7)
R_nb(8) = R_tv(8)/R_v(8)
R_nb(9) = R_tv(9)/R_v(9)
R_nb(10) = R_tv(10)/R_v(10)

--- Birth
R_BB(1) = R_BB(1) + R_vbb(1) + R_vbd(2)
R_BB(2) = R_BB(2) + R_vbb(2) + R_vbd(3)
R_BB(3) = R_BB(3) + R_vbb(3) + R_vbd(4)
R_BB(4) = R_BB(4) + R_vbb(4) + R_vbd(5)
R_BB(5) = R_BB(5) + R_vbb(5) + R_vbd(6)
R_BB(6) = R_BB(6) + R_vbb(6) + R_vbd(7)
R_BB(7) = R_BB(7) + R_vbb(7) + R_vbd(8)
R_BB(8) = R_BB(8) + R_vbb(8) + R_vbd(9)
R_BB(9) = R_BB(9) + R_vbb(9) + R_vbd(10)
R_BB(10) = R_BB(10) + R_vbb(10)

--- Death
R_DB(1) = R_DB(1) + R_vbd1(1) + R_vbd(1)
R_DB(2) = R_DB(2) + R_vbd1(2) + R_vbd(2)
R_DB(3) = R_DB(3) + R_vbd1(3) + R_vbd(3)
R_DB(4) = R_DB(4) + R_vbd1(4) + R_vbd(4)
R_DB(5) = R_DB(5) + R_vbd1(5) + R_vbd(5)
R_DB(6) = R_DB(6) + R_vbd1(6) + R_vbd(6)
R_DB(7) = R_DB(7) + R_vbd1(7) + R_vbd(7)
R_DB(8) = R_DB(8) + R_vbd1(8) + R_vbd(8)
R_DB(9) = R_DB(9) + R_vbd1(9) + R_vbd(9)
R_DB(10) = R_DB(10) + R_vbd1(10) + R_vbd(10)

END DO
END DO
END IF

--- Transformation of gas and liquid into foam
R_g(nc) = 2.0*Phi_mscal((35-1)*ncell+nc)*vfm(ip3)*vol(nc)*denm(ip3)
R_lq_av(nc) = 2.0*Phi_mscal((34-1)*ncell+nc)*vfm(ip3)*vol(nc)*denm(ip3)
R_tDgbt(nc) = 1.0e-35
R_lqt(nc) = 1.0e-35

--- Transformation of gas bubble to foam bubble
IF(vfm(ip1).GE.0.75.AND.vfm(ip2).GE.0.05) THEN
R_tDgbt(nc) = 0.999*vfm(ip1)*vol(nc)*denm(ip1)

--- Total liquid transformation
R_lqt(nc) = 0.0199*vfm(ip2)*vol(nc)*denm(ip2)
R_C_final(nc) = 1.0e-30
R_Fe_final(nc) = 1.0e-30
R_Si_final(nc) = 1.0e-30
R_Mn_final(nc) = 1.0e-30
R_P_final(nc) = 1.0e-30

END IF
c----------------------------------------------------------------------------------------------------------------
c-----Bubble coalescence in foam
c-----Film rupture inside foam
c----------------------------------------------------------------------------------------------------------------
IF(vfm(ip3).GT.vfrmin)THEN
  DO l_m=1,9
    DO l_i=1,l_m
      c-----Velocity of Drainage, R_cv=1,R_vd(I_i)=1.97e6*R_ap(I_i)
      c----------------------------------------------------------------------------------------------------------------
      c-----Probability of sharing the same film of bubble i and m
      R_FS(I_i,I_m)=R_nbf(I_i)/(R_nbf(1)+R_nbf(2)+R_nbf(3)+R_nbf(4)+R_nbf(5)+R_nbf(6)+R_nbf(7)+R_nbf(8)+R_nbf(9)+R_nbf(10))
      R_min_nbf(I_i,I_m)=min(R_nbf(I_i),R_nbf(I_m))
      c-----Coalescence rate of film
      R_crf(I_i,I_m)=5.78e05*(R_d(I_i)**2)*R_FS(I_i,I_m)
      IF(R_crf(I_i,I_m).GT.R_min_nbf(I_i,I_m))THEN
        R_crf(I_i,I_m)=R_min_nbf(I_i,I_m)
      END IF
      R_Xijf(I_i,I_m)=(1.0)-((2.0)**(I_m-I_i))
    END DO
  END DO
END IF
R_Xijf(I_i,I_m)=(1.0)-((2.0)**(I_m-I_i))

c----------------------------------------------------------------------------------------------------------------
c-----Scalar Value update for each bubble class
  c-----First Scalar value update
  R_vbcf1(1)=0.0
  R_vbcf2(1)=0.0
  R_vbcf3(1)=0.0
  R_vbcf4(1)=0.0
  c-----Second Scalar value update
  R_vbcf1(2)=0.0
  R_vbcf2(2)=0.0
  R_vbcf3(2)=0.0
  R_vbcf4(2)=0.0
  c-----Third Scalar value update
  R_vbcf1(3)=0.0
  R_vbcf2(3)=0.0
  R_vbcf3(3)=0.0
  R_vbcf4(3)=0.0
  c-----Fourth Scalar value update
  R_vbcf1(4)=0.0
  R_vbcf2(4)=0.0
  R_vbcf3(4)=0.0
  R_vbcf4(4)=0.0
  c-----Fifth Scalar value update
  R_vbcf1(5)=0.0
  R_vbcf2(5)=0.0
  R_vbcf3(5)=0.0
  R_vbcf4(5)=0.0
  c-----Sixth Scalar value update
  R_vbcf1(6)=0.0
  R_vbcf2(6)=0.0
  R_vbcf3(6)=0.0
  R_vbcf4(6)=0.0
  c-----Seventh Scalar value update
  R_vbcf1(7)=0.0
  R_vbcf2(7)=0.0
  R_vbcf3(7)=0.0
  R_vbcf4(7)=0.0
c-----Eighth Scalar value update
R_vbcf1(8)=0.0
R_vbcf2(8)=0.0
R_vbcf3(8)=0.0
R_vbcf4(8)=0.0
c-----Ninth Scalar value update
R_vbcf1(9)=0.0
R_vbcf2(9)=0.0
R_vbcf3(9)=0.0
R_vbcf4(9)=0.0
c-----Tenth Scalar value update
R_vbcf1(10)=0.0
R_vbcf2(10)=0.0
R_vbcf3(10)=0.0
R_vbcf4(10)=0.0
c-----Death of I_m for the birth of I_i
R_vbcf1(I_i)=R_Xijf(I_i,I_m)*R_crf(I_i,I_m)*R_v(I_m)
c-----Death of I_i that goes to I_i+1
IF (I_i==I_m) THEN
R_vbcf2(I_i)=0.0
ELSE
R_vbcf2(I_i)=(1.0-R_Xijf(I_i,I_m))*R_crf(I_i,I_m)*R_v(I_i)
END IF
c-----Death of I_m
R_vbcf3(I_i)=(1.0-R_Xijf(I_i,I_m))*R_crf(I_i,I_m)*R_v(I_m)
c-----Total death of I_m
R_vbcf4(I_m)=R_vbcf1(I_i)+R_vbcf3(I_i)
c----------------------------------------------------------------------------------------------------------------
R_vbctf(1)=R_vbcf2(1)+R_vbcf4(1)
R_vbctf(2)=R_vbcf2(2)+R_vbcf4(2)
R_vbctf(3)=R_vbcf2(3)+R_vbcf4(3)
R_vbctf(4)=R_vbcf2(4)+R_vbcf4(4)
R_vbctf(5)=R_vbcf2(5)+R_vbcf4(5)
R_vbctf(6)=R_vbcf2(6)+R_vbcf4(6)
R_vbctf(7)=R_vbcf2(7)+R_vbcf4(7)
R_vbctf(8)=R_vbcf2(8)+R_vbcf4(8)
R_vbctf(9)=R_vbcf2(9)+R_vbcf4(9)
R_vbctf(10)=R_vbcf2(10)+R_vbcf4(10)
c----------------------------------------------------------------------------------------------------------------
IF (R_vbctf(I_i).GT.R_tvf(I_i)) THEN
R_vbctf(I_i)=R_tvf(I_i)
END IF
c----------------------------------------------------------------------------------------------------------------
IF (R_vbctf(I_m).GT.R_tvf(I_m)) THEN
R_vbctf(I_m)=R_tvf(I_m)
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Scalar Value update for the birth of each bubble class due to death of other class
R_tvf(1)=R_tvf(1)-R_vbctf(I_i)
R_tvf(2)=R_tvf(2)-R_vbctf(I_i)
R_tvf(3)=R_tvf(3)-R_vbctf(I_i)
R_tvf(4)=R_tvf(4)-R_vbctf(I_i)
R_tvf(5)=R_tvf(5)-R_vbctf(I_i)
R_tvf(6)=R_tvf(6)-R_vbctf(I_i)
R_tvf(7)=R_tvf(7)-R_vbctf(I_i)
R_tvf(8)=R_tvf(8)-R_vbctf(I_i)
R_tvf(9)=R_tvf(9)-R_vbctf(I_i)
R_tvf(10)=R_tvf(10)-R_vbctf(I_i)
\[ R_{tvf}(8) = R_{tvf}(8) - R_{vbcf}(8) \]
\[ R_{tvf}(9) = R_{tvf}(9) - R_{vbcf}(9) \]
\[ R_{tvf}(10) = R_{tvf}(10) - R_{vbcf}(10) \]

\[ R_{nbf}(1) = \frac{R_{tvf}(1)}{R_v(1)} \]
\[ R_{nbf}(2) = \frac{R_{tvf}(2)}{R_v(2)} \]
\[ R_{nbf}(3) = \frac{R_{tvf}(3)}{R_v(3)} \]
\[ R_{nbf}(4) = \frac{R_{tvf}(4)}{R_v(4)} \]
\[ R_{nbf}(5) = \frac{R_{tvf}(5)}{R_v(5)} \]
\[ R_{nbf}(6) = \frac{R_{tvf}(6)}{R_v(6)} \]
\[ R_{nbf}(7) = \frac{R_{tvf}(7)}{R_v(7)} \]
\[ R_{nbf}(8) = \frac{R_{tvf}(8)}{R_v(8)} \]
\[ R_{nbf}(9) = \frac{R_{tvf}(9)}{R_v(9)} \]
\[ R_{nbf}(10) = \frac{R_{tvf}(10)}{R_v(10)} \]

\[ R_{DCF}(1) = R_{DCF}(1) + R_{vbcf2}(1) + R_{vbcf4}(1) \]
\[ R_{DCF}(2) = R_{DCF}(2) + R_{vbcf2}(2) + R_{vbcf4}(2) \]
\[ R_{DCF}(3) = R_{DCF}(3) + R_{vbcf2}(3) + R_{vbcf4}(3) \]
\[ R_{DCF}(4) = R_{DCF}(4) + R_{vbcf2}(4) + R_{vbcf4}(4) \]
\[ R_{DCF}(5) = R_{DCF}(5) + R_{vbcf2}(5) + R_{vbcf4}(5) \]
\[ R_{DCF}(6) = R_{DCF}(6) + R_{vbcf2}(6) + R_{vbcf4}(6) \]
\[ R_{DCF}(7) = R_{DCF}(7) + R_{vbcf2}(7) + R_{vbcf4}(7) \]
\[ R_{DCF}(8) = R_{DCF}(8) + R_{vbcf2}(8) + R_{vbcf4}(8) \]
\[ R_{DCF}(9) = R_{DCF}(9) + R_{vbcf2}(9) + R_{vbcf4}(9) \]
\[ R_{DCF}(10) = R_{DCF}(10) + R_{vbcf2}(10) + R_{vbcf4}(10) \]

\[ R_{BCF}(1) = R_{BCF}(1) + R_{vbcf1}(1) \]
\[ R_{BCF}(2) = R_{BCF}(2) + R_{vbcf1}(2) + R_{vbcf2}(1) + R_{vbcf3}(1) \]
\[ R_{BCF}(3) = R_{BCF}(3) + R_{vbcf1}(3) + R_{vbcf2}(2) + R_{vbcf3}(2) \]
\[ R_{BCF}(4) = R_{BCF}(4) + R_{vbcf1}(4) + R_{vbcf2}(3) + R_{vbcf3}(3) \]
\[ R_{BCF}(5) = R_{BCF}(5) + R_{vbcf1}(5) + R_{vbcf2}(4) + R_{vbcf3}(4) \]
\[ R_{BCF}(6) = R_{BCF}(6) + R_{vbcf1}(6) + R_{vbcf2}(5) + R_{vbcf3}(5) \]
\[ R_{BCF}(7) = R_{BCF}(7) + R_{vbcf1}(7) + R_{vbcf2}(6) + R_{vbcf3}(6) \]
\[ R_{BCF}(8) = R_{BCF}(8) + R_{vbcf1}(8) + R_{vbcf2}(7) + R_{vbcf3}(7) \]
\[ R_{BCF}(9) = R_{BCF}(9) + R_{vbcf1}(9) + R_{vbcf2}(8) + R_{vbcf3}(8) \]
\[ R_{BCF}(10) = R_{BCF}(10) + R_{vbcf2}(9) + R_{vbcf3}(9) \]

END DO
END DO
END IF

\[ R_{kgh}(nc) = \text{Phi}_mscal((35-1) \cdot ncell + nc) \]
\[ R_{foam}(nc) = vfm(ip3) \cdot \text{vol}(nc) \cdot \text{denm}(ip3) \]
\[ R_{g(nc)} = 2.0 \cdot \text{Phi}_mscal((35-1) \cdot ncell + nc) \cdot vfm(ip3) \cdot \text{vol}(nc) \cdot \text{denm}(ip3) \]
\[ R_{lq_av(nc)} = 2.0 \cdot \text{Phi}_mscal((34-1) \cdot ncell + nc) \cdot vfm(ip3) \cdot \text{vol}(nc) \cdot \text{denm}(ip3) \]

\[ R_{lq_f(nc)} = 0.0283 \cdot vfm(ip3) \cdot \text{vol}(nc) \cdot \text{denm}(ip3) \]
IF[R_{lq_f(nc)} < R_{lq_av(nc)}] THEN
R_lq_f(nc)=R_lq_av(nc)
END IF
R_tdgf(nc)=0.699*vfm(ip3)*vol(nc)*denm(ip3)
R_g_av(nc)=R_g(nc)
IF(R_tdgf(nc).GT.R_g_av(nc))THEN
  R_tdgf(nc)=R_g_av(nc)
END IF
R_tfg(nc)=R_tDgbt(nc)-R_tdgf(nc)
R_tfl(nc)=R_lqt(nc)-R_lq_f(nc)
R_tfoam(nc)=R_foam(nc)+R_tfg(nc)+R_tfl(nc)
IF(R_tfoam(nc).GT.0.0)THEN
  R_gf(nc)=0.5*(R_g(nc)+R_tfg(nc))/R_tfoam(nc)
  IF(R_gf(nc).GT.0.45)THEN
    R_gf(nc)=0.45
  END IF
  R_S(23,nc)=(0.5-R_gf(nc))-Phi_mscal((34-1)*ncell+nc)
  R_S(24,nc)=R_gf(nc)-Phi_mscal((35-1)*ncell+nc)
END IF
ELSE
  R_lq_f(nc)=0.0
  R_tdgf(nc)=0.0
  R_gf(nc)=0.45
END IF
c-----foam and liquid for mph
R_fm_lq(nc)=R_lq_f(nc)
R_lq_fm(nc)=R_lqt(nc)
c-----liquid and gas
c-----Foam and gas for mph
R_fm_g(nc)=R_tdgf(nc)
R_g_fm(nc)=R_tDgbt(nc)
R_gfr(nc)=R_gf(nc)
c----------------------------------------------------------------------------------------------------------------
R_fm_lq_com(nc)=R_fm_lq(nc)
R_lq_fm_com(nc)=R_lq_fm(nc)
R_fm_g_com(nc)=R_fm_g(nc)
R_g_fm_com(nc)=R_g_fm(nc)
R_gfr_com(nc)=R_gfr(nc)
c----------------------------------------------------------------------------------------------------------------
R_t=TIME
c----------------------------------------------------------------------------------------------------------------
IF(vfm(ip2).GE.vfrmin)THEN
c------Variable description
R_Fe_b(nc)=Phi_mscal((14-1)*ncell+nc)
R_C_b(nc)=Phi_mscal((15-1)*ncell+nc)
R_Si_b(nc)=Phi_mscal((16-1)*ncell+nc)
R_Mn_b(nc)=Phi_mscal((17-1)*ncell+nc)
R_P_b(nc)=Phi_mscal((18-1)*ncell+nc)
R_Fe_b1(nc)=R_Fe_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_C_b1(nc)=R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_Si_b1(nc)=R_Si_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_Mn_b1(nc)=R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_P_b1(nc)=R_P_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_FeO_b(nc)=Phi_mscal((19-1)*ncell+nc)
R_SiO2_b(nc)=Phi_mscal((20-1)*ncell+nc)
R_P2O5_b(nc)=Phi_mscal((21-1)*ncell+nc)
\[ R_{\text{MnO}_b}(\text{nc}) = \Phi_{\text{mscal}}((22-1)\times n_{\text{cell}} + \text{nc}) \]
\[ R_S_b(\text{nc}) = \Phi_{\text{mscal}}((23-1)\times n_{\text{cell}} + \text{nc}) \]
\[ R_{\text{FeO}_b1}(\text{nc}) = R_{\text{FeO}_b}(\text{nc}) \times v_{\text{fm}}(ip2) \times \text{vol}(\text{nc}) \times \text{denm}(ip2) \]
\[ R_{\text{SiO}_2_b1}(\text{nc}) = R_{\text{SiO}_2_b}(\text{nc}) \times v_{\text{fm}}(ip2) \times \text{vol}(\text{nc}) \times \text{denm}(ip2) \]
\[ R_{\text{P}_2\text{O}_5_b1}(\text{nc}) = R_{\text{P}_2\text{O}_5_b}(\text{nc}) \times v_{\text{fm}}(ip2) \times \text{vol}(\text{nc}) \times \text{denm}(ip2) \]
\[ R_{\text{MnO}_b1}(\text{nc}) = R_{\text{MnO}_b}(\text{nc}) \times v_{\text{fm}}(ip2) \times \text{vol}(\text{nc}) \times \text{denm}(ip2) \]

--- Reacted element masses initialization

\[ R_{L_{av}}C(\text{nc}) = 1.0 \times 10^{-30} \]
\[ R_{L_{av}}Fe(\text{nc}) = 1.0 \times 10^{-30} \]
\[ R_{L_{av}}P(\text{nc}) = 1.0 \times 10^{-30} \]
\[ R_{L_{av}}Si(\text{nc}) = 1.0 \times 10^{-30} \]
\[ R_{L_{av}}Mn(\text{nc}) = 1.0 \times 10^{-30} \]
\[ R_{L_{av}}FeO(\text{nc}) = 1.0 \times 10^{-30} \]
\[ R_{L_{av}}MnO(\text{nc}) = 1.0 \times 10^{-30} \]
\[ R_{L_{av}}SiO_2(\text{nc}) = 1.0 \times 10^{-30} \]
\[ R_{L_{av}}P_2O_5(\text{nc}) = 1.0 \times 10^{-30} \]

--- Amount of silicon and oxygen for reaction in gas and liquid

\[ R_{\text{Si}}_{Fickrate}(\text{nc}) = (0.00407) \times (R_{\text{Si}_b}(\text{nc}) - 0.00001) \times v_{\text{fm}}(ip2) \times \text{vol}(\text{nc}) \times \text{denm}(ip2) \]

IF (\( R_{\text{Si}}_{Fickrate}(\text{nc}) \leq 1.0 \times 10^{-30} \)) THEN
\[ R_{\text{Si}}_{Fickrate}(\text{nc}) = 1.0 \times 10^{-30} \]
END IF

\[ R_{O_2\_av\_g}(\text{nc}) = 2.0 \times \Phi_{\text{mscal}}((11-1)\times n_{\text{cell}} + \text{nc}) \times v_{\text{fm}}(ip1) \times \text{vol}(\text{nc}) \times \text{denm}(ip1) \]

--- Chemical reaction between Silicon and Oxygen

\[ R_{\text{Si}}_{av\_l}(\text{nc}) = R_{\text{Si}_b}(\text{nc}) \times v_{\text{fm}}(ip2) \times \text{vol}(\text{nc}) \times \text{denm}(ip2) \]
\[ R_{\text{Si}}_{req\_O_2} = R_{O_2\_av\_g}(\text{nc}) \times (0.875) \]

IF (\( R_{\text{Si}}_{req\_O_2} > R_{\text{Si}}_{av\_l}(\text{nc}) \)) THEN
\[ R_{\text{Si}}_{used\_O_2}(\text{nc}) = R_{\text{Si}}_{av\_l}(\text{nc}) \]
ELSE
\[ R_{\text{Si}}_{used\_O_2}(\text{nc}) = R_{\text{Si}}_{req\_O_2} \]
END IF

--- Amount of carbon and oxygen for reaction in gas and liquid

\[ R_{\text{C}}_{Fickrate}(\text{nc}) = (0.00164) \times (R_{\text{C}_b}(\text{nc}) - 0.000703) \times v_{\text{fm}}(ip2) \times \text{vol}(\text{nc}) \times \text{denm}(ip2) \]

IF (\( R_{\text{C}}_{Fickrate}(\text{nc}) \leq 1.0 \times 10^{-30} \)) THEN
\[ R_{\text{C}}_{Fickrate}(\text{nc}) = 1.0 \times 10^{-30} \]
END IF

--- Chemical reaction between Carbon and Oxygen

\[ R_{\text{C}}_{av\_l}(\text{nc}) = R_{\text{C}_b}(\text{nc}) \times v_{\text{fm}}(ip2) \times \text{vol}(\text{nc}) \times \text{denm}(ip2) \]
\[ R_{\text{C}}_{req\_O_2} = R_{O_2\_av\_g}(\text{nc}) \times (0.75) \]

IF (\( R_{\text{C}}_{req\_O_2} \gt R_{\text{C}}_{av\_l}(\text{nc}) \)) THEN
\[ R_{\text{C}}_{used\_O_2}(\text{nc}) = R_{\text{C}}_{av\_l}(\text{nc}) \]
ELSE
\[ R_{\text{C}}_{used\_O_2}(\text{nc}) = R_{\text{C}}_{req\_O_2} \]
END IF
IF (R_C_req_O2.GT.R_C_av_l(nc)) THEN
R_C_used_O2(nc)=R_C_av_l(nc)
ELSE
R_C_used_O2(nc)=R_C_req_O2
END IF

C-----Post combustion of CO to CO2

IF (TIME.GE.0.3e+03) THEN
R_CO_used_O2(nc)=(1.0e-20)
ELSE
R_CO_used_O2(nc)=(1.33*(100-(0.333*TIME)))*R_C_used_O2(nc)
END IF

C-----Chemical reaction between gas and liquid
C-----Amount of Manganese and oxygen for reaction in gas and liquid

IF (R_FeO_b(nc).LE.1.0e-30) THEN
R_FeO_b(nc)=1.0e-30
END IF
R_Mn_eq=(R_MnO_b(nc))/((R_FeO_b(nc))*11.427)
R_Mn_Fickrate(nc)=(0.021364)*(R_Mn_b(nc)-R_Mn_eq)*(vfm(ip2)*vol(nc)*denm(ip2))
END IF
R_O2_av_g(nc)=R_O2_av_g(nc)-(1.33*R_C_used_O2(nc))-(0.57*R_CO_used_O2(nc))
IF (R_O2_av_g(nc).LE.1.0e-30) THEN
R_O2_av_g(nc)=1.0e-30
END IF

C-----Chemical reaction between Manganese and Oxygen

R_Mn_av_l(nc)=R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_Mn_req_O2=R_O2_av_g(nc)*(3.4375)
IF (R_Mn_req_O2.GT.R_Mn_av_l(nc)) THEN
R_Mn_used_O2(nc)=R_Mn_av_l(nc)
ELSE
R_Mn_used_O2(nc)=R_Mn_req_O2
END IF

C-----Chemical reaction between gas and liquid
C-----Amount of Phosphorous and oxygen for reaction in gas and liquid

R_P_eq_1=(2.5*log10(R_FeO_b(nc)))+(0.5*log10(R_P2O5_b(nc)))-7.36
R_P_eq_2=10.0**(R_P_eq_1)
IF (R_P_eq_2.LE.0.02) THEN
R_P_eq_2=0.02
END IF
R_P_eq=(0.437*R_P2O5_b(nc))/(R_P_eq_2)
IF (R_P_eq.LE.0.00018) THEN
R_P_eq=0.00018
END IF
R_P_Fickrate(nc)=(0.047101)*(R_P_b(nc)-R_P_eq)*vfm(ip2)*vol(nc)*denm(ip2)
END IF
\[ R_{O2\text{-av}\_g(nc)} = R_{O2\_av\_g(nc)} - (0.29 \times R_{Mn\_used\_O2(nc)}) \]

\[ \text{IF} (R_{O2\_av\_g(nc)} \leq 1.0e^{-30}) \text{THEN} \]
\[ R_{O2\_av\_g(nc)} = 1.0e^{-30} \]
\[ \text{END IF} \]

\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ \text{c-----Chemical reaction between Phosphorous and Oxygen} \]
\[ \text{c----------------------------------------------------------------------------------------------------------------} \]

\[ R_{P\_av\_l(nc)} = R_{P\_b(nc)} \times \text{vfm(ip2)} \times \text{vol(ip2)} \times \text{denm(ip2)} \]

\[ R_{P\_req\_O2} = R_{O2\_av\_g(nc)} \times (0.775) \]

\[ \text{IF} (R_{P\_req\_O2} \gt R_{P\_av\_l(nc)}) \text{THEN} \]
\[ R_{P\_used\_O2(nc)} = R_{P\_av\_l(nc)} \]
\[ \text{ELSE} \]
\[ R_{P\_used\_O2(nc)} = R_{P\_req\_O2} \]
\[ \text{END IF} \]

\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ \text{c-----Chemical reaction between gas and liquid} \]
\[ \text{c-----Amount of Iron and oxygen for reaction in gas and liquid} \]
\[ \text{c----------------------------------------------------------------------------------------------------------------} \]

\[ R_{O2\_av\_g(nc)} = R_{O2\_av\_g(nc)} - (1.29 \times R_{P\_used\_O2(nc)}) \]

\[ \text{IF} (R_{O2\_av\_g(nc)} \leq 1.0e^{-30}) \text{THEN} \]
\[ R_{O2\_av\_g(nc)} = 1.0e^{-30} \]
\[ \text{END IF} \]

\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ \text{R_{Fe\_Fickrate(nc)}} = (R_{O2\_av\_g(nc)} - R_{Mn\_used\_O2(nc)} - R_{P\_used\_O2(nc)} - R_{C\_used\_O2(nc)} - R_{Si\_used\_O2(nc)}) \times 112/32 \]

\[ \text{IF} (R_{Fe\_Fickrate(nc)} \leq 1.0e^{-30}) \text{THEN} \]
\[ R_{Fe\_Fickrate(nc)} = 1.0e^{-30} \]
\[ \text{END IF} \]

\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ \text{c-----Chemical reaction between Iron and Oxygen} \]
\[ \text{c----------------------------------------------------------------------------------------------------------------} \]

\[ R_{Fe\_av\_l(nc)} = R_{Fe\_b(nc)} \times \text{vfm(ip2)} \times \text{vol(nc)} \times \text{denm(ip2)} \]

\[ R_{Fe\_req\_O2} = R_{O2\_av\_g(nc)} \times (3.50) \]

\[ \text{IF} (R_{Fe\_req\_O2} \gt R_{Fe\_av\_l(nc)}) \text{THEN} \]
\[ R_{Fe\_used\_O2(nc)} = R_{Fe\_av\_l(nc)} \]
\[ \text{ELSE} \]
\[ R_{Fe\_used\_O2(nc)} = R_{Fe\_req\_O2} \]
\[ \text{END IF} \]

\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ \text{c-----Chemical reaction between Silicon and P2O5} \]
\[ \text{c----------------------------------------------------------------------------------------------------------------} \]

\[ R_{Si\_av\_l(nc)} = R_{Si\_av\_l(nc)} - R_{Si\_used\_O2(nc)} \]

\[ \text{IF} (R_{Si\_av\_l(nc)} \leq 1.0e^{-30}) \text{THEN} \]
\[ R_{Si\_av\_l(nc)} = 1.0e^{-30} \]
\[ \text{END IF} \]

\[ R_{P2O5\_av\_l(nc)} = R_{P2O5\_b(nc)} \times \text{vfm(ip2)} \times \text{vol(nc)} \times \text{denm(ip2)} + (2.29 \times R_{P\_used\_O2(nc)}) \]

\[ \text{IF} (R_{P2O5\_av\_l(nc)} \leq 1.0e^{-30}) \text{THEN} \]
\[ R_{P2O5\_av\_l(nc)} = 1.0e^{-30} \]
\[ \text{END IF} \]

\[ R_{Si\_req\_P2O5} = R_{P2O5\_av\_l(nc)} \times (0.493) \]

\[ \text{IF} (R_{Si\_req\_P2O5} \gt R_{Si\_av\_l(nc)}) \text{THEN} \]
\[ R_{Si\_used\_P2O5(nc)} = R_{Si\_av\_l(nc)} \]
\[ \text{ELSE} \]
\[ R_{Si\_used\_P2O5(nc)} = R_{Si\_req\_P2O5} \]
\[ \text{END IF} \]

\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
c-----Chemical reaction between Carbon and P2O5

R_C_av_L(nc)=R_C_av_L(nc)-R_C_used_O2(nc)
IF (R_C_av_L(nc).LE.1.0e-30) THEN
  R_C_av_L(nc)=1.0e-30
END IF
R_P2O5_av_L(nc)=R_P2O5_av_L(nc)-(R_Si_used_P2O5(nc)*2.03)
IF (R_P2O5_av_L(nc).LE.1.0e-30) THEN
  R_P2O5_av_L(nc)=1.0e-30
END IF
R_C_req_P2O5=R_P2O5_av_L(nc)*0.423
IF (R_C_req_P2O5.GT.R_C_av_L(nc)) THEN
  R_C_used_P2O5(nc)=R_C_av_L(nc)
ELSE
  R_C_used_P2O5(nc)=R_C_req_P2O5
END IF

c-----Chemical reaction between Manganese and P2O5

R_Mn_av_L(nc)=R_Mn_av_L(nc)-R_Mn_used_O2(nc)
IF (R_Mn_av_L(nc).LE.1.0e-30) THEN
  R_Mn_av_L(nc)=1.0e-30
END IF
R_P2O5_av_L(nc)=R_P2O5_av_L(nc)-(R_C_used_P2O5(nc)*2.37)
IF (R_P2O5_av_L(nc).LE.1.0e-30) THEN
  R_P2O5_av_L(nc)=1.0e-30
END IF
R_Mn_req_P2O5=R_P2O5_av_L(nc)*(1.937)
IF (R_Mn_req_P2O5.GT.R_Mn_av_L(nc)) THEN
  R_Mn_used_P2O5(nc)=R_Mn_av_L(nc)
ELSE
  R_Mn_used_P2O5(nc)=R_Mn_req_P2O5
END IF

c-----Chemical reaction between Silicon and FeO

R_Si_av_L(nc)=R_Si_av_L(nc)-R_Si_used_P2O5(nc)
IF (R_Si_av_L(nc).LE.1.0e-30) THEN
  R_Si_av_L(nc)=1.0e-30
END IF
R_FeO_av_L(nc)=R_FeO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+(1.29*R_Fe_used_O2(nc))
IF (R_FeO_av_L(nc).LE.1.0e-30) THEN
  R_FeO_av_L(nc)=1.0e-30
END IF
R_Si_req_FeO=R_FeO_av_L(nc)*(0.194)
IF (R_Si_req_FeO.GT.R_Si_av_L(nc)) THEN
  R_Si_used_FeO(nc)=R_Si_av_L(nc)
ELSE
  R_Si_used_FeO(nc)=R_Si_req_FeO
END IF

c-----Chemical reaction between Iron and P2O5

R_Fe_av_L(nc)=R_Fe_av_L(nc)+(R_Si_used_FeO(nc)*4.0)-R_Fe_used_O2(nc)
IF (R_Fe_av_L(nc).LE.1.0e-30) THEN
  R_Fe_av_L(nc)=1.0e-30
END IF
R_P2O5_av_l(nc)=R_P2O5_av_l(nc)-(0.516*R_Mn_used_P2O5(nc))
IF(R_P2O5_av_l(nc).LE.1.0e-30) THEN
  R_P2O5_av_l(nc)=1.0e-30
END IF
R_Fe_req_P2O5=R_P2O5_av_l(nc)*(1.97)
IF (R_Fe_req_P2O5.GT.R_Fe_av_l(nc)) THEN
  R_Fe_used_P2O5(nc)=R_Fe_av_l(nc)
ELSE
  R_Fe_used_P2O5(nc)=R_Fe_req_P2O5
END IF

R_C_av_l(nc)=R_C_av_l(nc)-R_C_used_P2O5(nc)
IF (R_C_av_l(nc).LE.1.0e-30) THEN
  R_C_av_l(nc)=1.0e-30
END IF

R_FeO_av_l(nc)=R_FeO_av_l(nc)+(R_Fe_used_P2O5(nc)*1.29)-(R_Si_used_FeO(nc)*5.14)
IF (R_FeO_av_l(nc).LE.1.0e-30) THEN
  R_FeO_av_l(nc)=1.0e-30
END IF

R_Si_av_l(nc)=R_Si_av_l(nc)-R_Si_used_FeO(nc)
IF (R_Si_av_l(nc).LE.1.0e-30) THEN
  R_Si_av_l(nc)=1.0e-30
END IF

R_MnO_av_l(nc)=R_MnO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
x+(1.29*R_Mn_used_P2O5(nc))+1.29*R_Mn_used_O2(nc)
IF (R_MnO_av_l(nc).LE.1.0e-30) THEN
  R_MnO_av_l(nc)=1.0e-30
END IF

R_C_av_l(nc)=R_C_av_l(nc)-R_C_used_FeO(nc)
IF (R_C_av_l(nc).LE.1.0e-30) THEN
  R_C_av_l(nc)=1.0e-30
END IF

R_MnO_av_l(nc)=R_MnO_av_l(nc)-(5.07*R_Si_used_MnO(nc))
IF (R_MnO_av_l(nc).LE.1.0e-30) THEN
  R_MnO_av_l(nc)=1.0e-30
END IF
END IF
R_C_req_MnO=R_MnO_av_l(nc)*0.169
IF (R_C_req_MnO.GT.R_C_av_l(nc)) THEN
R_C_used_MnO(nc)=R_C_av_l(nc)
ELSE
R_C_used_MnO(nc)=R_C_req_MnO
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Manganese and FeO
c----------------------------------------------------------------------------------------------------------------
R_Mn_av_l(nc)=R_Mn_av_l(nc)+(R_C_used_MnO(nc)*4.58)x+(R_Si_used_MnO(nc)*3.93)-R_Mn_used_P2O5(nc)
IF (R_Mn_av_l(nc).LE.1.0e-30) THEN
R_Mn_av_l(nc)=1.0e-30
END IF
R_FeO_av_l(nc)=R_FeO_av_l(nc)-(R_C_used_FeO(nc)*6.0)
IF (R_FeO_av_l(nc).LE.1.0e-30) THEN
R_FeO_av_l(nc)=1.0e-30
END IF
R_Mn_req_FeO=R_FeO_av_l(nc)*(0.764)
IF (R_Mn_req_FeO.GT.R_Mn_av_l(nc)) THEN
R_Mn_used_FeO(nc)=R_Mn_av_l(nc)
ELSE
R_Mn_used_FeO(nc)=R_Mn_req_FeO
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Finalising the amount of Carbon reacted.
c----------------------------------------------------------------------------------------------------------------
R_CRate=(R_C_used_O2(nc)+R_C_used_P2O5(nc)+R_C_used_FeO(nc)+R_C_used_MnO(nc))
R_C_final(nc)=min(R_CRate,R_C_Fickrate(nc))
IF (R_C_final(nc).LE.1.0e-30) THEN
R_C_final(nc)=1.0e-30
END IF
R_C_final_1=R_C_final(nc)
c----------------------------------------------------------------------------------------------------------------
c-----Finalising the effect of Carbon reacted on other compounds.
c----------------------------------------------------------------------------------------------------------------
IF (R_C_used_O2(nc).GT.R_C_final_1) THEN
R_C_O2(nc)=R_C_final_1
ELSE
R_C_O2(nc)=R_C_used_O2(nc)
END IF
R_C_final_2=R_C_final_1-R_C_O2(nc)
IF (R_C_used_P2O5(nc).GT.R_C_final_2) THEN
R_C_P2O5(nc)=R_C_final_2
ELSE
R_C_P2O5(nc)=R_C_used_P2O5(nc)
END IF
R_C_final_3=R_C_final_2-R_C_P2O5(nc)
IF (R_C_used_FeO(nc).GT.R_C_final_3) THEN
R_C_FeO(nc)=R_C_final_3
ELSE
R_C_FeO(nc)=R_C_used_FeO(nc)
END IF
END IF
R_C_final_4=R_C_final_3-R_C_FeO(nc)

IF (R_C_used_MnO(nc).GT.R_C_final_4) THEN
R_C_MnO(nc)=R_C_final_4
ELSE
R_C_MnO(nc)=R_C_used_MnO(nc)
END IF

R_c_rate(nc)=R_C_O2(nc)

R_SiRate=(R_Si_used_O2(nc)+R_Si_used_P2O5(nc)+R_Si_used_FeO(nc)+R_Si_used_MnO(nc))
R_Si_final(nc)=min(R_SiRate,R_Si_Fickrate(nc))
R_Si_com(nc)=R_Si_final(nc)
IF(R_Si_final(nc).LE.1.0e-30)THEN
R_Si_final(nc)=0.0
END IF

R_Si_final_1=R_Si_final(nc)

R_Si_O2(nc)=R_Si_final_1-R_Si_O2(nc)

R_Si_P2O5(nc)=R_Si_used_P2O5(nc)

R_Si_final_2=R_Si_final_1-R_Si_P2O5(nc)

R_Si_FeO(nc)=R_Si_used_FeO(nc)

R_Si_final_3=R_Si_final_2-R_Si_FeO(nc)

R_Si_MnO(nc)=R_Si_used_MnO(nc)

R_Si_final_4=R_Si_final_3-R_Si_MnO(nc)

R_FeRate=(R_Fe_used_O2(nc)+R_Fe_used_P2O5(nc))
R_Fe_final(nc)=min(R_FeRate,R_Fe_Fickrate(nc))
IF(R_Fe_final(nc).LE.1.0e-30)THEN
R_Fe_final(nc)=1.0e-30
END IF

R_Fe_final_1=R_Fe_final(nc)
c----------------------------------------------------------------------------------------------------------------
c-----Finalising the effect of Iron reacted on other compounds.
c----------------------------------------------------------------------------------------------------------------
IF (R_Fe_used_O2(nc).GT.R_Fe_final_1) THEN
  R_Fe_O2(nc)=R_Fe_final_1
ELSE
  R_Fe_O2(nc)=R_Fe_used_O2(nc)
END IF

c----Finalising the amount of Phosphorous reacted.
R_PRate=R_P_used_O2(nc)
R_P_final(nc)=min(R_PRate,R_P_Fickrate(nc))
IF (R_P_final(nc).LE.1.0e-30) THEN
  R_P_final(nc)=1.0e-30
END IF
R_P_final(nc)=R_P_O2(nc)

c----------------------------------------------------------------------------------------------------------------
c-----Finalising the amount of Manganese reacted.
R_MnRate=(R_Mn_used_O2(nc)+R_Mn_used_P2O5(nc)+R_Mn_used_FeO(nc))
R_Mn_final(nc)=min(R_MnRate,R_Mn_Fickrate(nc))
IF (R_Mn_final(nc).LE.1.0e-30) THEN
  R_Mn_final(nc)=1.0e-30
END IF
R_Mn_final_1=R_Mn_final(nc)

c----Finalising the effect of Manganese reacted on other compounds.
IF (R_Mn_used_O2(nc).GT.R_Mn_final_1) THEN
  R_Mn_O2(nc)=R_Mn_final_1
ELSE
  R_Mn_O2(nc)=R_Mn_used_O2(nc)
END IF

c----------------------------------------------------------------------------------------------------------------
ELSE
  R_C_FeO(nc)=1.0e-30
  R_Si_FeO(nc)=1.0e-30
  R_Mn_FeO(nc)=1.0e-30
  R_Si_MnO(nc)=1.0e-30
  R_C_MnO(nc)=1.0e-30
  R_C_P2O5(nc)=1.0e-30
  R_Si_P2O5(nc)=1.0e-30
  R_Fe_P2O5(nc)=1.0e-30
  R_Mn_P2O5(nc)=1.0e-30
  R_C_final(nc)=1.0e-30
  R_Fe_final(nc)=1.0e-30
  R_Si_final(nc)=1.0e-30
  R_Mn_final(nc)=1.0e-30
  R_P_final(nc)=1.0e-30
  R_c_rate(nc)=1.0e-30
END IF

R_L_av_C(nc)=R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)-R_C_final(nc)
IF(R_L_av_C(nc).LE.1.0e-30)THEN
  R_L_av_C(nc)=1.0e-30
END IF

R_L_av_Fe(nc)=R_Fe_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_L_av_Fe(nc)=R_Fe_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+(R_C_FeO(nc)*4.67)+(R_Si_FeO(nc)*4.0)+(R_Mn_FeO(nc)*1.02)
IF(R_L_av_Fe(nc).LE.1.0e-30)THEN
  R_L_av_Fe(nc)=1.0e-30
END IF

R_L_av_Mn(nc)=R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)-R_Mn_final(nc)
R_L_av_Mn(nc)=R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+(R_C_MnO(nc)*4.58)+(R_Si_MnO(nc)*3.93)
IF(R_L_av_Mn(nc).LE.1.0e-30)THEN
  R_L_av_Mn(nc)=1.0e-30
END IF

R_L_av_P(nc)=R_P_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_L_av_P(nc)=R_P_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)-(R_Fe_final(nc)*1.29)-(R_C_FeO(nc)*6.0)-(R_Si_FeO(nc)*5.14)-(R_Mn_FeO(nc)*1.31)
IF(R_L_av_P(nc).LE.1.0e-30)THEN
  R_L_av_P(nc)=1.0e-30
END IF

R_L_av_Si(nc)=R_Si_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_L_av_Si(nc)=R_Si_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)-(R_Fe_final(nc)*1.29)-(R_Si_FeO(nc)*6.0)-(R_Si_MnO(nc)*5.14)-(R_Mn_MnO(nc)*1.31)
IF(R_L_av_Si(nc).LE.1.0e-30)THEN
  R_L_av_Si(nc)=1.0e-30
END IF

R_L_av_SiO2(nc)=R_SiO2_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+(R_Si_final(nc)*2.14)
IF(R_L_av_SiO2(nc).LE.1.0e-30)THEN
  R_L_av_SiO2(nc)=1.0e-30
END IF

R_L_av_MnO(nc)=R_MnO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_L_av_MnO(nc)=R_MnO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+(R_Si_final(nc)*5.07)+(R_C_MnO(nc)*5.92)
IF(R_L_av_MnO(nc).LE.1.0e-30)THEN
  R_L_av_MnO(nc)=1.0e-30
END IF
R_L_av_MnO(nc)=1.0e-30

END IF
R_L_av_P2O5(nc)=R_P2O5_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
=R(R_P_final(nc)*2.29)-(R_C_P2O5(nc)*2.367)
+{(R_Si_P2O5(nc)*2.028)-(R_Fe_P2O5(nc)*0.507)-(R_Mn_P2O5(nc)*0.516)
IF(R_L_av_P2O5(nc).LE.1.0e-30)THEN
R_L_av_P2O5(nc)=1.0e-30
END IF

R_L_av_Tot(nc)=vfm(ip2)*vol(nc)*denm(ip2)

IF(R_Fe_final(nc).GT.1.0e-30)
THEN
R_Fe_fr(nc)=(R_L_av_Fe(nc)/R_L_av_Tot(nc))
IF(R_Fe_fr(nc).LE.1.0e-30)
THEN
R_Fe_fr(nc)=1.0e-30
END IF
R_Fe_b2(nc)=(R_Fe_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF(R_Fe_b2(nc).LE.1.0e-30)
THEN
R_S(25,nc)=1.0e-30
ELSE
R_S(25,nc)=R_Fe_b1(nc)-R_Fe_b2(nc)
END IF
IF(R_S(25,nc).LE.0.0)
THEN
R_S(25,nc)=1.0e-30
ELSE
R_S(25,nc)=1.0e-35
R_Fe_b2(nc)=1.0e-35
END IF

IF(R_C_final(nc).GT.1.0e-30)
THEN
R_C_fr(nc)=(R_L_av_C(nc)/R_L_av_Tot(nc))
IF(R_C_fr(nc).LE.1.0e-30)
THEN
R_C_fr(nc)=1.0e-30
END IF
R_C_b2(nc)=(R_C_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF(R_C_b2(nc).GT.R_C_b1(nc))
THEN
R_C_b2(nc)=R_C_b1(nc)
END IF
IF(R_C_b2(nc).LE.1.0e-30)
THEN
R_S(26,nc)=1.0e-30
ELSE
R_S(26,nc)=R_C_b1(nc)-R_C_b2(nc)
END IF
IF(R_S(26,nc).LE.0.0)
THEN
R_S(26,nc)=1.0e-30
ELSE
R_S(26,nc)=1.0e-35
R_C_b2(nc)=1.0e-35
END IF

IF(R_Si_final(nc).GT.1.0e-30)
THEN
R_Si_fr(nc)=(R_L_av_Si(nc)/R_L_av_Tot(nc))
IF(R_Si_fr(nc).LE.1.0e-30)
THEN
R_Si_fr(nc)=1.0e-30

END IF
R_Si_b2(nc)=(R_Si_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_Si_b2(nc).GT.R_Si_b1(nc)) THEN
  R_Si_b2(nc)=R_Si_b1(nc)
END IF
IF (R_Si_b2(nc).LE.1.0e-30) THEN
  R_S(27,nc)=1.0e-30
ELSE
  R_S(27,nc)=R_Si_b1(nc)-R_Si_b2(nc)
END IF
IF (R_S(27,nc).LE.0.0) THEN
  R_S(27,nc)=1.0e-30
END IF
ELSE
  R_S(27,nc)=1.0e-35
  R_Si_b2(nc)=1.0e-35
END IF

----------------------------------------------------------------------------------------------------------------
IF (R_Mn_final(nc).GT.1.0e-30) THEN
  R_Mn_fr(nc)=(R_L_av_Mn(nc)/R_L_av_Tot(nc))
  IF (R_Mn_fr(nc).LE.1.0e-30) THEN
    R_Mn_fr(nc)=1.0e-30
  END IF
  IF (R_Mn_fr(nc).GT.R_Mn_b1(nc)) THEN
    R_Mn_fr(nc)=R_Mn_b1(nc)
  END IF
  R_Mn_b2(nc)=(R_Mn_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
  IF (R_Mn_b2(nc).LE.1.0e-30) THEN
    R_S(28,nc)=1.0e-30
  ELSE
    R_S(28,nc)=R_Mn_b1(nc)-R_Mn_b2(nc)
  END IF
  IF (R_S(28,nc).LE.0.0) THEN
    R_S(28,nc)=1.0e-30
  END IF
ELSE
  R_S(28,nc)=1.0e-35
  R_Si_b2(nc)=1.0e-35
END IF

----------------------------------------------------------------------------------------------------------------
IF (R_P_final(nc).GT.1.0e-30) THEN
  R_P_fr(nc)=(R_L_av_P(nc)/R_L_av_Tot(nc))
  IF (R_P_fr(nc).LE.1.0e-30) THEN
    R_P_fr(nc)=1.0e-30
  END IF
  IF (R_P_fr(nc).GT.R_P_b1(nc)) THEN
    R_P_fr(nc)=R_P_b1(nc)
  END IF
  R_P_b2(nc)=(R_P_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
  IF (R_P_b2(nc).LE.1.0e-30) THEN
    R_S(29,nc)=1.0e-30
  ELSE
    R_S(29,nc)=R_P_b1(nc)-R_P_b2(nc)
  END IF
  IF (R_S(29,nc).LE.0.0) THEN
    R_S(29,nc)=1.0e-30
  END IF
ELSE
  R_S(29,nc)=1.0e-35
  R_Si_b2(nc)=1.0e-35
END IF

----------------------------------------------------------------------------------------------------------------
IF (R_L_av_FeO(nc).GT.1.0e-30) THEN
  R_FeO_fr(nc)=R_L_av_FeO(nc)/R_L_av_Tot(nc)
IF (R_FeO_fr(nc).LE.1.0e-30) THEN
  R_FeO_fr(nc)=1.0e-30
END IF
IF (R_FeO_fr(nc).GT.1.0) THEN
  R_FeO_fr(nc)=1.0
END IF
R_FeO_b2(nc)=(R_FeO_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_FeO_b1(nc).LE.1.0e-30) THEN
  R_S(30,nc)=1.0e-30
ELSE
  R_S(30,nc)=R_FeO_b2(nc)-R_FeO_b1(nc)
END IF
IF (R_S(30,nc).LE.0.0) THEN
  R_S(30,nc)=1.0e-30
END IF
ELSE
  R_S(30,nc)=1.0e-35
  R_FeO_b2(nc)=1.0e-35
END IF

C----------------------------------------------------------------------------------------------------------------
IF (R_L_av_SiO2(nc).GT.1.0e-30) THEN
  R_SiO2_fr(nc)=(R_L_av_SiO2(nc)/R_L_av_Tot(nc))
IF (R_SiO2_fr(nc).LE.1.0e-30) THEN
  R_SiO2_fr(nc)=1.0e-30
END IF
IF (R_SiO2_fr(nc).GE.1.0) THEN
  R_SiO2_fr(nc)=1.0
END IF
R_SiO2_b2(nc)=(R_SiO2_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_SiO2_b1(nc).LE.1.0e-30) THEN
  R_S(31,nc)=1.0e-30
ELSE
  R_S(31,nc)=R_SiO2_b2(nc)-R_SiO2_b1(nc)
END IF
IF (R_S(31,nc).LE.0.0) THEN
  R_S(31,nc)=1.0e-30
END IF
ELSE
  R_S(31,nc)=1.0e-35
  R_SiO2_b2(nc)=1.0e-35
END IF

C----------------------------------------------------------------------------------------------------------------
IF (R_L_av_P2O5(nc).GT.1.0e-30) THEN
  R_P2O5_fr(nc)=(R_L_av_P2O5(nc)/R_L_av_Tot(nc))
IF (R_P2O5_fr(nc).LE.1.0e-30) THEN
  R_P2O5_fr(nc)=1.0e-30
END IF
IF (R_P2O5_fr(nc).GT.1.0) THEN
  R_P2O5_fr(nc)=1.0
END IF
R_P2O5_b2(nc)=(R_P2O5_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_P2O5_b1(nc).LE.1.0e-30) THEN
  R_S(32,nc)=1.0e-30
ELSE
  R_S(32,nc)=1.0e-35
  R_P2O5_b2(nc)=1.0e-35
END IF

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R_S(32,nc)=R_P2O5_b2(nc)-R_P2O5_b1(nc)
END IF
IF (R_S(32,nc).LE.0.0) THEN
  R_S(32,nc)=1.0e-30
END IF
ELSE
  R_S(32,nc)=1.0e-35
  R_P2O5_b2(nc)=1.0e-35
END IF

R_S(33,nc)=R_MnO_b2(nc)-R_MnO_b1(nc)
IF (R_S(33,nc).LE.0.0) THEN
  R_S(33,nc)=1.0e-30
END IF
ELSE
  R_S(32,nc)=1.0e-35
  R_MnO_b2(nc)=1.0e-35
END IF

R_t=TIME

R_CO_av=2.0*Phi_mscal((12-ncell+nc)*vfm(ip1)*vol(nc)*denm(ip1)
R_CO2_g=2.0*Phi_mscal((13-1)*ncell+nc)*vfm(ip1)*vol(nc)*denm(ip1)
R_O_CO_t=vfm(ip1)*vol(nc)*denm(ip1)
R_CO_r=2.34*R_C_final(nc)
R_CO2_rd(nc)=(100.0-0.167*R_t)*R_CO_r
R_CO_rem(nc)=R_CO_r-R_CO2_rd(nc)
IF (R_CO_rem(nc).GT.R_CO_r) THEN
  R_CO_rem(nc)=R_CO_r
END IF
IF (R_CO_rem(nc).LE.1.0e-30) THEN
  R_CO_rem(nc)=1.0e-30
END IF
R_COfr(nc)=0.5*(R_CO_av+R_CO_rem(nc))/(R_O_CO_t+R_CO_r)
IF (R_COfr(nc).GT.0.5) THEN
  R_COfr(nc)=0.5
END IF
R_COfe(nc)=0.5-R_COfr(nc)

R_S(22,nc)=((0.5-R_COfr(nc))-Phi_mscal((11-1)*ncell+nc))vfm(ip1)=vol(nc)*denm(ip1)
END IF
IF (R_CO_rem(nc).LE.1.0e-30) THEN
  R_CO_rem(nc)=1.0e-30
END IF
R_COfr(nc)=0.5*(R_CO_av+R_CO_rem(nc))/(R_O_CO_t+R_CO_r)
IF (R_COfr(nc).GT.0.5) THEN
  R_COfr(nc)=0.5
END IF
R_COfe(nc)=0.5-R_COfr(nc)

R_S(22,nc)=((0.5-R_COfr(nc))=Phi_mscal((11-1)*ncell+nc))vfm(ip1)*vol(nc)*denm(ip1)
IF (R_S(22,nc).LT.1.0e-30) THEN
  R_S(22,nc)=1.0e-30
END IF
R_S(21,nc)=(R_COfr(nc)-Phi_mscal((12-1)*ncell+nc))*vfm(ip1)*vol(nc)*denm(ip1)
IF(R_S(21,nc).LT.1.0e-30)
THEN
  R_S(21,nc)=1.0e-30
END IF
R_S(34,nc)=1.0e-30

R_O2_rate2(nc)=R_S(25,nc)+R_S(26,nc)+R_S(27,nc)+R_S(28,nc)+R_S(29,nc)
R_O2_rate1(nc)=R_S(30,nc)+R_S(31,nc)+R_S(32,nc)+R_S(33,nc)
R_c_rate1(nc)=R_S(21,nc)
R_c_rate2(nc)=R_S(22,nc)

R_bubble=Phi_mscal((31-1)*ncell+nc)

R_S(1,nc)=(R_BB(1)-R_DB(1)+R_BC(1)-R_DC(1))*denm(ip1)
R_S(2,nc)=(R_BB(2)-R_DB(2)+R_BC(2)-R_DC(2))*denm(ip1)
R_S(3,nc)=(R_BB(3)-R_DB(3)+R_BC(3)-R_DC(3))*denm(ip1)
R_S(4,nc)=(R_BB(4)-R_DB(4)+R_BC(4)-R_DC(4))*denm(ip1)
R_S(5,nc)=(R_BB(5)-R_DB(5)+R_BC(5)-R_DC(5))*denm(ip1)
R_S(6,nc)=(R_BB(6)-R_DB(6)+R_BC(6)-R_DC(6))*denm(ip1)
R_S(7,nc)=(R_BB(7)-R_DB(7)+R_BC(7)-R_DC(7))*denm(ip1)
R_S(8,nc)=(R_BB(8)-R_DB(8)+R_BC(8)-R_DC(8))*denm(ip1)
R_S(9,nc)=(R_BB(9)-R_DB(9)+R_BC(9)-R_DC(9))*denm(ip1)
R_S(10,nc)=(R_BB(10)-R_DB(10)+R_BC(10)-R_DC(10))*denm(ip1)

R_S(11,nc)=(R_BCF(1)-R_DCF(1))
R_S(12,nc)=(R_BCF(2)-R_DCF(2))
R_S(13,nc)=(R_BCF(3)-R_DCF(3))
R_S(14,nc)=(R_BCF(4)-R_DCF(4))
R_S(15,nc)=(R_BCF(5)-R_DCF(5))
R_S(16,nc)=(R_BCF(6)-R_DCF(6))
R_S(17,nc)=(R_BCF(7)-R_DCF(7))
R_S(18,nc)=(R_BCF(8)-R_DCF(8))
R_S(19,nc)=(R_BCF(9)-R_DCF(9))

IF(R_bubble.LE.0.9)
THEN
  R_S(20,nc)=(R_BCF(10)-R_DCF(10))
ELSE
  R_S(20,nc)=0.0
END IF

R_S(20,nc)=1.0e-30

END IF

R_S(34,nc)=1.0e-30

C-----Source term for each scalar
C-----Source term for gas bubble in gas phase
R_S(1,nc)=(R_BB(1)-R_DB(1)+R_BC(1)-R_DC(1))*denm(ip1)
R_S(2,nc)=(R_BB(2)-R_DB(2)+R_BC(2)-R_DC(2))*denm(ip1)
R_S(3,nc)=(R_BB(3)-R_DB(3)+R_BC(3)-R_DC(3))*denm(ip1)
R_S(4,nc)=(R_BB(4)-R_DB(4)+R_BC(4)-R_DC(4))*denm(ip1)
R_S(5,nc)=(R_BB(5)-R_DB(5)+R_BC(5)-R_DC(5))*denm(ip1)
R_S(6,nc)=(R_BB(6)-R_DB(6)+R_BC(6)-R_DC(6))*denm(ip1)
R_S(7,nc)=(R_BB(7)-R_DB(7)+R_BC(7)-R_DC(7))*denm(ip1)
R_S(8,nc)=(R_BB(8)-R_DB(8)+R_BC(8)-R_DC(8))*denm(ip1)
R_S(9,nc)=(R_BB(9)-R_DB(9)+R_BC(9)-R_DC(9))*denm(ip1)
R_S(10,nc)=(R_BB(10)-R_DB(10)+R_BC(10)-R_DC(10))*denm(ip1)

C-----Source term for gas bubble in foam phase
R_S(11,nc)=(R_BCF(1)-R_DCF(1))
R_S(12,nc)=(R_BCF(2)-R_DCF(2))
R_S(13,nc)=(R_BCF(3)-R_DCF(3))
R_S(14,nc)=(R_BCF(4)-R_DCF(4))
R_S(15,nc)=(R_BCF(5)-R_DCF(5))
R_S(16,nc)=(R_BCF(6)-R_DCF(6))
R_S(17,nc)=(R_BCF(7)-R_DCF(7))
R_S(18,nc)=(R_BCF(8)-R_DCF(8))
R_S(19,nc)=(R_BCF(9)-R_DCF(9))

IF(R_bubble.LE.0.9)
THEN
  R_S(20,nc)=(R_BCF(10)-R_DCF(10))
ELSE
  R_S(20,nc)=0.0
END IF

C-----Source term for chemical composition in foam
END DO

C-----Loop over internal cells
C-----Sources update for scalar 1 phase 1
C

IF (isc==1) THEN
  DO ip = nsp(mat),nep(mat)
    sum1(ip)= sum1(ip)+(R_S(1,ip)/dt)
  END DO
END IF

C-----Sources for scalar 2 phase 1
C

IF (isc==2) THEN
  DO ip = nsp(mat),nep(mat)
    sum1(ip)=sum1(ip)+(R_S(2,ip)/dt)
  END DO
END IF

c----Sources for scalar 3 phase 1

IF (isc==3) THEN
  DO ip = nsp(mat),nep(mat)
     sum1(ip)= sum1(ip)+(R_S(3,ip)/dt)
  END DO
END IF

END IF

END IF

END IF

END IF

END IF

END IF

END IF

END IF

END IF

END IF

END IF

END IF

END IF

END IF
END IF

c-----Sources for scalar 10 phase 1

IF (isc==10) THEN
  DO ip = nsp(mat),nep(mat)
    sum1(ip)= sum1(ip)+(R_S(10,ip)/dt)
  END DO
END IF

c-----Sources for scalar 11 O2 phase 1

IF (isc==11) THEN
  DO ip = nsp(mat),nep(mat)
    sum1(ip)= sum1(ip)+(R_S(22,ip)/dt)
  END DO
END IF

C-----Sources for scalar 12 CO phase 1

IF (isc==12) THEN
  DO ip = nsp(mat),nep(mat)
    SUM1(IP)= SUM1(IP)+(R_S(21,IP)/DT)
  END DO
END IF

C-----Sources for scalar 13 CO2 phase 1

IF (isc==13) THEN
  DO ip = nsp(mat),nep(mat)
    IF (TIME.LE.0.3e+03)
      THEN
      SUM1(IP)= SUM1(IP)+(R_S(34,IP)/DT)
    ELSE
      END IF
  END DO
END IF

C-----Sources for scalar 1 Fe phase 2

IF (isc==14) THEN
  DO ip = nsp(mat),nep(mat)
    IP2=IP+NCCELL
    IF (R_S(25,IP).LE.0.0)
      THEN
      R_S(25,IP)=0.0
    ELSE
      END IF
    SUM1(IP2)= SUM1(IP2)-(R_S(25,IP)/DT)
  END DO
END IF

C-----Sources for scalar 2 C phase 2

IF (isc==15) THEN
  DO ip = nsp(mat),nep(mat)
    IP2=IP+NCCELL
    IF (R_S(26,IP).LE.0.0)
      THEN
    END IF
  END DO
END IF
R_S(26,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)-(R_S(26,ip)/dt)
END DO
END IF

C-----Sources for scalar 3 Si phase 2
C----------------------------------------------------------------------------------------------------------------
IF (isc==16) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(27,ip).LE.0.0) THEN
R_S(27,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)-(R_S(27,ip)/dt)
END DO
END IF
C----------------------------------------------------------------------------------------------------------------
C-----Sources for scalar 4 Mn phase 2
C----------------------------------------------------------------------------------------------------------------
IF (isc==17) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(28,ip).LE.0.0) THEN
R_S(28,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)-(R_S(28,ip)/dt)
END DO
END IF
C----------------------------------------------------------------------------------------------------------------
C-----Sources for scalar 5 P phase 2
C----------------------------------------------------------------------------------------------------------------
IF (isc==18) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(29,ip).LE.0.0) THEN
R_S(29,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)-(R_S(29,ip)/dt)
END DO
END IF
C----------------------------------------------------------------------------------------------------------------
C-----Sources for scalar 6 FeO phase 2
C----------------------------------------------------------------------------------------------------------------
IF (isc==19) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(30,ip).LE.0.0) THEN
R_S(30,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)+(R_S(30,ip)/dt)
END DO
END IF
C----------------------------------------------------------------------------------------------------------------
C-----Sources for scalar 7 SiO2 phase 2
C----------------------------------------------------------------------------------------------------------------
IF (isc==20) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(31,ip).LE.0.0) THEN
R_S(31,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)+(R_S(31,ip)/dt)
END DO
END IF

c-----Sources for scalar 8 P2O5 phase 2

IF (isc==21) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(32,ip).LE.0.0) THEN
R_S(32,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)+(R_S(32,ip)/dt)
END DO
END IF

c-----Sources for scalar 9 MnO phase 2

IF (isc==22) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(33,ip).LE.0.0) THEN
R_S(33,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)
END DO
END IF

c-----Sources for scalar 10 S phase 2

IF (isc==23) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
sum1(ip2)= sum1(ip2)
END DO
END IF

c-----Sources for scalar 1 Bubble phase 3

IF (isc==24) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(11,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
END DO
END IF

IF (isc==25) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(12,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
END DO
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Sources for scalar 3 Bubble phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==26) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(13,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
END DO
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Sources for scalar 4 Bubble phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==27) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(14,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
END DO
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Sources for scalar 5 Bubble phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==28) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(15,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
END DO
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Sources for scalar 6 Bubble phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==29) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(16,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
END DO
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Sources for scalar 7 Bubble phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==30) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(17,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
END DO
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Sources for scalar 8 Bubble phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==31) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(18,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
END IF

C-----Sources for scalar 9 Bubble phase 3
C----------------------------------------------------------------------------------------------------------------
IF (isc==32) THEN
  DO ip = nsp(mat),nep(mat)
    ip3=ip+ncell+ncell
    sum1(ip3)= sum1(ip3)+(R_S(19,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
  END DO
END IF

C-----Sources for scalar 10 Bubble phase 3
C----------------------------------------------------------------------------------------------------------------
IF (isc==33) THEN
  DO ip = nsp(mat),nep(mat)
    ip3=ip+ncell+ncell
    sum1(ip3)= sum1(ip3)+(R_S(20,ip)*vol(ip)*vfm(ip3)*denm(ip3)/dt)
  END DO
END IF

C-----Sources for scalar 11 liquid, phase 3
C----------------------------------------------------------------------------------------------------------------
IF (isc==34) THEN
  DO ip = nsp(mat),nep(mat)
    ip3=ip+ncell+ncell
    sum1(ip3)= sum1(ip3)+(R_S(23,ip)*vfm(ip3)*vol(ip)*denm(ip3))/dt)
  END DO
END IF

C-----Sources for scalar 11 gas phase 3
C----------------------------------------------------------------------------------------------------------------
IF (isc==35) THEN
  DO ip = nsp(mat),nep(mat)
    ip3=ip+ncell+ncell
    sum1(ip3)= sum1(ip3)+(R_S(24,ip)*vfm(ip3)*vol(ip)*denm(ip3))/dt)
  END DO
END IF
RETURN
END SUBROUTINE usesc_mscal
• User subroutine to calculate sources in interfacial mass exchange

SUBROUTINE usemph(ieq,iva,mat)

C======================================================================
C    description: user subroutine for sources for interfacial exchange and general sources like body forces
C    author: Anuththara Kirindigoda Hewage (2070065)
C    date: 01/10/2015
C======================================================================
USE comm1
USE comm2
USE comm0
INCLUDE 'comdp.inc'
INCLUDE 'com90.inc'
INCLUDE 'SwiftIO_FortranFunctions.inc'
mat=1
C----Volume fraction equation interfacial sources
C==============================================================================
IF(ieq == ipvf) THEN
  DO i_p1=nsp(mat),nep(mat)
    i_p2=i_p1+ncell
    i_p3=i_p1+ncell+ncell
    C-----Source terms update for mass exchange
    sum1(i_p1)= sum1(i_p1)+((R_c_rate1(i_p1)/dt)-(R_c_rate2(i_p1)/dt)
    x +(R_fm_g(i_p1)-R_g_fm(i_p1))/dt
    x+(R_O2_rate1(i_p1)/dt)-(R_O2_rate2(i_p1)/dt)
    x+(R_fm_lq(i_p1)-R_lq_fm(i_p1))/dt
    C==============================================================================
  END DO
END IF
RETURN
END SUBROUTINE
• User subroutine to calculate the density of the foam phase

SUBROUTINE useden(mat,mph)
  c=====================================================================
  c     description: user subroutine for changing the density
  c     author: Anuththara Kirindigoda Hewage (2070065)
  c     date: 01/10/2015
  c=====================================================================
  c-----modules
  USE comm1
  USE comm2
  USE cthmod, ONLY: ymfrac
  USE comm0
  c----------------------------------------------------------------------------------------------------------------
  INCLUDE 'comdp.inc'
  INCLUDE 'com90.inc'
  INCLUDE 'SwiftIO_FortranFunctions.inc'
  INTEGER, INTENT(in) :: mat,mph
  c----------------------------------------------------------------------------------------------------------------
  DO ip=nsp(mat),nep(mat)
    ip1=ip
    ip2=ip+ncell
    ip3=ip+ncell+ncell
    denm(ip1)=denm(ip1)
    denm(ip2)=denm(ip2)
    denm(ip3)=2.0*R_gfr(ip)*denm(ip1)+(1.0-2.0*R_gfr(ip))*denm(ip2)
  c----------------------------------------------------------------------------------------------------------------
  END DO
  RETURN
END SUBROUTINE
• **User subroutine to calculate the viscosity of the foam phase**

**Subroutine** usevis(mat,mph)

C=====================================================================
C     description: user subroutine for changing the viscosity
C     author: Anuththara Kirindigoda Hewage (2070065)
C     date: 01/10/2015
C=====================================================================
C-----modules
USE comm1
USE comm2
USE cthmod, ONLY: ymfrac
USE comm0
INCLUDE 'comdp.inc'
INCLUDE 'com90.inc'
INCLUDE 'SwiftIO_FortranFunctions.inc'
INTEGER, INTENT(in) :: mat,mph
C----------------------------------------------------------------------------------------------------------------
DO ip=nsp(mat),nep(mat)
ip1=ip
ip2=ip+ncell
ip3=ip+ncell+ncell
vimm(ip1)=vimm(ip1)
vimm(ip2)=vimm(ip2)
vimm(ip3)=2.0*R_gfr(ip)*vimm(ip1)+(1.0-2.0*R_gfr(ip))*vimm(ip2)
C----------------------------------------------------------------------------------------------------------------
END DO
RETURN
END SUBROUTINE usevis
A7. Subroutines used in CFD three phases model with updated foaming model

- User subroutine to calculate sources in scalar equation

**SUBROUTINE** usesc_mscal(mat,isc,mph)

---

**Author:** Anuththara Kirindigoda Hewage (2070065)

**Date:** 30/08/2016

**Project:** Updated foam model

---

**USE** comm1

**USE** comm2

**USE** comm0

**INCLUDE** 'comdp.inc'

**INCLUDE** 'com90.inc'

**INCLUDE** 'SwiftIO_FortranFunctions.inc'

**INTEGER**, **INTENT**(in) :: mat,isc,mph

---

**REAL**, **DIMENSION**(1:24,NCELL):: R_S

**REAL**, **DIMENSION**(NCELL):: R_lqt,R_tDgbt,R_tdgf,R_lq_f,R_tfl,R_foam

**REAL**, **DIMENSION**(NCELL):: R_g,R_lqt_av,R_tfg,R_tfoam,R_gf,R_g_av

**REAL**, **DIMENSION**(NCELL):: R_COfr,R_gf_av,R_fm_lq_com,R_lq_fm_com

**REAL**, **DIMENSION**(1:10):: R_tv,R_tvf,R_BCF,R_DCF,R_BC,R_DC,R_d,R_v

**REAL**, **DIMENSION**(1:10):: R_fb,R_fb_c,R_fb_n,R_fb_nb

**REAL**, **DIMENSION**(1:10):: R_BB,R_DB,R_vbb,R_vbd1,R_nb,R_nbfo,R_vbctf

**REAL**, **DIMENSION**(1:10):: R_dr,R_Cf,R_zita,R_chaiC,R_cfq,R_vbd

**REAL**, **DIMENSION**(1:10):: R_vbc1,R_vbc2,R_vbc3,R_vbc4

**REAL**, **DIMENSION**(1:10):: R_vbcf1,R_vbcf2,R_vbcf3,R_vbcf4

**REAL**, **DIMENSION**(1:10,1:10):: R_ccarea,R_TCR,R_colef,R_tij

**REAL**, **DIMENSION**(1:10,1:10):: R_str,R_gf,R_mn,R_nf,R_nfbo,R_vbct

---

**REAL**, **DIMENSION**(1:10,1:10):: R_rbj,R_FS,R_crf,R_Xijf

---

**REAL**, **DIMENSION**(NCELL):: R_fm_g_com,R_g_fm_com,R_gfr_com,R_ifn,R_iff

**REAL**, **DIMENSION**(NCELL):: R_L_final_1,R_L_final_2,R_L_final_3,R_L_final_4

**REAL**, **DIMENSION**(NCELL):: R_C_final_1,R_C_final_2,R_C_final_3,R_C_final_4

**REAL**, **DIMENSION**(NCELL):: R_Si_final_1,R_Si_final_2,R_Si_final_3,R_Si_final_4

**REAL**, **DIMENSION**(NCELL):: R_Fe_final_1,R_Fe_final_2,R_Mn_final_1,R_Mn_final_2
REAL, DIMENSION (NCELL):: R_Fe_used_O2, R_P2O5_av_l, R_Si_used_P2O5
REAL, DIMENSION (NCELL):: R_Mn_used_P2O5, R_Feo_av_l, R_Si_used_FeO
REAL, DIMENSION (NCELL):: R_Fe_used_P2O5, R_C_used_FeO, R_MnO_av_l
REAL, DIMENSION (NCELL):: R_Si_used_MnO, R_C_used_MnO, R_Mn_used_FeO
REAL, DIMENSION (NCELL):: R_Si_O2, R_Fe_O2, R_Mn_O2, R_C_O2, R_P_O2
REAL, DIMENSION (NCELL):: R_C_P2O5, R_C MnO, R_C FeO, R_C_used_P2O5
REAL, DIMENSION (NCELL):: R_Mn_P2O5, R_Mn FeO, R_Fe fr, R_MnO fr
REAL, DIMENSION (NCELL):: R_FeO b, R_MnO b, R_FeO b used, R_MnO b used
REAL, DIMENSION (NCELL):: R_FeO fr, R_MnO fr, R_FeO fr used, R_MnO fr used
REAL, DIMENSION (NCELL):: R_P2O5 b1, R_MnO b1, R_FeO b1, R_MnO b2, R_FeO b2
REAL, DIMENSION (NCELL):: R_C b, R_P b, R_SiO2 b, R_C b1, R_P b1
REAL, DIMENSION (NCELL):: R_SiO2 b, R_C b2, R_P b2, R_SiO2 b2
REAL, DIMENSION (NCELL):: R_C b1, R_P b1, R_SiO2 b1, R_C b2, R_P b2
REAL, DIMENSION (NCELL):: R_C b, R_P b, R_SiO2 b, R_C b1, R_P b1
REAL, DIMENSION (NCELL):: R_SiO2 b, R_C b2, R_P b2, R_SiO2 b2
REAL, DIMENSION (NCELL):: R_C b, R_P b, R_SiO2 b, R_C b1, R_P b1
REAL, DIMENSION (NCELL):: R_SiO2 b, R_C b2, R_P b2, R_SiO2 b2

--- Bubble volume, diameter and length of plateau border

R_v(1) = 65.416E-09
R_v(2) = 130.833E-09
R_v(3) = 261.6667E-09
R_v(4) = 523.333E-09
R_v(5) = 1046.667E-09
R_v(6) = 209.333E-08
R_v(7) = 418.667E-08
R_v(8) = 837.333E-08
R_v(9) = 1674.67E-07
R_v(10) = 3349.933E-07

--- Bubble diameter

R_d(1) = 2.500E-03
R_d(2) = 3.149E-03
R_d(3) = 3.968E-03
R_d(4) = 5.000E-03
R_d(5) = 6.299E-03
R_d(6) = 7.937E-03
R_d(7) = 1.000E-02
R_d(8) = 1.2599E-02
R_d(9) = 1.5874E-02
R_d(10) = 2.000E-02

--- Bubble break up, Coalescence model and population balance

DO nc = nsp(mat), nep(mat)
i p1 = nc
ip2 = nc + ncell
ip3 = nc + ncell + ncell
IF (edm(ip2).LT.1.0e-06) THEN
edm(ip2)=1.0e-06

END IF
R_ld=(8.42e-05)/(edm(ip2)**0.25)
c---volume of each scalar in each cell

c---Scalar in gas phase
c---gas bubble
R_tv(1)=Phi_mscal((1-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(2)=Phi_mscal((2-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(3)=Phi_mscal((3-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(4)=Phi_mscal((4-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(5)=Phi_mscal((5-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(6)=Phi_mscal((6-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(7)=Phi_mscal((7-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(8)=Phi_mscal((8-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(9)=Phi_mscal((9-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(10)=Phi_mscal((10-1)*ncell+nc)*vfm(ip1)*vol(nc)
c-----Scalar in foam phase
c-----bubble
R_tvf(1)=Phi_mscal((24-1)*ncell+nc)
R_tvf(2)=Phi_mscal((25-1)*ncell+nc)
R_tvf(3)=Phi_mscal((26-1)*ncell+nc)
R_tvf(4)=Phi_mscal((27-1)*ncell+nc)
R_tvf(5)=Phi_mscal((28-1)*ncell+nc)
R_tvf(6)=Phi_mscal((29-1)*ncell+nc)
R_tvf(7)=Phi_mscal((30-1)*ncell+nc)
R_tvf(8)=Phi_mscal((31-1)*ncell+nc)
R_tvf(9)=Phi_mscal((32-1)*ncell+nc)
R_tvf(10)=Phi_mscal((33-1)*ncell+nc)
c-----liquid in foam
c-----Number of gas bubble in each cell in gas phase
R_nb(1)=R_tv(1)/R_v(1)
R_nb(2)=R_tv(2)/R_v(2)
R_nb(3)=R_tv(3)/R_v(3)
R_nb(4)=R_tv(4)/R_v(4)
R_nb(5)=R_tv(5)/R_v(5)
R_nb(6)=R_tv(6)/R_v(6)
R_nb(7)=R_tv(7)/R_v(7)
R_nb(8)=R_tv(8)/R_v(8)
R_nb(9)=R_tv(9)/R_v(9)
R_nb(10)=R_tv(10)/R_v(10)
c-----Number of foam bubble in each cell in foam phase
R_nbf(1)=R_tvf(1)/R_v(1)
R_nbf(2)=R_tvf(2)/R_v(2)
R_nbf(3)=R_tvf(3)/R_v(3)
R_nbf(4)=R_tvf(4)/R_v(4)
R_nbf(5)=R_tvf(5)/R_v(5)
R_nbf(6)=R_tvf(6)/R_v(6)
R_nbf(7)=R_tvf(7)/R_v(7)
R_nbf(8)=R_tvf(8)/R_v(8)
R_nbf(9)=R_tvf(9)/R_v(9)
R_nbf(10)=R_tvf(10)/R_v(10)
c-----Initialization for Birth and death term for break up
R_DB(1)=0.0
R_DB(2)=0.0
R_DB(3)=0.0
R_DB(4)=0.0
R_DB(5)=0.0
R_DB(6)=0.0
R_DB(7)=0.0
R_DB(8)=0.0
R_DB(9)=0.0
R_DB(10)=0.0
R_BB(1)=0.0
R_BB(2)=0.0
R_BB(3)=0.0
R_BB(4)=0.0
R_BB(5)=0.0
R_BB(6)=0.0
R_BB(7)=0.0
R_BB(8)=0.0
R_BB(9)=0.0
R_BB(10)=0.0

c-----Initialization for Birth and Death term for Coalescence in gas phase
R_DC(1)=0.0
R_DC(2)=0.0
R_DC(3)=0.0
R_DC(4)=0.0
R_DC(5)=0.0
R_DC(6)=0.0
R_DC(7)=0.0
R_DC(8)=0.0
R_DC(9)=0.0
R_DC(10)=0.0
R_BC(1)=0.0
R_BC(2)=0.0
R_BC(3)=0.0
R_BC(4)=0.0
R_BC(5)=0.0
R_BC(6)=0.0
R_BC(7)=0.0
R_BC(8)=0.0
R_BC(9)=0.0
R_BC(10)=0.0

c-----Initialization for Birth and Death term for Coalescence in foam phase
R_DCF(1)=0.0
R_DCF(2)=0.0
R_DCF(3)=0.0
R_DCF(4)=0.0
R_DCF(5)=0.0
R_DCF(6)=0.0
R_DCF(7)=0.0
R_DCF(8)=0.0
R_DCF(9)=0.0
R_DCF(10)=0.0
R_BCF(1)=0.0
R_BCF(2)=0.0
R_BCF(3)=0.0
R_BCF(4)=0.0
R_BCF(5)=0.0
R_BCF(6)=0.0
R_BCF(7)=0.0
R_BCF(8)=0.0
R_BCF(9)=0.0
R_BCF(10)=0.0

----------------------------------------------------------------------------------------------------------------
c-----Bubble coalescence
c-----Bubble Coalescence model by Prince and Blanch
c-----Birth of bubble class i+1 due to coalescence of bubble class i to N-1
c----------------------------------------------------------------------------------------------------------------
IF(vfm(ip1).LT.0.75) THEN
  DO i_i=1,9
    DO i_j=1,i_i
      R_ccarea(i_i,i_j)=((R_d(i_i)+R_d(i_j))**2.0)
    END DO
  END DO
  R_TCR(i_i,i_j)=0.089*R_nb(i_i)*R_nb(i_j)*R_ccarea(i_i,i_j)*
    (edm(ip2))**0.333)*((R_d(i_i)**0.666+R_d(i_j)**0.666)**0.5)
  R_min_nb(i_i,i_j)=min(R_nb(i_i),R_nb(i_j))
  R_TCR(i_i,i_j)=max(R_TCR(i_i,i_j),R_min_nb(i_i,i_j))
END IF

----------------------------------------------------------------------------------------------------------------
c-----Scalar Value update for each bubble class
  R_vbc1(1)=0.0
  R_vbc2(1)=0.0
  R_vbc3(1)=0.0
  R_vbc4(1)=0.0
  R_vbc1(2)=0.0
  R_vbc2(2)=0.0
  R_vbc3(2)=0.0
  R_vbc4(2)=0.0
  R_vbc1(3)=0.0
  R_vbc2(3)=0.0
  R_vbc3(3)=0.0
  R_vbc4(3)=0.0
  R_vbc1(4)=0.0
  R_vbc2(4)=0.0
  R_vbc3(4)=0.0
  R_vbc4(4)=0.0
  R_vbc1(5)=0.0
  R_vbc2(5)=0.0
  R_vbc3(5)=0.0
  R_vbc4(5)=0.0
c-----Sixth Scalar value update
R_vbc1(6)=0.0
R_vbc2(6)=0.0
R_vbc3(6)=0.0
R_vbc4(6)=0.0

c-----Seventh Scalar value update
R_vbc1(7)=0.0
R_vbc2(7)=0.0
R_vbc3(7)=0.0
R_vbc4(7)=0.0

c-----Eighth Scalar value update
R_vbc1(8)=0.0
R_vbc2(8)=0.0
R_vbc3(8)=0.0
R_vbc4(8)=0.0

c-----Ninth Scalar value update
R_vbc1(9)=0.0
R_vbc2(9)=0.0
R_vbc3(9)=0.0
R_vbc4(9)=0.0

c-----Tenth Scalar value update
R_vbc1(10)=0.0
R_vbc2(10)=0.0
R_vbc3(10)=0.0
R_vbc4(10)=0.0

c-----Death of I_i for the birth of I_j
R_vbc1(I_i)=R_Xij(I_i,I_j)*R_CR(I_i,I_j)*R_v(I_j)

c-----Death of I_i that goes to I_i+1
IF
(I_i==I_j)
THEN
R_vbc2(I_i)=0.0
ELSE
R_vbc2(I_i)=(1.0-R_Xij(I_i,I_j))*R_CR(I_i,I_j)*R_v(I_i)
END IF

c-----Death of I_j that goes to I_i+1
R_vbc3(I_i)=(1.0-R_Xij(I_i,I_j))*R_CR(I_i,I_j)*R_v(I_j)

c-----Total death of I_j
R_vbc4(I_j)=R_vbc1(I_i)+ R_vbc3(I_i)

c-----Number of bubble update
R_tv(1)=R_tv(1)-(R_vbc2(1)+R_vbc4(1))
R_tv(2)=R_tv(2)-(R_vbc2(2)+R_vbc4(2))
R_tv(3)=R_tv(3)-(R_vbc2(3)+R_vbc4(3))
R_tv(4)=R_tv(4)-(R_vbc2(4)+R_vbc4(4))
R_tv(5)=R_tv(5)-(R_vbc2(5)+R_vbc4(5))
R_tv(6)=R_tv(6)-(R_vbc2(6)+R_vbc4(6))
R_tv(7)=R_tv(7)-(R_vbc2(7)+R_vbc4(7))
R_tv(8)=R_tv(8)-(R_vbc2(8)+R_vbc4(8))
R_tv(9)=R_tv(9)-(R_vbc2(9)+R_vbc4(9))
R_tv(10)=R_tv(10)-(R_vbc2(10)+R_vbc4(10))

c-----
R_nb(1)=R_tv(1)/R_v(1)
R_nb(2)=R_tv(2)/R_v(2)
R_nb(3)=R_tv(3)/R_v(3)
R_nb(4)=R_tv(4)/R_v(4)
R_nb(5)=R_tv(5)/R_v(5)
R_nb(6)=R_tv(6)/R_v(6)
R_nb(7)=R_tv(7)/R_v(7)
R_nb(8)=R_tv(8)/R_v(8)
R_nb(9)=R_tv(9)/R_v(9)
R_nb(10)=R_tv(10)/R_v(10)

R_DC(1)=R_DC(1)+R_vbc2(1)+R_vbc4(1)
R_DC(2)=R_DC(2)+R_vbc2(2)+R_vbc4(2)
R_DC(3)=R_DC(3)+R_vbc2(3)+R_vbc4(3)
R_DC(4)=R_DC(4)+R_vbc2(4)+R_vbc4(4)
R_DC(5)=R_DC(5)+R_vbc2(5)+R_vbc4(5)
R_DC(6)=R_DC(6)+R_vbc2(6)+R_vbc4(6)
R_DC(7)=R_DC(7)+R_vbc2(7)+R_vbc4(7)
R_DC(8)=R_DC(8)+R_vbc2(8)+R_vbc4(8)
R_DC(9)=R_DC(9)+R_vbc2(9)+R_vbc4(9)
R_DC(10)=R_DC(10)+R_vbc2(10)+R_vbc4(10)

R_BC(1)=R_BC(1)+R_vbc1(1)
R_BC(2)=R_BC(2)+R_vbc1(2)+R_vbc2(1)+R_vbc3(1)
R_BC(3)=R_BC(3)+R_vbc1(3)+R_vbc2(2)+R_vbc3(2)
R_BC(4)=R_BC(4)+R_vbc1(4)+R_vbc2(3)+R_vbc3(3)
R_BC(6)=R_BC(6)+R_vbc1(6)+R_vbc2(5)+R_vbc3(5)
R_BC(7)=R_BC(7)+R_vbc1(7)+R_vbc2(6)+R_vbc3(6)
R_BC(8)=R_BC(8)+R_vbc1(8)+R_vbc2(7)+R_vbc3(7)
R_BC(9)=R_BC(9)+R_vbc1(9)+R_vbc2(8)+R_vbc3(8)
R_BC(10)=R_BC(10)+R_vbc2(9)+R_vbc3(9)

R_BR(I_k,I_i)=R_cfq(I_k)*R_pb(I_k,I_i)
IF (R_ld.GE.R_d(I_k)) THEN
R_BR(I_k,I_i)=0.0
END IF

R_pb(I_k,l_i)=EXP(-R_chaiC(I_k))

R_cfq(I_k)=8.22e14*((R_d(I_k)+R_ld)**2.0)*vfm(ip2)*(edm(ip2)**2.0)*R_nb(I_k)
IF (R_cfq(I_k).GT.R_nb(I_k)) THEN
R_cfq(I_k)=R_nb(I_k)
END IF

R_br(I_k,l_i)=R_cfq(I_k)*R_pb(I_k,l_i)
IF (R_ld.GE.R_d(I_k)) THEN
R_BR(I_k,l_i)=0.0
END IF

DO I_i=1,9
DO I_k=I_i+1,10

R_dr(I_k)=R_d(I_k)/R_d(I_k)
R_Cf(I_k)=(R_dr(I_k)**2.0-1.0)+(1.0-(R_dr(I_k)**3.0)**0.666)
R_zita(I_k)=(11.4/R_d(I_k))*((edm(ip2)*vimm(ip2))**(-0.25))

R_chaiC(I_k)=(6.21e-05*R_Cf(I_k))/((edm(ip2)**0.666) *(R_d(I_k)**1.66)*(R_zita(I_k)**3.66))

R_pb(I_k,I_i)=EXP(-R_chaiC(I_k))

R_cfq(I_k)=8.22e14*((R_d(I_k)+R_ld)**2.0)*vfm(ip2)*(edm(ip2)**2.0)*R_nb(I_k)
IF (R_cfq(I_k).GT.R_nb(I_k)) THEN
R_cfq(I_k)=R_nb(I_k)
END IF

R_BR(I_k,I_i)=R_cfq(I_k)*R_pb(I_k,I_i)
IF (R_ld.GE.R_d(I_k)) THEN
R_BR(I_k,I_i)=0.0
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Scalar Value update for the birth of each bubble class due to death of other class
c----------------------------------------------------------------------------------------------------------------
R_vbb(1)=0.0
R_vbb(2)=0.0
R_vbb(3)=0.0
R_vbb(4)=0.0
R_vbb(5)=0.0
R_vbb(6)=0.0
R_vbb(7)=0.0
R_vbb(8)=0.0
R_vbb(9)=0.0
R_vbb(10)=0.0
R_vbb(I_i)=R_BR(I_k,I_i)*R_v(I_i)
c----------------------------------------------------------------------------------------------------------------
c-----Scalar Value update for the birth of each bubble class due to death of other class
c----------------------------------------------------------------------------------------------------------------
R_Xik(I_k,I_i)=(2.0)**(1.0+I_i-I_k)
c-----First Scalar value update
R_vbd1(1)=0.0
R_vbd(1)=0.0
c-----Second Scalar value update
R_vbd1(2)=0.0
R_vbd(2)=0.0
c-----Third Scalar value update
R_vbd1(3)=0.0
R_vbd(3)=0.0
c-----Fourth Scalar value update
R_vbd1(4)=0.0
R_vbd(4)=0.0
c-----Fifth Scalar value update
R_vbd1(5)=0.0
R_vbd(5)=0.0
c-----Sixth Scalar value update
R_vbd1(6)=0.0
R_vbd(6)=0.0
c-----Seventh Scalar value update
R_vbd1(7)=0.0
R_vbd(7)=0.0
c-----Eighth Scalar value update
R_vbd1(8)=0.0
R_vbd(8)=0.0
c-----Ninth Scalar value update
R_vbd1(9)=0.0
R_vbd(9)=0.0
c-----Tenth Scalar value update
R_vbd1(10)=0.0
R_vbd(10)=0.0
c-----Scalar of birth
R_vbd1(I_k)=R_BR(I_k,I_i)*R_v(I_i)
R_vbd(I_k)=R_Xik(I_k,I_i)*R_BR(I_k,I_i)*(R_v(I_k)-R_v(I_i))
c----------------------------------------------------------------------------------------------------------------
R_tv(1)=R_tv(1)-(R_vbd1(1)+R_vbd(1))
R_tv(2)=R_tv(2)-(R_vbd1(2)+R_vbd(2))
R_tv(3)=R_tv(3)-(R_vbd1(3)+R_vbd(3))
R_tv(4)=R_tv(4)-(R_vbd1(4)+R_vbd(4))
R_tv(5)=R_tv(5)-(R_vbd1(5)+R_vbd(5))
R_tv(6)=R_tv(6)-(R_vbd1(6)+R_vbd(6))
R_tv(7)=R_tv(7)-(R_vbd1(7)+R_vbd(7))
R_tv(8)=R_tv(8)-(R_vbd1(8)+R_vbd(8))
R_tv(9)=R_tv(9)-(R_vbd1(9)+R_vbd(9))
R_tv(10)=R_tv(10)-(R_vbd1(10)+R_vbd(10))

C----Number of bubble update
R_nb(1)=R_tv(1)/R_v(1)
R_nb(2)=R_tv(2)/R_v(2)
R_nb(3)=R_tv(3)/R_v(3)
R_nb(4)=R_tv(4)/R_v(4)
R_nb(5)=R_tv(5)/R_v(5)
R_nb(6)=R_tv(6)/R_v(6)
R_nb(7)=R_tv(7)/R_v(7)
R_nb(8)=R_tv(8)/R_v(8)
R_nb(9)=R_tv(9)/R_v(9)
R_nb(10)=R_tv(10)/R_v(10)

C----Birth
R_BB(1)=R_BB(1)+R_vbb(1)+R_vbd(2)
R_BB(2)=R_BB(2)+R_vbb(2)+R_vbd(3)
R_BB(3)=R_BB(3)+R_vbb(3)+R_vbd(4)
R_BB(4)=R_BB(4)+R_vbb(4)+R_vbd(5)
R_BB(5)=R_BB(5)+R_vbb(5)+R_vbd(6)
R_BB(6)=R_BB(6)+R_vbb(6)+R_vbd(7)
R_BB(7)=R_BB(7)+R_vbb(7)+R_vbd(8)
R_BB(8)=R_BB(8)+R_vbb(8)+R_vbd(9)
R_BB(9)=R_BB(9)+R_vbb(9)+R_vbd(10)
R_BB(10)=R_BB(10)+R_vbb(10)

C----Death
R_DB(1)=R_DB(1)+R_vbd1(1)+R_vbd(1)
R_DB(2)=R_DB(2)+R_vbd1(2)+R_vbd(2)
R_DB(3)=R_DB(3)+R_vbd1(3)+R_vbd(3)
R_DB(4)=R_DB(4)+R_vbd1(4)+R_vbd(4)
R_DB(5)=R_DB(5)+R_vbd1(5)+R_vbd(5)
R_DB(6)=R_DB(6)+R_vbd1(6)+R_vbd(6)
R_DB(7)=R_DB(7)+R_vbd1(7)+R_vbd(7)
R_DB(8)=R_DB(8)+R_vbd1(8)+R_vbd(8)
R_DB(9)=R_DB(9)+R_vbd1(9)+R_vbd(9)
R_DB(10)=R_DB(10)+R_vbd1(10)+R_vbd(10)

END DO
END DO
END IF

C----------------------------------------------------------------------------------------------------------------
R_foam(nc)=vfm(ip3)*vol(nc)*denm(ip3)
R_g(nc)=2.0*Phi_mscal((35-1)*ncell+nc)*vfm(ip3)*vol(nc)*denm(ip3)
R_lq_av(nc)=2.0*Phi_mscal((34-1)*ncell+nc)*vfm(ip3)*vol(nc)*denm(ip3)
C----------------------------------------------------------------------------------------------------------------
R_tDgbt(nc)=1.0e-35
R_lqt(nc)=1.0e-35
R_rg(nc)=1.0e-35
R_rlq(nc)=1.0e-35
C-----Transformation of gas and liquid into foam
IF(vfm(ip1).GE.0.75.AND.vfm(ip2).GE.0.05)THEN
C-----Transformation of gas bubbles to foam bubbles
R_tDgbt(nc)=0.999*vfm(ip1)*vol(nc)*denm(ip1)
R_rg(nc)=0.001*vfm(ip1)*vol(nc)*denm(ip1)
c-----Total liquid tranformation
R_lqt(nc)=0.0199*vfm(ip2)*vol(nc)*denm(ip2)
R_rlq(nc)=0.9801*vfm(ip2)*vol(nc)*denm(ip2)
R_rlq_m(nc)=0.1*0.1*vol(nc)*denm(ip2)
IF(R_rlq(nc).GE.R_rlq_m(nc))THEN
  R_rlq(nc)=R_rlq_m(nc)
END IF

R_C_final(nc)=1.0e-30
R_Fe_final(nc)=1.0e-30
R_Si_final(nc)=1.0e-30
R_Mn_final(nc)=1.0e-30
R_P_final(nc)=1.0e-30
ELSE
  R_tDgbt(nc)=1.0e-35
  R_lqt(nc)=1.0e-35
  R_rg(nc)=1.0e-35
  R_rlq(nc)=1.0e-35
END IF
R_g(nc)=R_g(nc)+R_tDgbt(nc)+R_rg(nc)
R_lq_av(nc)=R_lq_av(nc)+R_lqt(nc)+R_rlq(nc)
R_foam(nc)=R_foam(nc)+R_tDgbt(nc)+R_lqt(nc)+R_rg(nc)+R_rlq(nc)

IF(vfm(ip3).GT.vfrmin)THEN
  DO i_m=1,9
    DO i_i=1,i_m
      c-----Velocity of Drainage,R_cv=1,R_vd(I_i)=1.97e6*R_ap(I_i)
    END DO
  END DO
  c-----Bubble coalescence in foam
  c-----Film rupture inside foam
  c----------------------------------------------------------------------------------------------------------------
  c-----Probability of sharing the same film of bubble i and m
  R_FS(I_i,I_m)=R_nbf(I_i)/(R_nbf(1)+R_nbf(2)+R_nbf(3)+R_nbf(4)
  +R_nbf(5)+R_nbf(6)+R_nbf(7)+R_nbf(8)+R_nbf(9)+R_nbf(10))
  R_min_nbf(I_i,I_m)=min(R_nbf(I_i),R_nbf(I_m))
  c-----Coalescence rate of film
  R_crf(I_i,I_m)=5.78e05*(R_d(I_i)**2)*R_FS(I_i,I_m)
  IF(R_crf(I_i,I_m).GT.R_min_nbf(I_i,I_m))THEN
    R_crf(I_i,I_m)=R_min_nbf(I_i,I_m)
  END IF
  R_Xijf(I_i,I_m)=(1.0)-((2.0)**(I_m-I_i))
  c----------------------------------------------------------------------------------------------------------------
  c-----Scalar Value update for each bubble class
  c-----First Scalar value update
  R_vbcf1(1)=0.0
  R_vbcf2(1)=0.0
  R_vbcf3(1)=0.0
  R_vbcf4(1)=0.0
  c-----Second Scalar value update
  R_vbcf1(2)=0.0
  R_vbcf2(2)=0.0
  R_vbcf3(2)=0.0
  R_vbcf4(2)=0.0
  c-----Third Scalar value update
  R_vbcf1(3)=0.0
  R_vbcf2(3)=0.0
R_vbctf(7)=R_vbcf2(7)+R_vbcf4(7)  
R_vbctf(8)=R_vbcf2(8)+R_vbcf4(8)  
R_vbctf(9)=R_vbcf2(9)+R_vbcf4(9)  
R_vbctf(10)=R_vbcf2(10)+R_vbcf4(10)

IF(R_vbctf(I_i).GT.R_tvf(I_i))THEN 
  R_vbctf(I_i)=R_tvf(I_i)
END IF

IF(R_vbctf(I_m).GT.R_tvf(I_m))THEN 
  R_vbctf(I_m)=R_tvf(I_m)
END IF

c-----Scalar Value update for the birth of each bubble class due to death of other class

c-----Number of bubble update
R_tvf(1)=R_tvf(1)-R_vbctf(1)  
R_tvf(2)=R_tvf(2)-R_vbctf(2)  
R_tvf(3)=R_tvf(3)-R_vbctf(3)  
R_tvf(4)=R_tvf(4)-R_vbctf(4)  
R_tvf(5)=R_tvf(5)-R_vbctf(5)  
R_tvf(6)=R_tvf(6)-R_vbctf(6)  
R_tvf(7)=R_tvf(7)-R_vbctf(7)  
R_tvf(8)=R_tvf(8)-R_vbctf(8)  
R_tvf(9)=R_tvf(9)-R_vbctf(9)  
R_tvf(10)=R_tvf(10)-R_vbctf(10)

c-----Death due to coalescence

R_DCF(1)=R_DCF(1)+R_vbcf2(1)+R_vbcf4(1)  
R_DCF(2)=R_DCF(2)+R_vbcf2(2)+R_vbcf4(2)  
R_DCF(3)=R_DCF(3)+R_vbcf2(3)+R_vbcf4(3)  
R_DCF(4)=R_DCF(4)+R_vbcf2(4)+R_vbcf4(4)  
R_DCF(5)=R_DCF(5)+R_vbcf2(5)+R_vbcf4(5)  
R_DCF(6)=R_DCF(6)+R_vbcf2(6)+R_vbcf4(6)  
R_DCF(7)=R_DCF(7)+R_vbcf2(7)+R_vbcf4(7)  
R_DCF(8)=R_DCF(8)+R_vbcf2(8)+R_vbcf4(8)  
R_DCF(9)=R_DCF(9)+R_vbcf2(9)+R_vbcf4(9)  
R_DCF(10)=R_DCF(10)+R_vbcf2(10)+R_vbcf4(10)

c-----Birth due to coalescence and transformation

R_BCF(1)=R_BCF(1)+R_vbcf1(1)  
R_BCF(2)=R_BCF(2)+R_vbcf1(2)+R_vbcf2(1)+R_vbcf3(1)  
R_BCF(3)=R_BCF(3)+R_vbcf1(3)+R_vbcf2(2)+R_vbcf3(2)  
R_BCF(4)=R_BCF(4)+R_vbcf1(4)+R_vbcf2(3)+R_vbcf3(3)  
R_BCF(5)=R_BCF(5)+R_vbcf1(5)+R_vbcf2(4)+R_vbcf3(4)  
R_BCF(6)=R_BCF(6)+R_vbcf1(6)+R_vbcf2(5)+R_vbcf3(5)  
R_BCF(7)=R_BCF(7)+R_vbcf1(7)+R_vbcf2(6)+R_vbcf3(6)  
R_BCF(8)=R_BCF(8)+R_vbcf1(8)+R_vbcf2(7)+R_vbcf3(7)  
R_BCF(9)=R_BCF(9)+R_vbcf1(9)+R_vbcf2(8)+R_vbcf3(8)  
R_BCF(10)=R_BCF(10)+R_vbcf2(10)+R_vbcf3(10)

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R_BCF(5)=R_BCF(5)+R_vbcf1(5)+R_vbcf2(4)+R_vbcf3(4)
R_BCF(6)=R_BCF(6)+R_vbcf1(6)+R_vbcf2(5)+R_vbcf3(5)
R_BCF(7)=R_BCF(7)+R_vbcf1(7)+R_vbcf2(6)+R_vbcf3(6)
R_BCF(8)=R_BCF(8)+R_vbcf1(8)+R_vbcf2(7)+R_vbcf3(7)
R_BCF(9)=R_BCF(9)+R_vbcf1(9)+R_vbcf2(8)+R_vbcf3(8)
R_BCF(10)=R_BCF(10)+R_vbcf2(9)+R_vbcf3(9)
END DO
END DO
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Liquid in foam calculation

R_g(nc)=R_g(nc)+R_tDgbt(nc)+R_rg(nc)
R_lq_av(nc)=R_lq_av(nc)+R_lqt(nc)+R_rlq(nc)
R_foam(nc)=R_foam(nc)+R_tDgbt(nc)+R_lqt(nc)+R_rg(nc)+R_rlq(nc)
IF(R_foam(nc).GE.vfrmin)THEN
  R_lq_r(nc)=R_lq_av(nc)/R_foam(nc)
  IF(R_lq_r(nc).LT.1.0e-30)THEN
    R_lq_r(nc)=1.0
  END IF
  IF(R_lq_r(nc).GE.1.0)THEN
    R_lq_r(nc)=1.0
  END IF
ELSE
  R_lq_r(nc)=1.0e-35
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Drainage of foam.

IF(vfm(ip3).GT.vfrmin.AND.R_lq_r(nc).GE.0.1)THEN
  R_k(nc)=6.7e-04*0.0074*R_lq_r(nc)**(1.5)
  R_drain(nc)=3.12e-08*9.81*6980*R_k(nc)/6.1e-03
  IF(R_drain(nc).GT.R_lq_av(nc))THEN
    R_drain(nc)=R_lq_av(nc)
  END IF
  IF(R_drain(nc).LT.0.0)THEN
    R_drain(nc)=1.0e-35
  END IF
ELSE
  R_drain(nc)=1.0e-35
END IF

c-------------------------------
R_g(nc)=R_g(nc)
R_lq_av(nc)=R_lq_av(nc)-R_drain(nc)
R_foam(nc)=R_foam(nc)-R_drain(nc)
IF(R_foam(nc).LT.1.0e-30)THEN
  R_foam(nc)=1.0e-30
END IF
IF(R_foam(nc).GE.vfrmin)THEN
  R_lq_r(nc)=R_lq_av(nc)/R_foam(nc)
  IF(R_lq_r(nc).LT.1.0e-30)THEN
    R_lq_r(nc)=1.0
  END IF
  IF(R_lq_r(nc).GE.1.0)THEN
    R_lq_r(nc)=1.0
  END IF
ELSE
  R_lq_r(nc)=1.0e-35
END IF
ELSE
R_lq_r(nc)=1.0e-35
END IF

IF(vfm(ip3).GE.0.15.AND.R_lq_r(nc).LT.0.1) THEN

c-----Mass transfer
R_lq_f(nc)=0.0283*vfm(ip3)*vol(nc)*denm(ip3)
IF(R_lq_f(nc).GT.R_lq_av(nc)) THEN
R_lq_f(nc)=R_lq_av(nc)
END IF
R_tdgf(nc)=0.699*vfm(ip3)*vol(nc)*denm(ip3)
R_g_av(nc)=R_g(nc)
IF(R_tdgf(nc).GT.R_g_av(nc)) THEN
R_tdgf(nc)=R_g_av(nc)
END IF

R_g(nc)=R_g(nc)-R_tdgf(nc)
R_lq_av(nc)=R_lq_av(nc)-R_lq_f(nc)
R_foam(nc)=R_foam(nc)-R_tdgf(nc)-R_lq_f(nc)
IF(R_foam(nc).LT.1.0e-30) THEN
R_foam(nc)=1.0e-30
END IF

IF(R_foam(nc).GT.1.0e-20) THEN
R_gf(nc)=0.5*(R_g(nc)/R_foam(nc))
END IF
IF(R_gf(nc).GT.0.45) THEN
R_gf(nc)=0.45
END IF
R_S(23,nc)=(0.5-R_gf(nc))-Phi_mscal((34-1)*ncell+nc)
R_S(24,nc)=R_gf(nc)-Phi_mscal((35-1)*ncell+nc)

ELSE
R_lq_f(nc)=1.0e-35
R_tdgf(nc)=1.0e-35
R_g(nc)=R_g(nc)
R_lq_av(nc)=R_lq_av(nc)
R_foam(nc)=R_foam(nc)
IF(R_foam(nc).LT.1.0e-30) THEN
R_foam(nc)=1.0e-30
END IF

IF(R_foam(nc).GT.1.0e-20) THEN
R_gf(nc)=0.5*(R_g(nc)/R_foam(nc))
END IF
IF(R_gf(nc).GT.0.45) THEN
R_gf(nc)=0.45
END IF
R_S(23,nc) = (0.5 - R_gf(nc)) - Phi_mscal((34-1)*ncell+nc)
R_S(24,nc) = R_gf(nc) - Phi_mscal((35-1)*ncell+nc)

--- Foam and liquid for mph
R_fm_lq(nc) = R_drain(nc)
R_lq_fm(nc) = R_lqt(nc) + R_rltq(nc)

--- Liquid and gas

--- Foam and gas for mph
R_fm_g(nc) = (1.0e-20)
R_g_fm(nc) = R_tDgbt(nc) + R_rg(nc)
END IF

IF (vfm(ip2) .LE. vfrmin.AND.vfm(ip3).GE.0.15) THEN
R_gfr(nc) = R_gf(nc)
ELSE
R_gfr(nc) = 0.45
END IF

--- Variable description
R_Fe_b(nc) = Phi_mscal((14-1)*ncell+nc)
R_C_b(nc) = Phi_mscal((15-1)*ncell+nc)
R_Si_b(nc) = Phi_mscal((16-1)*ncell+nc)
R_Mn_b(nc) = Phi_mscal((17-1)*ncell+nc)
R_P_b(nc) = Phi_mscal((18-1)*ncell+nc)
R_Fe_b1(nc) = R_Fe_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)
R_C_b1(nc) = R_C_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)
R_Si_b1(nc) = R_Si_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)
R_Mn_b1(nc) = R_Mn_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)
R_P_b1(nc) = R_P_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)
R_FeO_b(nc) = Phi_mscal((19-1)*ncell+nc)
R_SiO2_b(nc) = Phi_mscal((20-1)*ncell+nc)
R_P2O5_b(nc) = Phi_mscal((21-1)*ncell+nc)
R_MnO_b(nc) = Phi_mscal((22-1)*ncell+nc)
R_S_b(nc) = Phi_mscal((23-1)*ncell+nc)
R_FeO_b1(nc) = R_FeO_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)
R_SiO2_b1(nc) = R_SiO2_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)
R_P2O5_b1(nc) = R_P2O5_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)
R_MnO_b1(nc) = R_MnO_b(nc) * vfm(ip2) * vol(nc) * denm(ip2)

--- Reacted element masses initialization
R_L_av_C(nc) = 1.0e-30
R_L_av_Fe(nc) = 1.0e-30
R_L_av_P(nc) = 1.0e-30
R_L_av_Si(nc) = 1.0e-30
R_L_av_Mn(nc) = 1.0e-30
R_L_av_FeO(nc) = 1.0e-30
R_L_av_MnO(nc) = 1.0e-30
R_L_av_SiO2(nc) = 1.0e-30
R_L_av_P2O5(nc) = 1.0e-30
c----------------------------------------------------------------------------------------------------------------
R_O2_av_g(nc)=2.0*Phi_mscal((11-1)*ncell+nc)*vfm(ip1)*vol(nc)*denm(ip1)
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between gas and liquid
c-----Amount of silicon and oxygen for reaction in gas and liquid
c----------------------------------------------------------------------------------------------------------------
R_Si_Fickrate(nc)=(0.00407)*((R_Si_b(nc)-0.00001)*vfm(ip2)*vol(nc)*denm(ip2))
IF(R_Si_Fickrate(nc).LE.1.0e-30)THEN
R_Si_Fickrate(nc)=1.0e-30
END IF
R_O2_av_g(nc)=Phi_mscal((11-1)*ncell+nc)*vfm(ip1)*vol(nc)*denm(ip1)
IF(R_O2_av_g(nc).LE.1.0e-30)THEN
R_O2_av_g(nc)=1.0e-30
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Silicon and Oxygen
c----------------------------------------------------------------------------------------------------------------
R_Si_av_l(nc)=R_Si_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_Si_req_O2=R_O2_av_g(nc)*(0.875)
IF (R_Si_req_O2.GT.R_Si_av_l(nc)) THEN
R_Si_used_O2(nc)=R_Si_av_l(nc)
ELSE
R_Si_used_O2(nc)=R_Si_req_O2
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Amount of carbon and oxygen for reaction in gas and liquid
c----------------------------------------------------------------------------------------------------------------
R_C_Fickrate(nc)=(0.00164)*(R_C_b(nc)-0.000703)*vfm(ip2)*vol(nc)*denm(ip2)
IF(R_C_Fickrate(nc).LE.1.0e-30)THEN
R_C_Fickrate(nc)=1.0e-30
END IF
R_O2_av_g(nc)=R_O2_av_g(nc)-(1.14*R_Si_used_O2(nc))
IF(R_O2_av_g(nc).LE.1.0e-30)THEN
R_O2_av_g(nc)=1.0e-30
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Carbon and Oxygen
c----------------------------------------------------------------------------------------------------------------
R_C_av_l(nc)=R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_C_req_O2 =R_O2_av_g(nc)*(0.75)
IF (R_C_req_O2.GT.R_C_av_l(nc)) THEN
R_C_used_O2(nc)=R_C_av_l(nc)
ELSE
R_C_used_O2(nc)=R_C_req_O2
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Post combustion of CO to CO2
c----------------------------------------------------------------------------------------------------------------
IF(TIME.GE.0.3e+03) THEN
R_CO_used_O2(nc)=(1.0e-20)
ELSE
R_CO_used_O2(nc)=(1.33*(100-(0.333*TIME)))*R_C_used_O2(nc)
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between gas and liquid
c-----Amount of Manganese and oxygen for reaction in gas and liquid
IF (R_FeO_b(nc).LE.1.0e-30) THEN
  R_FeO_b(nc)=1.0e-30
END IF
R_Mn_eq=(R_MnO_b(nc)/((R_FeO_b(nc))*11.427))
R_Mn_Fickrate(nc)=(0.021364)*(R_Mn_b(nc)-R_Mn_eq)*(vfm(ip2)*vol(nc)*denm(ip2))
IF (R_Mn_Fickrate(nc).LE.1.0e-30) THEN
  R_Mn_Fickrate(nc)=1.0e-30
END IF
R_O2_av_g(nc)=R_O2_av_g(nc)-(1.33*R_C_used_O2(nc))-(0.57*R_CO_used_O2(nc))
IF (R_O2_av_g(nc).LE.1.0e-30) THEN
  R_O2_av_g(nc)=1.0e-30
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Manganese and Oxygen

c----------------------------------------------------------------------------------------------------------------
R_Mn_av_l(nc)=R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_Mn_req_O2=R_O2_av_g(nc)*(3.4375)
IF (R_Mn_req_O2.GT.R_Mn_av_l(nc)) THEN
  R_Mn_used_O2(nc)=R_Mn_av_l(nc)
ELSE
  R_Mn_used_O2(nc)=R_Mn_req_O2
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between gas and liquid

c-----Chemical reaction between Phosphorous and Oxygen

c-----Chemical reaction between gas and liquid

R_P_eq_1=(2.5*log10(R_FeO_b(nc)))+(0.5*log10(R_P2O5_b(nc)))-7.36
R_P_eq_2=10.0**(R_P_eq_1)
IF (R_P_eq_2.LE.0.02) THEN
  R_P_eq_2=0.02
END IF
R_P_eq=(0.437*R_P2O5_b(nc))/R_P_eq_2
IF (R_P_eq.LE.0.00018) THEN
  R_P_eq=0.00018
END IF
R_P_Fickrate(nc)=(0.047101)*(R_P_b(nc)-R_P_eq)*vfm(ip2)*vol(nc)*denm(ip2)
IF (R_P_Fickrate(nc).LE.1.0e-30) THEN
  R_P_Fickrate(nc)=1.0e-30
END IF
R_O2_av_g(nc)=R_O2_av_g(nc)-(0.29*R_Mn_used_O2(nc))
IF (R_O2_av_g(nc).LE.1.0e-30) THEN
  R_O2_av_g(nc)=1.0e-30
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Phosphorous and Oxygen

c----------------------------------------------------------------------------------------------------------------
R_P_av_l(nc)=R_P_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_P_req_O2=R_O2_av_g(nc)*(0.775)
IF (R_P_req_O2.GT.R_P_av_l(nc)) THEN
  R_P_used_O2(nc)=R_P_av_l(nc)
ELSE
  R_P_used_O2(nc)=R_P_req_O2
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between gas and liquid
!Amount of Iron and oxygen for reaction in gas and liquid

\[ R_{O2\text{, av, g}}(nc) = R_{O2\text{, av, g}}(nc) - (1.29 * R_{P\text{, used, O2}}(nc)) \]

\[ \text{IF } (R_{O2\text{, av, g}}(nc) \leq 1.0e-30) \text{ THEN } \]
\[ R_{O2\text{, av, g}}(nc) = 1.0e-30 \]
\[ \text{END IF} \]

\[ R_{Fe\text{, Fickrate}}(nc) = (R_{O2\text{, av, g}}(nc) - R_{Mn\text{, used, O2}}(nc) - R_{P\text{, used, O2}}(nc) - R_{C\text{, used, O2}}(nc) - R_{Si\text{, used, O2}}(nc)) * 112/32 \]

\[ \text{IF } (R_{Fe\text{, Fickrate}}(nc) \leq 1.0e-30) \text{ THEN } \]
\[ R_{Fe\text{, Fickrate}}(nc) = 1.0e-30 \]
\[ \text{END IF} \]

\[ \text{Chemical reaction between Iron and Oxygen} \]

\[ R_{Fe\text{, av, l}}(nc) = R_{Fe\text{, b}}(nc) * vfm(ip2) * vol(nc) * denm(ip2) \]
\[ R_{Fe\text{, req, O2}} = R_{O2\text{, av, g}}(nc) * 3.50 \]

\[ \text{IF } (R_{Fe\text{, req, O2}} > R_{Fe\text{, av, l}}(nc)) \text{ THEN } \]
\[ R_{Fe\text{, used, O2}}(nc) = R_{Fe\text{, av, l}}(nc) \]
\[ \text{ELSE} \]
\[ R_{Fe\text{, used, O2}}(nc) = R_{Fe\text{, req, O2}} \]
\[ \text{END IF} \]

\[ \text{Chemical reaction between Silicon and P2O5} \]

\[ R_{Si\text{, av, l}}(nc) = R_{Si\text{, av, l}}(nc) - R_{Si\text{, used, O2}}(nc) \]

\[ \text{IF } (R_{Si\text{, av, l}}(nc) \leq 1.0e-30) \text{ THEN } \]
\[ R_{Si\text{, av, l}}(nc) = 1.0e-30 \]
\[ \text{END IF} \]

\[ R_{P2O5\text{, av, l}}(nc) = R_{P2O5\text{, b}}(nc) * vfm(ip2) * vol(nc) * denm(ip2) + (2.29 * R_{P\text{, used, O2}}(nc)) \]

\[ \text{IF } (R_{P2O5\text{, av, l}}(nc) \leq 1.0e-30) \text{ THEN } \]
\[ R_{P2O5\text{, av, l}}(nc) = 1.0e-30 \]
\[ \text{END IF} \]

\[ R_{Si\text{, req, P2O5}} = R_{P2O5\text{, av, l}}(nc) * 0.493 \]

\[ \text{IF } (R_{Si\text{, req, P2O5}} > R_{Si\text{, av, l}}(nc)) \text{ THEN } \]
\[ R_{Si\text{, used, P2O5}(nc) = R_{Si\text{, av, l}}(nc) \]
\[ \text{ELSE} \]
\[ R_{Si\text{, used, P2O5}(nc) = R_{Si\text{, req, P2O5}} \]
\[ \text{END IF} \]

\[ \text{Chemical reaction between Carbon and P2O5} \]

\[ R_{C\text{, av, l}}(nc) = R_{C\text{, av, l}}(nc) - R_{C\text{, used, O2}}(nc) \]

\[ \text{IF } (R_{C\text{, av, l}}(nc) \leq 1.0e-30) \text{ THEN } \]
\[ R_{C\text{, av, l}}(nc) = 1.0e-30 \]
\[ \text{END IF} \]

\[ R_{P2O5\text{, av, l}}(nc) = R_{P2O5\text{, av, l}}(nc) - (R_{Si\text{, used, P2O5}(nc) * 2.03}) \]

\[ \text{IF } (R_{P2O5\text{, av, l}}(nc) \leq 1.0e-30) \text{ THEN } \]
\[ R_{P2O5\text{, av, l}}(nc) = 1.0e-30 \]
\[ \text{END IF} \]

\[ R_{C\text{, req, P2O5}} = R_{P2O5\text{, av, l}}(nc) * 0.423 \]

\[ \text{IF } (R_{C\text{, req, P2O5}} > R_{C\text{, av, l}}(nc)) \text{ THEN } \]
\[ R_{C\text{, used, P2O5}(nc) = R_{C\text{, av, l}}(nc) \]
\[ \text{ELSE} \]
\[ R_{C\text{, used, P2O5}(nc) = R_{C\text{, req, P2O5}} \]
\[ \text{END IF} \]
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Manganese and P2O5
R_Mn_av_l(nc)=R_Mn_av_l(nc)-R_Mn_used_O2(nc)
IF(R_Mn_av_l(nc).LE.1.0e-30)THEN
  R_Mn_av_l(nc)=1.0e-30
END IF
R_P2O5_av_l(nc)=R_P2O5_av_l(nc)-(R_C_used_P2O5(nc)*2.37)
IF(R_P2O5_av_l(nc).LE.1.0e-30)THEN
  R_P2O5_av_l(nc)=1.0e-30
END IF
R_Mn_req_P2O5=R_P2O5_av_l(nc)*(1.937)
IF(R_Mn_req_P2O5.GT.R_Mn_av_l(nc))THEN
  R_Mn_used_P2O5(nc)=R_Mn_av_l(nc)
ELSE
  R_Mn_used_P2O5(nc)=R_Mn_req_P2O5
END IF

R_Si_av_l(nc)=R_Si_av_l(nc)-R_Si_used_P2O5(nc)
IF(R_Si_av_l(nc).LE.1.0e-30)THEN
  R_Si_av_l(nc)=1.0e-30
END IF
R_FeO_av_l(nc)=R_FeO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+(1.29*R_Fe_used_O2(nc))
IF(R_FeO_av_l(nc).LE.1.0e-30)THEN
  R_FeO_av_l(nc)=1.0e-30
END IF
R_Si_req_FeO=R_FeO_av_l(nc)*(0.194)
IF(R_Si_req_FeO.GT.R_Si_av_l(nc))THEN
  R_Si_used_FeO(nc)=R_Si_av_l(nc)
ELSE
  R_Si_used_FeO(nc)=R_Si_req_FeO
END IF

R_C_av_l(nc)=R_C_av_l(nc)-R_C_used_P2O5(nc)
IF(R_C_av_l(nc).LE.1.0e-30)THEN
  R_C_av_l(nc)=1.0e-30
END IF
R_Fe_av_l(nc)=R_Fe_av_l(nc)+(R_Si_used_FeO(nc)*4.0)-R_Fe_used_O2(nc)
IF(R_Fe_av_l(nc).LE.1.0e-30)THEN
  R_Fe_av_l(nc)=1.0e-30
END IF
R_P2O5_av_l(nc)=R_P2O5_av_l(nc)-(0.516*R_Mn_used_P2O5(nc))
IF(R_P2O5_av_l(nc).LE.1.0e-30)THEN
  R_P2O5_av_l(nc)=1.0e-30
END IF
R_Fe Req_P2O5=R_P2O5_av_l(nc)*(1.97)
IF(R_Fe Req_P2O5.GT.R_Fe_av_l(nc))THEN
  R_Fe_used_P2O5(nc)=R_Fe_av_l(nc)
ELSE
  R_Fe_used_P2O5(nc)=R_Fe Req_P2O5
END IF

R_C av_l(nc)=R_C av_l(nc)-R_C used_P2O5(nc)
IF(R_C av_l(nc).LE.1.0e-30)THEN
R_C_av_l(nc)=1.0e-30
END IF
R_FeO_av_l(nc)=R_FeO_av_l(nc)+(R_Fe_used_P2O5(nc)*1.29)-(R_Si_used_FeO(nc)*5.14)
IF(R_FeO_av_l(nc).LE.1.0e-30) THEN
R_FeO_av_l(nc)=1.0e-30
END IF
R_C_req_FeO=R_FeO_av_l(nc)*0.167
IF(R_C_req_FeO.GT.R_C_av_l(nc)) THEN
R_C_used_FeO(nc)=R_C_av_l(nc)
ELSE
R_C_used_FeO(nc)=R_C_req_FeO
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Silicon and MnO
c----------------------------------------------------------------------------------------------------------------
R_Si_av_l(nc)=R_Si_av_l(nc)-R_Si_used_FeO(nc)
IF(R_Si_av_l(nc).LE.1.0e-30) THEN
R_Si_av_l(nc)=1.0e-30
END IF
R_MnO_av_l(nc)=R_MnO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+1.29*R_Mn_used_P2O5(nc)+1.29*R_Mn_used_O2(nc)
IF(R_MnO_av_l(nc).LE.1.0e-30) THEN
R_MnO_av_l(nc)=1.0e-30
END IF
R_Si_req_MnO=R_MnO_av_l(nc)*(0.197)
IF(R_Si_req_MnO.GT.R_Si_av_l(nc)) THEN
R_Si_used_MnO(nc)=R_Si_av_l(nc)
ELSE
R_Si_used_MnO(nc)=R_Si_req_MnO
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Carbon and MnO
c----------------------------------------------------------------------------------------------------------------
R_C_av_l(nc)=R_C_av_l(nc)-R_C_used_FeO(nc)
IF(R_C_av_l(nc).LE.1.0e-30) THEN
R_C_av_l(nc)=1.0e-30
END IF
R_MnO_av_l(nc)=R_MnO_av_l(nc)-(5.07*R_Si_used_MnO(nc))
IF(R_MnO_av_l(nc).LE.1.0e-30) THEN
R_MnO_av_l(nc)=1.0e-30
END IF
R_C_req_MnO=R_MnO_av_l(nc)*0.169
IF(R_C_req_MnO.GT.R_C_av_l(nc)) THEN
R_C_used_MnO(nc)=R_C_av_l(nc)
ELSE
R_C_used_MnO(nc)=R_C_req_MnO
END IF
c----------------------------------------------------------------------------------------------------------------
c-----Chemical reaction between Manganese and FeO
c----------------------------------------------------------------------------------------------------------------
R_Mn_av_l(nc)=R_Mn_av_l(nc)+(R_C_used_MnO(nc)*4.58)+R_Si_used_MnO(nc)*3.93)-R_Mn_used_P2O5(nc)
IF(R_Mn_av_l(nc).LE.1.0e-30) THEN
R_Mn_av_l(nc)=1.0e-30
END IF
R_FeO_av_l(nc)=R_FeO_av_l(nc)-(R_C_used_FeO(nc)*6.0)
IF(R_FeO_av_l(nc).LE.1.0e-30) THEN
  R_FeO_av_l(nc)=1.0e-30
END IF
R_Mn_req_FeO=R_FeO_av_l(nc)*(0.764)
IF(R_Mn_req_FeO.GT.R_Mn_av_l(nc)) THEN
  R_Mn_used_FeO(nc)=R_Mn_av_l(nc)
ELSE
  R_Mn_used_FeO(nc)=R_Mn_req_FeO
END IF

c----------------------------------------------------------------------------------------------------------------
c-----Finalising the amount of Carbon reacted.
c----------------------------------------------------------------------------------------------------------------
R_CRate=(R_C_used_O2(nc)+R_C_used_P2O5(nc)+R_C_used_FeO(nc)+R_C_used_MnO(nc))
R_C_final(nc)=min(R_CRate,R_C_Fickrate(nc))
IF(R_C_final(nc).LE.1.0e-30) THEN
  R_C_final(nc)=1.0e-30
END IF
R_C_final_1=R_C_final(nc)

C-----Finalising the effect of Carbon reacted on other compounds.
C-----
IF (R_C_used_O2(nc).GT.R_C_final_1) THEN
  R_C_O2(nc)=R_C_final_1
ELSE
  R_C_O2(nc)=R_C_used_O2(nc)
END IF
R_C_final_2=R_C_final_1-R_C_O2(nc)
IF (R_C_used_P2O5(nc).GT.R_C_final_2) THEN
  R_C_P2O5(nc)=R_C_final_2
ELSE
  R_C_P2O5(nc)=R_C_used_P2O5(nc)
END IF
R_C_final_3=R_C_final_2-R_C_P2O5(nc)
IF (R_C_used_FeO(nc).GT.R_C_final_3) THEN
  R_C_FeO(nc)=R_C_final_3
ELSE
  R_C_FeO(nc)=R_C_used_FeO(nc)
END IF
R_C_final_4=R_C_final_3-R_C_FeO(nc)
IF (R_C_used_MnO(nc).GT.R_C_final_4) THEN
  R_C_MnO(nc)=R_C_final_4
ELSE
  R_C_MnO(nc)=R_C_used_MnO(nc)
END IF
R_c_rate(nc)=R_C_O2(nc)

C----------------------------------------------------------------------------------------------------------------
c-----Finalising the amount of Silicon reacted.
c----------------------------------------------------------------------------------------------------------------
R_SiRate=(R_Si_used_O2(nc)+R_Si_used_P2O5(nc)+R_Si_used_FeO(nc)+R_Si_used_MnO(nc))
R_Si_final(nc)=min(R_SiRate,R_Si_Fickrate(nc))
IF(R_Si_final(nc).LE.1.0e-30) THEN
  R_Si_final(nc)=0.0
END IF
R_Si_final_1=R_Si_final(nc)

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IF (R_Si_used_O2(nc).GT.R_Si_final_1) THEN
R_Si_O2(nc)=R_Si_final_1
ELSE
R_Si_O2(nc)=R_Si_used_O2(nc)
END IF

----------------------------------------------------------------------------------------------------------------

R_Si_final_2=R_Si_final_1-R_Si_O2(nc)
IF (R_Si_used_P2O5(nc).GT.R_Si_final_2) THEN
R_Si_P2O5(nc)=R_Si_final_2
ELSE
R_Si_P2O5(nc)=R_Si_used_P2O5(nc)
END IF

----------------------------------------------------------------------------------------------------------------

R_Si_final_3=R_Si_final_2-R_Si_P2O5(nc)
IF (R_Si_used_FeO(nc).GT.R_Si_final_3) THEN
R_Si_FeO(nc)=R_Si_final_3
ELSE
R_Si_FeO(nc)=R_Si_used_FeO(nc)
END IF

----------------------------------------------------------------------------------------------------------------

R_Si_final_4=R_Si_final_3-R_Si_FeO(nc)
IF (R_Si_used_MnO(nc).GT.R_Si_final_4) THEN
R_Si_MnO(nc)=R_Si_final_4
ELSE
R_Si_MnO(nc)=R_Si_used_MnO(nc)
END IF

----------------------------------------------------------------------------------------------------------------

R_Fe_rate=(R_Fe_used_O2(nc)+R_Fe_used_P2O5(nc))
R_Fe_final(nc)=min(R_Fe_rate,R_Fe_Fickrate(nc))
IF (R_Fe_final(nc).LE.1.0e-30) THEN
R_Fe_final(nc)=1.0e-30
END IF

----------------------------------------------------------------------------------------------------------------

IF (R_Fe_used_O2(nc).GT.R_Fe_final_1) THEN
R_Fe_O2(nc)=R_Fe_final_1
ELSE
R_Fe_O2(nc)=R_Fe_used_O2(nc)
END IF

----------------------------------------------------------------------------------------------------------------

R_Fe_final_2=R_Fe_final_1-R_Fe_O2(nc)
IF (R_Fe_used_P2O5(nc).GT.R_Fe_final_2) THEN
R_Fe_P2O5(nc)=R_Fe_final_2
ELSE
R_Fe_P2O5(nc)=R_Fe_used_P2O5(nc)
END IF

----------------------------------------------------------------------------------------------------------------
c-----Finalising the amount of Phosphorous reacted.
c----------------------------------------------------------------------------------------------------------------
R_PRate=R_P_used_O2(nc)
R_P_final(nc)=min(R_PRate,R_P_Fickrate(nc))
IF(R_P_final(nc).LE.1.0e-30)THEN
R_P_final(nc)=1.0e-30
END IF
R_P_final(nc)=R_P_O2(nc)
c----------------------------------------------------------------------------------------------------------------
c-----Finalising the amount of Manganese reacted.
c----------------------------------------------------------------------------------------------------------------
R_MnRate=(R_Mn_used_O2(nc)+R_Mn_used_P2O5(nc)+R_Mn_used_FeO(nc))
R_Mn_final(nc)=min(R_MnRate,R_Mn_Fickrate(nc))
IF(R_Mn_final(nc).LE.1.0e-30)THEN
R_Mn_final(nc)=1.0e-30
END IF
R_Mn_final_1=R_Mn_final(nc)
c----------------------------------------------------------------------------------------------------------------
c-----Finalising the effect of Manganese reacted on other compounds.
c----------------------------------------------------------------------------------------------------------------
IF (R_Mn_used_O2(nc).GT.R_Mn_final_1) THEN
R_Mn_O2(nc)=R_Mn_final_1
ELSE
R_Mn_O2(nc)=R_Mn_used_O2(nc)
END IF
R_Mn_final_2=R_Mn_final_1-R_Mn_O2(nc)
IF (R_Mn_used_P2O5(nc).GT.R_Mn_final_2) THEN
R_Mn_P2O5(nc)=R_Mn_final_2
ELSE
R_Mn_P2O5(nc)=R_Mn_used_P2O5(nc)
END IF
R_Mn_final_3=R_Mn_final_2-R_Mn_P2O5(nc)
IF (R_Mn_used_FeO(nc).GT.R_Mn_final_3) THEN
R_Mn_FeO(nc)=R_Mn_final_3
ELSE
R_Mn_FeO(nc)=R_Mn_used_FeO(nc)
END IF
ELSE
R_C_FeO(nc)=1.0e-30
R_Si_FeO(nc)=1.0e-30
R_Mn_FeO(nc)=1.0e-30
R_Si_MnO(nc)=1.0e-30
R_C_MnO(nc)=1.0e-30
R_C_P2O5(nc)=1.0e-30
R_Si_P2O5(nc)=1.0e-30
R_Fe_P2O5(nc)=1.0e-30
R_Mn_P2O5(nc)=1.0e-30
R_C_final(nc)=1.0e-30
R_Fe_final(nc)=1.0e-30
R_Si_final(nc)=1.0e-30
R_Mn_final(nc)=1.0e-30
R_P_final(nc)=1.0e-30
R_c_rate(nc)=1.0e-30
END IF

R_L_av_C(nc)=R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)-R_C_final(nc)
IF (R_L_av_C(nc).LE.1.0e-30) THEN
R_L_av_C(nc)=1.0e-30
END IF

R_L_av_Fe(nc)=R_Fe_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
- R_Fe_final(nc)+R_C_FeO(nc)*4.67)+(R_Si_FeO(nc)*4.0)+(R_Mn_FeO(nc)*1.02)
IF (R_L_av_Fe(nc).LE.1.0e-30) THEN
R_L_av_Fe(nc)=1.0e-30
END IF

R_L_av_Mn(nc)=R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)-R_Mn_final(nc)
+ (R_C_MnO(nc)*4.58)+(R_Si_MnO(nc)*3.93)
IF (R_L_av_Mn(nc).LE.1.0e-30) THEN
R_L_av_Mn(nc)=1.0e-30
END IF

R_L_av_P(nc)=R_P_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
- R_P_final(nc)+(R_C_P2O5(nc)*1.06)+(R_Si_P2O5(nc)*0.886)
+ (R_Fe_P2O5(nc)*0.22)+(R_Mn_P2O5(nc)*0.225)
IF (R_L_av_P(nc).LE.1.0e-30) THEN
R_L_av_P(nc)=1.0e-30
END IF

R_L_av_Si(nc)=R_Si_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
- R_Si_final(nc)
IF (R_L_av_Si(nc).LE.1.0e-30) THEN
R_L_av_Si(nc)=1.0e-30
END IF

R_L_av_FeO(nc)=R_FeO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
+ (R_Fe_final(nc)*1.29)-(R_C_FeO(nc)*6.0)-(R_Si_FeO(nc)*5.14)-(R_Mn_FeO(nc)*1.31)
IF (R_L_av_FeO(nc).LE.1.0e-30) THEN
R_L_av_FeO(nc)=1.0e-30
END IF

R_L_av_SiO2(nc)=R_SiO2_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+R_Si_final(nc)*2.14
IF (R_L_av_SiO2(nc).LE.1.0e-30) THEN
R_L_av_SiO2(nc)=1.0e-30
END IF

R_L_av_MnO(nc)=R_MnO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
- (R_Mn_final(nc)*1.29)-(R_Si_MnO(nc)*5.07)-(R_C_MnO(nc)*5.92)
IF (R_L_av_MnO(nc).LE.1.0e-30) THEN
R_L_av_MnO(nc)=1.0e-30
END IF

R_L_av_P2O5(nc)=R_P2O5_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
- (R_P_final(nc)*2.29)-(R_C_P2O5(nc)*2.367)
- (R_Si_P2O5(nc)*2.028)-(R_Fe_P2O5(nc)*0.507)-(R_Mn_P2O5(nc)*0.516)
IF (R_L_av_P2O5(nc).LE.1.0e-30) THEN
R_L_av_P2O5(nc)=1.0e-30
END IF

R_L_av_Tot(nc)=vfm(ip2)*vol(nc)*denm(ip2)

END IF
R_Fe_b2(nc)=(R_Fe_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_Fe_b2(nc).LE.1.0e-30) THEN
R_S(25,nc)=1.0e-30
ELSE
R_S(25,nc)=R_Fe_b1(nc)-R_Fe_b2(nc)
END IF
IF (R_S(25,nc).LE.0.0) THEN
R_S(25,nc)=1.0e-30
END IF
ELSE
R_S(25,nc)=1.0e-35
R_Fe_b2(nc)=1.0e-35
END IF
C----------------------------------------------------------------------------------------------------------------
IF (R_C_final(nc).GT.1.0e-30) THEN
R_C_fr(nc)=(R_L_av_C(nc)/R_L_av_Tot(nc))
IF (R_C_fr(nc).LE.1.0e-30) THEN
R_C_fr(nc)=1.0e-30
END IF
R_C_b2(nc)=(R_C_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_C_b2(nc).GT.R_C_b1(nc)) THEN
R_C_b2(nc)=R_C_b1(nc)
END IF
IF (R_C_b2(nc).LE.1.0e-30) THEN
R_S(26,nc)=1.0e-30
ELSE
R_S(26,nc)=R_C_b1(nc)-R_C_b2(nc)
END IF
IF (R_S(26,nc).LE.0.0) THEN
R_S(26,nc)=1.0e-30
END IF
ELSE
R_S(26,nc)=1.0e-35
R_C_b2(nc)=1.0e-35
END IF
C----------------------------------------------------------------------------------------------------------------
IF (R_Si_final(nc).GT.1.0e-30) THEN
R_Si_fr(nc)=(R_L_av_Si(nc)/R_L_av_Tot(nc))
IF (R_Si_fr(nc).LE.1.0e-30) THEN
R_Si_fr(nc)=1.0e-30
END IF
R_Si_b2(nc)=(R_Si_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_Si_b2(nc).GT.R_Si_b1(nc)) THEN
R_Si_b2(nc)=R_Si_b1(nc)
END IF
IF (R_Si_b2(nc).LE.1.0e-30) THEN
R_S(27,nc)=1.0e-30
ELSE
R_S(27,nc)=R_Si_b1(nc)-R_Si_b2(nc)
END IF
IF (R_S(27,nc).LE.0.0) THEN
R_S(27,nc)=1.0e-30
END IF
ELSE
R_S(27,nc)=1.0e-35
R_Si_b2(nc)=1.0e-35
IF (R_Mn_final(nc).GT.1.0e-30) THEN
R_Mn_fr(nc)=(R_L_av_Mn(nc)/R_L_av_Tot(nc))
ENDIF
IF (R_Mn_fr(nc).LE.1.0e-30) THEN
R_Mn_fr(nc)=1.0e-30
ENDIF
IF (R_Mn_fr(nc).GT.R_Mn_b1(nc)) THEN
R_Mn_fr(nc)=R_Mn_b1(nc)
ENDIF
R_Mn_b2(nc)=(R_Mn_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_Mn_b2(nc).LE.1.0e-30) THEN
R_S(28,nc)=1.0e-30
ELSE
R_S(28,nc)=R_Mn_b1(nc)-R_Mn_b2(nc)
ENDIF
ENDIF
IF (R_S(28,nc).LE.0.0) THEN
R_S(28,nc)=1.0e-30
ENDIF
IF (R_P_final(nc).GT.1.0e-30) THEN
R_P_fr(nc)=(R_L_av_P(nc)/R_L_av_Tot(nc))
ENDIF
IF (R_P_fr(nc).LE.1.0e-30) THEN
R_P_fr(nc)=1.0e-30
ENDIF
IF (R_P_fr(nc).GT.R_P_b1(nc)) THEN
R_P_fr(nc)=R_P_b1(nc)
ENDIF
R_P_b2(nc)=(R_P_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_P_b2(nc).LE.1.0e-30) THEN
R_S(29,nc)=1.0e-30
ELSE
R_S(29,nc)=R_P_b1(nc)-R_P_b2(nc)
ENDIF
ENDIF
IF (R_S(29,nc).LE.0.0) THEN
R_S(29,nc)=1.0e-30
ENDIF
IF (R_L_av_FeO(nc).GT.1.0e-30) THEN
R_FeO_fr(nc)=(R_L_av_FeO(nc)/R_L_av_Tot(nc))
ENDIF
IF (R_FeO_fr(nc).LE.1.0e-30) THEN
R_FeO_fr(nc)=1.0e-30
ENDIF
IF (R_FeO_fr(nc).GE.1.0) THEN
R_FeO_fr(nc)=1.0
ENDIF
R_FeO_b2(nc)=(R_FeO_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_FeO_b2(nc).LE.1.0e-30) THEN
R_S(30,nc)=1.0e-30
ELSE
R_S(30,nc)=R_FeO_b2(nc)-R_FeO_b1(nc)
ENDIF
ENDIF
IF (R_S(30,nc).LE.0.0) THEN
R_S(30,nc)=1.0e-30
ENDIF
END IF
ELSE
R_S(30,nc)=1.0e-35
R_FeO_b2(nc)=1.0e-35
END IF

IF (R_L_av_SiO2(nc).GT.1.0e-30) THEN
R_SiO2_fr(nc)=(R_L_av_SiO2(nc)/R_L_av_Tot(nc))
IF (R_SiO2_fr(nc).LE.1.0e-30) THEN
R_SiO2_fr(nc)=1.0e-30
END IF
IF (R_SiO2_fr(nc).GE.1.0) THEN
R_SiO2_fr(nc)=1.0
END IF
R_SiO2_b2(nc)=(R_SiO2_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_SiO2_b1(nc).LE.1.0e-30) THEN
R_S(31,nc)=1.0e-30
ELSE
R_S(31,nc)=R_SiO2_b2(nc)-R_SiO2_b1(nc)
END IF
IF (R_S(31,nc).LE.0.0) THEN
R_S(31,nc)=1.0e-30
END IF
ELSE
R_S(31,nc)=1.0e-35
R_SiO2_b2(nc)=1.0e-35
END IF

C----------------------------------------------------------------------------------------------------------------

IF (R_L_av_P2O5(nc).GT.1.0e-30) THEN
R_P2O5_fr(nc)=(R_L_av_P2O5(nc)/R_L_av_Tot(nc))
IF (R_P2O5_fr(nc).LE.1.0e-30) THEN
R_P2O5_fr(nc)=1.0e-30
END IF
IF (R_P2O5_fr(nc).GE.1.0) THEN
R_P2O5_fr(nc)=1.0
END IF
R_P2O5_b2(nc)=(R_P2O5_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_P2O5_b1(nc).LE.1.0e-30) THEN
R_S(32,nc)=1.0e-30
ELSE
R_S(32,nc)=R_P2O5_b2(nc)-R_P2O5_b1(nc)
END IF
IF (R_S(32,nc).LE.0.0) THEN
R_S(32,nc)=1.0e-30
END IF
ELSE
R_S(32,nc)=1.0e-35
R_P2O5_b2(nc)=1.0e-35
END IF

C----------------------------------------------------------------------------------------------------------------

IF (R_L_av_MnO(nc).GT.1.0e-30) THEN
R_MnO_fr(nc)=(R_L_av_MnO(nc)/R_L_av_Tot(nc))
IF (R_MnO_fr(nc).LE.1.0e-30) THEN
R_MnO_fr(nc)=1.0e-30
END IF
IF (R_MnO_fr(nc).GE.1.0) THEN
\[ R_{\text{MnO}_{\text{fr}}}(nc) = 1.0 \]
\[ \text{END IF} \]
\[ R_{\text{MnO}_{\text{b2}}}(nc) = (R_{\text{MnO}_{\text{fr}}}(nc) \times vfm(ip2) \times vol(nc) \times denm(ip2)) \]
\[ \text{IF} \ (R_{\text{MnO}_{\text{b1}}}(nc) \leq 1.0e-30) \text{THEN} \]
\[ R_S(33,nc) = 1.0e-30 \]
\[ \text{ELSE} \]
\[ R_S(33,nc) = R_{\text{MnO}_{\text{b2}}}(nc) - R_{\text{MnO}_{\text{b1}}}(nc) \]
\[ \text{END IF} \]
\[ \text{IF} \ (R_S(33,nc) \leq 0.0) \text{THEN} \]
\[ R_S(33,nc) = 1.0e-30 \]
\[ \text{ELSE} \]
\[ R_S(32,nc) = 1.0e-35 \]
\[ R_{\text{MnO}_{\text{b2}}}(nc) = 1.0e-35 \]
\[ \text{ELSE} \]
\[ R_{\text{t}} = \text{TIME} \]
\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ R_{\text{CO}_{\text{av}}} = 2.0 \times \Phi_{\text{mscal}}((12-1) \times ncell+nc) \times vfm(ip1) \times vol(nc) \times denm(ip1) \]
\[ R_{\text{CO}_{2} \_g} = 2.0 \times \Phi_{\text{mscal}}((13-1) \times ncell+nc) \times vfm(ip1) \times vol(nc) \times denm(ip1) \]
\[ R_{\text{O}_{\text{CO}} \_t} = vfm(ip1) \times vol(nc) \times denm(ip1) \]
\[ R_{\text{CO}} \_r = 2.34 \times R_{\text{C}_{\text{final}}}(nc) \]
\[ R_{\text{CO2}_{\_rd}}(nc) = (100.0 - 0.167 \times R_{\text{t}}) \times R_{\text{CO}} \_r \]
\[ R_{\text{CO}_{\_rem}}(nc) = R_{\text{CO}} \_r - R_{\text{CO2}_{\_rd}}(nc) \]
\[ \text{IF} \ (R_{\text{CO}_{\_rem}}(nc) > R_{\text{CO}} \_r) \text{THEN} \]
\[ R_{\text{CO}_{\_rem}}(nc) = R_{\text{CO}} \_r \]
\[ \text{IF} \ (R_{\text{CO}_{\_rem}}(nc) \leq 1.0e-30) \text{THEN} \]
\[ R_{\text{CO}_{\_rem}}(nc) = 1.0e-30 \]
\[ R_{\text{COfr}}(nc) = 0.5 \times (R_{\text{CO}_{\av}} + R_{\text{CO}_{\rem}}(nc)) / (R_{\text{O}_{\text{CO}} \_t} + R_{\text{CO}} \_r) \]
\[ \text{IF} \ (R_{\text{COfr}}(nc) > 0.5) \text{THEN} \]
\[ R_{\text{COfr}}(nc) = 0.5 \]
\[ R_{\text{COfe}}(nc) = 0.5 - R_{\text{COfr}}(nc) \]
\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ R_{\text{S}}(22,nc) = ((0.5 - R_{\text{COfr}}(nc)) - \Phi_{\text{mscal}}((11-1) \times ncell+nc)) \times vfm(ip1) \times vol(nc) \times denm(ip1) \]
\[ \text{IF} \ (R_{\text{S}}(22,nc) < 1.0e-30) \text{THEN} \]
\[ R_{\text{S}}(22,nc) = 1.0e-30 \]
\[ R_{\text{S}}(21,nc) = (R_{\text{COfr}}(nc) - \Phi_{\text{mscal}}((12-1) \times ncell+nc)) \times vfm(ip1) \times vol(nc) \times denm(ip1) \]
\[ \text{IF} \ (R_{\text{S}}(21,nc) < 1.0e-30) \text{THEN} \]
\[ R_{\text{S}}(21,nc) = 1.0e-30 \]
\[ R_{\text{S}}(34,nc) = 1.0e-30 \]
\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ R_{\text{O2}_{\text{rate2}}}(nc) = R_{\text{S}}(25,nc) + R_{\text{S}}(26,nc) + R_{\text{S}}(27,nc) + R_{\text{S}}(28,nc) + R_{\text{S}}(29,nc) \]
\[ R_{\text{O2}_{\text{rate1}}}(nc) = R_{\text{S}}(30,nc) + R_{\text{S}}(31,nc) + R_{\text{S}}(32,nc) + R_{\text{S}}(33,nc) \]
\[ R_{\text{c}_{\text{rate1}}}(nc) = R_{\text{S}}(21,nc) \]
\[ R_{\text{c}_{\text{rate2}}}(nc) = R_{\text{S}}(22,nc) \]
\[ \text{c----------------------------------------------------------------------------------------------------------------} \]
\[ R_{\text{bubble}} = \Phi_{\text{mscal}}((31-1) \times ncell+nc) \]
\[ \text{c-----Source term for each scalar} \]
\[ \text{c-----Source term for gas bubble in gas phase} \]
\[ R_{\text{S}}(1,nc) = (R_{\text{BB}(1)} - R_{\text{DB}(1)} + R_{\text{BC}(1)} - R_{\text{DC}(1)}) \times denm(ip1) \]
\[ R_{\text{S}}(2,nc) = (R_{\text{BB}(2)} - R_{\text{DB}(2)} + R_{\text{BC}(2)} - R_{\text{DC}(2)}) \times denm(ip1) \]
R_S(3,nc)=(R_BB(3)-R_DB(3)+R_BC(3)-R_DC(3))*denm(ip1)
R_S(4,nc)=(R_BB(4)-R_DB(4)+R_BC(4)-R_DC(4))*denm(ip1)
R_S(5,nc)=(R_BB(5)-R_DB(5)+R_BC(5)-R_DC(5))*denm(ip1)
R_S(6,nc)=(R_BB(6)-R_DB(6)+R_BC(6)-R_DC(6))*denm(ip1)
R_S(7,nc)=(R_BB(7)-R_DB(7)+R_BC(7)-R_DC(7))*denm(ip1)
R_S(8,nc)=(R_BB(8)-R_DB(8)+R_BC(8)-R_DC(8))*denm(ip1)
R_S(9,nc)=(R_BB(9)-R_DB(9)+R_BC(9)-R_DC(9))*denm(ip1)
R_S(10,nc)=(R_BB(10)-R_DB(10)+R_BC(10)-R_DC(10))*denm(ip1)

C-----Source term for gas bubble in foam phase
R_tvf(1)=Phi_mscal((24-1)*ncell+nc)
R_tvf(2)=Phi_mscal((25-1)*ncell+nc)
R_tvf(3)=Phi_mscal((26-1)*ncell+nc)
R_tvf(4)=Phi_mscal((27-1)*ncell+nc)
R_tvf(5)=Phi_mscal((28-1)*ncell+nc)
R_tvf(6)=Phi_mscal((29-1)*ncell+nc)
R_tvf(7)=Phi_mscal((30-1)*ncell+nc)
R_tvf(8)=Phi_mscal((31-1)*ncell+nc)
R_tvf(9)=Phi_mscal((32-1)*ncell+nc)
R_tvf(10)=Phi_mscal((33-1)*ncell+nc)
R_gfcrf(nc)=Phi_mscal((35-1)*ncell+nc)
R_lq_frf(nc)=Phi_mscal((34-1)*ncell+nc)

C----------------------------------------------------------------------------------------------------------------
IF (R_tvf(1).GE.0.5)THEN
R_tvf(1)=0.5
END IF
IF (R_tvf(2).GE.0.5)THEN
R_tvf(2)=0.5
END IF
IF (R_tvf(3).GE.0.5)THEN
R_tvf(3)=0.5
END IF
IF (R_tvf(4).GE.0.5)THEN
R_tvf(4)=0.5
END IF
IF (R_tvf(5).GE.0.5)THEN
R_tvf(5)=0.5
END IF
IF (R_tvf(6).GE.0.5)THEN
R_tvf(6)=0.5
END IF
IF (R_tvf(7).GE.0.5)THEN
R_tvf(7)=0.5
END IF
IF (R_tvf(8).GE.0.5)THEN
R_tvf(8)=0.5
END IF
IF (R_tvf(9).GE.0.5)THEN
R_tvf(9)=0.5
END IF
IF (R_tvf(10).GE.0.5)THEN
R_tvf(10)=0.5
END IF
IF (R_gfrf(nc).GE.0.5)THEN
R_g(nc)=0.5
END IF
IF (R_lq_frf(nc).GE.0.5)THEN
\[ R_{lq \_av}(nc)=0.5 \]

**END IF**

\[ R_{fb}(1)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(2)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(3)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(4)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(5)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(6)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(7)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(8)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(9)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb}(10)=2.0*R_{tvf}(10)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{g}(nc)=2.0*R_{gfrf}(nc)*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{lq \_av}(nc)=2.0*R_{lq \_frf}(nc)*vfm(ip3)*vol(nc)*denm(ip3) \]

**END IF**

\[ R_{fb \_c}(1)=(R_{BCF}(1)-R_{DCF}(1))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(2)=(R_{BCF}(2)-R_{DCF}(2))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(3)=(R_{BCF}(3)-R_{DCF}(3))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(4)=(R_{BCF}(4)-R_{DCF}(4))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(5)=(R_{BCF}(5)-R_{DCF}(5))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(6)=(R_{BCF}(6)-R_{DCF}(6))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(7)=(R_{BCF}(7)-R_{DCF}(7))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(8)=(R_{BCF}(8)-R_{DCF}(8))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(9)=(R_{BCF}(9)-R_{DCF}(9))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{fb \_c}(10)=(R_{BCF}(10)-R_{DCF}(10))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{gf \_c}(nc)=(R_{gf}(nc)-R_{gfrf}(nc))*vfm(ip3)*vol(nc)*denm(ip3) \]
\[ R_{lq \_c}(nc)=(0.5-R_{gf}(nc)-R_{lq \_frf}(nc))*vfm(ip3)*vol(nc)*denm(ip3) \]

**END IF**

\[ R_{fb \_n}(1)=R_{fb \_c}(1)+R_{fb}(1) \]
\[ R_{fb \_n}(2)=R_{fb \_c}(2)+R_{fb}(2) \]
\[ R_{fb \_n}(3)=R_{fb \_c}(3)+R_{fb}(3) \]
\[ R_{fb \_n}(4)=R_{fb \_c}(4)+R_{fb}(4) \]
\[ R_{fb \_n}(5)=R_{fb \_c}(5)+R_{fb}(5) \]
\[ R_{fb \_n}(6)=R_{fb \_c}(6)+R_{fb}(6) \]
\[ R_{fb \_n}(7)=R_{fb \_c}(7)+R_{fb}(7) \]
\[ R_{fb \_n}(8)=R_{fb \_c}(8)+R_{fb}(8) \]
\[ R_{fb \_n}(9)=R_{fb \_c}(9)+R_{fb}(9) \]
\[ R_{fb \_n}(10)=R_{fb \_c}(10)+R_{fb}(10) \]
\[ R_{lq \_n}(nc)=R_{lq \_c}(nc)+R_{lq \_av}(nc) \]
\[ R_{gf \_n}(nc)=R_{gf \_c}(nc)+R_{g}(nc) \]

**END IF**

\[ \text{IF}(R_{fb \_n}(1).LT.1.0e-30) \text{THEN} \]
\[ R_{fb \_c}(1)=1.0e-30 \]
\[ \text{END IF} \]
\[ \text{IF}(R_{fb \_n}(2).LT.1.0e-30) \text{THEN} \]
\[ R_{fb \_c}(2)=1.0e-30 \]
\[ \text{END IF} \]
\[ \text{IF}(R_{fb \_n}(3).LT.1.0e-30) \text{THEN} \]
\[ R_{fb \_c}(3)=1.0e-30 \]
\[ \text{END IF} \]
\[ \text{IF}(R_{fb \_n}(4).LT.1.0e-30) \text{THEN} \]
\[ R_{fb \_c}(4)=1.0e-30 \]
\[ \text{END IF} \]
\[ \text{IF}(R_{fb \_n}(5).LT.1.0e-30) \text{THEN} \]
\[ R_{fb \_c}(5)=1.0e-30 \]

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IF (R_fb_n(6).LT.1.0e-30) THEN
R_fb_c(6)=1.0e-30
END IF
IF (R_fb_n(7).LT.1.0e-30) THEN
R_fb_c(7)=1.0e-30
END IF
IF (R_fb_n(8).LT.1.0e-30) THEN
R_fb_c(8)=1.0e-30
END IF
IF (R_fb_n(9).LT.1.0e-30) THEN
R_fb_c(9)=1.0e-30
END IF
IF (R_fb_n(10).LT.1.0e-30) THEN
R_fb_c(10)=1.0e-30
END IF
IF (R_lf_n(nc).LT.1.0e-30) THEN
R_lf_c(nc)=1.0e-30
END IF
IF (R_gf_n(nc).LT.1.0e-30) THEN
R_gf_c(nc)=1.0e-30
END IF

R_tot_fn(nc)=R_fb_n(1)+R_fb_n(2)+R_fb_n(3)+R_fb_n(4)+R_fb_n(5)+R_fb_n(6)+R_fb_n(7)+R_fb_n(8)+R_fb_n(9)+R_fb_n(10)+R_gf_n(nc)+R_lf_n(nc)
IF (R_tot_fn(nc).LT.1.0e-30) THEN
R_tot_fn(nc)=1.0e-30
END IF

R_fb_nb(1)=0.5*(R_fb_c(1))/R_tot_fn(nc)
R_fb_nb(2)=0.5*(R_fb_c(2))/R_tot_fn(nc)
R_fb_nb(3)=0.5*(R_fb_c(3))/R_tot_fn(nc)
R_fb_nb(4)=0.5*(R_fb_c(4))/R_tot_fn(nc)
R_fb_nb(5)=0.5*(R_fb_c(5))/R_tot_fn(nc)
R_fb_nb(6)=0.5*(R_fb_c(6))/R_tot_fn(nc)
R_fb_nb(7)=0.5*(R_fb_c(7))/R_tot_fn(nc)
R_fb_nb(8)=0.5*(R_fb_c(8))/R_tot_fn(nc)
R_fb_nb(9)=0.5*(R_fb_c(9))/R_tot_fn(nc)
R_fb_nb(10)=0.5*(R_fb_c(10))/R_tot_fn(nc)
R_gf_nb(nc)=0.5*(R_gf_c(nc))/R_tot_fn(nc)
R_lf_nb(nc)=0.5*(R_lf_c(nc))/R_tot_fn(nc)
IF (R_tot_fn(nc).GT.0.0) THEN
R_fb_nb(1)=0.5*(R_fb_c(1))/R_tot_fn(nc)
R_fb_nb(2)=0.5*(R_fb_c(2))/R_tot_fn(nc)
R_fb_nb(3)=0.5*(R_fb_c(3))/R_tot_fn(nc)
R_fb_nb(4)=0.5*(R_fb_c(4))/R_tot_fn(nc)
R_fb_nb(5)=0.5*(R_fb_c(5))/R_tot_fn(nc)
R_fb_nb(6)=0.5*(R_fb_c(6))/R_tot_fn(nc)
R_fb_nb(7)=0.5*(R_fb_c(7))/R_tot_fn(nc)
R_fb_nb(8)=0.5*(R_fb_c(8))/R_tot_fn(nc)
R_fb_nb(9)=0.5*(R_fb_c(9))/R_tot_fn(nc)
R_fb_nb(10)=0.5*(R_fb_c(10))/R_tot_fn(nc)
R_gf_nb(nc)=0.5*(R_gf_c(nc))/R_tot_fn(nc)
R_lf_nb(nc)=0.5*(R_lf_c(nc))/R_tot_fn(nc)
IF (R_gf_nb(nc).GT.0.49) THEN
R_gf_nb(nc)=0.49
END IF

R_S(11,nc)=(R_fb_nb(1)*vfm(ip3)*vol(nc)*denm(ip3))
R_S(12,nc)=(R_fb_nb(2)*vfm(ip3)*vol(nc)*denm(ip3))
R_S(13,nc)=(R_fb_nb(3)*vfm(ip3)*vol(nc)*denm(ip3))
R_S(14,nc)=(R_fb_nb(4)*vfm(ip3)*vol(nc)*denm(ip3))
R_S(15,nc)=(R_fb_nb(5)*vfm(ip3)*vol(nc)*denm(ip3))
R_S(16,nc)=(R_fb_nb(6)*vfm(ip3)*vol(nc)*denm(ip3))
R_S(17,nc)=(R_fb_nb(7)*vfm(ip3)*vol(nc)*denm(ip3))
R_S(18,nc)=(R_fb_nb(8)*vfm(ip3)*vol(nc)*denm(ip3))
R_S(19,nc)=(R_fb_nb(9)*vfm(ip3)*vol(nc)*denm(ip3))
IF (R_bubble.LE.0.9) THEN
R_S(20,nc)=(R_fb_nb(10)*vfm(ip3)*vol(nc)*denm(ip3))
ELSE
R_S(20,nc)=0.0
END IF
END IF
END DO

c-----loop over internal cells
c-----sources update for scalar 1 phase 1

IF (isc==1) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)= sum1(ip)+(R_S(1,ip)/dt)
END DO
END IF

c-----Sources for scalar 2 phase 1

IF (isc==2) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)=sum1(ip)+(R_S(2,ip)/dt)
END DO
END IF

c-----sources for scalar 3 phase 1

IF (isc==3) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)=sum1(ip)+(R_S(3,ip)/dt)
END DO
END IF

c-----sources for scalar 4 phase 1

IF (isc==4) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)=sum1(ip)+(R_S(4,ip)/dt)
END DO
END IF

c-----sources for scalar 5 phase 1

IF (isc==5) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)=sum1(ip)+(R_S(5,ip)/dt)
END DO
END IF

c-----sources for scalar 6 phase 1

IF (isc==6) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)=sum1(ip)+(R_S(6,ip)/dt)
END DO
END IF

c-----sources for scalar 7 phase 1
IF (isc==7) THEN
DO ip = nsp(mat),nep(mat)
sum1(ip)= sum1(ip)+(R_S(7,ip)/dt)
END DO
END IF

IF (isc==8) THEN
DO ip = nsp(mat),nep(mat)
sum1(ip)= sum1(ip)+(R_S(8,ip)/dt)
END DO
END IF

IF (isc==9) THEN
DO ip = nsp(mat),nep(mat)
sum1(ip)= sum1(ip)+(R_S(9,ip)/dt)
END DO
END IF

IF (isc==10) THEN
DO ip = nsp(mat),nep(mat)
sum1(ip)= sum1(ip)+(R_S(10,ip)/dt)
END DO
END IF

IF (isc==11) THEN
DO ip = nsp(mat),nep(mat)
sum1(ip)= sum1(ip)+(R_S(22,ip)/dt)
END DO
END IF

IF (isc==12) THEN
DO ip = nsp(mat),nep(mat)
sum1(ip)= sum1(ip)+(R_S(21,ip)/dt)
END DO
END IF

IF (isc==13) THEN
DO ip = nsp(mat),nep(mat)
IF (TIME.LE.0.3e+03) THEN
sum1(ip)= sum1(ip)+(R_S(34,ip)/dt)
ELSE
sum1(ip)= sum1(ip)
END IF
END IF
END DO
END IF

c-----sources for scalar 1 Fe phase 2

IF (isc==14) THEN
  DO ip = nsp(mat),nep(mat)
    ip2=ip+ncell
    IF (R_S(25,ip).LE.0.0) THEN
      R_S(25,ip)=0.0
    END IF
    sum1(ip2)= sum1(ip2)-(R_S(25,ip)/dt)
  END DO
END IF

END IF

END IF

END IF

c-----sources for scalar 3 Si phase 2

IF (isc==16) THEN
  DO ip = nsp(mat),nep(mat)
    ip2=ip+ncell
    IF (R_S(27,ip).LE.0.0) THEN
      R_S(27,ip)=0.0
    END IF
    sum1(ip2)= sum1(ip2)-(R_S(27,ip)/dt)
  END DO
END IF

END IF

END IF

c-----sources for scalar 5 P phase 2

IF (isc==18) THEN
  DO ip = nsp(mat),nep(mat)
    ip2=ip+ncell
    IF (R_S(29,ip).LE.0.0) THEN
      R_S(29,ip)=0.0
    END IF
    sum1(ip2)= sum1(ip2)-(R_S(29,ip)/dt)
  END DO
END IF

END IF
IF (R_S(29,ip).LE.0.0) THEN
R_S(29,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)-(R_S(29,ip)/dt)
END DO
END IF

c-----sources for scalar 6 FeO phase 2

IF (isc==19) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(30,ip).LE.0.0) THEN
R_S(30,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)+(R_S(30,ip)/dt)
END DO
END IF

c-----sources for scalar 7 SiO2 phase 2

IF (isc==20) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(31,ip).LE.0.0) THEN
R_S(31,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)+(R_S(31,ip)/dt)
END DO
END IF

c-----sources for scalar 8 P2O5 phase 2

IF (isc==21) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(32,ip).LE.0.0) THEN
R_S(32,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)+(R_S(32,ip)/dt)
END DO
END IF

C-----sources for scalar 9 MnO phase 2

IF (isc==22) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(33,ip).LE.0.0) THEN
R_S(33,ip)=0.0
END IF
sum1(ip2)= sum1(ip2)+(R_S(33,ip)/dt)
END DO
END IF

C-----sources for scalar 10 S phase 2
IF (isc==23) THEN
   DO ip = nsp(mat),nep(mat)
      ip2=ip+ncell
      sum1(ip2)= sum1(ip2)
   END DO
END IF

-----sources for scalar 1 Bubble phase 3

IF (isc==24) THEN
   DO ip = nsp(mat),nep(mat)
      ip3=ip+ncell+ncell
      sum1(ip3)= sum1(ip3)+(R_S(11,ip)/dt)
   END DO
END IF

-----sources for scalar 2 Bubble phase 3

IF (isc==25) THEN
   DO ip = nsp(mat),nep(mat)
      ip3=ip+ncell+ncell
      sum1(ip3)= sum1(ip3)+(R_S(12,ip)/dt)
   END DO
END IF

-----sources for scalar 3 Bubble phase 3

IF (isc==26) THEN
   DO ip = nsp(mat),nep(mat)
      ip3=ip+ncell+ncell
      sum1(ip3)= sum1(ip3)+(R_S(13,ip)/dt)
   END DO
END IF

-----sources for scalar 4 Bubble phase 3

IF (isc==27) THEN
   DO ip = nsp(mat),nep(mat)
      ip3=ip+ncell+ncell
      sum1(ip3)= sum1(ip3)+(R_S(14,ip)/dt)
   END DO
END IF

-----sources for scalar 5 Bubble phase 3

IF (isc==28) THEN
   DO ip = nsp(mat),nep(mat)
      ip3=ip+ncell+ncell
      sum1(ip3)= sum1(ip3)+(R_S(15,ip)/dt)
   END DO
END IF

-----sources for scalar 6 Bubble phase 3

IF (isc==29) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(16,ip)/dt)
END DO
END IF
C-----sources for scalar 7 Bubble phase 3
C------------------------------------------------------------------------------------------

IF (isc==30) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(17,ip)/dt)
END DO
END IF
C------------------------------------------------------------------------------------------

C-----sources for scalar 8 Bubble phase 3
C------------------------------------------------------------------------------------------

IF (isc==31) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(18,ip)/dt)
END DO
END IF
C------------------------------------------------------------------------------------------

C-----sources for scalar 9 Bubble phase 3
C------------------------------------------------------------------------------------------

IF (isc==32) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(19,ip)/dt)
END DO
END IF
C------------------------------------------------------------------------------------------

C-----sources for scalar 10 Bubble phase 3
C------------------------------------------------------------------------------------------

IF (isc==33) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(20,ip)/dt)
END DO
END IF
C------------------------------------------------------------------------------------------

C-----sources for scalar 11 liquid, phase 3
C------------------------------------------------------------------------------------------

IF (isc==34) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)+(R_S(23,ip)*vfm(ip3)*vol(ip)*denm(ip3))/dt
END DO
END IF
C------------------------------------------------------------------------------------------

C-----sources for scalar 11 gas phase 3
C------------------------------------------------------------------------------------------

IF (isc==35) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
User subroutine to calculate sources in interfacial mass exchange

SUBROUTINE usemph(ieq,iva,mat)
  c==============================================================
  c    description: user subroutine for sources for interfacial exchange and general sources like body forces
  c    author: Anuththara Kirindigoda Hewage (2070065)
  c    date: 01/10/2015
  c==============================================================
USE comm1
USE comm2
USE comm0
INCLUDE 'comdp.inc'
INCLUDE 'com90.inc'
INCLUDE 'SwiftIO_FortranFunctions.inc'
mat=1
  c----Volume fraction equation interfacial sources
  c==============================================================
IF(ieq == ipvf) THEN
DO i_p1=nsp(mat),nep(mat)
  i_p2=i_p1+ncell
  i_p3=i_p1+ncell+ncell
  c----Source terms update for mass exchange
  sum1(i_p1) = sum1(i_p1)+(R_c_rate1(i_p1)/dt)-(R_c_rate2(i_p1)/dt)
  sum1(i_p2) = sum1(i_p2)+(R_O2_rate1(i_p1)/dt)-(R_O2_rate2(i_p1)/dt)
  sum1(i_p3) = sum1(i_p3)-(R_FM_g(i_p1)-R_g_FM(i_p1)+
                        R_FM_lq(i_p1)-R_lq_FM(i_p1))/dt
  c==============================================================
END DO
END IF
RETURN
END SUBROUTINE usemph
• **User subroutine to calculate the density of the foam phase**

```fortran
SUBROUTINE useden(mat,mph)

C=====================================================================
C     description: user subroutine for changing the density
C     author: Anuththara Kirindigoda Hewage (2070065)
C     date: 01/10/2015
C=====================================================================

C-----modules
USE comm1
USE comm2
USE cthmod, ONLY: ymfrac
USE comm0

C------------------------------------------------------------------------
INCLUDE 'comdp.inc'
INCLUDE 'com90.inc'
INCLUDE 'SwiftIO_FortranFunctions.inc'
INTEGER, INTENT(in) :: mat,mph
C------------------------------------------------------------------------
DO ip=nsp(mat),nep(mat)
ip1=ip
ip2=ip+ncell
ip3=ip+ncell+ncell
denm(ip1)=0.233
denm(ip2)=6980.0
denm(ip3)=678.0
IF(R_gfr(ip).LT.0.01) THEN
  R_gfr(ip)=0.45
ENDIF
denm(ip1)=denm(ip1)
denm(ip2)=denm(ip2)
denm(ip3)=2.0*R_gfr(ip)*denm(ip1)+(1.0-2.0*R_gfr(ip))*denm(ip2)
C------------------------------------------------------------------------
END DO
RETURN
END SUBROUTINE useden
```
• User subroutine to calculate the viscosity of the foam phase

Subroutine usevis(mat,mph)

description: user subroutine for changing the viscosity
author: Anuththara Kirindigoda Hewage (2070065)
date: 01/10/2015

modules
USE comm1
USE comm2
USE cthmod, ONLY: ymfrac
USE comm0
INCLUDE 'comdp.inc'
INCLUDE 'com90.inc'
INCLUDE 'SwiftIO_FortranFunctions.inc'
INTEGER, INTENT(in) :: mat,mph

DO ip=nsp(mat),nep(mat)
ip1=ip
ip2=ip+ncell
ip3=ip+ncell+ncell
vimm(ip1)=vimm(ip1)
vimm(ip2)=vimm(ip2)
vimm(ip3)=2.0*R_gfr(ip)*vimm(ip1)+(1.0-2.0*R_gfr(ip))*vimm(ip2)
END DO
RETURN
END SUBROUTINE usevis
A8. CFD model results used to generate the result graphs in Chapter 7

- Measurements of slag foam height from the CFD model
  Foam height measurement was obtained at three different positions as the foam height was not same in the radial direction from the center of the model. The average of the three height measurements was taken as the final foam height, which was used in the analysis and is tabulated below.

Table A9: Slag foam height measurements with time

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Foam height (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td>0.99552</td>
</tr>
<tr>
<td>120</td>
<td>1.10207</td>
</tr>
<tr>
<td>180</td>
<td>1.29479</td>
</tr>
<tr>
<td>240</td>
<td>1.13182</td>
</tr>
<tr>
<td>300</td>
<td>1.21182</td>
</tr>
<tr>
<td>360</td>
<td>1.18526</td>
</tr>
<tr>
<td>420</td>
<td>1.04885</td>
</tr>
<tr>
<td>480</td>
<td>1.13477</td>
</tr>
<tr>
<td>540</td>
<td>1.02811</td>
</tr>
<tr>
<td>600</td>
<td>0.94515</td>
</tr>
</tbody>
</table>
A9. Graphical results of evolving four phases in the four phases model (Chapter 7)

<table>
<thead>
<tr>
<th>Time (s)</th>
<th>Gas phase</th>
<th>Liquid phase</th>
<th>Slag phase</th>
<th>Slag foam phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>60</td>
<td><img src="image1.png" alt="" /></td>
<td><img src="image2.png" alt="" /></td>
<td><img src="image3.png" alt="" /></td>
<td><img src="image4.png" alt="" /></td>
</tr>
<tr>
<td>120</td>
<td><img src="image5.png" alt="" /></td>
<td><img src="image6.png" alt="" /></td>
<td><img src="image7.png" alt="" /></td>
<td><img src="image8.png" alt="" /></td>
</tr>
<tr>
<td>180</td>
<td><img src="image9.png" alt="" /></td>
<td><img src="image10.png" alt="" /></td>
<td><img src="image11.png" alt="" /></td>
<td><img src="image12.png" alt="" /></td>
</tr>
</tbody>
</table>
Figure A 7: Evolving volume fraction of four phases with time
A10. Subroutines used in CFD four phases model

- User subroutine to calculate sources in scalar equation

SUBROUTINE usesc_mscal(mat,isc,mph)

C=====================================================================
C     author: Anuththara Kirindigoda Hewage
C     date: 01/10/2016
C     project: Four phase model
C----------------------------------------------------------------------------------------------------------------
USE comm1
USE comm2
USE comm0
INCLUDE 'com93.inc'
INCLUDE 'SwiftIO_FortranFunctions.inc'
INTEGER, INTENT(in) :: mat,isc,mph
INTEGER::I_i,I_j,I_k,I_m,nc,ip,ip1,ip2,ip3,ip4
REAL, DIMENSION(1:33,NCELL)::R_S
REAL, DIMENSION(1:10)::R_tv,R_tvf,R_BCF,R_DCF,R_dr,R_Cf,R_zita
REAL, DIMENSION(1:10,1:10)::R_bb,R_DB,R_vbb,R_vbd1,R_nb,R_nbf,R_chaiC
REAL, DIMENSION(1:10,1:10)::R_BC,R_DC,R_d,R_v,R_vbctf,R_cfq,R_vbd
REAL, DIMENSION(1:10):=R_vbc1,R_vbc2,R_vbc3,R_vbc4
REAL, DIMENSION(1:10):=R_vbcf1,R_vbcf2,R_vbcf3,R_vbcf4
REAL, DIMENSION(1:10):=R_xij,R_pb,R_corr,R_BR,R_xik,R_FS,R_xijf
REAL, DIMENSION(1:10):=R_tauij,R_min_nb,R_min_nbfr,R_crf
REAL, DIMENSION(NCELL):=R_Fe_final,R_Si_final,R_Mn_final,R_C_final
REAL, DIMENSION(NCELL):=R_L_av_Fe,R_L_av_C,R_L_av_Si
REAL, DIMENSION(NCELL):=R_L_av_Mn,R_L_av_P,R_CRate,R_de,R_tfs
REAL, DIMENSION(NCELL):=R_S_av_FeO,R_S_av_SiO2,R_S_av_P2O5
REAL, DIMENSION(NCELL):=R_S_av_MnO,R_S_av_CaO,R_S_av_MgO,R_C_O2
REAL, DIMENSION(NCELL):=R_S_av_Tot,R_L_r_Tot,R_L_S_Tot
REAL, DIMENSION(NCELL):=R_MnO_Cr,R_MnO_Sir,R_P2O5_Cr
REAL, DIMENSION(NCELL):=R_MnO_Sir,R_MnO_P2O5,Sir,P2O5_Mnr
REAL, DIMENSION(NCELL):=R_MnO_P2O5,Sir,P2O5_Mnr
REAL, DIMENSION(NCELL):=R_FeRate,R_SiRate,R_MnRate,R_PRate
REAL, DIMENSION(NCELL):=R_lqt,R_tDgbt,R_tdgf,R_lq_f,R_lqf,R_tfl,R_St
REAL, DIMENSION(NCELL):=R_foam,R_g,R_lqt_av,R_tfg,R_S_av_f,R_S_f
REAL, DIMENSION(NCELL):=R_tfoam,R_gf,R_g_av,R_lq_av,R_COfr,R_gf_av
C----------------------------------------------------------------------------------------------------------------
REAL::R_CO_av,R_CO_r,R_Id,R_O_CO_t,R_bubble,R_O2_a,R_P_req_O2
REAL::R_P_eq,R_Mn_eq,R_Mn_req,R_Mn_req_P2O5,R_Mn_req_FeO
REAL::R_C_req_O2,R_C_req_P2O5,R_C_req_MnO,R_C_req_FeO
REAL::R_Si_req_O2,R_Si_req_P2O5,R_Si_req_MnO,R_Si_req_FeO
REAL::R_Fe_final_1,R_Fe_final_2,R_vfmin,R_Mn_final_1,R_Mn_final_2
REAL, DIMENSION(NCELL):=R_O2_av_g,R_Si_Fickrate,R_Si_av_l,R_C_P2O5
REAL, DIMENSION(NCELL):=R_Si_used_O2,R_C_Fickrate,R_C_av_l,R_C_MnO
REAL, DIMENSION(NCELL):=R_C_used_O2,R_P_Fickrate,R_P_av_l,R_C_FeO
REAL, DIMENSION(NCELL):=R_P_used_O2,R_Mn_Fickrate,R_Mn_av_l,R_Si_b3
REAL, DIMENSION(NCELL):=R_Mn_used_O2,R_Fe_Fickrate,R_Fe_av_l
REAL, DIMENSION(NCELL):=R_Fe_used_O2,R_P_final,R_L_av_S_R_Fe_P2O5
REAL, DIMENSION(NCELL):=R_P2O5_av_l,R_Si_used_P2O5,R_C_used_P2O5
REAL, DIMENSION(NCELL):=R_Mn_used_P2O5,R_FeO_av_l,R_Si_used_FeO
REAL, DIMENSION(NCELL):=R_Fe_used_P2O5,R_C_used_FeO,R_MnO_av_l
REAL, DIMENSION(NCELL):=R_Si_used_MnO,R_C_used_MnO,R_Mn_used_FeO
REAL, DIMENSION(NCELL):: R_Mn_P2O5, R_Mn_FeO, R_Si_FeO, R_Si_MnO
REAL, DIMENSION(NCELL):: R_Mn_used_O2_1, R_C_used_O2_1, R_P_used_O2_1
REAL, DIMENSION(NCELL):: R_P_O2, R_Mn_O2, R_Fe_b, R_Mn_b, R_Si_P2O5
REAL, DIMENSION(NCELL):: R_C_b, R_P_b, R_Si_b, R_Fe_used_O2_1
REAL, DIMENSION(NCELL):: R_Si_b_com, R_S_b_com, R_Fe_b_com, R_CaO_b1
REAL, DIMENSION(NCELL):: R_C_b_l, R_P_b_l, R_Si_b_l, R_Fe_b_l, R_Mn_b_l
REAL, DIMENSION(NCELL):: R_liq_fr, R_FeO_b_l, R_SiO2_b_l, R_mchange
REAL, DIMENSION(NCELL):: R_sC_b1, R_sP_b1, R_sMn_b1, R_sSi_b1, R_sFe_b1
REAL, DIMENSION(NCELL):: R_sC_b, R_sP_b, R_sMn_b, R_sSi_b, R_sFe_b
REAL, DIMENSION(NCELL):: R_sP2O5_b1, R_sMnO_b1, R_sSiO2_b1, R_sFeO_b1
REAL, DIMENSION(NCELL):: R_sP2O5_b, R_sMnO_b, R_sSiO2_b, R_sFeO_b
REAL, DIMENSION(NCELL):: R_FeO_lq, R_SiO2_lq, R_FeO_b, R_SiO2_b
REAL, DIMENSION(NCELL):: R_FeO_b_l, R_SiO2_b_l, R_mchange
REAL, DIMENSION(NCELL):: R_sC_b1, R_sP_b1, R_sMn_b1, R_sSi_b1, R_sFe_b1
REAL, DIMENSION(NCELL):: R_sC_b, R_sP_b, R_sMn_b, R_sSi_b, R_sFe_b
REAL, DIMENSION(NCELL):: R_SiO2_b1, d3, v3, R_FeO_b2, R_SiO2_b2, R_Si_O2
REAL, DIMENSION(NCELL):: R_FeO_b1, R_FeO_b2, R_FeO_b1, R_FeO_b2
REAL, DIMENSION(NCELL):: R_sCaO_b1, R_sMgO_b1, R_sCaO_b, R_sMgO_b
REAL, DIMENSION(NCELL):: R_s_fe, R_s_C, R_s_P, R_s_Mn, R_s_Si, R_s_Fe
REAL, DIMENSION(NCELL):: R_s_liq, R_s_gas, R_FeO_b, R_SiO2_b, R_FeO_b1, R_SiO2_b1
REAL, DIMENSION(NCELL):: R_C_R, R_P_R, R_Si_R, R_Fe_R, R_Mn_R
REAL, DIMENSION(NCELL):: R_s_C, R_s_P, R_s_Mn, R_s_Si, R_s_Fe
REAL, DIMENSION(NCELL):: R_s_P2O5, R_s_MnO, R_s_SiO2, R_s_FeO
REAL, DIMENSION(NCELL):: R_s_P2O5_l, R_s_MnO_l, R_s_SiO2_l, R_s_FeO_l
REAL, DIMENSION(NCELL):: R_C_b, R_P_b, R_Si_b, R_Fe_b, R_Mn_b
REAL, DIMENSION(NCELL):: R_FeO_b, R_SiO2_b, R_P2O5_b, R_MnO_b, R_FeO_b
REAL, DIMENSION(NCELL):: R_L_av_FeO, R_L_av_SiO2, R_L_av_MnO, R_MgO_b1
REAL, DIMENSION(NCELL):: R_FeO_lq, R_SiO2_lq, R_FeO_b, R_SiO2_b
REAL, DIMENSION (NCELL):: R_sC_final_1, R_sC_final_2, R_sC_final_3
REAL, DIMENSION (NCELL):: R_sC_O2, R_sC_P2O5, R_sC_MnO, R_sC_FeO, R_mslag
REAL, DIMENSION (NCELL):: R_sSi_final_1, R_sSi_final_2, R_sSi_final_3
REAL, DIMENSION (NCELL):: R_sSi_P2O5, R_sSi_MnO, R_sSi_FeO, R_sSi_O2
REAL, DIMENSION (NCELL):: R_sFe_final_1, R_sFe_final_2, R_sFe_P2O5, R_qb
REAL, DIMENSION (NCELL):: R_sMn_final_1, R_sMn_final_2, R_sMn_final_3
REAL, DIMENSION (NCELL):: R_sMn_P2O5, R_sMn_FeO, R_sMn_O2, R_sFeO2, R_u
REAL, DIMENSION (NCELL):: R_sC_final_4, R_sC_final_1, R_sC_final_2, R_sC_final
REAL, DIMENSION (NCELL):: R_sSi_final_4, R_sC_final_4, R_sC_final, R_N
REAL, DIMENSION (NCELL):: R_sP_final, R_sC_used_P2O5, R_sFe_used_P2O5
REAL, DIMENSION (NCELL):: R_S_av_C, R_S_av_Fe, R_S_av_Mn, R_s_liquid
REAL, DIMENSION (NCELL):: R_sFe_b2, R_sSi_b2, R_sP_b2, R_sMn_b2, R_sc_b2
REAL, DIMENSION (NCELL):: R_sFe_fr, R_sc_fr, R_sSi_fr, R_sp_fr, R_sMn_fr
REAL, DIMENSION (NCELL):: R_sFeO_fr, R_sSiO2_fr, R_sP2O5_fr, R_sMnO_fr
REAL, DIMENSION (NCELL):: R_S_av_P, R_S_av_Si, R_S_frt, R_s_slag, R_sliq_fr
REAL, DIMENSION (NCELL):: R_S_av_P, R_S_av_Si, R_S_frt, R_s_slag, R_sliq_fr
REAL, DIMENSION (NCELL):: R_S_av_P, R_S_av_Si, R_S_frt, R_s_slag, R_sliq_fr
REAL, DIMENSION (NCELL):: R_S_av_P, R_S_av_Si, R_S_frt, R_s_slag, R_sliq_fr
REAL, DIMENSION (NCELL):: R_S_av_P, R_S_av_Si, R_S_frt, R_s_slag, R_sliq_fr
REAL, DIMENSION (NCELL):: R_S_av_P, R_S_av_Si, R_S_frt, R_s_slag, R_sliq_fr

c----------------------------------------------------------------------------------------------------------------
c----- Bubble volume, diameter and length of plateau border
c----------------------------------------------------------------------------------------------------------------

R_v(1)=65.416E-09
R_v(2)=130.833E-09
R_v(3)=261.6667E-09
R_v(4)=523.333E-09
R_v(5)=1046.667E-09
R_v(6)=209.333E-08
R_v(7)=418.667E-08
R_v(8)=837.333E-08
R_v(9)=167.467E-07
R_v(10)=334.933E-07
c----- Bubble diameter
R_d(1)=2.500E-03
R_d(2)=3.149E-03
R_d(3)=3.968E-03
R_d(4)=5.000E-03
R_d(5)=6.299E-03
R_d(6)=7.937E-03
R_d(7)=10.000E-03
R_d(8)=12.599E-03
R_d(9)=15.874E-03
R_d(10)=20.000E-03
c----- Bubble break up, Coalescence model and population balance
c----------------------------------------------------------------------------------------------------------------

DO nc=nsp(mat), nep(mat)
ip1=nc
ip2=nc+ncell
ip3=nc+ncell+ncell
ip4=nc+ncell+ncell+ncell
IF(edm(ip2).LT.1.0e-06)THEN
  edm(ip2)=1.0e-06
END IF
R_ld=(8.42e-05)/(edm(ip2)**0.25)
c----- volume of each scalar in each cell

c----- Scalar in gas phase
c----- gas bubble
R_tv(1) = Phi_mscal((1-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(2) = Phi_mscal((2-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(3) = Phi_mscal((3-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(4) = Phi_mscal((4-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(5) = Phi_mscal((5-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(6) = Phi_mscal((6-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(7) = Phi_mscal((7-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(8) = Phi_mscal((8-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(9) = Phi_mscal((9-1)*ncell+nc)*vfm(ip1)*vol(nc)
R_tv(10) = Phi_mscal((10-1)*ncell+nc)*vfm(ip1)*vol(nc)

c----- Scalar in foam phase
c----- bubble
R_tvf(1) = Phi_mscal((39-1)*ncell+nc)
R_tvf(2) = Phi_mscal((40-1)*ncell+nc)
R_tvf(3) = Phi_mscal((41-1)*ncell+nc)
R_tvf(4) = Phi_mscal((42-1)*ncell+nc)
R_tvf(5) = Phi_mscal((43-1)*ncell+nc)
R_tvf(6) = Phi_mscal((44-1)*ncell+nc)
R_tvf(7) = Phi_mscal((45-1)*ncell+nc)
R_tvf(8) = Phi_mscal((46-1)*ncell+nc)
R_tvf(9) = Phi_mscal((47-1)*ncell+nc)
R_tvf(10) = Phi_mscal((48-1)*ncell+nc)

c----- Number of gas bubble in each cell in gas phase
R_nb(1) = R_tv(1)/R_v(1)
R_nb(2) = R_tv(2)/R_v(2)
R_nb(3) = R_tv(3)/R_v(3)
R_nb(4) = R_tv(4)/R_v(4)
R_nb(5) = R_tv(5)/R_v(5)
R_nb(6) = R_tv(6)/R_v(6)
R_nb(7) = R_tv(7)/R_v(7)
R_nb(8) = R_tv(8)/R_v(8)
R_nb(9) = R_tv(9)/R_v(9)
R_nb(10) = R_tv(10)/R_v(10)

c----- Number of foam bubble in each cell in foam phase
R_nbf(1) = R_tvf(1)/R_v(1)
R_nbf(2) = R_tvf(2)/R_v(2)
R_nbf(3) = R_tvf(3)/R_v(3)
R_nbf(4) = R_tvf(4)/R_v(4)
R_nbf(5) = R_tvf(5)/R_v(5)
R_nbf(6) = R_tvf(6)/R_v(6)
R_nbf(7) = R_tvf(7)/R_v(7)
R_nbf(8) = R_tvf(8)/R_v(8)
R_nbf(9) = R_tvf(9)/R_v(9)
R_nbf(10) = R_tvf(10)/R_v(10)

c----- Initialization for Birth and death term for break up
R_DB(1) = 0.0
R_DB(2) = 0.0
R_DB(3) = 0.0
R_DB(4) = 0.0
R_DB(5) = 0.0
R_DB(6) = 0.0
R_DB(7) = 0.0
R_DB(8)=0.0
R_DB(9)=0.0
R_DB(10)=0.0
R_BB(1)=0.0
R_BB(2)=0.0
R_BB(3)=0.0
R_BB(4)=0.0
R_BB(5)=0.0
R_BB(6)=0.0
R_BB(7)=0.0
R_BB(8)=0.0
R_BB(9)=0.0
R_BB(10)=0.0

c----- Initialization for Birth and Death term for Coalescence in gas phase
R_DC(1)=0.0
R_DC(2)=0.0
R_DC(3)=0.0
R_DC(4)=0.0
R_DC(5)=0.0
R_DC(6)=0.0
R_DC(7)=0.0
R_DC(8)=0.0
R_DC(9)=0.0
R_DC(10)=0.0
R_BC(1)=0.0
R_BC(2)=0.0
R_BC(3)=0.0
R_BC(4)=0.0
R_BC(5)=0.0
R_BC(6)=0.0
R_BC(7)=0.0
R_BC(8)=0.0
R_BC(9)=0.0
R_BC(10)=0.0

R_DCF(1)=0.0
R_DCF(2)=0.0
R_DCF(3)=0.0
R_DCF(4)=0.0
R_DCF(5)=0.0
R_DCF(6)=0.0
R_DCF(7)=0.0
R_DCF(8)=0.0
R_DCF(9)=0.0
R_DCF(10)=0.0
R_BCF(1)=0.0
R_BCF(2)=0.0
R_BCF(3)=0.0
R_BCF(4)=0.0
R_BCF(5)=0.0
R_BCF(6)=0.0
R_BCF(7)=0.0
R_BCF(8)=0.0
R_BCF(9)=0.0
R_BCF(10)=0.0

C---- Initialization for Birth and Death term for Coalescence in foam phase
R_DCF(1)=0.0
R_DCF(2)=0.0
R_DCF(3)=0.0
R_DCF(4)=0.0
R_DCF(5)=0.0
R_DCF(6)=0.0
R_DCF(7)=0.0
R_DCF(8)=0.0
R_DCF(9)=0.0
R_DCF(10)=0.0
R_BCF(1)=0.0
R_BCF(2)=0.0
R_BCF(3)=0.0
R_BCF(4)=0.0
R_BCF(5)=0.0
R_BCF(6)=0.0
R_BCF(7)=0.0
R_BCF(8)=0.0
R_BCF(9)=0.0
R_BCF(10)=0.0
c-----Start of bubble coalescence

c-----Bubble Coalescence model by Prince and Blanch

**Birth of bubble class i+1 due to coalescence of bubble class i to N-1**

```fortran
IF(vfm(ip1).LT.0.75)THEN
  DO  I_i=1,9
    DO  I_j=1,I_i
      R_ccarea(I_i,I_j)=((R_d(I_i)+R_d(I_j))**2.0)
      c-----Turbulent collision rate R_TCR
      R_TCR(I_i,I_j)=0.089*R_nb(I_i)*R_nb(I_j)*R_ccarea(I_i,I_j)*
      ((edm(ip2)**0.333)*((R_d(I_i)**0.666+R_d(I_j)**0.666)**0.5)
      c-----Min number of bubble calculation
      R_min_nb(I_i,I_j)=min(R_nb(I_i),R_nb(I_j))
      c-----Total coalescence
      IF(R_TCR(I_i,I_j).GT.R_min_nb(I_i,I_j))THEN
        R_TCR(I_i,I_j)=R_min_nb(I_i,I_j)
      END IF
      c-----coalescence efficnecy,log(ho/hf=4)
      R_rbij(I_i,I_j)=(0.5)*(((1.0/R_d(I_i))+(1.0/R_d(I_j)))**(-1.0))
      R_taij(I_i,I_j)=((1.0/edm(ip2))**0.333)*((R_rbij(I_i,I_j))**0.33)
      R_tij(I_i,I_j)=26151.6*(R_rbij(I_i,I_j)**3.0)
    END DO
  END DO
  R_colef(I_i,I_j)=EXP(-R_tij(I_i,I_j)/R_taij(I_i,I_j))
  c-----Total coalescence rate due to turbulence, Buoyancy and laminar shear collision
  R_CR(I_i,I_j)=R_TCR(I_i,I_j)*R_colef(I_i,I_j)
  R_Xij(I_i,I_j)=(1.0)-((2.0)**(I_j-I_i))
END IF
```

c-----Scalar Value update for each bubble class

c-----First Scalar value update
R_vbc1(1)=0.0
R_vbc2(1)=0.0
R_vbc3(1)=0.0
R_vbc4(1)=0.0

c-----Second Scalar value update
R_vbc1(2)=0.0
R_vbc2(2)=0.0
R_vbc3(2)=0.0
R_vbc4(2)=0.0

c-----Third Scalar value update
R_vbc1(3)=0.0
R_vbc2(3)=0.0
R_vbc3(3)=0.0
R_vbc4(3)=0.0

c-----Fourth Scalar value update
R_vbc1(4)=0.0
R_vbc2(4)=0.0
R_vbc3(4)=0.0
R_vbc4(4)=0.0

c-----Fifth Scalar value update
R_vbc1(5)=0.0
R_vbc2(5)=0.0
R_vbc3(5)=0.0
R_vbc4(5)=0.0

c-----Sixth Scalar value update
R_vbc1(6)=0.0
R_vbc2(6)=0.0
R_vbc3(6)=0.0
R_vbc4(6)=0.0
c-----Seventh Scalar value update
R_vbc1(7)=0.0
R_vbc2(7)=0.0
R_vbc3(7)=0.0
R_vbc4(7)=0.0
c-----Eighth Scalar value update
R_vbc1(8)=0.0
R_vbc2(8)=0.0
R_vbc3(8)=0.0
R_vbc4(8)=0.0
c-----Ninth Scalar value update
R_vbc1(9)=0.0
R_vbc2(9)=0.0
R_vbc3(9)=0.0
R_vbc4(9)=0.0
c-----Tenth Scalar value update
R_vbc1(10)=0.0
R_vbc2(10)=0.0
R_vbc3(10)=0.0
R_vbc4(10)=0.0
c-----Death of I_j for the birth of I_i
R_vbc1(I_i)=R_Xij(I_i,I_j)*R_CR(I_i,I_j)*R_v(I_j)
c-----Death of I_i that goes to I_i+1
IF (I_i==I_j) THEN
R_vbc2(I_i)=0.0
ELSE
R_vbc2(I_i)=(1.0-R_Xij(I_i,I_j))*R_CR(I_i,I_j)*R_v(I_i)
END IF
c-----Death of I_j that goes to I_i+1
R_vbc3(I_i)=(1.0-R_Xij(I_i,I_j))*R_CR(I_i,I_j)*R_v(I_j)
c-----Total death of I_j
R_vbc4(I_j)=R_vbc1(I_i)+R_vbc3(I_i)
c-----Number of bubble update
R_tv(1)=R_tv(1)-(R_vbc2(1)+R_vbc4(1))
R_tv(2)=R_tv(2)-(R_vbc2(2)+R_vbc4(2))
R_tv(3)=R_tv(3)-(R_vbc2(3)+R_vbc4(3))
R_tv(4)=R_tv(4)-(R_vbc2(4)+R_vbc4(4))
R_tv(5)=R_tv(5)-(R_vbc2(5)+R_vbc4(5))
R_tv(6)=R_tv(6)-(R_vbc2(6)+R_vbc4(6))
R_tv(7)=R_tv(7)-(R_vbc2(7)+R_vbc4(7))
R_tv(8)=R_tv(8)-(R_vbc2(8)+R_vbc4(8))
R_tv(9)=R_tv(9)-(R_vbc2(9)+R_vbc4(9))
R_tv(10)=R_tv(10)-(R_vbc2(10)+R_vbc4(10))
c----------------------------------------------------------------------------------------------------------------
R_nb(1)=R_tv(1)/R_v(1)
R_nb(2)=R_tv(2)/R_v(2)
R_nb(3)=R_tv(3)/R_v(3)
R_nb(4)=R_tv(4)/R_v(4)
R_nb(5)=R_tv(5)/R_v(5)
R_nb(6)=R_tv(6)/R_v(6)
R_nb(7)=R_tv(7)/R_v(7)
R_nb(8)=R_tv(8)/R_v(8)
R_nb(9)=R_tv(9)/R_v(9)
\[ R_{\text{nb}}(10) = \frac{R_{\text{tv}}(10)}{R_{\text{v}}(10)} \]

\[ R_{\text{DC}}(1) = R_{\text{DC}}(1) + R_{\text{vbc2}}(1) + R_{\text{vbc4}}(1) \]
\[ R_{\text{DC}}(2) = R_{\text{DC}}(2) + R_{\text{vbc2}}(2) + R_{\text{vbc4}}(2) \]
\[ R_{\text{DC}}(3) = R_{\text{DC}}(3) + R_{\text{vbc2}}(3) + R_{\text{vbc4}}(3) \]
\[ R_{\text{DC}}(4) = R_{\text{DC}}(4) + R_{\text{vbc2}}(4) + R_{\text{vbc4}}(4) \]
\[ R_{\text{DC}}(5) = R_{\text{DC}}(5) + R_{\text{vbc2}}(5) + R_{\text{vbc4}}(5) \]
\[ R_{\text{DC}}(6) = R_{\text{DC}}(6) + R_{\text{vbc2}}(6) + R_{\text{vbc4}}(6) \]
\[ R_{\text{DC}}(7) = R_{\text{DC}}(7) + R_{\text{vbc2}}(7) + R_{\text{vbc4}}(7) \]
\[ R_{\text{DC}}(8) = R_{\text{DC}}(8) + R_{\text{vbc2}}(8) + R_{\text{vbc4}}(8) \]
\[ R_{\text{DC}}(9) = R_{\text{DC}}(9) + R_{\text{vbc2}}(9) + R_{\text{vbc4}}(9) \]
\[ R_{\text{DC}}(10) = R_{\text{DC}}(10) + R_{\text{vbc2}}(10) + R_{\text{vbc4}}(10) \]

\[ R_{\text{BC}}(1) = R_{\text{BC}}(1) + R_{\text{vbc1}}(1) \]
\[ R_{\text{BC}}(2) = R_{\text{BC}}(2) + R_{\text{vbc1}}(2) + R_{\text{vbc2}}(1) + R_{\text{vbc3}}(1) \]
\[ R_{\text{BC}}(3) = R_{\text{BC}}(3) + R_{\text{vbc1}}(3) + R_{\text{vbc2}}(2) + R_{\text{vbc3}}(2) \]
\[ R_{\text{BC}}(4) = R_{\text{BC}}(4) + R_{\text{vbc1}}(4) + R_{\text{vbc2}}(3) + R_{\text{vbc3}}(3) \]
\[ R_{\text{BC}}(5) = R_{\text{BC}}(5) + R_{\text{vbc1}}(5) + R_{\text{vbc2}}(4) + R_{\text{vbc3}}(4) \]
\[ R_{\text{BC}}(6) = R_{\text{BC}}(6) + R_{\text{vbc1}}(6) + R_{\text{vbc2}}(5) + R_{\text{vbc3}}(5) \]
\[ R_{\text{BC}}(7) = R_{\text{BC}}(7) + R_{\text{vbc1}}(7) + R_{\text{vbc2}}(6) + R_{\text{vbc3}}(6) \]
\[ R_{\text{BC}}(8) = R_{\text{BC}}(8) + R_{\text{vbc1}}(8) + R_{\text{vbc2}}(7) + R_{\text{vbc3}}(7) \]
\[ R_{\text{BC}}(9) = R_{\text{BC}}(9) + R_{\text{vbc1}}(9) + R_{\text{vbc2}}(8) + R_{\text{vbc3}}(8) \]
\[ R_{\text{BC}}(10) = R_{\text{BC}}(10) + R_{\text{vbc2}}(9) + R_{\text{vbc3}}(9) \]

END DO
END DO

---

--- Bubble break up model by Luo and Svendsen
--- Birth of bubble class \( i \) due to break up of bubble class \( i+1 \) to \( N \)
---

DO 
I_i=1,9
DO 
I_k=I_i+1,10
--- Coefficient of surface area increase
R_dr(I_k)=R_d(I_i)/R_d(I_k)
R_Cf(I_k)=((R_dr(I_k)**2.0)-1.0)+((1.0-(R_dr(I_k)**3.0)**0.666)
--- Dimensionless size of eddy
R_zita(I_k)=(11.4/R_d(I_k))*((edm(ip2)*vimm(ip2))**(-0.25))
--- Critical dimensionless energy for break up
R_chaiC(I_k)=(6.21e-05*R_Cf(I_k))/((edm(ip2)**0.666)*(R_d(I_k)**1.66)*(R_zita(I_k)**3.66))
--- Probability of bubble size \( k \) colliding with eddy lamda breaking up into size \( i \)
R_pb(I_k,I_i)=EXP(-R_chaiC(I_k))
--- Collision frequency of bubble class \( k \) with \( pi=3.14 \) eddy size lamda
R_cfq(I_k)=8.22e14*((R_d(I_k)+R_ld)**2.0)*vfm(ip2)*(edm(ip2)**2.0)*R_nb(I_k)
IF(R_cfq(I_k).GT.R_nb(I_k))THEN
R_cfq(I_k)=R_nb(I_k)
END IF
--- Break up rate of bubble class \( k \) into class \( i \)
IF (R_pb(I_k,I_i).GT.1.0)THEN
R_pb(I_k,I_i)=1.0
END IF
R_BR(I_k,I_i)=R_cfq(I_k)*R_pb(I_k,I_i)
IF (R_ld.GE.R_d(I_k))THEN
R_BR(I_k,I_i)=0.0
END IF
---
--- Scalar Value update for the birth of each bubble class due to death of other class
---

---
\[ R_{vbb}(1) = 0.0 \]
\[ R_{vbb}(2) = 0.0 \]
\[ R_{vbb}(3) = 0.0 \]
\[ R_{vbb}(4) = 0.0 \]
\[ R_{vbb}(5) = 0.0 \]
\[ R_{vbb}(6) = 0.0 \]
\[ R_{vbb}(7) = 0.0 \]
\[ R_{vbb}(8) = 0.0 \]
\[ R_{vbb}(9) = 0.0 \]
\[ R_{vbb}(10) = 0.0 \]
\[ R_{vbb}(l_i) = R_{BR}(l_k, l_i) * R_v(l_i) \]

---

Scalar Value update for the birth of each bubble class due to death of other class

\[ R_{Xik}(l_k, l_i) = (2.0)^{(1 + l_i - l_k)} \]

--- First Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Second Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Third Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Fourth Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Fifth Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Sixth Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Seventh Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Eighth Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Ninth Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

--- Tenth Scalar value update
\[ R_{vbd}(1) = 0.0 \]
\[ R_{vbd}(2) = 0.0 \]

Scalar of birth
\[ R_{vbd}(l_k) = R_{BR}(l_k, l_i) * R_v(l_i) \]
\[ R_{vbd}(l_k) = R_{Xik}(l_k, l_i) * R_{BR}(l_k, l_i) * (R_v(l_k) - R_v(l_i)) \]

---

\[ R_{tv}(1) = R_{tv}(1) - (R_{vbd}(1) + R_{vbd}(2)) \]
\[ R_{tv}(2) = R_{tv}(2) - (R_{vbd}(1) + R_{vbd}(2)) \]
\[ R_{tv}(3) = R_{tv}(3) - (R_{vbd}(2) + R_{vbd}(3)) \]
\[ R_{tv}(4) = R_{tv}(4) - (R_{vbd}(2) + R_{vbd}(3)) \]
\[ R_{tv}(5) = R_{tv}(5) - (R_{vbd}(3) + R_{vbd}(4)) \]
\[ R_{tv}(6) = R_{tv}(6) - (R_{vbd}(2) + R_{vbd}(3)) \]
\[ R_{tv}(7) = R_{tv}(7) - (R_{vbd}(3) + R_{vbd}(4)) \]
\[ R_{tv}(8) = R_{tv}(8) - (R_{vbd1}(8) + R_{vbd}(8)) \]
\[ R_{tv}(9) = R_{tv}(9) - (R_{vbd1}(9) + R_{vbd}(9)) \]
\[ R_{tv}(10) = R_{tv}(10) - (R_{vbd1}(10) + R_{vbd}(10)) \]

--- Number of bubble update
\[ R_{nb}(1) = R_{tv}(1) / R_v(1) \]
\[ R_{nb}(2) = R_{tv}(2) / R_v(2) \]
\[ R_{nb}(3) = R_{tv}(3) / R_v(3) \]
\[ R_{nb}(4) = R_{tv}(4) / R_v(4) \]
\[ R_{nb}(5) = R_{tv}(5) / R_v(5) \]
\[ R_{nb}(6) = R_{tv}(6) / R_v(6) \]
\[ R_{nb}(7) = R_{tv}(7) / R_v(7) \]
\[ R_{nb}(8) = R_{tv}(8) / R_v(8) \]
\[ R_{nb}(9) = R_{tv}(9) / R_v(9) \]
\[ R_{nb}(10) = R_{tv}(10) / R_v(10) \]

--- Birth
\[ R_{BB}(1) = R_{BB}(1) + R_{vbb}(1) + R_{vbd}(2) \]
\[ R_{BB}(2) = R_{BB}(2) + R_{vbb}(2) + R_{vbd}(3) \]
\[ R_{BB}(3) = R_{BB}(3) + R_{vbb}(3) + R_{vbd}(4) \]
\[ R_{BB}(4) = R_{BB}(4) + R_{vbb}(4) + R_{vbd}(5) \]
\[ R_{BB}(5) = R_{BB}(5) + R_{vbb}(5) + R_{vbd}(6) \]
\[ R_{BB}(6) = R_{BB}(6) + R_{vbb}(6) + R_{vbd}(7) \]
\[ R_{BB}(7) = R_{BB}(7) + R_{vbb}(7) + R_{vbd}(8) \]
\[ R_{BB}(8) = R_{BB}(8) + R_{vbb}(8) + R_{vbd}(9) \]
\[ R_{BB}(9) = R_{BB}(9) + R_{vbb}(9) + R_{vbd}(10) \]
\[ R_{BB}(10) = R_{BB}(10) + R_{vbb}(10) \]

--- Death
\[ R_{DB}(1) = R_{DB}(1) + R_{vbd1}(1) + R_{vbd}(1) \]
\[ R_{DB}(2) = R_{DB}(2) + R_{vbd1}(2) + R_{vbd}(2) \]
\[ R_{DB}(3) = R_{DB}(3) + R_{vbd1}(3) + R_{vbd}(3) \]
\[ R_{DB}(4) = R_{DB}(4) + R_{vbd1}(4) + R_{vbd}(4) \]
\[ R_{DB}(5) = R_{DB}(5) + R_{vbd1}(5) + R_{vbd}(5) \]
\[ R_{DB}(6) = R_{DB}(6) + R_{vbd1}(6) + R_{vbd}(6) \]
\[ R_{DB}(7) = R_{DB}(7) + R_{vbd1}(7) + R_{vbd}(7) \]
\[ R_{DB}(8) = R_{DB}(8) + R_{vbd1}(8) + R_{vbd}(8) \]
\[ R_{DB}(9) = R_{DB}(9) + R_{vbd1}(9) + R_{vbd}(9) \]
\[ R_{DB}(10) = R_{DB}(10) + R_{vbd1}(10) + R_{vbd}(10) \]

END DO
END DO
END IF

--- Foam formation from gas and slag

--- Transformation of gas and liquid into foam
IF(vfm(ip1).GE.0.75.AND.vfm(ip3).GE.0.05) THEN
R_{tDgbt}(nc)=0.999*vfm(ip1)*vol(nc)*denm(ip1)
ENDIF
\( R_{\text{reG}}(nc) = 0.001 \times vfm(ip1) \times \text{vol}(nc) \times \text{denm}(ip1) \)

IF \( R_{\text{reG}}(nc) \lt 1.0 \times 10^{-30} \) THEN
\( R_{\text{reG}}(nc) = 1.0 \times 10^{-30} \)
END IF

--- Total slag transformation
\( R_{\text{St}}(nc) = 0.0199 \times vfm(ip3) \times \text{vol}(nc) \times \text{denm}(ip3) \)
\( R_{\text{reS}}(nc) = 0.9801 \times vfm(ip3) \times \text{vol}(nc) \times \text{denm}(ip3) \)

--- Total liquid transformation
\( R_{\text{tqt}}(nc) = vfm(ip2) \times \text{vol}(nc) \times \text{denm}(ip2) \)
\( R_{\text{C\_final}}(nc) = 1.0 \times 10^{-30} \)
\( R_{\text{Fe\_final}}(nc) = 1.0 \times 10^{-30} \)
\( R_{\text{Si\_final}}(nc) = 1.0 \times 10^{-30} \)
\( R_{\text{Mn\_final}}(nc) = 1.0 \times 10^{-30} \)
\( R_{\text{P\_final}}(nc) = 1.0 \times 10^{-30} \)
ELSE
\( R_{\text{tDgbt}}(nc) = 1.0 \times 10^{-30} \)
\( R_{\text{tqt}}(nc) = 1.0 \times 10^{-30} \)
\( R_{\text{St}}(nc) = 1.0 \times 10^{-30} \)
\( R_{\text{reG}}(nc) = 1.0 \times 10^{-30} \)
\( R_{\text{reS}}(nc) = 1.0 \times 10^{-30} \)
END IF
\( R_{\text{g}}(nc) = R_{\text{g}}(nc) + R_{\text{tDgbt}}(nc) + R_{\text{reG}}(nc) \)
\( R_{\text{lq}}(nc) = R_{\text{lq}}(nc) + R_{\text{tqt}}(nc) \)
\( R_{\text{s}}(nc) = R_{\text{s}}(nc) + R_{\text{St}}(nc) + R_{\text{reS}}(nc) \)
\( R_{\text{foam}}(nc) = R_{\text{foam}}(nc) + R_{\text{g}}(nc) + R_{\text{lq}}(nc) + R_{\text{s}}(nc) \)

--- Bubble coalescence in foam
--- Film rupture inside foam

IF \( vfm(ip4) \gt \text{vrmin} \) THEN
DO \( i_m = 1, 9 \)
  DO \( i_i = 1, i_m \)
    --- Probability of sharing the same film of bubble \( i \) and \( m \)
    \( R_{\text{FS}}(i_i, i_m) = R_{\text{nbf}}(i_i) / (R_{\text{nbf}}(1) + R_{\text{nbf}}(2) + R_{\text{nbf}}(3) + R_{\text{nbf}}(4) + R_{\text{nbf}}(5) + R_{\text{nbf}}(6) + R_{\text{nbf}}(7) + R_{\text{nbf}}(8) + R_{\text{nbf}}(9) + R_{\text{nbf}}(10)) \)
    \( R_{\text{min\_nbf}}(i_i, i_m) = \text{min}(R_{\text{nbf}}(i_i), R_{\text{nbf}}(i_m)) \)
    --- Coalescence rate of film
    \( R_{\text{crf}}(i_i, i_m) = 5.78 \times 10^5 \times (R_{d}(i_i) \times 2.0) \times R_{\text{FS}}(i_i, i_m) \)
    IF \( R_{\text{crf}}(i_i, i_m) \gt R_{\text{min\_nbf}}(i_i, i_m) \) THEN
      \( R_{\text{crf}}(i_i, i_m) = R_{\text{min\_nbf}}(i_i, i_m) \)
    END IF
    --- Scalar Value update for each bubble class
    --- First Scalar value update
    \( R_{\text{vbcf1}}(1) = 0.0 \)
    \( R_{\text{vbcf2}}(1) = 0.0 \)
    \( R_{\text{vbcf3}}(1) = 0.0 \)
    \( R_{\text{vbcf4}}(1) = 0.0 \)
    --- Second Scalar value update
    \( R_{\text{vbcf1}}(2) = 0.0 \)
    \( R_{\text{vbcf2}}(2) = 0.0 \)
    \( R_{\text{vbcf3}}(2) = 0.0 \)
    \( R_{\text{vbcf4}}(2) = 0.0 \)
    --- Third Scalar value update
  END DO
END DO
--- Scalar Value update for each bubble class
--- First Scalar value update
\( R_{\text{vbcf1}}(1) = 0.0 \)
\( R_{\text{vbcf2}}(1) = 0.0 \)
\( R_{\text{vbcf3}}(1) = 0.0 \)
\( R_{\text{vbcf4}}(1) = 0.0 \)
--- Second Scalar value update
\( R_{\text{vbcf1}}(2) = 0.0 \)
\( R_{\text{vbcf2}}(2) = 0.0 \)
\( R_{\text{vbcf3}}(2) = 0.0 \)
\( R_{\text{vbcf4}}(2) = 0.0 \)
--- Third Scalar value update
R_vbcf1(3)=0.0
R_vbcf2(3)=0.0
R_vbcf3(3)=0.0
R_vbcf4(3)=0.0

c-----Fourth Scalar value update
R_vbcf1(4)=0.0
R_vbcf2(4)=0.0
R_vbcf3(4)=0.0
R_vbcf4(4)=0.0

c-----Fifth Scalar value update
R_vbcf1(5)=0.0
R_vbcf2(5)=0.0
R_vbcf3(5)=0.0
R_vbcf4(5)=0.0

c-----Sixth Scalar value update
R_vbcf1(6)=0.0
R_vbcf2(6)=0.0
R_vbcf3(6)=0.0
R_vbcf4(6)=0.0

c-----Seventh Scalar value update
R_vbcf1(7)=0.0
R_vbcf2(7)=0.0
R_vbcf3(7)=0.0
R_vbcf4(7)=0.0

c-----Eighth Scalar value update
R_vbcf1(8)=0.0
R_vbcf2(8)=0.0
R_vbcf3(8)=0.0
R_vbcf4(8)=0.0

c-----Ninth Scalar value update
R_vbcf1(9)=0.0
R_vbcf2(9)=0.0
R_vbcf3(9)=0.0
R_vbcf4(9)=0.0

c-----Tenth Scalar value update
R_vbcf1(10)=0.0
R_vbcf2(10)=0.0
R_vbcf3(10)=0.0
R_vbcf4(10)=0.0

c-----Death of I_m for the birth of I_i
R_vbcf1(I_i)=R_Xijf(I_i,I_m)*R_crf(I_i,I_m)*R_v(I_m)
c-----Death of I_i that goes to I_i+1
IF(I_i==I_m) THEN
R_vbcf2(I_i)=0.0
ELSE
R_vbcf2(I_i)=(1.0-R_Xijf(I_i,I_m))*R_crf(I_i,I_m)*R_v(I_i)
END IF

c-----Death of I_m
R_vbcf3(I_i)=(1.0-R_Xijf(I_i,I_m))*R_crf(I_i,I_m)*R_v(I_m)
c-----Total death of I_m
R_vbcf4(I_m)=R_vbcf1(I_i)+R_vbcf3(I_i)

R_vbcf1(1)=R_vbcf2(1)+R_vbcf4(1)
R_vbcf2(2)=R_vbcf2(2)+R_vbcf4(2)
R_vbcf3(3)=R_vbcf2(3)+R_vbcf4(3)
R_vbcf4(4)=R_vbcf2(4)+R_vbcf4(4)
\[
R_{vbctf}(5) = R_{vbcf2}(5) + R_{vbcf4}(5) \\
R_{vbctf}(6) = R_{vbcf2}(6) + R_{vbcf4}(6) \\
R_{vbctf}(7) = R_{vbcf2}(7) + R_{vbcf4}(7) \\
R_{vbctf}(8) = R_{vbcf2}(8) + R_{vbcf4}(8) \\
R_{vbctf}(9) = R_{vbcf2}(9) + R_{vbcf4}(9) \\
R_{vbctf}(10) = R_{vbcf2}(10) + R_{vbcf4}(10)
\]

\[
\text{IF} (R_{vbctf}(I_i) \gt R_{tvf}(I_i)) \text{THEN} \\
R_{vbctf}(I_i) = R_{tvf}(I_i) \\
\text{END IF}
\]

\[
\text{IF} (R_{vbctf}(I_m) \gt R_{tvf}(I_m)) \text{THEN} \\
R_{vbctf}(I_m) = R_{tvf}(I_m) \\
\text{END IF}
\]

\[
\text{c-----Scalar Value update for the birth of each bubble class due to death of other class} \\
\text{c-----Number of bubble update} \\
R_{tvf}(1) = R_{tvf}(1) - R_{vbctf}(1) \\
R_{tvf}(2) = R_{tvf}(2) - R_{vbctf}(2) \\
R_{tvf}(3) = R_{tvf}(3) - R_{vbctf}(3) \\
R_{tvf}(4) = R_{tvf}(4) - R_{vbctf}(4) \\
R_{tvf}(5) = R_{tvf}(5) - R_{vbctf}(5) \\
R_{tvf}(6) = R_{tvf}(6) - R_{vbctf}(6) \\
R_{tvf}(7) = R_{tvf}(7) - R_{vbctf}(7) \\
R_{tvf}(8) = R_{tvf}(8) - R_{vbctf}(8) \\
R_{tvf}(9) = R_{tvf}(9) - R_{vbctf}(9) \\
R_{tvf}(10) = R_{tvf}(10) - R_{vbctf}(10)
\]

\[
\text{c-----Death due to coalescence} \\
R_{DCF}(1) = R_{DCF}(1) + R_{vbcf2}(1) + R_{vbcf4}(1) \\
R_{DCF}(2) = R_{DCF}(2) + R_{vbcf2}(2) + R_{vbcf4}(2) \\
R_{DCF}(3) = R_{DCF}(3) + R_{vbcf2}(3) + R_{vbcf4}(3) \\
R_{DCF}(4) = R_{DCF}(4) + R_{vbcf2}(4) + R_{vbcf4}(4) \\
R_{DCF}(5) = R_{DCF}(5) + R_{vbcf2}(5) + R_{vbcf4}(5) \\
R_{DCF}(6) = R_{DCF}(6) + R_{vbcf2}(6) + R_{vbcf4}(6) \\
R_{DCF}(7) = R_{DCF}(7) + R_{vbcf2}(7) + R_{vbcf4}(7) \\
R_{DCF}(8) = R_{DCF}(8) + R_{vbcf2}(8) + R_{vbcf4}(8) \\
R_{DCF}(9) = R_{DCF}(9) + R_{vbcf2}(9) + R_{vbcf4}(9) \\
R_{DCF}(10) = R_{DCF}(10) + R_{vbcf2}(10) + R_{vbcf4}(10)
\]

\[
\text{c-----Birth due to coalescence and transformation} \\
R_{BCF}(1) = R_{BCF}(1) + R_{vbcf1}(1) \\
R_{BCF}(2) = R_{BCF}(2) + R_{vbcf1}(2) + R_{vbcf2}(1) + R_{vbcf3}(1) \\
R_{BCF}(3) = R_{BCF}(3) + R_{vbcf1}(3) + R_{vbcf2}(2) + R_{vbcf3}(2) \\
R_{BCF}(4) = R_{BCF}(4) + R_{vbcf1}(4) + R_{vbcf2}(3) + R_{vbcf3}(3) \\
R_{BCF}(5) = R_{BCF}(5) + R_{vbcf1}(5) + R_{vbcf2}(4) + R_{vbcf3}(4) \\
R_{BCF}(6) = R_{BCF}(6) + R_{vbcf1}(6) + R_{vbcf2}(5) + R_{vbcf3}(5)
\]
\[ R_{BCF}(7) = R_{BCF}(7) + R_{vbcf1}(7) + R_{vbcf2}(6) + R_{vbcf3}(6) \]
\[ R_{BCF}(8) = R_{BCF}(8) + R_{vbcf1}(8) + R_{vbcf2}(7) + R_{vbcf3}(7) \]
\[ R_{BCF}(9) = R_{BCF}(9) + R_{vbcf1}(9) + R_{vbcf2}(8) + R_{vbcf3}(8) \]
\[ R_{BCF}(10) = R_{BCF}(10) + R_{vbcf2}(9) + R_{vbcf3}(9) \]
\[ END DO \]
\[ END DO \]
\[ END IF \]

\[ R_g(nc) = R_g(nc) + R_{Tdgbt}(nc) + R_{reG}(nc) \]
\[ R_{lq_{av}(nc)} = R_{lq_{av}(nc)} + R_{lq_{frt}(nc)} \]
\[ R_{S_{av}(nc)} = R_{S_{av}(nc)} + R_{St(nc)} + R_{reS(nc)} \]
\[ R_{foam(nc)} = R_{foam(nc)} + R_{g(nc)} + R_{lq_{av}(nc)} + R_{S_{av}(nc)} \]

\[ c\text{----Foam drainage} \]
\[ R_{lq_{drain}(nc)} = (R_{lq_{av}(nc)} + R_{S_{av}(nc)}) / R_{foam(nc)} \]
\[ R_{lqdrain(nc)} = (R_{lq_{av}(nc)} + R_{S_{av}(nc)}) / R_{foam(nc)} \]

\[ IF (vfm(ip4).GT.vfrmin) THEN \]
\[ R_{N(nc)} = (R_{nbf(1)} + R_{nbf(1)} + R_{nbf(1)} + R_{nbf(1)} + R_{nbf(1)}) / 10.00 \]
\[ R_u(nc) = (8.836e-09*denm(ip4))/vimm(ip4) \]
\[ R_{qb(nc)} = 0.20*0.00044*10.0*3.12*0.00000001*R_u(nc)*R_N(nc) \]
\[ R_{drain(nc)} = R_{qb(nc)}/(vol(nc)*denm(ip4)) \]
\[ IF (R_{drain(nc).GT.(R_{lq_{av}(nc) + R_{S_{av}(nc)}))) THEN \]
\[ R_{drain(nc)} = R_{lq_{av}(nc)} + R_{S_{av}(nc)} \]
\[ END IF \]
\[ ELSE \]
\[ R_{drain(nc)} = 1.0e-30 \]
\[ END IF \]

\[ c\text{----Amount of slag drainage} \]
\[ R_{sldrain(nc)} = (R_{S_{av}(nc)} / R_{foam(nc)}) * R_{drain(nc)} \]
\[ IF (R_{sldrain(nc).LT.1.0e-30) THEN \]
\[ R_{sldrain(nc)} = 1.0e-30 \]
\[ END IF \]
\[ IF (R_{sldrain(nc).GE.R_{S_{av}(nc)})) THEN \]
\[ R_{sldrain(nc)} = R_{S_{av}(nc)} \]
\[ END IF \]

\[ c\text{----Foam drainage} \]
\[ R_{lq_{drain}(nc)} = (R_{lq_{av}(nc)} + R_{S_{av}(nc)} + R_{lq_{frt}(nc)}) / R_{foam(nc)} \]
\[ IF (vfm(ip3).LE.vfrmin.AND.R_{lq_{frt}(nc).LT.0.10) THEN \]
\[ R_{tdgfrt(nc)} = 0.699 * R_{foam(nc)} \]
\[ IF (R_{tdgfrt(nc).GT.R_{g(nc)}) THEN \]
\[ R_{tdgfrt(nc)} = R_{g(nc)} \]
\[ END IF \]

\[ END IF \]
R_S_f(nc) = (4.22e-07/vimm(ip3)) * R_foam(nc)
IF (R_S_f(nc) > R_S_av(nc)) THEN
  R_S_f(nc) = R_S_av(nc)
END IF

R_lq_f(nc) = R_lq_av(nc)
IF (R_lq_f(nc) > R_lqt(nc)) THEN
  R_lq_f(nc) = R_lqt(nc)
END IF

R_g(nc) = R_g(nc) + R_tDgbt(nc) + R_reG(nc) - R_tdgf(nc)
R_lq_av(nc) = R_lq_av(nc) + R_lqt(nc) - R_lqdrain(nc) - R_lq_f(nc)
R_S_av(nc) = R_S_av(nc) + R_St(nc) + R_reS(nc) - R_sldrain(nc) - R_S_f(nc)
R_foam(nc) = R_foam(nc) + R_g(nc) + R_lq_av(nc) + R_S_av(nc)

IF (R_foam(nc) > 1.0e-20) THEN
  R_gf(nc) = 0.5 * R_g(nc) / R_foam(nc)
  IF (R_gf(nc) > 0.40) THEN
    R_gf(nc) = 0.40
  END IF
  R_slagf(nc) = 0.5 * R_S_av(nc) / R_foam(nc)
  IF (R_slagf(nc) > 0.40) THEN
    R_slagf(nc) = 0.40
  END IF
  R_liquidf(nc) = 0.5 * R_lq_av(nc) / R_foam(nc)
  IF (R_liquidf(nc) > 0.40) THEN
    R_liquidf(nc) = 0.40
  END IF
ELSE
  R_gf(nc) = 1.0e-30
  R_slagf(nc) = 1.0e-30
  R_liquidf(nc) = 1.0e-30
END IF

R_S(23,nc) = R_liquidf(nc) - Phi_mscal((49-1)*ncell+nc)
IF (R_S(23,nc) <= 0.0) THEN
  R_S(23,nc) = 1.0e-30
END IF

R_S(24,nc) = R_gf(nc) - Phi_mscal((50-1)*ncell+nc)
IF (R_S(24,nc) <= 0.0) THEN
  R_S(24,nc) = 1.0e-30
END IF

R_S(34,nc) = R_slagf(nc) - Phi_mscal((51-1)*ncell+nc)
IF (R_S(34,nc) <= 0.0) THEN
  R_S(34,nc) = 1.0e-30
END IF

--- liquid and gas
--- Foam and gas for mph
IF(R_gf(nc).GT.0.40) THEN
    R_gf(nc)=0.40
END IF
R_fm_g(nc)=R_tdgf(nc)
R_g_fm(nc)=R_tDgbt(nc)+R_reG(nc)
R_gfr(nc)=R_gf(nc)
R_fm_S(nc)=R_St(nc)+R_reS(nc)
R_fm_lq(nc)=R_lq_f(nc)
ELSE
    R_tdgf(nc)=1.0e-30
    R_lq_f(nc)=1.0e-30
    R_S_f(nc)=1.0e-30
    c----------------------------------------------------------------------------------------------------------------
    R_g(nc)=R_g(nc)+R_tDgbt(nc)+R_reG(nc)
    R_lq_av(nc)=R_lq_av(nc)+R_lqt(nc)-R_lq_drain(nc)
    R_S_av(nc)=R_S_av(nc)+R_St(nc)+R_reS(nc)-R_sldrain(nc)
    R_foam(nc)=R_foam(nc)+R_g(nc)+R_lq_av(nc)+R_S_av(nc)
    c----------------------------------------------------------------------------------------------------------------
IF(R_foam(nc).GT.1.0e-20) THEN
    c----------------------------------------------------------------------------------------------------------------
    R_gf(nc)=0.5*(R_g(nc))/R_foam(nc)
    IF(R_gf(nc).GT.0.40) THEN
        R_gf(nc)=0.40
    END IF
    R_slagf(nc)=0.5*(R_S_av(nc))/R_foam(nc)
    IF(R_slf(nc).GT.0.40) THEN
        R_slf(nc)=0.40
    END IF
    R_liquidf(nc)=0.5*(R_lq_av(nc))/R_foam(nc)
    IF(R_liquidf(nc).GT.0.40) THEN
        R_liquidf(nc)=0.40
    END IF
    ELSE
        R_gf(nc)=1.0e-30
        R_slagf(nc)=1.0e-30
        R_liquidf(nc)=1.0e-30
    c----------------------------------------------------------------------------------------------------------------
    R_S(23,nc)=R_liquidf(nc)-Phi_mscal((49-1)*ncell+nc)
    IF(R_S(23,nc).LE.0.0) THEN
        R_S(23,nc)=1.0e-30
    END IF
    R_S(24,nc)=R_gf(nc)-Phi_mscal((50-1)*ncell+nc)
    IF(R_S(24,nc).LE.0.0) THEN
        R_S(24,nc)=1.0e-30
    END IF
    R_S(34,nc)=R_slagf(nc)-Phi_mscal((51-1)*ncell+nc)
    IF(R_S(34,nc).LE.0.0) THEN
        R_S(34,nc)=1.0e-30
    END IF
END IF
c-----liquid and gas

IF(R_gf(nc).GT.0.40) THEN
  R_gf(nc)=0.40
END IF

R_fm_g(nc)=1.0e-30
R_g_fm(nc)=R_tdgbt(nc)+R_reG(nc)
R_gfr(nc)=R_gf(nc)
R_fm_S(nc)=R_sl_drain(nc)
R_S_fm(nc)=R_ST(nc)+R_reS(nc)
R_fm_lq(nc)=R_lq_drain(nc)
R_lq_fm(nc)=R_lqt(nc)

END IF

C-----Variable description (Liquid)

R_Fe_b(nc)=Phi_mscal((14-1)*ncell+nc)
R_C_b(nc)=Phi_mscal((15-1)*ncell+nc)
R_Si_b(nc)=Phi_mscal((16-1)*ncell+nc)
R_Mn_b(nc)=Phi_mscal((17-1)*ncell+nc)
R_P_b(nc)=Phi_mscal((18-1)*ncell+nc)
R_FeO_b(nc)=Phi_mscal((20-1)*ncell+nc)
R_SiO2_b(nc)=Phi_mscal((21-1)*ncell+nc)
R_P2O5_b(nc)=Phi_mscal((23-1)*ncell+nc)
R_MnO_b(nc)=Phi_mscal((22-1)*ncell+nc)
R_CaO_b(nc)=Phi_mscal((24-1)*ncell+nc)
R_MgO_b(nc)=Phi_mscal((25-1)*ncell+nc)
R_S_b(nc)=Phi_mscal((19-1)*ncell+nc)
R_FeO_b(nc)=Phi_mscal((20-1)*ncell+nc)
R_SiO2_b(nc)=Phi_mscal((21-1)*ncell+nc)
R_P2O5_b(nc)=Phi_mscal((23-1)*ncell+nc)
R_MnO_b(nc)=Phi_mscal((22-1)*ncell+nc)
R_CaO_b(nc)=Phi_mscal((24-1)*ncell+nc)
R_MgO_b(nc)=Phi_mscal((25-1)*ncell+nc)
R_S_b(nc)=Phi_mscal((19-1)*ncell+nc)
R_FeO_b(nc)=Phi_mscal((20-1)*ncell+nc)
R_SiO2_b(nc)=Phi_mscal((21-1)*ncell+nc)
R_P2O5_b(nc)=Phi_mscal((23-1)*ncell+nc)
R_MnO_b(nc)=Phi_mscal((22-1)*ncell+nc)
R_CaO_b(nc)=Phi_mscal((24-1)*ncell+nc)
R_MgO_b(nc)=Phi_mscal((25-1)*ncell+nc)
R_S_b(nc)=Phi_mscal((19-1)*ncell+nc)

ELSE

R_m_liq(nc)=R_Fe_b(nc)+R_C_b(nc)+R_Si_b(nc)+R_P_b(nc)+R_Mn_b(nc)
R_s_lag(nc)=Phi_mscal((37-1)*ncell+nc)*vol(nc)*denm(ip3)
R_g_slag(nc)=Phi_mscal((38-1)*ncell+nc)*vol(nc)*denm(ip3)

IF(vfm(ip2).GE.0.10.AND.R_m_liq(nc).LE.0.75.AND.vfm(ip1).LT.0.10.AND.vfm(ip4).LE.0.01.AND.vfm(ip3).GE.0.10) THEN
  R_lq_s(nc)=vfm(ip2)*vol(nc)*denm(ip2)
  R_g_s(nc)=vfm(ip1)*vol(nc)*denm(ip1)
  R_f_s(nc)=vfm(ip4)*vol(nc)*denm(ip4)
ELSE
  R_lq_s(nc)=vfm(ip2)*vol(nc)*denm(ip2)
  R_g_s(nc)=vfm(ip1)*vol(nc)*denm(ip1)
  R_f_s(nc)=vfm(ip4)*vol(nc)*denm(ip4)
ENDIF
R_lq_s(nc)=1.0e-35
R_g_s(nc)=1.0e-35
R_f_s(nc)=1.0e-35

END IF

c--- slag(nc)=R_slag(nc)+R_lq_s(nc)+R_g_s(nc)+R_f_s(nc)
c
R_l_slag(nc)=R_l_slag(nc)+R_lq_s(nc)
c
c--- R_slag(nc)=R_g_slag(nc)+R_g_s(nc)

R_slag(nc)=R_slag(nc)+R_lq_s(nc)+R_g_s(nc)+R_f_s(nc)

R_g_slag(nc)=R_g_slag(nc)+R_g_s(nc)

R_l_slag(nc)=R_l_slag(nc)+R_lq_s(nc)

R_g_slag(nc)=R_g_slag(nc)+R_g_s(nc)

--- Variable description (Slag)

R_sFe_b(nc)=Phi_mscal((32-1)*ncell+nc)
R_sC_b(nc)=Phi_mscal((33-1)*ncell+nc)
R_sSi_b(nc)=Phi_mscal((34-1)*ncell+nc)
R_sMn_b(nc)=Phi_mscal((35-1)*ncell+nc)
R_sP_b(nc)=Phi_mscal((36-1)*ncell+nc)

R_sFe_b1(nc)=R_sFe_b(nc)*vfm(ip3)*vol(nc)*denm(ip3)
R_sC_b1(nc)=R_sC_b(nc)*vfm(ip3)*vol(nc)*denm(ip3)
R_sSi_b1(nc)=R_sSi_b(nc)*vfm(ip3)*vol(nc)*denm(ip3)
R_sMn_b1(nc)=R_sMn_b(nc)*vfm(ip3)*vol(nc)*denm(ip3)
R_sP_b1(nc)=R_sP_b(nc)*vfm(ip3)*vol(nc)*denm(ip3)

--- Scalars transported to slag from liquid

R_lisFe_b(nc)=Phi_mscal((14-1)*ncell+nc)
R_lisC_b(nc)=Phi_mscal((15-1)*ncell+nc)
R_lisSi_b(nc)=Phi_mscal((16-1)*ncell+nc)
R_lisMn_b(nc)=Phi_mscal((17-1)*ncell+nc)
R_lisP_b(nc)=Phi_mscal((18-1)*ncell+nc)

R_lisFe_b1(nc)=R_lisFe_b(nc)*R_lq_s(nc)
R_lisC_b1(nc)=R_lisC_b(nc)*R_lq_s(nc)
R_lisSi_b1(nc)=R_lisSi_b(nc)*R_lq_s(nc)
R_lisMn_b1(nc)=R_lisMn_b(nc)*R_lq_s(nc)
R_lisP_b1(nc)=R_lisP_b(nc)*R_lq_s(nc)
\[ R_{\text{lisP2O5\_b1}}(nc) = R_{\text{lisP2O5\_b}}(nc) R_{\text{lq\_s}}(nc) \]
\[ R_{\text{lisMnO\_b1}}(nc) = R_{\text{lisMnO\_b}}(nc) R_{\text{lq\_s}}(nc) \]
\[ R_{\text{lisCaO\_b1}}(nc) = R_{\text{lisCaO\_b}}(nc) R_{\text{lq\_s}}(nc) \]
\[ R_{\text{lisMgO\_b1}}(nc) = R_{\text{lisMgO\_b}}(nc) R_{\text{lq\_s}}(nc) \]
\[ R_{\text{liq\_slag\_s}}(nc) = R_{\text{sFe\_b1}}(nc) + R_{\text{sC\_b1}}(nc) + R_{\text{sSi\_b1}}(nc) + R_{\text{sMn\_b1}}(nc) + R_{\text{sP\_b1}}(nc) 
+ R_{\text{lisFe\_b1}}(nc) + R_{\text{lisC\_b1}}(nc) + R_{\text{lisSi\_b1}}(nc) + R_{\text{lisMn\_b1}}(nc) + R_{\text{lisP\_b1}}(nc) \]
\[ R_{\text{s\_slag\_s}}(nc) = R_{\text{sFeO\_b1}}(nc) + R_{\text{sSiO2\_b1}}(nc) + R_{\text{sP2O5\_b1}}(nc) 
+ R_{\text{lisFeO\_b}}(nc) + R_{\text{lisCaO\_b}}(nc) + R_{\text{lisSiO2\_b}}(nc) + R_{\text{lisMnO\_b}}(nc) 
+ R_{\text{lisP2O5\_b}}(nc) + R_{\text{lisMgO\_b}}(nc) R_{\text{lq\_s}}(nc) \]
\[ R_{\text{slag\_s}}(nc) = R_{\text{slag\_s}}(nc) + R_{\text{lq\_s}}(nc) + R_{\text{f\_s}}(nc) \]
\[ R_{\text{slag\_l}}(nc) = R_{\text{slag\_l}}(nc) + (R_{\text{lisFe\_b}}(nc) + R_{\text{lisC\_b}}(nc) 
+ R_{\text{lisSi\_b}}(nc) + R_{\text{lisMn\_b}}(nc) + R_{\text{lisP\_b}}(nc) ) R_{\text{lq\_s}}(nc) \]
\[ R_{\text{g\_slag\_s}}(nc) = R_{\text{g\_slag\_s}}(nc) + R_{\text{g\_s}}(nc) \]
\[ \text{IF} (R_{\text{liquidfr\_nc}} \geq 1.0) \text{THEN} \]
\[ R_{\text{liquidfr\_nc}} = 1.0 \]
\[ \text{END IF} \]

\[ \text{IF} (vfm(ip3) \geq 0.10 \text{AND} R_{\text{liquidfr\_nc}} > 0.90) \text{THEN} \]
\[ \text{R_{\text{s\_lq\_nc}} = R_{\text{l\_slag\_nc}} + R_{\text{f\_s\_nc}} \]}
\[ \text{IF} (R_{\text{s\_lq\_nc}} \leq 1.0e-30) \text{THEN} \]
\[ R_{\text{s\_lq\_nc}} = 1.0e-30 \]
\[ \text{END IF} \]
\[ R_{\text{s\_gas\_nc}} = R_{\text{g\_slag\_nc}} \]
\[ \text{IF} (R_{\text{s\_gas\_nc}} \leq 1.0e-30) \text{THEN} \]
\[ R_{\text{s\_gas\_nc}} = 1.0e-30 \]
\[ \text{END IF} \]
\[ \text{ELSE} \]
\[ R_{\text{s\_lq\_nc}} = 1.0e-30 \]
\[ R_{\text{s\_gas\_nc}} = 1.0e-30 \]
\[ \text{END IF} \]

\[ \text{IF} (R_{\text{s\_lq\_nc}} \leq 1.0e-30) \text{THEN} \]
\[ R_{\text{s\_lq\_nc}} = 1.0e-30 \]
\[ \text{END IF} \]
\[ \text{IF} (R_{\text{s\_gas\_nc}} \leq 1.0e-30) \text{THEN} \]
\[ R_{\text{s\_gas\_nc}} = 1.0e-30 \]
\[ \text{END IF} \]
\[ \text{IF} (R_{\text{lq\_s\_nc}} \leq 1.0e-30) \text{THEN} \]
\[ R_{\text{lq\_s\_nc}} = 1.0e-30 \]
\[ \text{END IF} \]
\[ \text{IF} (R_{\text{g\_s\_nc}} \leq 1.0e-30) \text{THEN} \]
\[ R_{\text{g\_s\_nc}} = 1.0e-30 \]
\[ \text{END IF} \]
\[ \text{IF} (R_{\text{lqf\_s\_nc}} \leq 1.0e-30) \text{THEN} \]
\[ R_{\text{lqf\_s\_nc}} = 1.0e-30 \]
\[ \text{END IF} \]

\[ R_{\text{slag\_nc}} = R_{\text{slag\_nc}} - R_{\text{s\_lq\_nc}} - R_{\text{s\_gas\_nc}} \]
\[ \text{IF} (R_{\text{slag\_nc}} \leq 1.0e-30) \text{THEN} \]
R_slag(nc)=1.0e-30
END IF
R_l_slag(nc)=R_l_slag(nc)-R_s_lq(nc)
IF(R_l_slag(nc).LE.1.0e-30) THEN
R_l_slag(nc)=1.0e-30
END IF
R_g_slag(nc)=R_g_slag(nc)-R_s_gas(nc)
IF(R_g_slag(nc).LE.1.0e-30) THEN
R_g_slag(nc)=1.0e-30
END IF
R_l_fr(nc)=R_l_slag(nc)/R_slag(nc)
IF(R_l_fr(nc).GE.1.0) THEN
R_l_fr(nc)=1.0
END IF
R_gas_fr(nc)=R_g_slag(nc)/R_slag(nc)
IF(R_g_s(nc).GE.1.0) THEN
R_g_s(nc)=1.0
END IF
R_s_fr(nc)=(R_slag(nc)-R_l_slag(nc)-R_g_slag(nc))/R_slag(nc)
IF(R_s_fr(nc).GE.1.0) THEN
R_s_fr(nc)=1.0
END IF
IF(R_s_fr(nc).LE.1.0e-30) THEN
R_s_fr(nc)=1.0e-30
END IF
R_S(44,nc)=(R_l_fr(nc)-Phi_mscal((37-1)*ncell+nc))*vfm(ip3)*vol(nc)*denm(ip3)
IF(R_S(44,nc).LE.1.0e-30) THEN
R_S(44,nc)=1.0e-30
END IF
R_S(45,nc)=(R_gas_fr(nc)-Phi_mscal((38-1)*ncell+nc))*vfm(ip3)*vol(nc)*denm(ip3)
IF(R_S(45,nc).LE.1.0e-30) THEN
R_S(45,nc)=1.0e-30
END IF
R_S(46,nc)=((R_l_fr(nc)-R_l_slag(nc)-R_g_slag(nc))/R_slag(nc))
IF(R_S(46,nc).LE.1.0e-30) THEN
R_S(46,nc)=1.0e-30
END IF
R_Fe_b(nc)=Phi_mscal((14-1)*ncell+nc)
R_C_b(nc)=Phi_mscal((15-1)*ncell+nc)
R_Si_b(nc)=Phi_mscal((16-1)*ncell+nc)
R_Mn_b(nc)=Phi_mscal((17-1)*ncell+nc)
R_Fe_b1(nc)=R_Fe_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
IF(R_Fe_b1(nc).LE.1.0e-30) THEN
R_Fe_b1(nc)=1.0e-30
END IF
$R_{C_b1(nc)} = R_{C_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2)$

**IF** $(R_{C_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{C_b1(nc)} = 1.0e-30$

**END IF**

$R_{Si_b1(nc)} = (R_{Si_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2))$

**IF** $(R_{Si_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{Si_b1(nc)} = 1.0e-30$

**END IF**

$R_{Mn_b1(nc)} = (R_{Mn_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2))$

**IF** $(R_{Mn_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{Mn_b1(nc)} = 1.0e-30$

**END IF**

$R_{P_b1(nc)} = (R_{P_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2))$

**IF** $(R_{P_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{P_b1(nc)} = 1.0e-30$

**END IF**

$R_{FeO_b(nc)} = \Phi_{mscal}((20-1) * ncell + nc)$

$R_{SiO2_b(nc)} = \Phi_{mscal}((21-1) * ncell + nc)$

$R_{P2O5_b(nc)} = \Phi_{mscal}((23-1) * ncell + nc)$

$R_{MnO_b(nc)} = \Phi_{mscal}((22-1) * ncell + nc)$

$R_{CaO_b(nc)} = \Phi_{mscal}((24-1) * ncell + nc)$

$R_{MgO_b(nc)} = \Phi_{mscal}((25-1) * ncell + nc)$

$R_{S_b(nc)} = \Phi_{mscal}((19-1) * ncell + nc)$

**----------------------------------------------------------------------------------------------------------------**

$R_{FeO_b1(nc)} = R_{FeO_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2)$

**IF** $(R_{FeO_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{FeO_b1(nc)} = 1.0e-30$

**END IF**

$R_{SiO2_b1(nc)} = R_{SiO2_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2)$

**IF** $(R_{SiO2_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{SiO2_b1(nc)} = 1.0e-30$

**END IF**

$R_{P2O5_b1(nc)} = R_{P2O5_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2)$

**IF** $(R_{P2O5_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{P2O5_b1(nc)} = 1.0e-30$

**END IF**

$R_{MnO_b1(nc)} = R_{MnO_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2)$

**IF** $(R_{MnO_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{MnO_b1(nc)} = 1.0e-30$

**END IF**

$R_{CaO_b1(nc)} = R_{CaO_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2)$

**IF** $(R_{CaO_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{CaO_b1(nc)} = 1.0e-30$

**END IF**

$R_{MgO_b1(nc)} = R_{MgO_b(nc)} * vfm(ip2) * vol(nc) * denm(ip2)$

**IF** $(R_{MgO_b1(nc)} \leq 1.0e-30)$ **THEN**

$R_{MgO_b1(nc)} = 1.0e-30$

**END IF**

**----------------------------------------------------------------------------------------------------------------**

**C----- Reacted element masses initialization**

$R_{C_FeO(nc)} = 1.0e-30$

$R_{Si_FeO(nc)} = 1.0e-30$

$R_{Mn_FeO(nc)} = 1.0e-30$

$R_{Si_MnO(nc)} = 1.0e-30$

$R_{C_MnO(nc)} = 1.0e-30$

$R_{C_P2O5(nc)} = 1.0e-30$
R_Si_P2O5(nc)=1.0e-30
R_Fe_P2O5(nc)=1.0e-30
R_Mn_P2O5(nc)=1.0e-30
R_C_final(nc)=1.0e-30
R_Fe_final(nc)=1.0e-30
R_Si_final(nc)=1.0e-30
R_Mn_final(nc)=1.0e-30
R_L_av_C(nc)=1.0e-30
R_L_av_Fe(nc)=1.0e-30
R_L_av_P(nc)=1.0e-30
R_L_av_Si(nc)=1.0e-30
R_L_av_Mn(nc)=1.0e-30

R_tgas(nc)=vfm(ip1)*vol(nc)*denm(ip1)
R_tgas(nc)=R_tgas(nc)-R_g_s(nc)+R_s_gas(nc)
R_O2_av_g(nc)=2.0*Phi_mscal((11-1)*ncell+nc)*R_tgas(nc)
IF(R_O2_av_g(nc).GE.1.0e-04)
THEN
R_Si_Fickrate(nc)=(0.40703)*((R_Si_b(nc)*vfm(ip2)*vol(nc)*denm(ip2))-0.00001)
IF(R_Si_Fickrate(nc).LE.1.0e-30)
THEN
R_Si_used_O2(nc)=R_Si_av_l(nc)
ELSE
R_Si_used_O2(nc)=R_Si_req_O2
END IF
R_O2_av_g(nc)=R_O2_av_g(nc)-(1.14*R_Si_used_O2(nc))
IF(R_O2_av_g(nc).LE.1.0e-30)
THEN
R_O2_av_g(nc)=1.0e-30
END IF

R_C_Fickrate(nc)=(0.16363)*((R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2))-0.000703)
IF(R_C_Fickrate(nc).LE.1.0e-30)
THEN
R_C_used_O2(nc)=R_C_av_l(nc)
ELSE
R_C_used_O2(nc)=R_C_req_O2
END IF

R_C_av_l(nc)=R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_C_req_O2=R_O2_av_g(nc)*(0.75)

R_C_Fickrate(nc)=0.16363*((R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2))-0.000703)
IF(R_C_Fickrate(nc).LE.1.0e-30)
THEN
R_C_Fickrate(nc)=1.0e-30
END IF
R_O2_av_g(nc)=R_O2_av_g(nc)-(1.14*R_Si_used_O2(nc))
IF(R_O2_av_g(nc).LE.1.0e-30)
THEN
R_O2_av_g(nc)=1.0e-30
END IF

R_C_av_l(nc)=R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_C_req_O2=R_O2_av_g(nc)*(0.75)
IF (R_C_req_O2.GT.R_C_av_l(nc)) THEN
R_C_used_O2(nc)=R_C_av_l(nc)
ELSE
R_C_used_O2(nc)=R_C_req_O2
END IF

c-----Chemical reaction between gas and liquid

R_FeO_b(nc)=1.0e-30
END IF
R_Mn_eq=(R_MnO_b(nc))/((R_FeO_b(nc))*3.297)
R_Mn_Fickrate(nc)=(0.042)*((R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2))-R_Mn_eq)
IF(R_Mn_Fickrate(nc).LE.1.0e-30)THEN
R_Mn_Fickrate(nc)=1.0e-30
END IF
R_O2_av_g(nc)=R_O2_av_g(nc)-(1.33*R_C_used_O2(nc))
IF(R_O2_av_g(nc).LE.1.0e-30)THEN
R_O2_av_g(nc)=1.0e-30
END IF

R_Mn_av_l(nc)=R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
R_Mn_req_O2=R_O2_av_g(nc)*(3.4375)
IF (R_Mn_req_O2.GT.R_Mn_av_l(nc)) THEN
R_Mn_used_O2(nc)=R_Mn_av_l(nc)
ELSE
R_Mn_used_O2(nc)=R_Mn_req_O2
END IF

R_P_eq_1=(2.5*log10(R_FeO_b(nc)))+(0.5*log10(R_P2O5_b(nc)))-1.39
R_P_eq_2=10.0**(R_P_eq_1)
IF(R_P_eq_2.LE.0.02)THEN
R_P_eq_2=0.02
END IF
R_P_eq=(0.437*R_P2O5_b(nc))/R_P_eq_2
IF(R_P_eq.LE.0.00018)THEN
R_P_eq=0.00018
END IF
R_P_Fickrate(nc)=(0.07)*((R_P_b1(nc)*vfm(ip2)*vol(nc)*denm(ip2))-R_P_eq)
IF(R_P_Fickrate(nc).LE.1.0e-30)THEN
R_P_Fickrate(nc)=1.0e-30
END IF
R_O2_av_g(nc)=R_O2_av_g(nc)-(0.29*R_Mn_used_O2(nc))
IF(R_O2_av_g(nc).LE.1.0e-30)THEN
R_O2_av_g(nc)=1.0e-30
END IF

R_P_av_l(nc)=R_P_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
\( R_{P \_req \_O2} = R_{O2 \_av \_g(nc)} \times 0.775 \)

**IF** \( R_{P \_req \_O2} > R_{P \_av \_l(nc)} \) **THEN**

\( R_{P \_used \_O2(nc)} = R_{P \_av \_l(nc)} \)

**ELSE**

\( R_{P \_used \_O2(nc)} = R_{P \_req \_O2} \)

**END IF**

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**:Chemical reaction between gas and liquid**

**:Amount of Iron and oxygen for reaction in gas and liquid**

\( R_{O2 \_av \_g(nc)} = R_{O2 \_av \_g(nc)} - (1.29 \times R_{P \_used \_O2(nc)}) \)

**IF** \( R_{O2 \_av \_g(nc)} \leq 1.0e-30 \) **THEN**

\( R_{O2 \_av \_g(nc)} = 1.0e-30 \)

**END IF**

\( R_{Fe \_Fickrate(nc)} = (R_{O2 \_av \_g(nc)} - R_{Mn \_used \_O2(nc)} - R_{P \_used \_O2(nc)} - R_{C \_used \_O2(nc)} - R_{Si \_used \_O2(nc)}) \)

**IF** \( R_{Fe \_Fickrate(nc)} \leq 1.0e-30 \) **THEN**

\( R_{Fe \_Fickrate(nc)} = 1.0e-30 \)

**END IF**

---

**:Chemical reaction between Iron and Oxygen**

\( R_{Fe \_av \_l(nc)} = R_{Fe \_b(nc)} \times \text{vfm(ip2)} \times \text{vol(nc)} \times \text{denm(ip2)} \)

\( R_{Fe \_req \_O2} = R_{O2 \_av \_g(nc)} \times 3.50 \)

**IF** \( R_{Fe \_req \_O2} > R_{Fe \_av \_l(nc)} \) **THEN**

\( R_{Fe \_used \_O2(nc)} = R_{Fe \_av \_l(nc)} \)

**ELSE**

\( R_{Fe \_used \_O2(nc)} = R_{Fe \_req \_O2} \)

**END IF**

---

**:Chemical reaction between Silicon and P2O5**

\( R_{Si \_av \_l(nc)} = R_{Si \_av \_l(nc)} - R_{Si \_used \_O2(nc)} \)

**IF** \( R_{Si \_av \_l(nc)} \leq 1.0e-30 \) **THEN**

\( R_{Si \_av \_l(nc)} = 1.0e-30 \)

**END IF**

\( R_{P2O5 \_av \_l(nc)} = R_{P2O5 \_b(nc)} \times \text{vfm(ip2)} \times \text{vol(nc)} \times \text{denm(ip2)} + (2.29 \times R_{P \_used \_O2(nc)}) \)

**IF** \( R_{P2O5 \_av \_l(nc)} \leq 1.0e-30 \) **THEN**

\( R_{P2O5 \_av \_l(nc)} = 1.0e-30 \)

**END IF**

\( R_{Si \_req \_P2O5} = R_{P2O5 \_av \_l(nc)} \times 0.493 \)

**IF** \( R_{Si \_req \_P2O5} > R_{Si \_av \_l(nc)} \) **THEN**

\( R_{Si \_used \_P2O5(nc)} = R_{Si \_av \_l(nc)} \)

**ELSE**

\( R_{Si \_used \_P2O5(nc)} = R_{Si \_req \_P2O5} \)

**END IF**

---

**:Chemical reaction between Carbon and P2O5**

\( R_{C \_av \_l(nc)} = R_{C \_av \_l(nc)} - R_{C \_used \_O2(nc)} \)

**IF** \( R_{C \_av \_l(nc)} \leq 1.0e-30 \) **THEN**

\( R_{C \_av \_l(nc)} = 1.0e-30 \)

**END IF**

\( R_{P2O5 \_av \_l(nc)} = R_{P2O5 \_av \_l(nc)} - (R_{Si \_used \_P2O5(nc)} \times 2.03) \)

**IF** \( R_{P2O5 \_av \_l(nc)} \leq 1.0e-30 \) **THEN**

\( R_{P2O5 \_av \_l(nc)} = 1.0e-30 \)
END IF
R_C_req_P2O5=R_P2O5_av_l(nc)*0.423
IF (R_C_req_P2O5.GT.R_C_av_l(nc)) THEN
R_C_used_P2O5(nc)=R_C_av_l(nc)
ELSE
R_C_used_P2O5(nc)=R_C_req_P2O5
END IF
C----------------------------------------------------------------------------------------------------------------
C-----Chemical reaction between Manganese and P2O5
C----------------------------------------------------------------------------------------------------------------
R_Mn_av_l(nc)=R_Mn_av_l(nc)-R_Mn_used_O2(nc)
IF (R_Mn_av_l(nc).LE.1.0e-30) THEN
R_Mn_av_l(nc)=1.0e-30
END IF
R_P2O5_av_l(nc)=R_P2O5_av_l(nc)-(R_C_used_P2O5(nc)*2.37)
IF (R_P2O5_av_l(nc).LE.1.0e-30) THEN
R_P2O5_av_l(nc)=1.0e-30
END IF
R_Mn_req_P2O5=R_P2O5_av_l(nc)*(1.937)
IF (R_Mn_req_P2O5.GT.R_Mn_av_l(nc)) THEN
R_Mn_used_P2O5(nc)=R_Mn_av_l(nc)
ELSE
R_Mn_used_P2O5(nc)=R_Mn_req_P2O5
END IF
C----------------------------------------------------------------------------------------------------------------
C-----Chemical reaction between Silicon and FeO
C----------------------------------------------------------------------------------------------------------------
R_Si_av_l(nc)=R_Si_av_l(nc)-R_Si_used_P2O5(nc)
IF (R_Si_av_l(nc).LE.1.0e-30) THEN
R_Si_av_l(nc)=1.0e-30
END IF
R_FeO_av_l(nc)=R_FeO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+(1.29*R_Fe_used_O2(nc))
IF (R_FeO_av_l(nc).LE.1.0e-30) THEN
R_FeO_av_l(nc)=1.0e-30
END IF
R_Si_req_FeO=R_FeO_av_l(nc)*(0.194)
IF (R_Si_req_FeO.GT.R_Si_av_l(nc)) THEN
R_Si_used_FeO(nc)=R_Si_av_l(nc)
ELSE
R_Si_used_FeO(nc)=R_Si_req_FeO
END IF
C----------------------------------------------------------------------------------------------------------------
C-----Chemical reaction between Iron and P2O5
C----------------------------------------------------------------------------------------------------------------
R_Fe_av_l(nc)=R_Fe_av_l(nc)+(R_Si_used_FeO(nc)*4.0)-R_Fe_used_O2(nc)
IF (R_Fe_av_l(nc).LE.1.0e-30) THEN
R_Fe_av_l(nc)=1.0e-30
END IF
R_Fe_av_l(nc)=R_Fe_av_l(nc)+(R_Si_used_FeO(nc)*4.0)-R_Fe_used_O2(nc)
IF (R_Fe_av_l(nc).LE.1.0e-30) THEN
R_Fe_av_l(nc)=1.0e-30
END IF
R_Fe_used_P2O5(nc)=R_Fe_av_l(nc)*1.97
IF (R_Fe_used_P2O5(nc).LT.R_Fe_av_l(nc)) THEN
R_Fe_used_P2O5(nc)=R_Fe_av_l(nc)
ELSE
R_Fe_used_P2O5(nc)=R_Fe_req_P2O5
END IF

C-----Chemical reaction between Carbon and FeO

R_C_av_l(nc)=R_C_av_l(nc)-R_C_used_P2O5(nc)
IF(R_C_av_l(nc).LE.1.0e-30) THEN
  R_C_av_l(nc)=1.0e-30
END IF
R_FeO_av_l(nc)=R_FeO_av_l(nc)-(R_Fe_used_P2O5(nc)*1.29)-(R_Si_used_FeO(nc)*5.14)
IF(R_FeO_av_l(nc).LE.1.0e-30) THEN
  R_FeO_av_l(nc)=1.0e-30
END IF
R_C_req_FeO=R_FeO_av_l(nc)*0.167
IF(R_C_req_FeO.GT.R_C_av_l(nc)) THEN
  R_C_used_FeO(nc)=R_C_av_l(nc)
ELSE
  R_C_used_FeO(nc)=R_C_req_FeO
END IF

C-----Chemical reaction between Silicon and MnO

R_Si_av_l(nc)=R_Si_av_l(nc)-R_Si_used_FeO(nc)
IF(R_Si_av_l(nc).LE.1.0e-30) THEN
  R_Si_av_l(nc)=1.0e-30
END IF
R_MnO_av_l(nc)=R_MnO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
+ (1.29*R_Mn_used_P2O5(nc)) + (1.29*R_Mn_used_O2(nc))
IF(R_MnO_av_l(nc).LE.1.0e-30) THEN
  R_MnO_av_l(nc)=1.0e-30
END IF
R_Si_req_MnO=R_MnO_av_l(nc)*(0.197)
IF(R_Si_req_MnO.GT.R_Si_av_l(nc)) THEN
  R_Si_used_MnO(nc)=R_Si_av_l(nc)
ELSE
  R_Si_used_MnO(nc)=R_Si_req_MnO
END IF

C-----Chemical reaction between Carbon and MnO

R_C_av_l(nc)=R_C_av_l(nc)-R_C_used_FeO(nc)
IF(R_C_av_l(nc).LE.1.0e-30) THEN
  R_C_av_l(nc)=1.0e-30
END IF
R_MnO_av_l(nc)=R_MnO_av_l(nc)-(5.07*R_Si_used_MnO(nc))
IF(R_MnO_av_l(nc).LE.1.0e-30) THEN
  R_MnO_av_l(nc)=1.0e-30
END IF
R_C_req_MnO=R_MnO_av_l(nc)*0.169
IF(R_C_req_MnO.GT.R_C_av_l(nc)) THEN
  R_C_used_MnO(nc)=R_C_av_l(nc)
ELSE
  R_C_used_MnO(nc)=R_C_req_MnO
END IF

C-----Chemical reaction between Manganese and FeO

R_MnO_av_l(nc)=R_MnO_av_l(nc)-(5.07*R_Si_used_MnO(nc))
IF(R_MnO_av_l(nc).LE.1.0e-30) THEN
  R_MnO_av_l(nc)=1.0e-30
END IF
R_C_req_MnO=R_MnO_av_l(nc)*0.169
IF(R_C_req_MnO.GT.R_C_av_l(nc)) THEN
  R_C_used_MnO(nc)=R_C_av_l(nc)
ELSE
  R_C_used_MnO(nc)=R_C_req_MnO
END IF

C-----Chemical reaction between Carbon and MnO
R_Mn_av_l(nc)=R_Mn_av_l(nc)+(R_C_used_MnO(nc)*4.58)
R_Mn_av_l(nc)=R_Mn_av_l(nc)+(R_Si_used_MnO(nc)*3.93)-R_Mn_used_P2O5(nc)
IF(R_Mn_av_l(nc).LE.1.0e-30)THEN
R_Mn_av_l(nc)=1.0e-30
END IF
R_FeO_av_l(nc)=R_FeO_av_l(nc)-(R_C_used_FeO(nc)*6.0)
IF(R_FeO_av_l(nc).LE.1.0e-30)THEN
R_FeO_av_l(nc)=1.0e-30
END IF
R_Mn_req_FeO=R_FeO_av_l(nc)*(0.764)
IF(R_Mn_req_FeO.GT.R_Mn_av_l(nc))THEN
R_Mn_used_FeO(nc)=R_Mn_av_l(nc)
ELSE
R_Mn_used_FeO(nc)=R_Mn_req_FeO
END IF

R_CRate(nc)=(R_C_used_O2(nc)+R_C_used_P2O5(nc)+R_C_used_FeO(nc)+R_C_used_MnO(nc))
R_C_final(nc)=min(R_CRate(nc),R_C_Fickrate(nc))
IF(R_C_final(nc).LE.1.0e-30)THEN
R_C_final(nc)=1.0e-30
END IF
R_C_final_1=R_C_final(nc)
IF(R_C_used_O2(nc).GT.R_C_final_1)THEN
R_C_O2(nc)=R_C_final_1
ELSE
R_C_O2(nc)=R_C_used_O2(nc)
END IF
R_C_final_2=R_C_final_1-R_C_O2(nc)
IF(R_C_used_P2O5(nc).GT.R_C_final_2)THEN
R_C_P2O5(nc)=R_C_final_2
ELSE
R_C_P2O5(nc)=R_C_used_P2O5(nc)
END IF
R_C_final_3=R_C_final_2-R_C_P2O5(nc)
IF(R_C_used_FeO(nc).GT.R_C_final_3)THEN
R_C_FeO(nc)=R_C_final_3
ELSE
R_C_FeO(nc)=R_C_used_FeO(nc)
END IF
R_C_final_4=R_C_final_3-R_C_FeO(nc)
IF(R_C_used_MnO(nc).GT.R_C_final_4)THEN
R_C_MnO(nc)=R_C_final_4
ELSE
R_C_MnO(nc)=R_C_used_MnO(nc)
END IF

R_C_final_1=R_C_final_1-R_C_O2(nc)
R_C_final_2=R_C_final_2-R_C_P2O5(nc)
R_C_final_3=R_C_final_3-R_C_FeO(nc)
R_C_final_4=R_C_final_4-R_C_MnO(nc)

c-----Finalising the amount of Silicon reacted.
\( R_{\text{SiRate}}(nc) = (R_{\text{Si_used_O2}}(nc) + R_{\text{Si_used_P2O5}}(nc) + R_{\text{Si_used_FeO}}(nc) + R_{\text{Si_used_MnO}}(nc)) \)

\( R_{\text{Si_final}}(nc) = \text{min}(R_{\text{SiRate}}(nc), R_{\text{Si_Fickrate}}(nc)) \)

\[ \text{IF} (R_{\text{Si_final}}(nc) \leq 1.0 \times 10^{-30}) \text{THEN} \]

\( R_{\text{Si_final}}(nc) = 0.0 \)

\[ \text{END IF} \]

\( R_{\text{Si_final_1}} = R_{\text{Si_final}}(nc) \)

\[ \text{END IF} \]

\[ \text{-----Finalising the effect of Silicon reacted on other compounds.} \]

\[ \text{-----Finalising the amount of Iron reacted.} \]

\( R_{\text{FeRate}}(nc) = (R_{\text{Fe_used_O2}}(nc) + R_{\text{Fe_used_P2O5}}(nc)) \)

\( R_{\text{Fe_final}}(nc) = \text{min}(R_{\text{FeRate}}(nc), R_{\text{Fe_Fickrate}}(nc)) \)

\[ \text{IF} (R_{\text{Fe_final}}(nc) \leq 1.0 \times 10^{-30}) \text{THEN} \]

\( R_{\text{Fe_final}}(nc) = 1.0 \times 10^{-30} \)

\[ \text{END IF} \]

\( R_{\text{Fe_final_1}} = R_{\text{Fe_final}}(nc) \)

\[ \text{-----Finalising the effect of Iron reacted on other compounds.} \]
R_Fe_P2O5(nc)=R_Fe_final_2
ELSE
R_Fe_P2O5(nc)=R_Fe_used_P2O5(nc)
END IF

c-----Finalising the amount of Phosphorous reacted.

R_PRate(nc)=R_P_used_O2(nc)
R_P_final(nc)=min(R_PRate(nc),R_P_Fickrate(nc))
IF(R_P_final(nc).LE.1.0e-30)THEN
R_P_final(nc)=1.0e-30
END IF

c-----Finalising the amount of Manganese reacted.

R_MnRate(nc)=(R_Mn_used_O2(nc)+R_Mn_used_P2O5(nc)+R_Mn_used_FeO(nc))
R_Mn_final(nc)=min(R_MnRate(nc),R_Mn_Fickrate(nc))
IF(R_Mn_final(nc).LE.1.0e-30)THEN
R_Mn_final(nc)=1.0e-30
END IF
R_Mn_final_1=R_Mn_final(nc)

c-----Finalising the effect of Manganese reacted on other compounds.

IF (R_Mn_used_O2(nc).GT.R_Mn_final_1) THEN
R_Mn_O2(nc)=R_Mn_final_1
ELSE
R_Mn_O2(nc)=R_Mn_used_O2(nc)
END IF

R_Mn_final_2=R_Mn_final_1-R_Mn_O2(nc)
IF (R_Mn_used_P2O5(nc).GT.R_Mn_final_2) THEN
R_Mn_P2O5(nc)=R_Mn_final_2
ELSE
R_Mn_P2O5(nc)=R_Mn_used_P2O5(nc)
END IF

R_Mn_final_3=R_Mn_final_2-R_Mn_P2O5(nc)
IF (R_Mn_used_FeO(nc).GT.R_Mn_final_3) THEN
R_Mn_FeO(nc)=R_Mn_final_3
ELSE
R_Mn_FeO(nc)=R_Mn_used_FeO(nc)
END IF

ELSE
R_C_FeO(nc)=1.0e-30
R_Si_FeO(nc)=1.0e-30
R_Mn_FeO(nc)=1.0e-30
R_Si_MnO(nc)=1.0e-30
R_C_MnO(nc)=1.0e-30
R_C_P2O5(nc)=1.0e-30
R_Si_P2O5(nc)=1.0e-30
R_Fe_P2O5(nc)=1.0e-30
R_Mn_P2O5(nc)=1.0e-30
R_C_final(nc)=1.0e-30
R_Fe_final(nc)=1.0e-30
R_Si_final(nc)=1.0e-30
R_Mn_final(nc)=1.0e-30
R_P_final(nc)=1.0e-30
R_C_O2(nc)=1.0e-30
END IF
END IF

R_L_av_C(nc)=R_C_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)-R_C_final(nc)

IF(R_L_av_C(nc).LE.1.0e-30) THEN
  R_L_av_C(nc)=1.0e-30
END IF

R_L_av_Fe(nc)=R_Fe_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
  +R_Fe_final(nc)+(R_C_FeO(nc)*4.67)+(R_Si_FeO(nc)*4.0)+(R_Mn_FeO(nc)*1.02)
IF(R_L_av_Fe(nc).LE.1.0e-30) THEN
  R_L_av_Fe(nc)=1.0e-30
END IF

R_L_av_Mn(nc)=R_Mn_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
  +(R_C_MnO(nc)*4.58)+(R_Si_MnO(nc)*3.93)
IF(R_L_av_Mn(nc).LE.1.0e-30) THEN
  R_L_av_Mn(nc)=1.0e-30
END IF

R_L_av_P(nc)=R_P_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
  +(R_C_P2O5(nc)*1.06)+(R_Si_P2O5(nc)*0.886)
  +(R_Fe_P2O5(nc)*0.22)+(R_Mn_P2O5(nc)*0.225)
IF(R_L_av_P(nc).LE.1.0e-30) THEN
  R_L_av_P(nc)=1.0e-30
END IF

R_L_av_Si(nc)=R_Si_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
IF(R_L_av_Si(nc).LE.1.0e-30) THEN
  R_L_av_Si(nc)=1.0e-30
END IF

R_L_av_FeO(nc)=R_FeO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
  +(R_Fe_final(nc)*1.29)-(R_C_FeO(nc)*6.0)-(R_Si_FeO(nc)*5.14)-(R_Mn_FeO(nc)*1.31)
IF(R_L_av_FeO(nc).LE.1.0e-30) THEN
  R_L_av_FeO(nc)=1.0e-30
END IF

R_L_av_SiO2(nc)=R_SiO2_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)+(R_Si_final(nc)*2.14)
IF(R_L_av_SiO2(nc).LE.1.0e-30) THEN
  R_L_av_SiO2(nc)=1.0e-30
END IF

R_L_av_MnO(nc)=R_MnO_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
  +(R_Mn_final(nc)*1.29)-(R_Si_MnO(nc)*5.07)-(R_C_MnO(nc)*5.92)
IF(R_L_av_MnO(nc).LE.1.0e-30) THEN
  R_L_av_MnO(nc)=1.0e-30
END IF

R_L_av_P2O5(nc)=R_P2O5_b(nc)*vfm(ip2)*vol(nc)*denm(ip2)
  +(R_P_final(nc)*2.29)-(R_C_P2O5(nc)*2.367)
  -(R_Si_P2O5(nc)*2.028)-(R_Fe_P2O5(nc)*0.507)-(R_Mn_P2O5(nc)*0.516)
IF(R_L_av_P2O5(nc).LE.1.0e-30) THEN
  R_L_av_P2O5(nc)=1.0e-30
END IF

R_L_av_Tot(nc)=vfm(ip2)*vol(nc)*denm(ip2)

----------------------------------------------------------------------------------------------------------------
IF (R_Fe_final(nc).GT.1.0e-30) THEN
  R_Fe_fr(nc)=(R_L_av_Fe(nc)/R_L_av_Tot(nc))
ELSE
  R_Fe_fr(nc)=1.0e-30
END IF
IF (R_Fe_fr(nc).LE.1.0e-30) THEN
  R_Fe_b2(nc)=(R_Fe_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
ELSE
  R_Fe_b2(nc)=1.0e-35
END IF
IF (R_Fe_b2(nc).LE.1.0e-30) THEN
  R_S(25,nc)=1.0e-30
ELSE
  R_S(25,nc)=R_Fe_b1(nc)-R_Fe_b2(nc)
ENDIF
IF (R_S(25,nc).LE.0.0) THEN
  R_S(25,nc)=1.0e-30
ELSE
  R_Fe_b2(nc)=1.0e-35
ENDIF

IF (R_C_final(nc).GT.1.0e-30) THEN
  R_C_fr(nc)=(R_L_av_C(nc)/R_L_av_Tot(nc))
ELSE
  R_C_fr(nc)=1.0e-30
END IF
IF (R_C_fr(nc).LE.1.0e-30) THEN
  R_C_b2(nc)=(R_C_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
ELSE
  R_C_b2(nc)=R_C_b1(nc)
END IF
IF (R_C_b2(nc).GT.R_C_b1(nc)) THEN
  R_C_b2(nc)=R_C_b1(nc)
ELSE
  R_S(26,nc)=R_C_b1(nc)-R_C_b2(nc)
ENDIF
IF (R_S(26,nc).LE.0.0) THEN
  R_S(26,nc)=1.0e-30
ELSE
  R_S(26,nc)=1.0e-35
ENDIF

IF (R_Si_final(nc).GT.1.0e-30) THEN
  R_Si_fr(nc)=(R_L_av_Si(nc)/R_L_av_Tot(nc))
ELSE
  R_Si_fr(nc)=1.0e-30
END IF
IF (R_Si_fr(nc).LE.1.0e-30) THEN
  R_Si_b2(nc)=(R_Si_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
ELSE
  R_Si_b2(nc)=R_Si_b1(nc)
END IF
IF (R_Si_b2(nc).GT.R_Si_b1(nc)) THEN
  R_Si_b2(nc)=R_Si_b1(nc)
ELSE
  R_S(27,nc)=R_Si_b1(nc)-R_Si_b2(nc)
ENDIF
IF (R_S(27,nc).LE.0.0) THEN
  R_S(27,nc)=1.0e-30
ELSE
  R_S(27,nc)=1.0e-35
ENDIF
\( R_S(27, nc) = 1.0e-30 \)
END IF
ELSE
\( R_Si_b2(nc) = 1.0e-35 \)
END IF

\begin{verbatim}
C----------------------------------------------------------------------------------------------------------------
IF (R_Mn_final(nc).GT.1.0e-30)
THEN
R_Mn_fr(nc)=(R_L_av_Mn(nc)/R_L_av_Tot(nc))
IF (R_Mn_fr(nc).LE.1.0e-30)
THEN
R_Mn_fr(nc)=1.0e-30
END IF
IF (R_Mn_fr(nc).GT.R_Mn_b1(nc))
THEN
R_Mn_fr(nc)=R_Mn_b1(nc)
END IF
R_Mn_b2(nc)=(R_Mn_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_Mn_b2(nc).LE.1.0e-30)
THEN
R_S(28,nc)=1.0e-30
ELSE
R_S(28,nc)=R_Mn_b1(nc)-R_Mn_b2(nc)
END IF
IF (R_S(28,nc).LE.0.0)
THEN
R_S(28,nc)=1.0e-30
END IF
ELSE
R_S(28,nc)=1.0e-35
R_Mn_b2(nc)=1.0e-35
END IF
C----------------------------------------------------------------------------------------------------------------
IF (R_P_final(nc).GT.1.0e-30)
THEN
R_P_fr(nc)=(R_L_av_P(nc)/R_L_av_Tot(nc))
IF (R_P_fr(nc).LE.1.0e-30)
THEN
R_P_fr(nc)=1.0e-30
END IF
IF (R_P_fr(nc).GT.R_P_b1(nc))
THEN
R_P_fr(nc)=R_P_b1(nc)
END IF
R_P_b2(nc)=(R_P_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_P_b2(nc).LE.1.0e-30)
THEN
R_S(29,nc)=1.0e-30
ELSE
R_S(29,nc)=R_P_b1(nc)-R_P_b2(nc)
END IF
IF (R_S(29,nc).LE.0.0)
THEN
R_S(29,nc)=1.0e-30
END IF
ELSE
R_S(29,nc)=1.0e-35
R_P_b2(nc)=1.0e-35
END IF
C----------------------------------------------------------------------------------------------------------------
IF (R_L_av_FeO(nc).GE.1.0e-30)
THEN
R_FeO_fr(nc)=(R_L_av_FeO(nc)/R_L_av_Tot(nc))
IF (R_FeO_fr(nc).LE.1.0e-30)
THEN
R_FeO_fr(nc)=1.0e-30
END IF
\end{verbatim}
IF (R_FeO_fr(nc).GE.1.0) THEN
    R_FeO_fr(nc)=1.0
END IF
R_FeO_b2(nc)=(R_FeO_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_FeO_b1(nc).LE.1.0e-30) THEN
    R_S(30,nc)=1.0e-30
ELSE
    R_S(30,nc)=R_FeO_b2(nc)-R_FeO_b1(nc)
END IF
IF (R_S(30,nc).LE.0.0) THEN
    R_S(30,nc)=1.0e-30
END IF
ELSE
    R_S(30,nc)=1.0e-35
    R_FeO_b2(nc)=1.0e-35
END IF

IF (R_L_av_SiO2(nc).GE.1.0e-30) THEN
    R_SiO2_fr(nc)=(R_L_av_SiO2(nc)/R_L_av_Tot(nc))
IF (R_SiO2_fr(nc).LE.1.0e-30) THEN
    R_SiO2_fr(nc)=1.0e-30
END IF
IF (R_SiO2_fr(nc).GE.1.0) THEN
    R_SiO2_fr(nc)=1.0
END IF
R_SiO2_b2(nc)=(R_SiO2_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_SiO2_b1(nc).LE.1.0e-30) THEN
    R_S(31,nc)=1.0e-30
ELSE
    R_S(31,nc)=R_SiO2_b2(nc)-R_SiO2_b1(nc)
END IF
IF (R_S(31,nc).LE.0.0) THEN
    R_S(31,nc)=1.0e-30
END IF
ELSE
    R_S(31,nc)=1.0e-35
    R_SiO2_b2(nc)=1.0e-35
END IF

IF (R_L_av_P2O5(nc).GE.1.0e-30) THEN
    R_P2O5_fr(nc)=(R_L_av_P2O5(nc)/R_L_av_Tot(nc))
IF (R_P2O5_fr(nc).LE.1.0e-30) THEN
    R_P2O5_fr(nc)=1.0e-30
END IF
IF (R_P2O5_fr(nc).GE.1.0) THEN
    R_P2O5_fr(nc)=1.0
END IF
R_P2O5_b2(nc)=(R_P2O5_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_P2O5_b1(nc).LE.1.0e-30) THEN
    R_S(32,nc)=1.0e-30
ELSE
    R_S(32,nc)=R_P2O5_b2(nc)-R_P2O5_b1(nc)
END IF
IF (R_S(32,nc).LE.0.0) THEN
    R_S(32,nc)=1.0e-30
END IF
ELSE
R_S(32,nc)=1.0e-35
R_P2O5_b2(nc)=1.0e-35
END IF

IF (R_L_av_MnO(nc).GE.1.0e-30)
THEN
R_MnO_fr(nc)=(R_L_av_MnO(nc)/R_L_av_Tot(nc))
IF (R_MnO_fr(nc).LE.1.0e-30)
THEN
R_MnO_fr(nc)=1.0e-30
END IF
IF (R_MnO_fr(nc).GE.1.0)
THEN
R_MnO_fr(nc)=1.0
END IF
R_MnO_b2(nc)=(R_MnO_fr(nc)*vfm(ip2)*vol(nc)*denm(ip2))
IF (R_MnO_b1(nc).LE.1.0e-30)
THEN
R_S(33,nc)=1.0e-30
ELSE
R_S(33,nc)=R_MnO_b2(nc)-R_MnO_b1(nc)
END IF
IF (R_S(33,nc).LE.0.0)
THEN
R_S(33,nc)=1.0e-30
END IF
ELSE
R_S(32,nc)=1.0e-35
R_P2O5_b2(nc)=1.0e-35
END IF

R_O2_rate2(nc)=R_S(25,nc)+R_S(26,nc)+R_S(27,nc)+R_S(28,nc)+R_S(29,nc)
R_O2_rate1(nc)=R_S(30,nc)+R_S(31,nc)+R_S(32,nc)+R_S(33,nc)
R_CO_r=2.34*R_C_final(nc)
R_CO_av=2.0*Phi_mscal((121)*ncell+nc)*vfm(ip1)*vol(nc)*denm(ip1)
R_CO_r=1.75*R_C_final(nc)
R_O_CO_t=vfm(ip1)*vol(nc)*denm(ip1)
R_COfr(nc)=0.5*(R_CO_av+R_CO_r)/(R_CO_r+R_O_CO_t)
IF (R_COfr(nc).GT.0.5)
THEN
R_COfr(nc)=0.5
END IF

R_S(22,nc)=((0.5-R_COfr(nc))-Phi_mscal((11-1)*ncell+nc))*vfm(ip1)*vol(nc)*denm(ip1)
R_S(21,nc)=(R_COfr(nc)-Phi_mscal((12-1)*ncell+nc))*vfm(ip1)*vol(nc)*denm(ip1)

R_c_rate(nc)=0.33*R_C_O2(nc)
R_O2_rate(nc)=0.33*R_C_O2(nc)

R_bubble=Phi_mscal((31-1)*ncell+nc)

R_S(1,nc)=(R_BB(1)-R_DB(1)+R_BC(1)-R_DC(1))*denm(ip1)
R_S(2,nc)=(R_BB(2)-R_DB(2)+R_BC(2)-R_DC(2))*denm(ip1)
R_S(3,nc)=(R_BB(3)-R_DB(3)+R_BC(3)-R_DC(3))*denm(ip1)
R_S(4,nc)=(R_BB(4)-R_DB(4)+R_BC(4)-R_DC(4))*denm(ip1)
R_S(5,nc)=(R_BB(5)-R_DB(5)+R_BC(5)-R_DC(5))*denm(ip1)
R_S(6,nc)=(R_BB(6)-R_DB(6)+R_BC(6)-R_DC(6))*denm(ip1)
R_S(7,nc)=(R_BB(7)-R_DB(7)+R_BC(7)-R_DC(7))*denm(ip1)
R_S(8,nc)=(R_BB(8)-R_DB(8)+R_BC(8)-R_DC(8))*denm(ip1)
\[ R_{S}(9,nc) = (R_{BB}(9) - R_{DB}(9) + R_{BC}(9) - R_{DC}(9)) \times \text{denm(ip1)} \]
\[ R_{S}(10,nc) = (R_{BB}(10) - R_{DB}(10) + R_{BC}(10) - R_{DC}(10)) \times \text{denm(ip1)} \]
\[ R_{S}(11,nc) = (R_{BCF}(1) - R_{DCF}(1)) \]
\[ R_{S}(12,nc) = (R_{BCF}(2) - R_{DCF}(2)) \]
\[ R_{S}(13,nc) = (R_{BCF}(3) - R_{DCF}(3)) \]
\[ R_{S}(14,nc) = (R_{BCF}(4) - R_{DCF}(4)) \]
\[ R_{S}(15,nc) = (R_{BCF}(5) - R_{DCF}(5)) \]
\[ R_{S}(16,nc) = (R_{BCF}(6) - R_{DCF}(6)) \]
\[ R_{S}(17,nc) = (R_{BCF}(7) - R_{DCF}(7)) \]
\[ R_{S}(18,nc) = (R_{BCF}(8) - R_{DCF}(8)) \]
\[ R_{S}(19,nc) = (R_{BCF}(9) - R_{DCF}(9)) \]
\[ \text{IF } (R_{\text{bubble}} \leq 0.9) \text{ THEN} \]
\[ R_{S}(20,nc) = (R_{BCF}(10) - R_{DCF}(10)) \]
\[ \text{ELSE} \]
\[ R_{S}(20,nc) = 0.0 \]
\[ \text{END IF} \]

\text{c-----Source term for gas bubble in foam phase} 
\text{END DO} 
\text{c-----mat=1} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{IF } (isc==1) \text{ THEN} 
\text{DO} \ ip = nsp(mat),nep(mat) 
\ text{sum1(ip)= sum1(ip)+(R}_{S}(1,ip)/dt) \text{ END DO} 
\text{END IF} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{c-----Sources for scalar 2 phase 1} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{IF } (isc==2) \text{ THEN} 
\text{DO} \ ip = nsp(mat),nep(mat) 
\ text{sum1(ip)= sum1(ip)+(R}_{S}(2,ip)/dt) \text{ END DO} 
\text{END IF} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{c-----Sources for scalar 3 phase 1} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{IF } (isc==3) \text{ THEN} 
\text{DO} \ ip = nsp(mat),nep(mat) 
\ text{sum1(ip)= sum1(ip)+(R}_{S}(3,ip)/dt) \text{ END DO} 
\text{END IF} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{c-----Sources for scalar 4 phase 1} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{IF } (isc==4) \text{ THEN} 
\text{DO} \ ip = nsp(mat),nep(mat) 
\ text{sum1(ip)= sum1(ip)+(R}_{S}(4,ip)/dt) \text{ END DO} 
\text{END IF} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{c-----Sources for scalar 5 phase 1} 
\text{c----------------------------------------------------------------------------------------------------------------} 
\text{IF } (isc==5) \text{ THEN} 
\text{DO} \ ip = nsp(mat),nep(mat) 
\ text{sum1(ip)= sum1(ip)+(R}_{S}(5,ip)/dt) \text{ END DO} 
\text{END IF}
END DO
END IF

C-----Sources for scalar 6 phase 1
C----------------------------------------------------------------------------------------------------------------
IF (isc==6) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)= sum1(ip)+R_S(6,ip)/dt
END DO
END IF

C-----Sources for scalar 7 phase 1
C----------------------------------------------------------------------------------------------------------------
IF (isc==7) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)= sum1(ip)+R_S(7,ip)/dt
END DO
END IF

C-----Sources for scalar 8 phase 1
C----------------------------------------------------------------------------------------------------------------
IF (isc==8) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)= sum1(ip)+R_S(8,ip)/dt
END DO
END IF

C-----Sources for scalar 9 phase 1
C----------------------------------------------------------------------------------------------------------------
IF (isc==9) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)= sum1(ip)+R_S(9,ip)/dt
END DO
END IF

C-----Sources for scalar 10 phase 1
C----------------------------------------------------------------------------------------------------------------
IF (isc==10) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)= sum1(ip)+R_S(10,ip)/dt
END DO
END IF

C-----Sources for scalar 11 O2 phase 1
C----------------------------------------------------------------------------------------------------------------
IF (isc==11) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)= sum1(ip)+R_S(22,ip)/dt
END DO
END IF

C-----Sources for scalar 12 CO phase 1
C----------------------------------------------------------------------------------------------------------------
IF (isc==12) THEN
DO ip = nsp(mat),nep(mat)
  sum1(ip)= sum1(ip)+R_S(21,ip)/dt
END DO
END DO
END IF

c------Sources for scalar 13 CO2 phase 1

IF (isc==13) THEN
DO ip = nsp(mat),nep(mat)
    sum1(ip)= sum1(ip)
END DO
END IF

c------Sources for scalar 1 Fe phase 2

IF (isc==14) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(25,ip).LE.0.0) THEN
    R_S(25,ip)=1.0e-30
ELSE
    sum1(ip2)= sum1(ip2)-(R_S(25,ip)/dt)
END IF
END DO
END IF

c------Sources for scalar 2 C phase 2

IF (isc==15) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(26,ip).LE.0.0) THEN
    R_S(26,ip)=1.0e-30
ELSE
    sum1(ip2)= sum1(ip2)-(R_S(26,ip)/dt)
END IF
END DO
END IF

c------Sources for scalar 3 Si phase 2

IF (isc==16) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(27,ip).LE.0.0) THEN
    R_S(27,ip)=1.0e-30
ELSE
    sum1(ip2)= sum1(ip2)-(R_S(27,ip)/dt)
END IF
END DO
END IF

c------Sources for scalar 4 Mn phase 2

IF (isc==17) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(28,ip).LE.0.0) THEN
R_S(28,ip)=1.0e-30
ELSE
sum1(ip2)= sum1(ip2)-(R_S(28,ip)/dt)
END IF
END DO
END IF

--- Sources for scalar 5 P phase 2
IF (isc==18) THEN
DO ip = nsp(mat),nep(mat)
ip2=ip+ncell
IF (R_S(29,ip).LE.0.0) THEN
R_S(29,ip)=1.0e-30
ELSE
sum1(ip2)= sum1(ip2)-(R_S(29,ip)/dt)
END IF
END DO
END IF

--- Sources for scalar 1 FeO phase 2
IF (isc==20) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell
sum1(ip2)= sum1(ip2)-(R_S(30,ip)/dt)
END DO
END IF

--- Sources for scalar 2 SiO2 phase 2
IF (isc==21) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell
sum1(ip2)= sum1(ip2)-(R_S(31,ip)/dt)
END DO
END IF

--- Sources for scalar 3 MnO phase 2
IF (isc==22) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell
sum1(ip2)= sum1(ip2)-(R_S(33,ip)/dt)
END DO
END IF

--- Sources for scalar 4 P2O5 phase 2
IF (isc==23) THEN  
DO ip = nsp(mat),nep(mat)  
ip3=ip+ncell  
sum1(ip2)= sum1(ip2)-(R_S(32,ip)/dt)  
END DO  
END IF  

C-----Sources for scalar 5 CaO phase 2  
C----------------------------------------------------------------------------------------------------------------

IF (isc==24) THEN  
DO ip = nsp(mat),nep(mat)  
ip3=ip+ncell  
sum1(ip2)= sum1(ip2)  
END DO  
END IF  

C-----Sources for scalar 6 MgO phase 2  
C----------------------------------------------------------------------------------------------------------------

IF (isc==25) THEN  
DO ip = nsp(mat),nep(mat)  
ip3=ip+ncell+ncell  
sum1(ip3)= sum1(ip3)  
END DO  
END IF  

C-----Sources for scalar 1 FeO phase 3  
C----------------------------------------------------------------------------------------------------------------

IF (isc==26) THEN  
DO ip = nsp(mat),nep(mat)  
ip3=ip+ncell+ncell  
sum1(ip3)= sum1(ip3)  
END DO  
END IF  

C-----Sources for scalar 2 SiO2 phase 3  
C----------------------------------------------------------------------------------------------------------------

IF (isc==27) THEN  
DO ip = nsp(mat),nep(mat)  
ip3=ip+ncell+ncell  
sum1(ip3)= sum1(ip3)  
END DO  
END IF  

C-----Sources for scalar 3 MnO phase 3  
C----------------------------------------------------------------------------------------------------------------

IF (isc==28) THEN  
DO ip = nsp(mat),nep(mat)  
ip3=ip+ncell+ncell  
sum1(ip3)= sum1(ip3)  
END DO  
END IF  

C-----Sources for scalar 4 P2O5 phase 3  
C----------------------------------------------------------------------------------------------------------------

IF (isc==29) THEN  
DO ip = nsp(mat),nep(mat)  

ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)
END DO
END IF

c-----Sources for scalar 5 CaO phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==30) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)
END DO
END IF

c-----Sources for scalar 6 MgO phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==31) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)
END DO
END IF

c-----Sources for scalar 7 Fe phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==32) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)
END DO
END IF

c-----Sources for scalar 8 C phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==33) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)
END DO
END IF

c-----Sources for scalar 9 Si phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==34) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)
END DO
END IF

c-----Sources for scalar 10 Mn phase 3
c----------------------------------------------------------------------------------------------------------------
IF (isc==35) THEN
DO ip = nsp(mat),nep(mat)
ip3=ip+ncell+ncell
sum1(ip3)= sum1(ip3)
END DO
END IF
c-----Sources for scalar 11 P phase 3

IF (isc==36) THEN
  DO  ip = nsp(mat),nep(mat)
      ip3=ip+ncell+ncell
      sum1(ip3)= sum1(ip3)
  END DO
END IF

END IF

END DO

END IF

END IF

c-----Sources for scalar 12 liquid phase 3

IF (isc==37) THEN
  DO  ip = nsp(mat),nep(mat)
      ip3=ip+ncell+ncell
      sum1(ip3)= sum1(ip3)+(R_S(44,ip)/dt)
  END DO
END IF

END IF

END DO

END IF

END IF

c-----Sources for scalar 13 gas phase 3

IF (isc==38) THEN
  DO  ip = nsp(mat),nep(mat)
      ip3=ip+ncell+ncell
      sum1(ip3)= sum1(ip3)+(R_S(45,ip)/dt)
  END DO
END IF

END IF

END DO

END IF

END IF

END IF

END IF

END IF

c-----Sources for scalar 1 Bubble phase 4

IF (isc==39) THEN
  DO  ip = nsp(mat),nep(mat)
      ip4=ip+ncell+ncell+ncell
      sum1(ip4)= sum1(ip4)+(R_S(11,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt)
  END DO
END IF

END IF

END DO

END IF

END IF

c-----Sources for scalar 2 Bubble phase 4

IF (isc==40) THEN
  DO  ip = nsp(mat),nep(mat)
      ip4=ip+ncell+ncell+ncell
      sum1(ip4)= sum1(ip4)+(R_S(12,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt)
  END DO
END IF

END IF

END DO

END IF

END IF

END IF

c-----Sources for scalar 3 Bubble phase 4

IF (isc==41) THEN
  DO  ip = nsp(mat),nep(mat)
      ip4=ip+ncell+ncell+ncell
      sum1(ip4)= sum1(ip4)+(R_S(13,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt)
  END DO
END IF

END IF

END DO

END IF
IF (isc==42) THEN
  DO  
ip = nsp(mat), nep(mat)
  ip4=i+ncell+ncell+ncell
  sum1(ip4)= sum1(ip4)+R_S(14,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt
  END DO
END IF

---Sources for scalar 5 Bubble phase 4

IF (isc==43) THEN
  DO  
ip = nsp(mat), nep(mat)
  ip4=i+ncell+ncell+ncell
  sum1(ip4)= sum1(ip4)+R_S(15,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt
  END DO
END IF

---Sources for scalar 6 Bubble phase 4

IF (isc==44) THEN
  DO  
ip = nsp(mat), nep(mat)
  ip4=i+ncell+ncell+ncell
  sum1(ip4)= sum1(ip4)+R_S(16,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt
  END DO
END IF

---Sources for scalar 7 Bubble phase 4

IF (isc==45) THEN
  DO  
ip = nsp(mat), nep(mat)
  ip4=i+ncell+ncell+ncell
  sum1(ip4)= sum1(ip4)+R_S(17,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt
  END DO
END IF

---Sources for scalar 8 Bubble phase 4

IF (isc==46) THEN
  DO  
ip = nsp(mat), nep(mat)
  ip4=i+ncell+ncell+ncell
  sum1(ip4)= sum1(ip4)+R_S(18,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt
  END DO
END IF

---Sources for scalar 9 Bubble phase 4

IF (isc==47) THEN
  DO  
ip = nsp(mat), nep(mat)
  ip4=i+ncell+ncell+ncell
  sum1(ip4)= sum1(ip4)+R_S(19,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt
  END DO
END IF

---Sources for scalar 10 Bubble phase 4

---End of sources for scalar 4 Bubble phase 4
---End of sources for scalar 5 Bubble phase 4
---End of sources for scalar 6 Bubble phase 4
---End of sources for scalar 7 Bubble phase 4
---End of sources for scalar 8 Bubble phase 4
---End of sources for scalar 9 Bubble phase 4
---End of sources for scalar 10 Bubble phase 4

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IF (isc==48) THEN
  DO ip = nsp(mat),nep(mat)
    ip4=ip+ncell+ncell+ncell
    sum1(ip4)= sum1(ip4)+(R_S(20,ip)*vol(ip)*vfm(ip4)*denm(ip4)/dt)
  END DO
END IF

C-----Sources for scalar 11 liquid, phase 4
C

IF (isc==49) THEN
  DO ip = nsp(mat),nep(mat)
    ip4=ip+ncell+ncell+ncell
    sum1(ip4)= sum1(ip4)+(R_S(23,ip)*vfm(ip4)*vol(ip)*denm(ip4))/dt
  END DO
END IF

C-----Sources for scalar 11 gas phase 4
C

IF (isc==50) THEN
  DO ip = nsp(mat),nep(mat)
    ip4=ip+ncell+ncell+ncell
    sum1(ip4)= sum1(ip4)+(R_S(24,ip)*vfm(ip4)*vol(ip)*denm(ip4))/dt
  END DO
END IF

C-----Sources for scalar 11 slag phase 4
C

IF (isc==51) THEN
  DO ip = nsp(mat),nep(mat)
    ip4=ip+ncell+ncell+ncell
    sum1(ip4)= sum1(ip4)+(R_S(34,ip)*vfm(ip4)*vol(ip)*denm(ip4))/dt
  END DO
END IF

RETURN
END SUBROUTINE usesc_mscal
• User subroutine to calculate sources in mass interfacial exchange

```
SUBROUTINE usemph(ieq,iva,mat)
   c=======================================================================
   USE comm1
   USE comm2
   USE comm0
   INCLUDE 'com93.inc'
   INCLUDE 'SwiftIO_FortranFunctions.inc'
   mat=1
   c-----Volume fraction equation interfacial sources
   IF(ieq == ipvf) THEN
      DO i_p1=nsp(mat),nep(mat)
         i_p2=i_p1+ncell
         i_p3=i_p1+ncell+ncell
         i_p4=i_p1+ncell+ncell+ncell
         c-----Source terms update for mass exchange
         sum1(i_p1)= sum1(i_p1)-(R_c_rate(i_p1)/dt)+(R_sl_g(i_p1)/dt)-(R_g_sl(i_p1)/dt)
            x+(R_fm_g(i_p1)-R_g_fm(i_p1))/dt
         c-----------------------------------------------------------------------
         sum1(i_p2)= sum1(i_p2)+(R_O2_rate(i_p1)/dt)+(R_sl_lq(i_p1)/dt)-(R_lq_sl(i_p1)/dt)
            x+(R_fm_lq(i_p1)-R_lq_fm(i_p1))/dt
         c-----------------------------------------------------------------------
         sum1(i_p3) = sum1(i_p3)-(R_sl_g(i_p1)/dt)+(R_g_sl(i_p1)/dt)-(R_sl_lq(i_p1)/dt)+
            (R_lq_sl(i_p1)/dt)+(R_fm_S(i_p1)-R_S_fm(i_p1))/dt
         c-----------------------------------------------------------------------
         sum1(i_p4) = sum1(i_p4)-(R_fm_g(i_p1)-R_g_fm(i_p1))/dt-(R_fm_lq(i_p1)-R_lq_fm(i_p1))/dt
            x-(R_fm_S(i_p1)-R_S_fm(i_p1))/dt
         c-----------------------------------------------------------------------
      END DO
      END IF
   RETURN
END SUBROUTINE
```
• User subroutine for calculating the density of slag foam

C======================================================================
SUBROUTINE useden(mat,mph)
C======================================================================
C     description: user subroutine for changing the density
C     author: Anuththara Kirindigoda Hewage
C     date: 01/10/2016
C     project: Four phases model
C======================================================================
USE comm1
USE comm2
USE cthmod, ONLY: ymfrac
USE comm0
INCLUDE 'com93.inc'
INCLUDE 'SwiftIO_FortranFunctions.inc'
INTEGER, INTENT(in) :: mat,mph

C----------------------------------------------------------------------------------------------------------------
DO ip=nsp(mat),nep(mat)
  ip1=ip
  ip2=ip+ncell
  ip3=ip+ncell+ncell
  ip4=ip+ncell+ncell+ncell
  denm(ip1)=denm(ip1)
  denm(ip2)=denm(ip2)
  denm(ip3)=denm(ip3)
  denm(ip1)=0.233
  denm(ip2)=6980
  denm(ip3)=3600

  denm(ip4)=(1.0-(2.0*R_slagf(ip))-(2.0-R_liquidf(ip)))*denm(ip1)
            + (2.0*R_slagf(ip))*denm(ip3)+(2.0*R_liquidf(ip))*denm(ip2)
  IF(denm(ip4).LE.0.0)THEN
    denm(ip4)=0.9*denm(ip1)
  END IF

C----------------------------------------------------------------------------------------------------------------
END DO
RETURN
END SUBROUTINE useden

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User subroutine for calculating the viscosity of slag foam

```fortran
C=====================================================================
subroutine usevis(mat,mph)
C=====================================================================
C     description: user subroutine for changing the viscosity
C     author: Anuththara Kirindigoda Hewage
C     date: 01/10/2016
C     project: Four phase model
C=====================================================================
C-----modules
USE comm1
USE comm2
USE cthmod, ONLY: ymfrac
USE comm0
INCLUDE 'com93.inc'
INCLUDE 'SwiftO_FortranFunctions.inc'
INTEGER, INTENT(in) :: mat, mph
C----------------------------------------------------------------------------------------------------------------
C-----Molecular viscosity of pure substances and their mixtures
C----------------------------------------------------------------------------------------------------------------
DO ip=nsp(mat),nep(mat)
  ip1=ip
  ip2=ip+ncell
  ip3=ip+ncell+ncell
  ip4=ip+ncell+ncell+ncell
  vimm(ip1)=vimm(ip1)
  vimm(ip2)=vimm(ip2)
  vimm(ip3)=vimm(ip3)
  vimm(ip1)=1.824e-011
  vimm(ip2)=1.01e-009
  vimm(ip3)=1.01e-009
C----------------------------------------------------------------------------------------------------------------
  IF(R_lqf_s(ip).LE.0.0) THEN
    R_lqf_s(ip)=1.0e-04
  END IF
  vimm(ip4)=(1.0-(2.0*R_slagf(ip))-(2.0-R_liquidf(ip)))*vimm(ip1)+(2.0*R_slagf(ip))*vimm(ip3)
    x+(2.0*R_liquidf(ip))*vimm(ip2)
  IF(vimm(ip4).LE.0.0) THEN
    vimm(ip4)=0.9*vimm(ip1)
  END IF
C----------------------------------------------------------------------------------------------------------------
END DO
RETURN
END SUBROUTINE
```

RETURN
END SUBROUTINE
usevis
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