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Developments in the Modelling of Oxygen Steelmaking

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Abstract

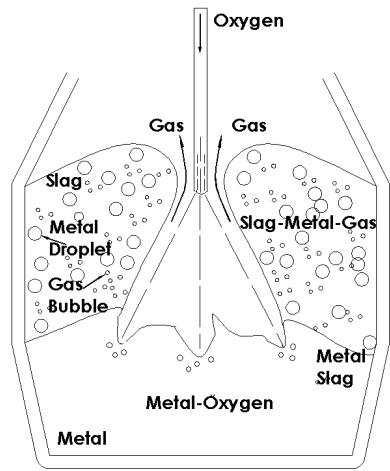
Steelmaking is a complex process involving simultaneous multi-phase interactions, chemical reactions, heat transfer and turbulent flow patterns at high temperatures. The severe operating conditions make it difficult to make measurements and directly observe the process. Mathematical modelling has been widely used to evaluate the process and improve understanding of the system and optimise process control. Three approaches to modelling the process, equilibrium modelling to predict the equilibrium chemistry of the process, kinetic modelling to analyse rate of chemical changes throughout the process, and computational fluid modelling to understand the fluid flow in the reactor, are discussed in this paper. The governing equations and the forms of numerical computational solution techniques for these models are described, and critically examined.

Introduction

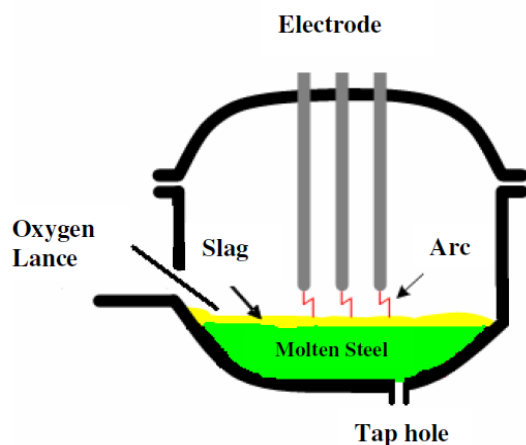
Steel is the most produced metal in the world, with over 1400 million metric tons (mmt) p.a made around the world, compared to approximately 30 mmt p.a. of aluminium. There are two major techniques to produce steel,

oxygen steelmaking and Electric Arc Furnace steelmaking (EAF). These processes are illustrated schematically in FIGURE 1. Oxygen steelmaking uses high speed pure oxygen to oxidize impurities from molten iron produced from a blast furnace. In the case of an EAF, scrap steel and other iron sources are heated up using gas burners and melted by high powered electric arcs. In EAF steelmaking, oxygen and carbon injection is used to oxidize impurities and form a foaming slag (molten oxide impurities) above the molten metal bath. While there are major differences in these production techniques, they both have high rates of production (>100 tonne/hour) and can produce high quality steel, though several other processes steps after steelmaking are required before casting.[1]

Table 1 lists the major reactions occurring in steelmaking processes. The refining reactions take place simultaneously between 1600 and 1700 °C. The majority of these reactions are exothermic reactions and subsequently no external heat is required in oxygen steelmaking, in fact, scrap is added to cool the process. In the case of electric arc furnace, electric energy is used for heating up the scrap from ambient temperatures.



(a)



(b)

FIGURE 1: Schematic representation of top-blowing oxygen steelmaking (a) and electric arc furnace (b)

Steelmaking processes are complex since they involve simultaneous multi-phase (solid-gas-liquid) interactions, chemical reactions, heat and mass transfer and complex flow patterns at high temperatures. The process is also highly transient, meaning that steady state assumptions commonly used by chemical engineers are often invalid.[2] The severe operating conditions make it difficult to make measurements and directly observe the process. This difficulty can be addressed by developing models, which make it possible to describe the complicated nature of the process itself and to understand the interconnection of important process variables. Simple empirical models have been developed in industry for the purposes of process control but they are not suitable for increasing

understanding or optimising the process beyond current operating regimes.[3] Neural networks,[4, 5] fuzzy logic[6, 7] and multivariate statistics[8-11] have also been used as process control tools in steelmaking operations but these “black box” models[12] suffer from the same limitations as simple empirical models, though they are likely to improve control and provide a basis for process optimisation within current operating

Table 1. Major reactions in oxygen steelmaking [13]

Oxygen pick up by the metal:	
$O_{2(g)} = [O]$	(1)
$CO_{2(g)} = CO_{(g)} + [O]$	(2)
$(FeO) = Fe + [O]$	(3)
$(Fe_2O_3) = 2(FeO) + [O]$	(4)
Oxidation of elements in the metal:	
$[C] + [O] = CO_{(g)}$	(5)
$Fe + [O] = (FeO)$	(6)
$[Si] + [O] = (SiO_2)$	(7)
$[Mn] + [O] = (MnO)$	(8)
$2[P] + 5[O] = (P_2O_5)$	(9)
Oxidation of compounds in the slag:	
$2(FeO) + \frac{1}{2}O_{2(g)} = (Fe_2O_3)$	(10)
$2(FeO) + CO_{2(g)} = (Fe_2O_3) + CO_{(g)}$	(11)
Flux reactions:	
$MgO_{(s)} = (MgO)$	(12)
$CaO_{(s)} = (CaO)$	(13)
Gas reactions:	
$CO_{(g)} + \frac{1}{2}O_{2(g)} = CO_{2(g)}$	(14)

regimes. Unfortunately, the physical complexity of the process means that a completely rigorous mathematical description of the process based on fundamental physics and chemistry is currently not possible. In many cases, only semi-empirical relationships are available to describe physical phenomena in processes like oxygen steelmaking.[14] Whilst, a fully scientific model (“white box” model) of oxygen steelmaking maybe impractical, more scientifically based modelling techniques can be applied to improve understanding, providing a basis to design more efficient furnaces and optimize the current technology.[3] However, in developing models for complex processes like oxygen steelmaking, it is important to compromise between the detail required, the

information available on empirical parameters, the inherent limits of the available mathematical tools and the computational time required to find solutions.[15]

There are various modelling techniques used to improve the understanding of the process. The common modelling techniques can be classified into three groups, shown schematically in FIGURE 2: Computational thermodynamics models are used to understand the limits of the system and partitioning of the impurities among the phases; computational fluid models are employed to understand the fluid flow patterns and interaction between the phases; and computational kinetics evaluate the concentration changes of each phase with time. As implied by the schematic representation in FIGURE 2, these techniques are interrelated and results from each model inform the development of other models. For example, computational fluid dynamics provides important parameters for understanding convective mass transfer. Similarly, thermodynamics models provide the limits for kinetic modelling. In this paper, we review these modelling techniques, using selected aspects of steelmaking operations to illustrate the general approach and highlighting limitations of the techniques developed to date.

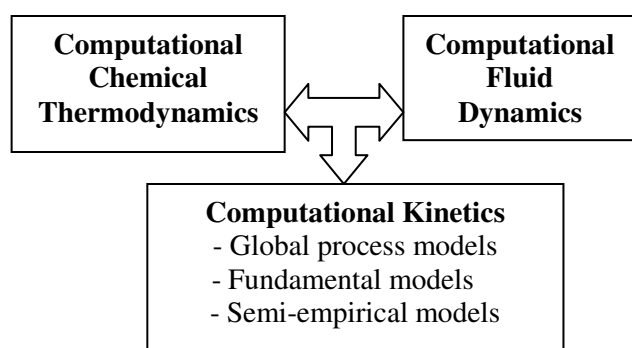


FIGURE 2: Modelling techniques used in steelmaking processes

Modelling techniques

Computational Chemical Thermodynamics

Computational chemical thermodynamics is a well established technique for understanding high temperature processes, many aspects of

materials science, the geology of the earth and even the chemistry of the stars.[16-20] Thermodynamic models provide information on the equilibrium distribution of species within the phases, the heat generated or consumed by these chemical reactions and behaviour of species in solution. Thermodynamic modelling is based on the 2nd law of Thermodynamics and equilibrium calculations are made using the Gibbs free energy minimization technique, which is developed from this law. The basis of the method is to minimize Gibbs free energy of the system at constant temperature and pressure using:[19]

$$G = \sum_i n_i \mu_i = \sum_i n_i (\mu_i^0 + RT \ln a_i) = \min \quad (15)$$

Here variables R , T , n_i refer to gas constant, temperature and mole of species i , respectively. μ_i^0 denotes the standard chemical potential and a_i refers to activity. Activity can be understood as representing “effective concentration” of a particular species and is an important thermodynamic quantity for quantifying the way species dissolve into each other. Chemical potential is the increase in Gibbs free energy of the system for an additional mole of species, i , and represents how a change in composition of the system effects the amount of energy introduced to the system at constant temperature and pressure.[21] Two constraints should be satisfied; n_i must be non-negative and total moles of the elements in the system must be equal to summation of moles of the species in each phase as given in Eq. (16).

$$\sum_{i=1}^k n_i a_{ji} = b_j \quad (16)$$

where a_{ji} is the number of g atoms of element j and b_j is the total atom of element j . This is a standard optimization problem that can be solved using the Lagrange method of unknown multipliers. Eq. (15) becomes:[20]

$$\theta = G + \sum_{i=1}^k \lambda_i \left(\sum_{j=1}^m a_{ji} n_i - b_j^0 \right) = 0 \quad (17)$$

where the λ_i are the Lagrange multipliers, one for each element. This allows each of the n_j to be treated independently, and it can be shown using multivariate calculus that the equilibrium condition is given by;

$$\frac{\partial \theta}{\partial n_j} = 0 \quad (18)$$

and

$$\frac{\partial \theta}{\partial \lambda_i} = 0 \quad (19)$$

These results in a set of $(m+k)$ equations with $(m+k)$ unknowns (all the n_i and λ_i terms) and may, therefore, be solved for each equilibrium concentrations of a particular species (n_i) as long as the chemical potentials are known as functions of the concentrations at the given temperature and pressure. The equations that required to be solved to obtain the composition of the system are not all linear in regards to the composition variables. A Newton-Raphson method is used to solve the equations using initial estimates of compositions n_j , and Lagrangian multipliers λ_i , for a given quantity of species n and temperature. [20, 22]

In developing thermodynamic models, the phases and possible species within the system need to be defined carefully. All the species defined in the system require thermochemical data such as heat capacity, enthalpy and entropy, as functions of temperature for pure species before Gibbs energy minimization techniques can be applied. Fortunately, large databases of critically evaluated thermodynamic data has been compiled by international recognised groups such as NASA and NPL. The appropriate solution models for each phase also need to be evaluated based on solution structure and behaviour. The initial quantities of species within the phases and operating conditions are then entered. The equilibrium calculations are evaluated based on the Gibbs energy minimization technique which is readily available in commercial thermochemical software. The most widely used packages are Thermo-Calc, Factsage, MTDData, Thermodata, HSC, Chemix and Gemini2.[19, 23] These software combine computational codes for

databases and equilibrium calculations to extend the applications in different metallurgical systems.[23, 24] For example, Chemix, Thermo-Calc and MTDData offers flexibility to chose a solution model such as polynomial, Redlich-Kister and Margules depending on the user's system. HSC currently has a limitation on the solution behaviour, as activity coefficients can only be entered as constant number or as a polynomial function of composition and temperature. Nevertheless, HSC has been widely used in industry because of its simplicity.[19] Once again, the balance between scientific rigor and finding practical solutions is evident in modelling of complex industrial systems such as steelmaking.

One of the major challenges in a thermodynamic model of steelmaking is the determination of an appropriate solution model for each phase in the steelmaking processes. Models of solution behaviour allow experimental results for particular systems to be generalised and make predictions of solution behaviour away from the conditions of the original empirical data set. However, the interactions between different species in a phase at different concentrations and temperatures are complex, and particularly in the case of phases where the basic molecular forms in the phase vary with concentration and temperature, it is hard to find a solution model that work well for all conditions. It remains one of the great scientific challenges to determine solution behaviour a priori i.e. calculate from basic physics without resorting to the current high level of empiricism. The major phases in the system are liquid iron, slag (molten oxides), gas, solid refractory, solid fluxing agents (e.g. limestone) and solid steel (scrap). In the case of liquid iron, a dilute solution model using empirically determined "interaction" parameters is well established and can be readily applied to these problems. The dilute solution model is based on Henry's Law, which assumes that the activity of solute has a linear relationship with concentration.[25] However, for slag, the solution behaviour of the phase is challenging to model because it's difficult to describe the complex molecular structure of slag itself,

makes the interpretation of experimental data troublesome.

Moreover, due to the lack of knowledge about the interaction between different metal oxides in slag results in further difficulties in developing robust thermodynamic models of slags.[24] However, the importance of molten oxide solution behaviour to materials science, geology and inorganic chemistry, has meant that a large body of work exists addressing these issues.[26, 27] Several models have been developed for multi-component oxide systems, these include ionic two sub-lattice, regular solution, cell, associated solution and modified quasichemical models.[28-36] Although the regular solution model is simple to employ, the cell and modified quasichemical models have been found more appropriate for studying steelmaking slags.[24]

Whilst, the modelling of molten oxides solution behaviour is complex and the reliance on empirical measurements is disappointing, computational chemical thermodynamic modelling is regarded as a great triumph, resulting in many useful and important predictions over many fields, including steelmaking.[37] For example, thermodynamic modelling has been successfully applied to the prediction of the distribution of sulphur in steelmaking reactions[38] using the techniques described above.

Computational Kinetics

Whilst, computational thermodynamics can predict the equilibrium composition of steelmaking reactions, these techniques can not predict how fast these reactions take place and what controls their rate. As a field of knowledge, “reaction kinetics” attempts to answer such questions. It is important to note that the term “reaction kinetics” is sometimes used to only describe the speed of molecular interactions during reaction, whereas we use the term to describe the overall process of the reaction, which may include mass transfer and other mechanisms; we reserve the term “inherent” kinetics to describe the actual molecular re-arrangement step. In many

systems, the overall kinetics is controlled by one or two steps of the process, which may not be the “inherent” kinetics. For example, the diffusion of sugar in a tea cup is clearly important to the rate of sugar dissolution, and stirring the cup speeds up the process not because stirring helps the inherent kinetics (it can't) but because the diffusion step is accelerated by the increased mixing (“mass transfer” is increased) Reaction kinetics provides information on the conditions that govern the rate at which a reaction will occur and can describe the mechanism by which the reaction proceeds. In general, computational kinetics is less developed than computational thermodynamics, with less commercial software and large databases available.

In steelmaking reactions, the inherent kinetics are not usually the rate limiting step as the high temperatures of steelmaking reactions favour very high inherent rates, thus the reactions kinetics are more likely to be controlled by transport of elements from/to the phase interphase. Generally speaking, reaction rates in steelmaking operations can be predicted using Fick's first law, which states that the rate of diffusion is proportional to the concentration gradient.[39, 40] The rate equation is written in terms of molar concentration:

$$J = -D \left(\frac{\partial C}{\partial x} \right) \quad (20)$$

where J is molar flux in x direction (mol/m²sec). C refers to molar concentration (mol/cm³) and D refers to diffusion coefficient (cm²/sec). To reduce the process variables to a manageable level, time is mainly chosen as the differential independent variable and spatial gradients are ignored. With this simplification, the dependent variable, bulk concentration, is not a function of position and the equation can be reduced to;

$$\frac{dC}{dt} = k \frac{A}{V} (C_b - C^*) \quad (21)$$

Here variables k, A and V are mass transfer constant, area and volume, respectively. The formulations of rate equation differ with the

physical properties and type of fluid flow over the surface of the reacting condensed phase. This equation with appropriate initial and boundary conditions can be solved to analyse the process itself or alternatively, various aspects of the process. In reality, the reduction of Fick 1st Law to the simple 1st order differential of Eq. (20) involves many gross simplifications. Recently, the authors of this paper have tried to address these issues through the development of transient kinetic theories, which deal with changes in interfacial area, mass transfer coefficients and concentration gradients.[41]

For example, global model of oxygen steelmaking including the kinetics of scrap melting, flux dissolution, slag chemistry, temperature profile of the system, formation and residence of metal droplets in the emulsion, kinetics of decarburization reaction in different reaction zones has been developed by the present authors.[42] In this model, total decarburization rate in the emulsion zone is obtained by the summation of decarburization rates of individual metal droplets. The generated droplets, whose residence time is smaller than given time-step, are returning from the emulsion zone. Based on this boundary condition, decarburization rate can be calculated using;

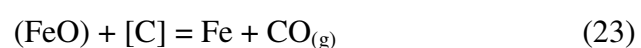
$$M_e \frac{dC}{dt} = \frac{\sum_{i=1}^n \frac{m_i}{100} (C_i^{t+\Delta t} - C_i^t)}{\Delta t} \quad (22)$$

Here the number of the droplets in the emulsion zone is represented by n , m_i is weight of a single droplet (kg) and C is the carbon content of droplet (mass%). The global model has been validated against industrial data.⁶⁶⁾

Process models [43-49] are developed to aim to express what steps a process consists of, or how they are to be performed. These models enable us to evaluate the key process variables such as concentration of impurities and temperature of liquid bath throughout the blow to understand the process better, design new techniques and optimize the process. Numerous of kinetic models have been proposed to predict process

variables that influencing the system such as scrap melting,[50-57] flux dissolution[58] and carbon removal reaction in the gas-slag-metal emulsion.[59-62]

Few of these models are fully based on the laws of physics formed by limited set of equations. Normally, a level of empiricism is introduced to provide a practical solution. For example, when liquid metal droplets are ejected to the emulsion phase due to the oxygen impingement onto the liquid bath at high speeds (> Mach 1), these droplets spend some time in emulsion and fall back to metal bath. Droplet generation enhances the reaction area significantly that increases the reaction rates of the process. Based on the previous studies,[62-65] it has been found that the residence time of a droplet varies from 0.2 to 120 seconds. It has been observed experimentally that this phenomenon is strongly related to the carbon removal reaction in the emulsion phase. The overall reaction is;



Carbon is oxidized via FeO reduction that forms carbon monoxide gas. If the rate of carbon removal is weak, the reaction product, CO gas escapes easily and detaches from the droplet as a result, the droplet maintains its original shape. After a critical point, defined as threshold decarburization rate, gas product is not able to escape from the droplet and stays in the metal droplet that the droplet becomes “bloated”. Brooks et al.[62] developed a mathematical model to predict the residence time of the droplets generated in the slag-gas-metal emulsion system under various operating conditions. In this model, a force balance was used to analyse the ballistic motion of a single droplet at vertical and horizontal coordinates. The motion of a single droplet is illustrated in FIGURE 3.

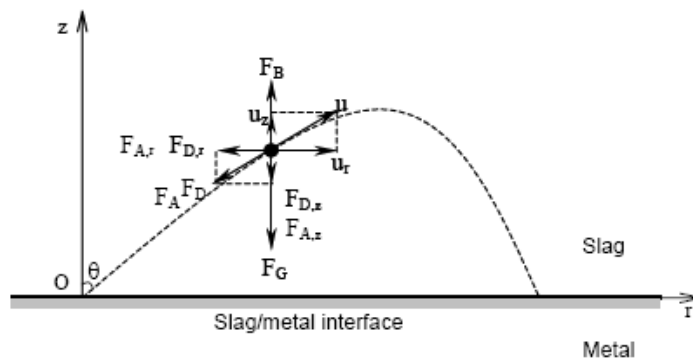


FIGURE 3: The schematic illustration of ballistic motion of a metal droplet in slag[62]

The relationship between the forces can be represented for horizontal and vertical coordinates in the following equations.[62]

for z direction:

$$\rho_d V_d \frac{du_z}{dt} = F_B - F_G - F_{D,z} - F_{A,z} \quad (24)$$

for r direction:

$$\rho_d V_d \frac{du_r}{dt} = -F_{D,r} - F_{A,r} \quad (25)$$

where u_z and u_r are the velocity of droplet for z and r directions, respectively. Variables ρ_d and V_d refer to density and volume of droplet. F_B , F_G , F_D and F_A are buoyancy, gravitation, drag and added mass forces, respectively. The numerical calculation is undertaken using the explicit forward differencing method. After differentiating, the trajectory of metal droplet for z and r directions can be obtained. As the trajectory at z direction approaches zero, the lapse time is calculated and defined as a residence time of a droplet.[62]

Up to this point, this model is based on basic laws of Newtonian physics. However, there is a lack of understanding on how the bloating behaviour of a droplet occurs in the emulsion. This phenomenon cannot have not yet been fully explained, so empirical relationships were introduced based on the experimental study by Molloseau and Fruehan.[60] It was observed that bloating behaviour occurs if FeO concentration in the slag is higher than 10 mass% in the emulsion phase. The threshold

decarburization rate is related to the FeO concentration in the emulsion phase using;

$$i_C^* = 2.86 \times 10^{-4} (\text{mass\%FeO}) \quad (26)$$

This model is able to predict the residence time of bloated and dense droplets using this simple correlation. The detail of this model was explained elsewhere.[62] This approach has been successfully applied to experimental results[60] and now being incorporated into industrial models.[66] In time, it may be possible to remove the current level of empiricism associated with the threshold decarburization rate. This example is typical of modelling of complex processes, where a mixture of basic physics and empiricism is used produce useful results and identify areas requiring more research. In this sense, model developments help us understand the gaps in our knowledge and point towards useful research directions.

Computational Fluid Dynamics

Computational fluid dynamics (CFD) is increasingly utilised in modelling the fluid flow behaviour of different industrial processes. In this approach, the equations that govern a process of interest are solved by means of computer based simulation. The advent of powerful digital computers has reduced the time required for the simulation process as well as opened up a new era in CFD application enabling modelling of many complex processes.

In steelmaking, oxygen is injected under supersonic condition of around Mach 2 inside the furnace.[71] Supersonic gas jets are preferred over subsonic jets because of high dynamic pressure associated with it which results in higher depth of penetration onto the liquid bath and better mixing of oxygen gas with liquid melt. Also as discussed earlier, the high speed oxygen jet produces droplets upon impingement on the liquid.[72] Since the environment inside the furnace is very harsh to make any measurement, a number of experimental [73-82] and some numerical studies [83-87] have been performed to help

understanding of fluid flow behaviour inside the furnace.

In our numerical studies of gas jet impinging on liquid bath, the unsteady continuity, momentum and energy equations are solved for pressure, velocity and temperature of the fluid flow. The equations are given below[88];

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_i}{\partial x_i} = 0 \quad (27)$$

where ρ is the density and U_i is the velocity of fluid flow in i^{th} direction.

Momentum equation:

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial (\rho U_i U_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial (\tau_{ij} - \overline{\rho u_i u_j})}{\partial x_j} + F \quad (28)$$

where P is the pressure of fluid, τ_{ij} is the molecular shear stress, $\overline{\rho u_i u_j}$ is the turbulent shear stress and F is the body force. For Newtonian fluid, the molecular shear stress is proportional to the rate of deformation. There are different turbulent models available for the calculation of turbulent shear stresses.[89, 90]

Energy equation:

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho E U_i + P U_i)}{\partial x_i} = -\frac{\partial (q_i + C_p \overline{\rho u_i t})}{\partial x_i} + \frac{\partial (\tau_{ij} U_j - \overline{\rho u_i u_j U_j})}{\partial x_i} \quad (29)$$

where E is the total energy, q_i is the conduction heat flux and is calculated by Fourier's law of heat conduction. The term $\overline{\rho u_i t}$ is the turbulent heat flux.[89]

These are partial differential equations and are solved by using finite volume method applying appropriate boundary conditions.[88]

FIGURE 4 shows a computational domain with boundary conditions for the simulation of gas jet impinging on liquid surface. Generally, velocity boundary condition is used at the inlet and static pressure boundary condition is used at the outlet. For the solid wall, the wall boundary condition was used in our model. The

deformation of the gas liquid interface due to the transfer of momentum of gas jet to the liquid surface is modelled by the following equation.[91]

$$P_l - P_g = \sigma \text{div} \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right) \quad (30)$$

where P_l , P_g are the liquid and gas side pressure and σ is the surface tension of liquid. Brackbill et al.[91] developed a continuum surface force model where this equation is included as a body force in the momentum equation. In order to determine the sharp gas liquid interface, the volume of fluid (VOF) technique[92] is used which solves an additional transport equation for the volume fraction α of tracked phase:

$$\frac{\partial \alpha}{\partial t} + u_j \frac{\partial \alpha}{\partial x_j} = 0 \quad (31)$$

$\alpha = 1$, cell is filled with tracked phase
 $\alpha = 0$, no tracked phase in this cell.
 $0 < \alpha < 1$ cell shares both phase.

After calculating the volume fraction in each cell, the density ρ and viscosity μ of the fluid in each cell are determined by a weighted average, as shown in following equations:

$$\rho = \rho_l \alpha_l + \rho_g (1 - \alpha_l) \quad (32)$$

$$\mu = \mu_l \alpha_l + \mu_g (1 - \alpha_l) \quad (33)$$

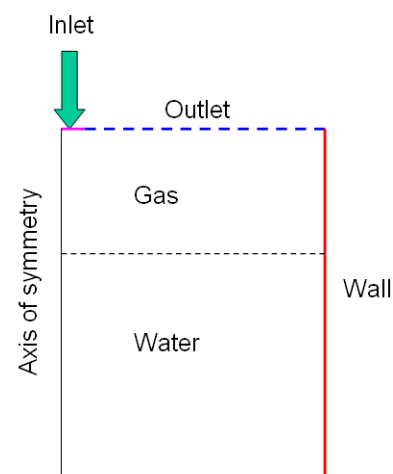


FIGURE 4: Computational domain with boundary conditions

where the subscripts l and g correspond to the liquid and gas phase, respectively. These properties are then used to solve the transport equations.

In finite volume method, the solution domain is subdivided into a number of cells and the partial differential equations are integrated over the volume of each cell in computational domain. The non-linear equations are discretised to make linear algebraic equations. Then the algebraic equations are solved iteratively using a suitable iterative technique.

Previous studies [85-87] have calculated the depth and diameter of depression created by the gas jet upon impingement on liquid bath. The depth of depression increases with increasing gas jet velocity and decreasing lance height as shown in FIGURE 5 [87]. The higher the depth of penetration, the better the mixing of oxygen gas and liquid metals which, in turn, increases the overall rate of reaction.

All of the previous numerical studies have assumed the gas phase as incompressible which is not the case in the real process. As a result, previous numerical solutions have under predicted the depth of depression when used for modelling of oxygen steelmaking[87]. This is one of the limitations of the numerical techniques described, it that it does not

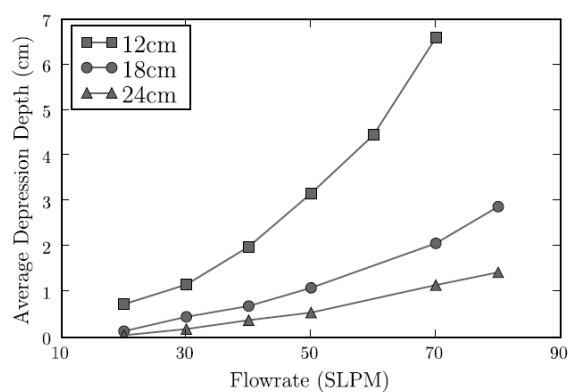


FIGURE 5: Depth of depression variation with changing flow rate and lance height

give stable solutions when one phase is highly compressible in multiphase flows. No numerical studies have been performed on

droplet generation rate because in order to simulate droplet generation, a very fine mesh is required which will result in a excessive computational time. Simulation of complex fluid dynamics [93] inside the furnace at isothermal condition has been carried out in some studies but the simulation of reactions is still a big challenge for CFD although models can simulate some simple reactions between gas phases. Among the advantages of numerical studies is that we can study non-isothermal conditions in the process whereas it is very difficult to do experimental studies at non-isothermal conditions. Some numerical studies at non-isothermal condition [83, 86] have been performed. The present authors have numerically simulated the supersonic oxygen jet behaviour at steelmaking temperatures [94]. It was found that the potential core length (the length up to which the axial gas velocity is equal to nozzle exit velocity) of the supersonic jet is higher at high ambient temperature and at steelmaking condition (1800K), it is 2.5 times higher than the potential core length at normal room temperature condition (285K), as shown in FIGURE 6. This was the first step towards developing non-isothermal modelling gas-jet impinging phenomenon in steelmaking. Studies are going on to simulate the fluid flow phenomenon such as depression depth, splashing at non-isothermal condition.

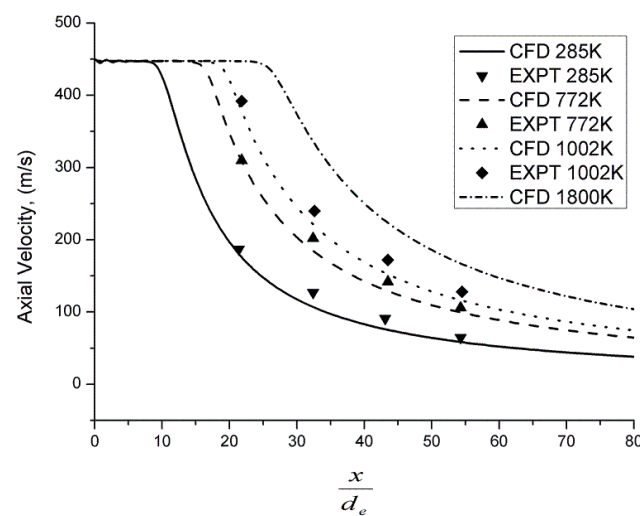


FIGURE 6: Velocity distribution of supersonic jet at different ambient temperatures.

These examples illustrate the advances in CFD modelling of complex processes such as Oxygen

steelmaking but also illustrate how significant work is still required to link the results of CFD models to chemical thermodynamics and kinetics.

Conclusions

In this paper, we reviewed how mathematical modelling has been used to analyse steelmaking processes. The modelling concepts were illustrated with examples drawn from the literature and studies by the authors. Steelmaking reactions occur under non-equilibrium conditions, thus predictions based on thermodynamics alone will be insufficient to understand and control the system. However, thermodynamics predictions can be used to predict the limits and direction of reactions occurring in the system. Models based on fundamental physics, for example, computational fluid dynamics, can be used to increase understanding of kinetic factors in the process but the use of empirical relationships is still required in many cases, either due to a lack of theory or difficulty in obtaining more fundamental data.

In summary, models provide powerful tools for making useful predictions, developing theoretical understanding of the system and provide a framework to advance our understanding. The complexity of steelmaking and problems associated with measuring and visualizing the phenomenon being studied necessitates the use of semi-empirical models and compromises between mathematical/scientific rigor and practical solutions being found.

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