MATHEMATICAL MODELLING OF BASIC OXYGEN STEEL MAKING PROCESS

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In

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By

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CERTIFICATE

*This is to certify that the work in this thesis report entitled "**Mathematical Modelling of Basic Oxygen Steel Making Process"** which is being submitted by **Ms. Vinita Kumari** (Roll no: 213MM2485) of Master of Technology, National Institute of Technology Rourkela, has been carried out under my supervision in partial fulfilment of the requirements for the degree of Master of Technology and is an original work.*

To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other University / Institute for the award of any Degree or Diploma.

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Vinita Kumari

ABSTRACT

A numerical model based on reaction thermodynamics has been developed to simulate basic oxygen steel making process for predicting hot metal composition inside Linz-Donawitz (LD) converter with respect to blowing time. This model also contributes towards the prediction of sloping phenomenon taken place during basic oxygen steel making process. Modelling of basic oxygen steel making process has significant utility as productivity and lining life of Basic Oxygen Steelmaking (BOS) is highly dependable upon mass, momentum, energy transfer and rigorous interaction among metal, slag and gaseous phases. Comprehensive thermodynamic model of basic oxygen steel making process has been developed to predict the bath composition and temperature as well as decarburization rate dynamically based on relevant blowing process parameters. One of the striking features of this developed model is the first time prediction of temperature variation depending on evolving bath composition and generated heat from bath composition dependent feasible reactions and their extent. Moreover, this numerical model does not require off gas analysis to maintain its dynamic nature of prediction. A true attempt for the benefit of steel industry is made for predicting slopping initiation time for particular blowing condition based on correlation with model predicted decarburization rate and critical decarburization rate for bloating of metal droplet. In connection to that, formation of foamy slag and sloping possibility have been studied using thermodynamic modelling followed by multiphase computational fluid dynamics (CFD) simulation technique. The CFD simulation has been carried out taking different turbulence models along with volume of fluid method (VOF) using ANSYS 15.0 software. CFD work demonstrates change in bath deformation profile during blowing period and also identifies the locations of different vortexes formed owing to supersonic oxygen jet penetration. Dynamic mathematical model of BOS has been interconnected with CFD simulation work for correlating fluid flow parameters with reaction behaviour inside BOS furnace. The results of developed model has been compared and validated with plant data. This work actually helps to understand basic oxygen steel making process in detail during the blowing period. Developed dynamic model can be used for LD converter having different capacities and accordingly this model's application is very significant and wide in primary steel making area.

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List of symbols and abbreviations used

ΔG	Change in Gibbs free energy
ΔG°	Change in Standard Gibbs free energy
K	Activity Coefficient
T	Temperature
ΔT	Change in Temperature
ΔS	Change in Entropy
Cp	Heat Capacity
ΔH	Change in Enthalpy
BOS	Basic Oxygen Steelmaking
wt. %	weight percentage

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Chapter1: Introduction

1. Overview of basic oxygen steelmaking

Steelmaking in simple terms can be defined as the process of refining or removal of unwanted elements and impurities from the hot metal produced from blast furnace (Fruehan, 1988, Ghosh and Chatterjee, 2008, Pehlke, 1982) and currently the world's major steel production is done via route of basic oxygen steelmaking. (Fruehan, 1988). It was only after World War II that the use of gaseous oxygen (instead of air) as the agent for purifying molten pig iron and scrap mixtures to produce steel by pneumatic processes received the attention of various researchers from Bessemer steelmaking process. (Pehlke, 1982)

The main functions of the BOS process are to remove impurities like carbon, phosphorous, manganese, sulphur and silicon from the hot metal, and to optimize the steel temperature so that any further treatment prior to casting can be performed with minimal reheating or cooling of the steel. (U.S. Patent no. US3301662 A)

The oxygen supplied to it causes oxidation of the impurities and iron, which either forms part of slag or escapes as CO or CO_2 gas. The heat required for the oxidation of impurities are derived itself from the exothermic oxidation reactions. The BOS process is also called autogenous, i.e. the required thermal energy is produced during the oxidation process.

The complete BOF process can be described as

1. Molten iron (hot metal) from a blast furnace is poured into a large container called a ladle lined by refractory. The first stage of steelmaking is the pre-treatment stage where the metal in the ladle is sent directly for basic oxygen steelmaking. The first

pre-treatment stage helps in refining of hot metal by removing impurities from steel like manganese, silicon, and phosphorus.

2. The process of filling the furnace with the raw materials of steel production is known as charging. It is very important for maintaining the proper charge balance, the ratio of hot metal to scrap. The BOS vessel is one-fifth filled with steel scrap. Molten iron from the ladle is added as required by the charge balance. A typical chemistry of hot metal charged into the BOS vessel is: 4% C, 0.2–0.8% Si, 0.08%–0.18% P, and 0.01–0.04% S. (Ghosh and Chatterjee, 2008)
3. The vessel is then made upright and a water-cooled lance is lowered down into the converter. The lance which blows oxygen with supersonic speed of around Mach 2 with 99% purity onto the steel and, ignites the carbon dissolved in the steel , converting it to form carbon monoxide and carbon dioxide, and thereby causing the temperature to rise to about 1700°C. This melts the scrap, dissolves the flux, and lowers the impurity content of the molten iron. It is this use of pure oxygen instead of air that improves upon the Bessemer process, as nitrogen (and other gases) in air do not react with the charge as oxygen does. Supersonic oxygen jet is blown through the water cooled lance.

   (Turkdogan, 1996).

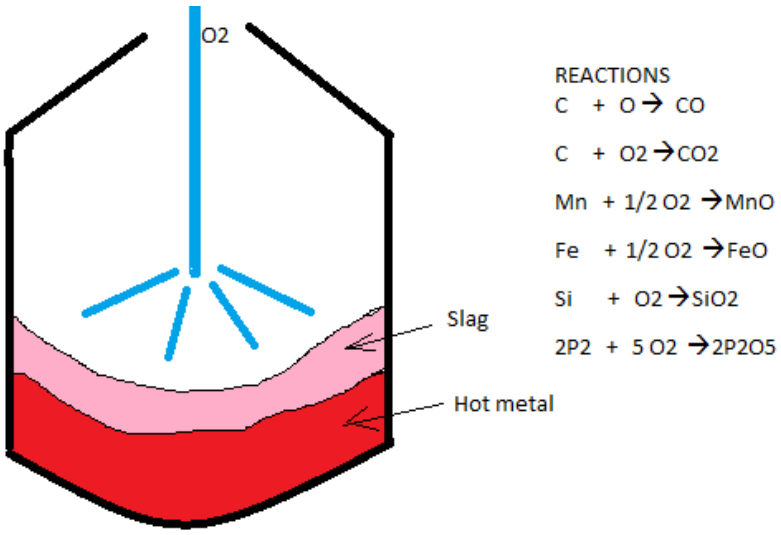


Fig 1. Oxygen steel making process

4. Fluxes which comprises of burnt lime or dolomite are fed into the LD convertor. It helps in absorbing impurities of the steelmaking process vessel to form slag. During blowing, the metal in the vessel forms an emulsion with the slag, which further facilitates the refining process.

The general chemistry of the steel produced is 0.3–0.6% C, 0.01–0.03% Si, 0.05–0.1% Mn 0.01–0.03% S and P. After the completion of blowing time, the BOS vessel is tilted again and the steel is poured into a giant ladle. This process is called *tapping of* steel. The steel is further refined in the ladle furnace, by adding alloying materials to give the steel more special properties as per customer's requirement.

The steel is desired to have 0.1–1% carbon content. Higher the carbon content of steel, the harder it is, as well as also more brittle and less flexible too.

Reactions inside the LD Converter

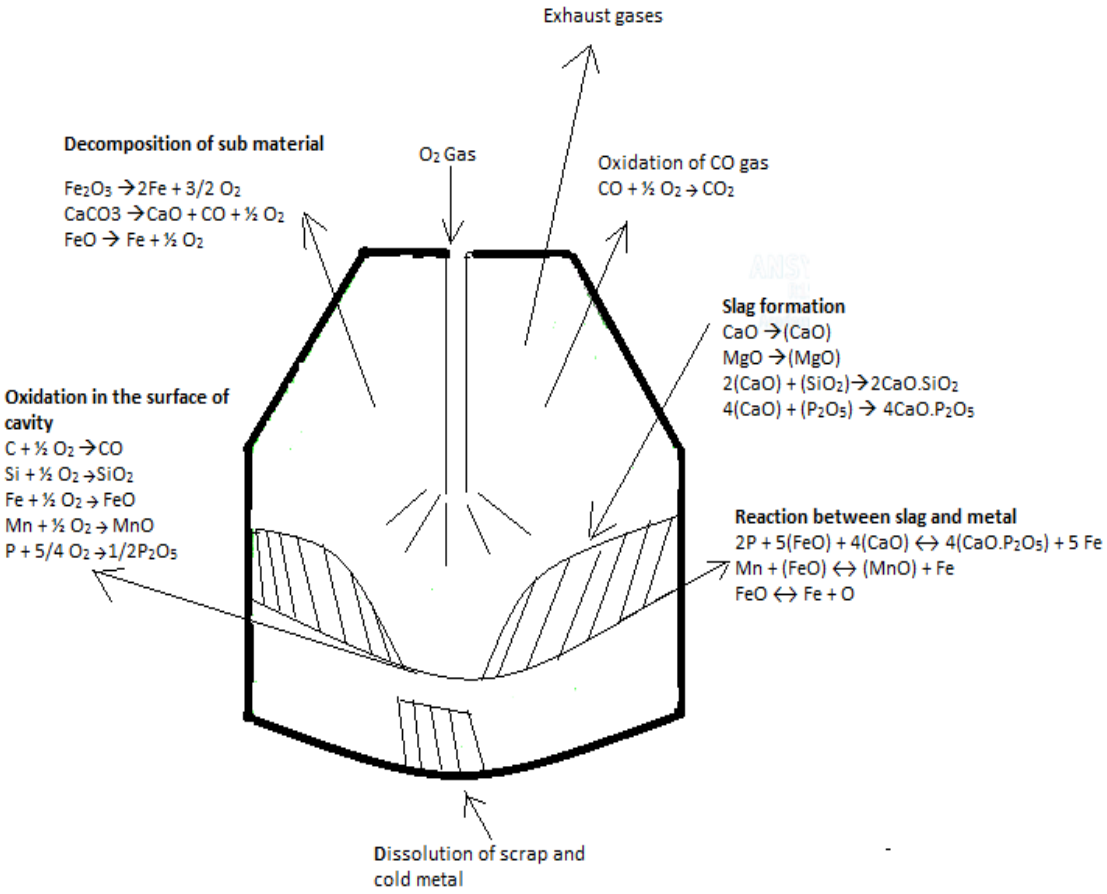


Fig 2. Schematic diagram of LD converter and its reactions

Chapter 2: BOS Modelling

2.1 Modelling and its types

Steelmaking is a complex process as it involves simultaneous multi-phase interactions, chemical reactions varying with temperature profile, heat transfer and turbulent flow patterns at high temperatures. This severity in the operating conditions makes it highly cumbersome process to make measurement and to observe its process parameters.

To remove this difficulty, mathematical modelling comes into play as it helps to evaluate the process along with helps in understanding the system. **(**Brooks, Dogan, Alam, Naser, and Rhamdhani, 2011)

In basic oxygen steelmaking process, there are basically two types of mathematical models available to simulate process behaviour

- Static
- Dynamic

- **STATIC MODEL**

It helps in predicting the end blow conditions of steels with the input data of weight, temperature and composition of steel whereas dynamic model describe the rate of change of bath and slag composition throughout the blowing stage and take variations in blowing conditions into account.(Sarkar, Gupta, Basu and Ballal, 2015)

It has been seen that static control fails to adjust the course of refining which includes multiple variations in the reactions, thus gives very limited accuracy .It is basically used to define the initial blowing and input conditions to get the desired final end point steel composition.

- **DYNAMIC MODELS**

Dynamic models of BOF should be such that it can predict the time dependent progress of the blow and be able to describe the real events happening in the bath. This can help the operator to have improved quality control of steel. Dynamic models help in prescribing the corrective action to ensure that the process achieves its final end target composition (Sarkar et al., 2015). The aspects of dynamic modelling of basic oxygen steel making process are well explored by researchers worldwide and majorities of their approaches can be described in three different model perspectives such as thermodynamic model, kinetic model and CFD model.

2.2 Thermodynamic modelling

Thermodynamic modelling usually includes the feasibility of each individual oxidation reaction and their subsequent effects for further purification of impurities. These provide information on the equilibrium distribution of species within the phases, behaviour of species in solution (i.e. activity) and also give information about the heat generated or consumed by these chemical reactions (Brooks et al, 2011).

Equilibrium calculations are made using the Gibbs free energy minimization technique in thermodynamic modelling as it is based on second law of thermodynamics. It includes mass balance, energy balance, calculation of enthalpies and calculation of moles of each species reacting and left in bath to give final bath composition.

In the development of thermodynamic models, one of the important parameters to be kept in mind is definition of all phases and possible species within the system. This also generates the need of thermochemical data such as heat capacity, enthalpy and entropy for pure species before the application of Gibbs free energy techniques. The most widely

used packages for this purpose are Thermo-Calc, Chemix, MT Data, Factsage Thermo-data, HSC, and Gemini2.(Wulandari et al. 2009; Gaye et al. 2001)

- **Decarburisation studies**

Decarburisation actually converts molten iron to molten steel. The process of decarburisation has been the interest of many researcher's since the beginning of steelmaking. One of such studies concluded that 70% of decarburisation occurs in the emulsion zone during the main part of the blow, and it decreases towards the end of the blow as droplets becomes denser. (Dogan, Brooks and Rhamdhani (2011).

Many researchers have developed a dynamic model for studying the decarburization rate and the accumulation rate of oxygen with respect to changing decarburization rate with the help of measured step response (Kattenbelt and Roffel, 2008). However they have assumed that the oxidation of manganese, phosphorous, and sulphur to be negligible during the main blow. This assumption may seem reasonable to make things simple. But in reality oxidation of manganese and phosphorous do have their impacts in changing the reaction thermodynamics by changing the available oxygen for the oxidation of carbon and in causing the overall temperature change of the bath.

Many researchers have experimented with small carbon containing iron droplet, dropping them into a slag (Gare et al., 1981; Mulholland et al.1973; Min et al. 1992).They have observed that the decarburization rate is a direct function of temperature, carbon concentration, and iron oxide concentration.

Many empirical relations have been derived and reported in literature for calculating the variation of C and O_2 content of bath in liquid metal as well as CO composition in the gas as the function of blow time, oxygen blow rate, gas purity and metal weight. (Chou, Pal and Reddy, 1993)

A model is developed consisting of an iron oxide and a carbon balance and an additional equation is given to describe the influence of the lance height and the oxygen blowing rate on the decarburization rate by Barron, Medina and Hilerio (2014). They have showed that as the oxygen blowing rate and the rate of addition of iron ore increases, it increases the oxygen content in bath. Thus more oxygen becomes available for its consumption by impurities, thus thereby decarburisation rate increases. They have also showed that increase in oxygen blowing rate along with decrease in lance height increases the amount of iron droplets generated in the slag. Their studies have also revealed the linearly dependence of decarburisation on oxygen flow rate. (Barron et al. 2014).

Ikeda and Matsuo (1982) have studied the relationships among the metal oxidation, the decarburization and the dephosphorization in stainless and carbon steel refining. They have found out that for decarburization reaction, refining under low CO partial pressure is favourable and for dephosphorization of carbon steel refining with slag of optimum iron oxide content and refining at low temperature are favourable.

In steel making silicon content, manganese content, oxygen injection rate, lance height and the bath temperature are the main factors influencing the decarburisation rate. (Min, and Fruehan 1992; Lee and Kolbeinsen, 2007; Chukwulebe et al., 2004; Ogawa, Yano, Kitamura and Hirata, 2001)

Emulsification studies

There has been many experimental studies that have shown the importance of emulsification behaviour in steelmaking process. The formation of CO bubble extends the interfacial area, helping in bath circulation and thus impacting the overall kinetics of the bath (Trentini, (1968); Meyer et al., (1968); Kozakevitch, (1969); Price (1974); Schoop et al., 1978; Cicutti et al.2000).

Many researchers have attempted to give an enlarged meaning to the emulsion theory to describe operating conditions of soft and hard blowing. (Costa, Canepa, Maga, and De March, 1980) .They have used classical linearization method of the thermodynamics of ir- reversible process assuming that each reaction rate is proportional to its affinity, to define the refining reaction kinetics occurring in industrial process.

Turkdogan (2000) have revealed with his plant data studies that, the iron content of oxide of slag has a decisive effect on steel dephosphorisation and desulphurisation. His studies also gave some inter relations between FeO, CaO and SiO_2 concentrations in the slag at the end of oxygen blowing.

Droplet generation studies

In oxygen steel making, metal droplets generated by impinging gas jet play a very significant role in metal processing operations, as they avail a large interfacial area of droplets which enhances the rate of heat transfer and chemical reactions. Thus it is imperative to consider droplet generation rate into account while developing the model. (Subagyo, Brooks, Coley and Irons, 2003)

Turner and Jahanshahi (1987) have found out with their series of experiments that the concentration of metal droplets in the upper phase increases with decreasing of lance height in the absence of bottom bubbling. They have found that the position of bubbles has a significant effect on the mass of metal droplets entrapped in the emulsion phase. One of their conclusions also included that with decreasing lance height, the relative change in metal droplet content of the emulsion phase decreases which is caused by bottom. They also provide an insight of drop generation in combined blowing processes. (Turner and Jahanshahi, 1987)

Drop generation has been investigated with the help of experiments by a gas jet impinging on a liquid surface by Standish and He, (1989). They have found out that

there are different mechanisms of drop generation in “dropping" and “swarming" regions, which result in different increase of drop generation rate .Impact of bottom blowing on the rate of droplet generation have also been studied by Standish et al (1989).

Studies on the role of external agitation

External agitation helps in homogenisation of bath and helps in removal of dissolved oxygen .It has been found out experimentally that for identical volumes of injected gas into the bath, mixing time is shorter in case of dispersed bubble agitation as compared to agitation induced by gas introduction through a single basal tuyere.(Das, Ray and Chatterjee 1989).

Modelling based on off gas analysis

There has been numerous attempts in developing mathematical model using the off gas data. In 2009, Evestedt and Medvedev have developed a method to give warning about the slopping phenomena using the off gas funnel. This method was quite reliable method of predicting the slopping phenomena as it processes the sound signal from microphone located at off gas funnel which gives the slag estimation. (Evestedt and Medvedev, 2009) Their model have provided a relationship between off-gas flow rate, pressure and the slag level to be estimated and it updates itself recursively with time. (Evestedt et al., 2009).However there is a further scope of improvement by devising a method of slopping prediction without the use of off gas analysis.

Li et.al (2010) have developed a BOF process model by analysing the effect of silicon, oxygen injection rate, oxygen lance height, manganese, and bath temperature on decarburization. However while studying the decarburisation rate they have not taken the role of iron oxide into consideration (Li et.al, 2010). Although they have significant impact on decarburisation rate. This leads to scope of further improvement in this regard.

In connection to that the possibility of blowing control based on exhaust gas data have also been studied by Iso et al. (1987). They have found out many inter relations between the amount of oxygen accumulated in LD converter (Calculated from the oxygen balance by using exhaust gas data) with the amount of FeO, Fe_2O_3 and MnO in the slag during blowing. Oxygen level has been used here as an indicator of progress of a reaction as it controls the P and Mn content of steel and the total iron content of slag at the end of the blow. (Iso et al., 1987)

Sarkar et.al (2015) have modelled the process dynamics by dividing the LD convertor into three separate continuous stirred tank reactors. Oxidation reactions have been assumed to be primarily taking place at the interface between the slag and the metal phases in the emulsion. And the mass transfer of FeO in the slag phase has been assumed to be rate controlling factor. However they have not modelled the initial part of the blow before the formation of emulsion. This model also does not give the complete information about bath and slag composition during the blow. Dephoshphorization have not been taken into account in this paper. Temperature change is assumed to vary linearly which is generally not in real case. This model also does not give clear n concise picture of process going within the bath.

Modelling based on change in Gibbs free energy

The attempts of BOS process modelling based on the distribution of blown oxygen among the elements of metal proportional to the fraction of Gibbs free energies for the oxidation of hot metal components have been reported in literatures (Chigwedu, Kempken and Pluschkell 2006). Deo and Shukla (2012) have calculated Gibbs free energy change for all the probable reactions of basic oxygen steel making process using FactSage database assuming system as fully mixed.

Jalkanen and Holappa (2004) have distributed the blown oxygen among the components of the metal phase and assumed to be controlled by the reaction affinity. The surface concentration of the oxidized component has been changed, and the consumption of the next small part of oxygen was considered for the new concentrations of metal phase components (Jalkanen and Holappa, 2004).

Hack et. al. (2007) have developed multi-zone process model of the LD converter steel making process using SimuSage modelling software. They have divided the converter process into different reaction zones. Inside these reaction zones, they have assumed thermochemical equilibrium. They have considered empirical dependences for simulating mass and energy exchange among the zones. Empirical dependences have been determined experimentally, considering several process conditions (e.g. blow rate, lance height, and other geometrical parameters).

2.2 Kinetic modelling

Thermodynamic modelling may give information about the equilibrium composition of species in the bath. But it is kinetic modelling which gives the information about the reaction kinetics or the rate of reactions occurring in the bath and tells "how fast a reaction" is occurring. Reaction kinetics provides information about the conditions that govern the rate of reactions occurring in the bath and provides information about the mechanism by which the reaction proceeds.

Many process models have been developed (Sharma et al 1987; Gaye and Lehmann 1997; Szekely, 1988; Asai and Muchi, 1970; Weeks, 1973; Knoop et al.1992; Modigell et al. 2001;Graveland-Gisolf et al., 2003) to give details about the steps that makes up a process, and how they are to be performed. These models help 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.

A mathematical model has been developed using the bloated droplet theory to predict decarburisation rate under full scale operating conditions by Dogan, Brooks and Rhamdhani, 2011. They have found out that emulsion zone increase as lance height is decreased. Their model have also showed the variation in residence time of ejected metal droplets. (Dogan, Brooks and Rhamdhani (2011).

Brook et al., (2005) have developed a model based on dense and bloated droplet theory based on ballistic motion principles which have been found to be useful for predicting the residence time of dense metal droplets in slag at the end stage of blow for top blown oxygen steelmaking.They have showed that if residence time of the dense droplets in slag is less than 1 second in top blown oxygen steelmaking, it would imply the poor kinetic condition at end stage of blow in top blown oxygen steel making.This bloated droplet model has been found to be excellent tool for predicting the kinetic behavior in top blown oxygen steelmaking during rigorous decarburization period of blowing.

With the help of kinetic experiments on oxidation of slag and molten iron (Pan, San, Ohirasawa and Mori, 1990), the effects of Si and P in the metal and slag on the oxidation reaction rate as well as the effect of mechanical stirring have been observed and subsequently a mathematical model is developed. Kitamura, Miyamoto, Shibata, Maruoka and Matsuo (2009) have developed a reaction model for hot metal dephosphorisation, considering the effect of di calcium silicate and lime dissolution rate for simulation of laboratory scale experiments by varying the slag composition, fluxing method and oxidiser addition. Christopher P. manning and Richard J. Fruehan, (2012) have investigated the rates of dephosphorisation and rephosphorisation of liquid iron with simulated steelmaking slag of liquid iron at 1873K experimentally. Thier results have indicated that the mass transfer

parameter of slag metal interface area and the overall mass transfer decrease as the reaction proceeds.

Molloseau and Fruehan, (2002) have studied the rate of reduction of FeO in the slag for $CaO\text{-}SiO_2\text{-}MgO$ by carbon in iron droplets .They have also studied the behaviour of metal droplets in slag with the help of X-ray fluoroscopy. They have found out that the droplet remained intact for FeO with concentration up to 10 wt. percent, and above this level of concentration, droplets emulsified in the slag as their surface area and reaction kinetics greatly increases. Attempts have been made by many researchers to model viscosity of slag (Zhang, Chou and Mills,2011), which will be help full for CFD modelling of steel making.

Pomfret and Grieveson,(1983) have studied the kinetics of slag metal reactions and developed a mathematical model to evaluate the slag metal reactions.

$$R = (k*(A/V))*\Delta C$$

Here R is the rate of reaction, k is a mass transfer coefficient .ΔC is driving force for mass transport .A represents is the reaction interface area and V the volume of the phase in which concentration is being measured. This equation have been analysed for different boundary conditions and rate determining steps and a conclusion was made that the rate-determining step is mass transport in the metal phase (Pomfret et al., 1983). Rhamdhani, Brooks, and Coley (2005) incorporated the interfacial area changes in kinetic equations in presence of emulsification process .They have analysed the kinetics by including time averaged interfacial areas in rate equations.

A sub mathematical model have been developed to predict the flux dissolution rate in oxygen steelmaking process. This model is good enough to predict the progress of flux dissolution and the amount of slag generation as a function of saturation concentration of CaO and MgO in the slag, gas flow rate of CO and the physical properties of slag. The

model revealed that if rate of addition of flux is increased, the amount of flux dissolved would also increase. (Dogan, Brooks and Rhamdhani, 2009)

Rhamdhani, Brooks, and Coley,(2006) have analysed the changes of interfacial area in metal slag reactions .Their studies have revealed that maximum change in interfacial area depends upon initial rate and change in free energy due to chemical reaction. They have found out the two main sources of increase in interfacial area i) flattening of droplet formed originally ii) separation of smaller droplets.

2.3. Computational Fluid Dynamics

It is the new era technology which helps in graphically showing fluid flow, swirls, turbulent motion, cavity formation etc. It is increasingly being utilised in the industry for modelling of different fluid flow behaviours in different complex process. The advent of powerful digital computers has reduced the time required for the simulation process. CFD have proved as an efficient simulation tool to many researchers. Many researchers have combined CFD simulation with physical model based studies of fluid flow inside LD converter to optimise bottom tuyeres configuration of the BOF vessel. (Singh et al., 2007)

Ersson et al. have studied impinging air jet on a water surface using numerical fluid flow techniques. They have also done CFD modelling of a top-blown converter coupled with equilibrium thermodynamic databases (ThermoCalc). (Ersson et al., 2008). Kundu and Pal (2012) have performed investigations on interaction of impinging oxygen jet with hot-metal bath using multiphase model. VOF model of Ansys Fluent is one of the important technique used to study fluid flow behaviour in multiphase CFD model. It is used to model free surface flows for multi fluid processing in metallurgical operations like slopping, skimming of slags etc.

The volume of fluid (VOF) technique can be considered as a simple an efficient method of numerically treating free boundaries embedded in a calculational mesh of Eulerian or Arbitrary Lagrangian -Eulerian cells. It is very useful method as it uses minimum stored information ,efficient in treating all complex intersecting free boundaries, and can be easily extended to all three dimensional calculations.(Hirt and Nichols 1981),(Liovic, Liow and Rudman 2001).

Schlüter et al. (2008*)* have developed a multiphase CFD model of a top blown converter where he studied splashing phenomena due to the impinging jet as well as the mixing time in the converter due to both bottom and top blowing. (Schlüter, Kempken, Odenthal, Reifferscheid and Vogl 2008). However in their model steel having carbon 3 mass % carbon results in no initial amount of slag, which is not possible in real practice. Another major drawback of the result from their model was the amount of FeO and SiO_2 produced which was negligible, therefore as per their model only gas (CO, CO_2) is created as the oxygen jet hits the steel bath. This leads to need of future developments in the model.

Johansen, 2001 studied the applications of multiphase flow in CFD, ranging from dispersed to separated flows to show the effects of free surface flows and wetting phenomena.

Ayub, Sohaib, Rafique, (2006) have conducted a time dependent CFD analysis of gas jets impinging on liquid surface to analyse the surface deformations like dimpling, splashing and penetration using three different multiphase models like the Eulerian model, the VOF model and the mixture model .They have used the standard k-ε model to account the turbulence in the continuous phase.

Sulasalmi, Kärnä, Fabritius and Savolainen, (2009) have developed a CFD model based on water model experiments to conduct simulations on slag entrainment and droplet formation. To track the interface between slag and steel, a multiphase VOF method has been

used by them and to track separate droplets and User Defined File (UDF) code was applied.

A CFD model have been developed by Alam, Naser, and Brooks (2012) to investigate the effect of a high ambient temperature field on behaviour of supersonic oxygen jet. Li, Wei and Yu, (2011) have developed a numerical model for top blown oxygen converter to study its effects on the characteristics of off gas like concentrations, temperature, flow rate and sensible heat flux on top-blown oxygen converter steelmaking process, a large amount of high-temperature off-gas is produced.

Alam, Naser, Brooks and Fontana, (2011) have developed a CFD model to simulate the liquid flow field and surface deformation caused by an impinging shrouded supersonic jet on a liquid bath from top blown oxygen steelmaking. They have found that the cavity surface area was the most influencing factor in the generation of droplets.

Barron, Medina and Hilerio, (2013) have studied the influence of viscosity on the efficiency of slag splashing with the help of transient CFD simulations as viscosity plays a major role in influencing slag splashing technique.

2.4 Coupled Model

Shukla, Deo, Millman, Snoeijer, Overbosch, and Kapilashrami, (2010) have developed a dynamic model based on thermodynamic approach .They have coupled the kinetics of scrap dissolution in their model and revealed that mixing was the major factor in deciding the course of any reaction which in turn depends upon oxygen flow rate ,height of lance and the nature of scrap.

Ersson et al., (2008) have developed a model coupling ThermoCalc database and CFD software to make dynamic simulations of top blown converter. For this, reactions between gas–steel, gas–slag, steel–slag and gas–steel–slag have been considered. Their theory

stated that a large amount of production of CO gas can actually hinder the decarburisation rate.

2.5 Technological gap

All the models that have been developed so far, none of them have been able to model phosphorous content dynamically capturing phosphorous reversal in the bath. Apart from that, all the models that have been developed so far, require input process characteristics parameter like off gas analysis during the blow. Then only those model are able to give the bath composition during blowing period. Updation of temperature due to the chemical reactions is also an area to be studied to get the concise idea of the feasible reactions and the composition of bath as change in Gibbs free energy is dependent on temperature. Considering all the above points, a software based on dynamic modelling that could give the updated values of bath composition just by giving input conditions would be great help towards safe automation of steel industry. In the perspective of total quality management (TQM), such type of predictive software can be very useful to meet stringent quality criteria for steel. There is a significant scope of optimizing the bottom nozzle configurations (number, dimension and location) and bottom purging gas flow rate for achieving better and fast refining of molten iron by physical modeling and numerical modeling of top blown and bottom purging LD converter. Coupled CFD – thermodynamic - kinetic model of BOF steel making process for predicting end point composition and temperature for a complete blow of LD converter is not available. Optimization of blowing process or blowing parameters to eliminate requirement of re-blow, is yet to be done accurately. Concrete understanding of inter-relation between reaction kinetics with fluid dynamics for basic oxygen steel making is not achieved.

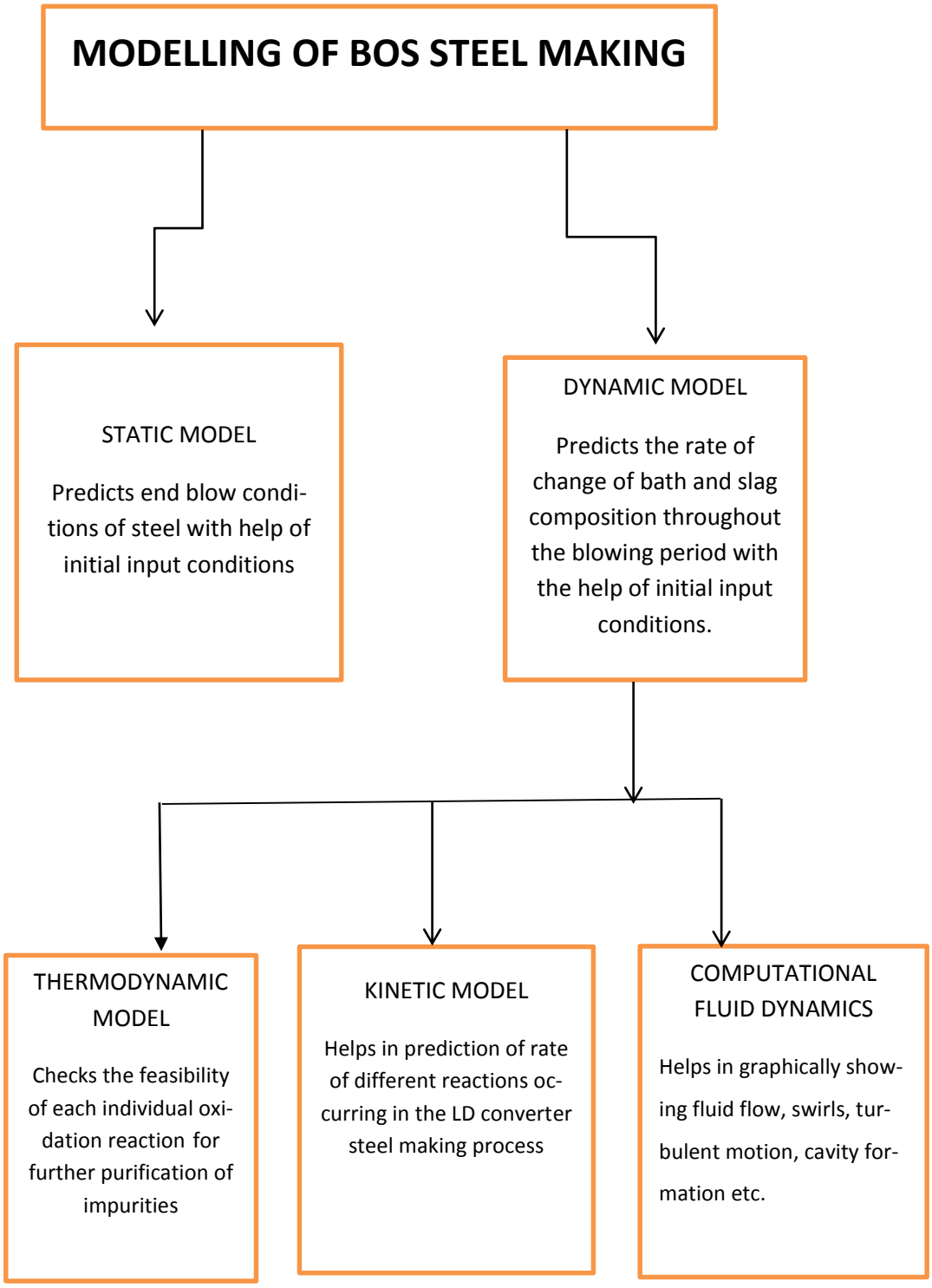


Fig 3: Modelling of BOS steelmaking

Chapter3: Description of the model

3.1 Thermodynamic model

The thermodynamic model presented here is divided in three parts.

- Blown oxygen driven gas metal reaction model
- FeO (of Slag) driven model
- Droplet generation model

3.1.1 Blown oxygen driven model uses oxygen directly taken from lance for the oxidation of its impurities in hot metal. Emulsion formation is not taken into account for the first minute of the blowing period as it requires some time to form.

- In this part , the oxygen derived directly from the lance is distributed in all the reactions as per the probabilistic ratio of Gibbs free energy of individual reaction to the total Gibbs free energy of the all the reactions. This tells the amount of oxygen consumed by each reaction. And also gives the idea as which reaction is dominating in the bath and to which extent.
- For the first minute of blowing period, we are using temperature dependent equations as given in book Turkdogan, 1996.

$$C + O \rightarrow CO \quad (1)$$

$$\Delta G = - 114400 - (85.8 \times T) \quad (2)$$

$$C + O_2 \rightarrow CO_2 \quad (3)$$

$$\Delta G = -395300 - (0.5 \times T) \quad (4)$$

$$Mn + O \rightarrow MnO \quad (5)$$

$$\Delta G = - 397000 + (81.1 \times T) \quad (6)$$

$$Fe + O \rightarrow FeO \quad (7)$$

$$\Delta G = -225500 + (41.3 \times T) \quad (8)$$

$$Si + O_2 \rightarrow SiO_2 \quad (9)$$

$$\Delta G = - 907100 + (175.7 \times T) \quad (10)$$

$$2P_2 + 5\ O_2 \rightarrow 2P_2O_5 \quad (11)$$

$$\Delta G = - 630000 + (422.5 \times T) \quad (12)$$

From mass balance, the oxides formed and the weight of each element remaining in bath is calculated and this in turn gives the steel composition of the bath.

- To update the value of ΔG for every reaction, we use

  $\Delta G = \Delta G° + RT \ln K$

- The term "Activity" used here can be understood as an "effective concentration" of a particular species and is an important thermodynamic quantity used for quantifying the way species mix and dissolve into each other (Brooks et al.,2011).Here

  K= activity coefficient = weight of individual oxide / total weight of oxide formed .

- Now, with the weight of each element remaining in bath, the number of moles of element used for the further reactions is calculated.
- Updation of temperature is done by using the formula

  ΔT = total enthalpy/total Cp.

- We add this ΔT with the previous temperature to give the updated temp in every minute.
- Heat capacity (Cp) of each reactant is found out by using the formula

  $\Delta S = \Delta H / T = Cp / T$
- Enthalpy values are taken from Turkdogan, 1996.
- Total weight of steel is calculated by adding weight of each elements remaining in bath. Weight percentage of each element = weight remaining of each element in bath/ total weight of steel.

3.1.2 Slag driven model

Here FeO from slag is used for the further purification of hot metal. Oxygen required for oxidation of further elements is derived from FeO.

$FeO \rightarrow Fe + [O]$

Meyer et al. (1968) have also concluded that direct reaction between the oxygen jet is less important than slag–metal decarburization in the emulsion of slag and metal.as major part of refining of hot metal is done in this slag metal zone only.

- In this part of model we have used probalistic oxygen distribution in all the reaction except for CO2 formation reaction.
- Again mass balance is used to calculate the weight of element remaining in bath after the formation of its respective oxide.
- Thus weight of each element remaining in bath is updated always. It is a coupled model which goes back and forth again and again to update its value, making it 'Dynamic' in true sense.

3.1.3 Droplet generation model

The model have presented here makes the use of droplet generation to aid in purification process of hot metal. Many attempts have been reported in literature where the behaviour of metal droplets in slag metal gas emulsion has been experimentally investigated. Subagyo et al. (2003) have developed a mathematical model which revealed that droplet generation rate was strongly dependent on blowing number (ratio of ratio of inertial to surface tension and buoyancy forces).

Sarkar et al. (2015) have showed the variation between lance height and droplet generation rate with the blowing time.

- Using the droplet generated from that paper, we have calculated weight of each purified element of steel assuming each droplet get 10% purified during its residence time.
- This 10% purified droplet weight is considered and updated bath composition accordingly. We also add iron ore to aid in emulsion formation as it increases the FeO content for the slag driven model. This also in turn helps in further purification process.

3.2 Assumptions made

1. We have assumed only 10% of the droplets get purified during its residence time.
2. We takes into account of distribution of oxygen as per probability of reaction based on Gibbs free energy.
3. We have taken oxygen efficiency as 30%, assuming 70% of oxygen do not hit the bath surface and just escapes out of the converter.
4. We have taken a specific lime sequence for modelling and have not modelled lime dissolution and scrap melting.

3.3 Flow chart of thermodynamic model

3.3.1 Flowchart of oxygen driven model

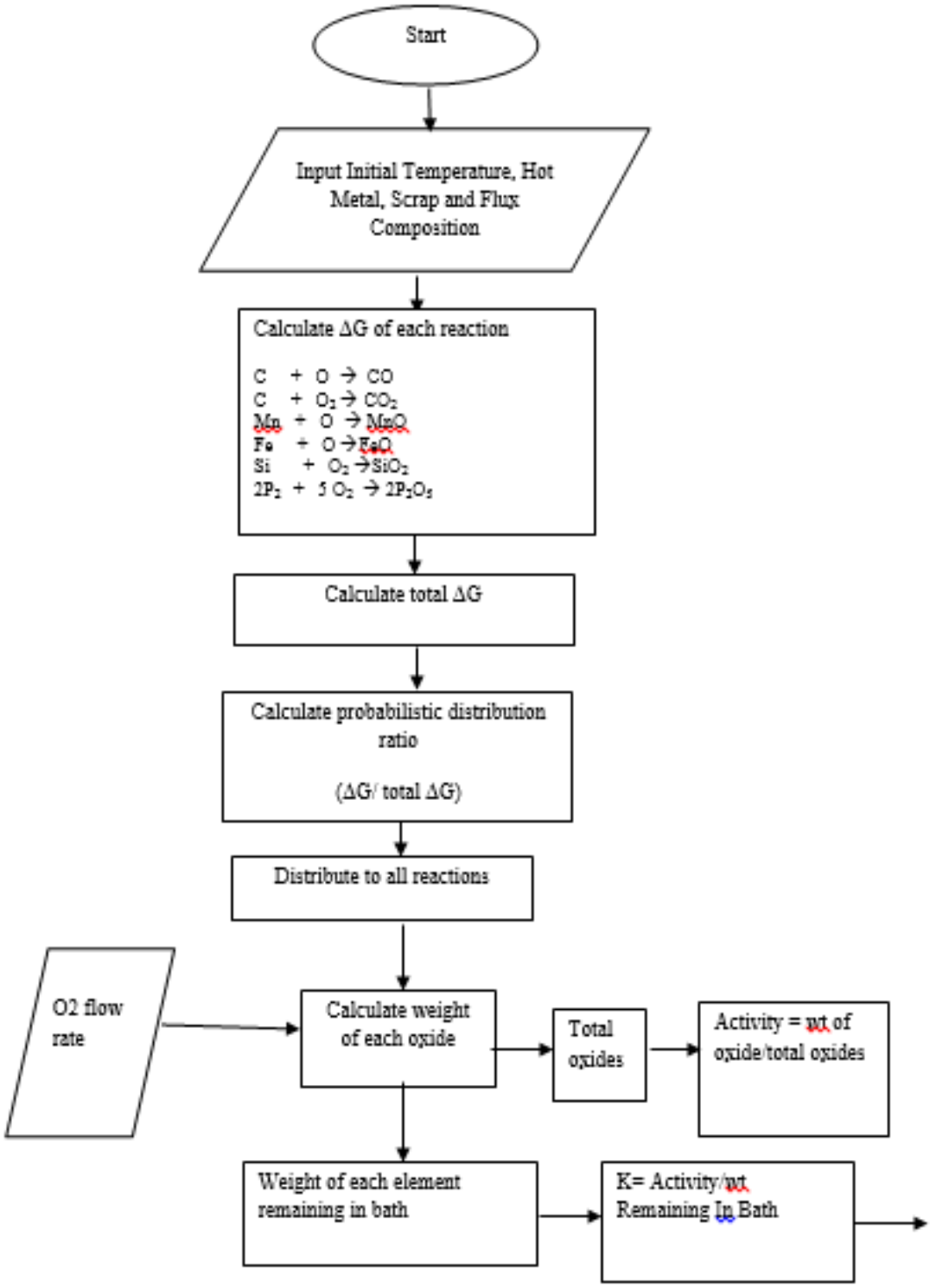


Fig 4: Flowchart of oxygen driven model

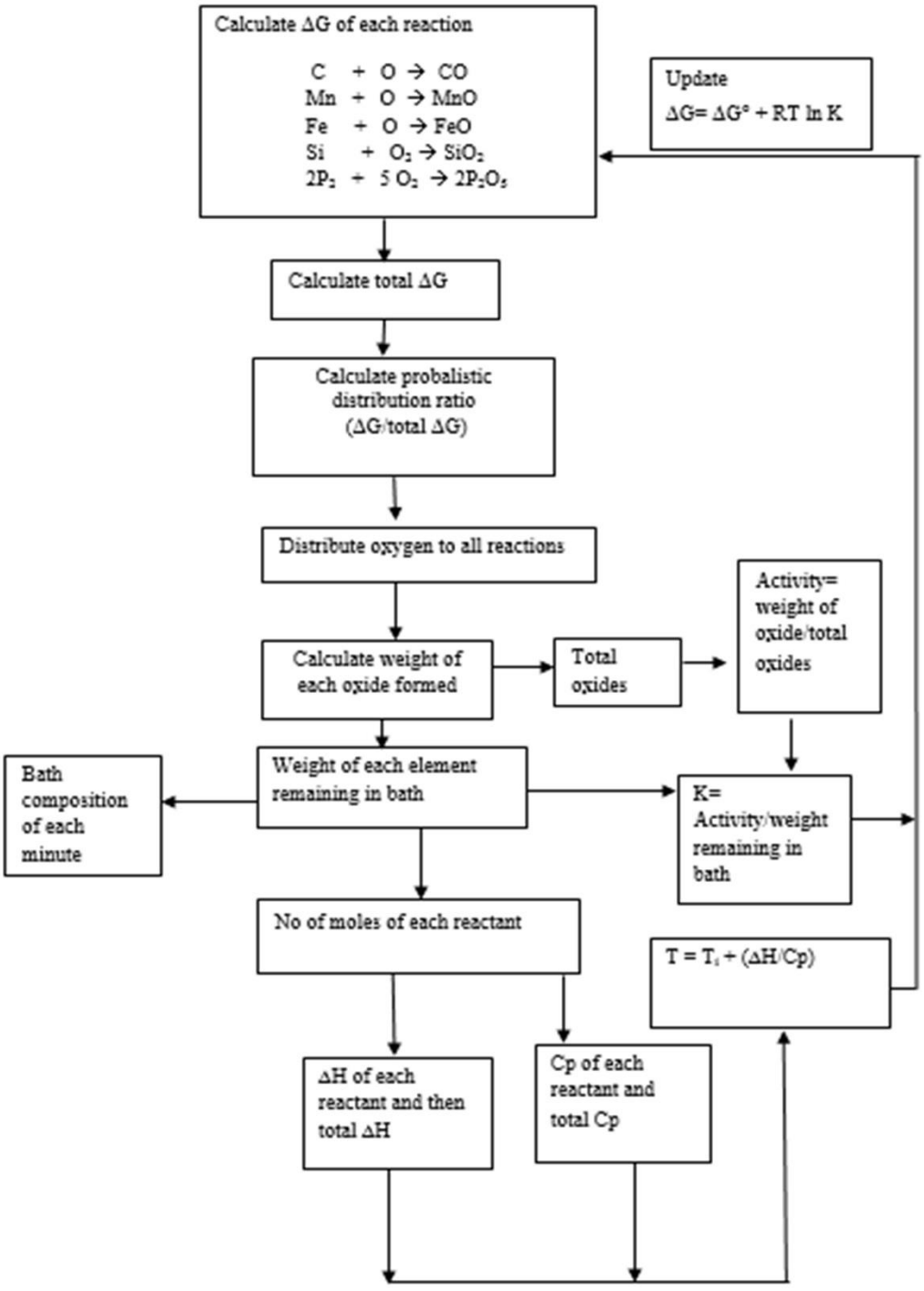


Fig 5: Flowchart of slag driven model

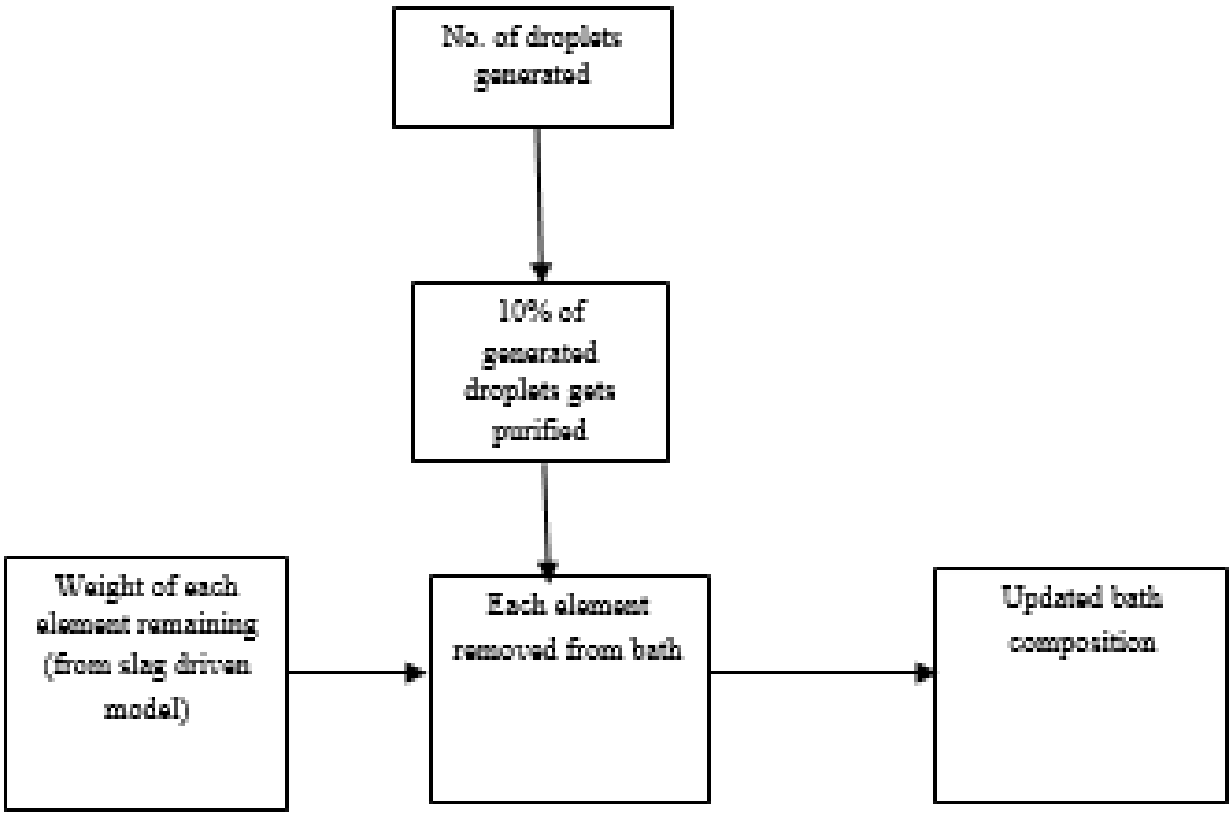


Fig 6: Flowchart of droplet generation model

3.4 CFD MODEL

The efficiency of basic oxygen steel making process depends on mass, momentum, energy transfer and dynamic interaction among ions, atoms, molecules in the bath. So, concrete understanding of bath fluid dynamics inside basic oxygen furnace is important for optimization of reaction kinetics inside the bath and maximization of LD converter lining life. Inter-relation between reaction kinetics with fluid dynamics for basic oxygen steel making is not understood completely till date. Therefore realistic prediction of **spitting** and **slopping** based on interdependency among fluid flow behaviour, mass transfer phenomena and energy transfer is yet to be achieved. Computational fluid dynamics (CFD) modelling helps in evaluating different fluid flow parameters during simulated blowing (impossible to measure in real LD converter during blowing period) and by finding the correlation between fluid dynamics and reaction kinetics.

A 2D BOF two phase model is numerically simulated by using computational fluid dynamics. For CFD analysis, ANSYS 15 software is used. FLUENT is the ANSYS solver to solve the fluid related problems. The solver is based on Finite Volume method. Before CFD simulation, domain is discretized into a finite set of control volumes.

There are some steps to solve ventilation simulation as following –

1. Problem identification
2. Pre-Processing
3. Solution
4. Post-Processing

Figure represents different steps of solving problem using CFD analysis

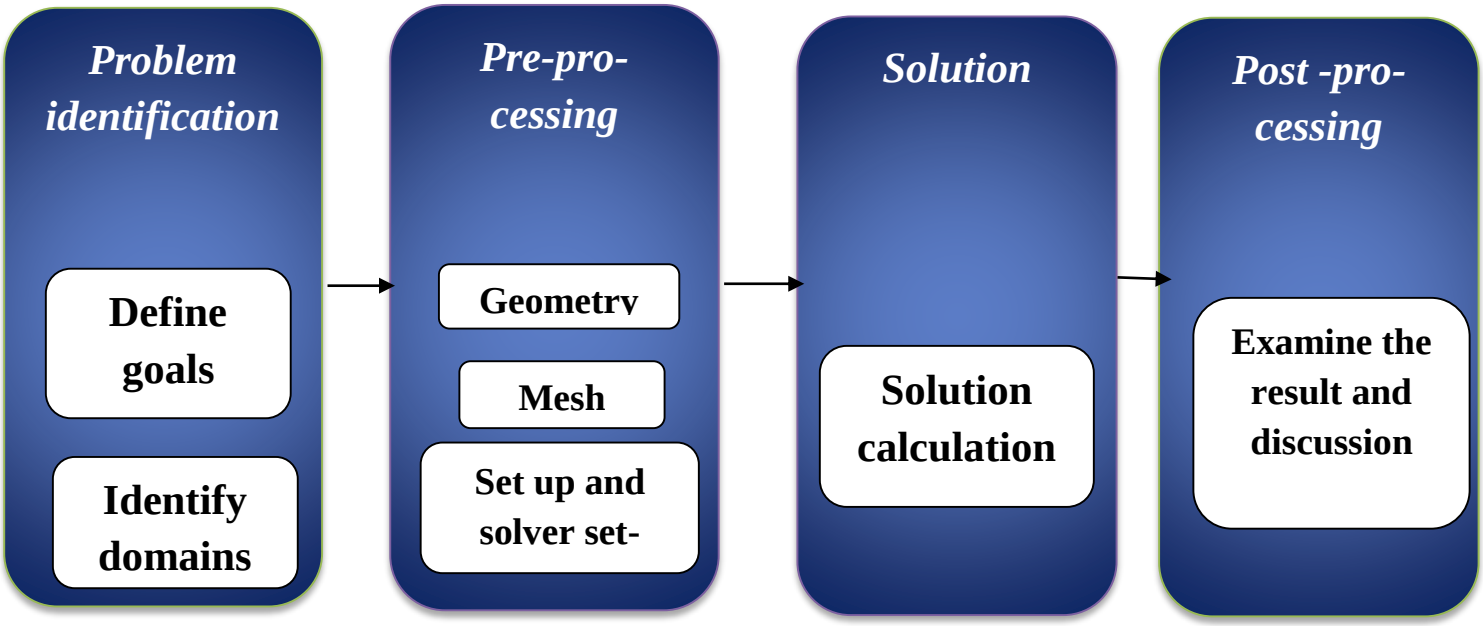


Fig. 7 - Steps in CFD solver

3.4.1 Problem identification-

Define goals – Identification of goals as per the problem is done as the first step here. The ultimate objective was to study the fluid flow behaviour inside the BOF furnace and to predict the slopping time.

Identify domain – In this section, we identify the domain of our problem. In BOF modelling, different domains like inlet, outlet, wall or free surface are being identified.

3.4.2 Pre-processing

It is the initial stage of modelling. The geometry of the LD converter or BOF of basic oxygen steelmaking process is developed using design modular of the ANSYS 15 software. Then the model is meshed or discretized into smaller domain by mesh module. After completing the meshing, the model is simulated using the FLUENT solver in ANSYS 15. The different parameters used for the simulation are set according to fluid model,

material properties, boundary conditions, solving techniques, turbulence model, criterion etc.

A. There are three steps to be followed in pre-processing -
    a. Geometry drawing
    b. Meshing
    c. Solver and set up settings

3.4.3 Geometry Drawing

Geometry drawing is done in the design modular. A 2D model of the BOF of basic oxygen steelmaking process is drawn. The sketch and complete geometry with dimensions are shown in the figure3.2 and 3.3 given below and the complete geometry with the different named section sections are shown in the figure 3.3 below.

- **Dimension of the Object -**

The Dimension of BOF model is taken from Kundu and Pal, 2012.

The Dimensions are-

Table1: Characteristic parameters of industrial and model LD converter

Parameters	Physical LD converter	Model LD converter
Mouth diameter	3.5	3.5
Barrel diameter	8.4	8.4
Oxygen flow rate (Nm^3/min)	360-450	450
Lance hole diameter(m)	0.4	0.4
Tonnage(ton)	300	300

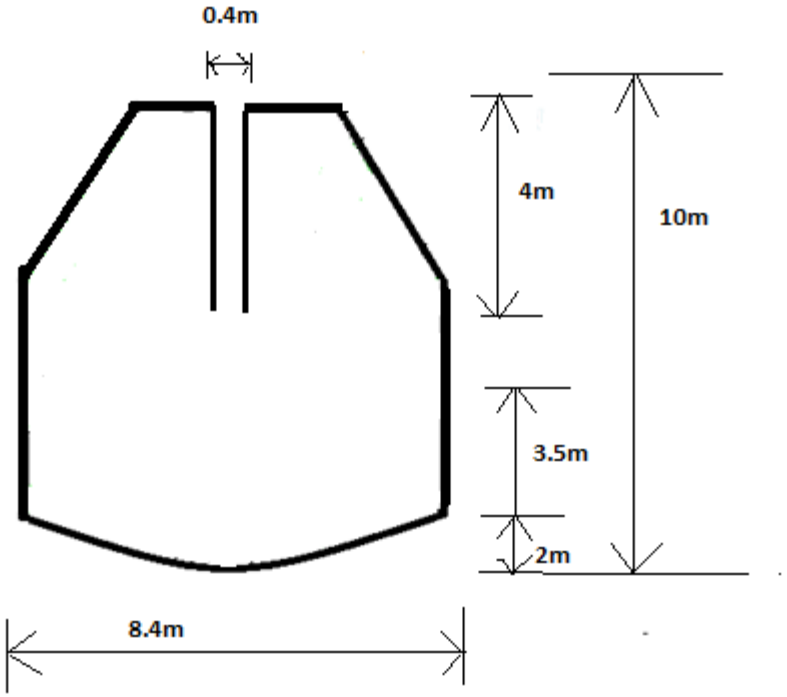


Fig7. Dimensions of 2D geometry

The 2-D geometry is prepared in the following way-

- ❖ WORKBENCH is used to prepare the Geometry
- ❖ In WORKBENCH select ‘X-Y’ Plane and click on ‘Look at’ to look at the plane
- ❖ Select Sketching in left hand side tree
- ❖ Select ‘DRAW’ and click on it and then choose ‘POLYLINE’ to draw the Rhombus in ‘X-Y’ Plane
- ❖ Select ‘CONSTRAINT’ from the tree in the left side and choose first ‘EQUAL DISTANCE’ then ‘EQUAL LENGTH’ and then click on the vertical line in the Rhombus.
- ❖ Select ‘DIMENSION’ from the tree under ‘SKETCHING’ and select ‘HORIZONTAL’, ‘VERTICAL’, ‘RADIUS’ to draw the dimension
- ❖ It can also be drawn by selecting ‘GENERAL’ under the ‘DIMENSION’.

- Dimension are shown in the bottom left part of the tree, click on particular dimension to change it.
- Click on ‘GENERATE’ to generate the sketch.
- Now for 2-D we have to make a ‘surface body’ from the sketch
- Go to the ‘CONCEPT’ in the top of the bar and select ‘surface from the sketches’ select the base plane by clicking the on the sketch and then generate.
- It will generate one surface body.

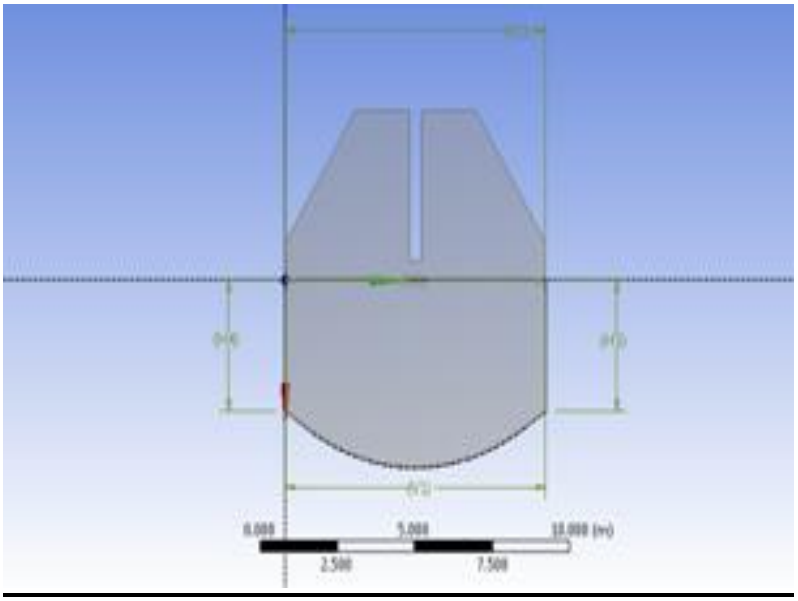


Fig 8: Surface body generated

3.4.4 GRID Formation (MESHING) –

- CFD uses numerical technique to solve equations, so it requires a Discretization of variables, for this we have to create meshing or grid.
- After preparing geometry go to meshing, right click on meshing and click edit or it can also be done by double clicking on meshing
- In meshing click on generate mesh option to create the default mesh and make it fine
- Create 'NAMED SECTION' for geometry
- In this, we have created 5 named section namely –
  - Velocity Inlet
  - Top part
  - wall
  - Bottom part
  - Outlet

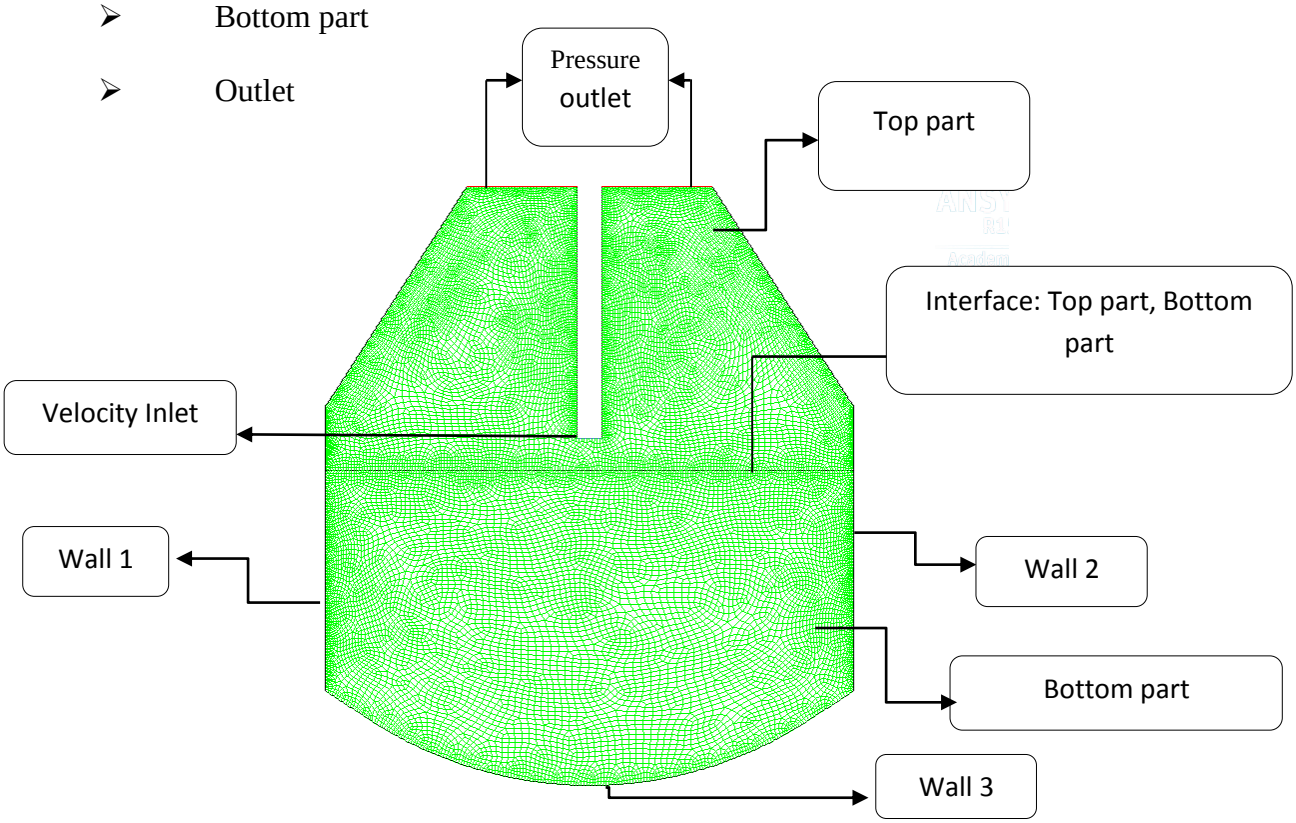


Fig 9. Meshing of 2D BOF model

Solution

Before starting the fluent solver we have to launch set up. In this we have set up double precision serial option. After that we have open the Solver i.e. FLUENT. In this we have to do the following things-

- First check the mesh and the report quality.
- Then display the mesh.
- Remember 'NOT TO SELECT THE SOLID INTERIOR PART' when running the 3- D case, which is created by default.
- Then select the modal, different for different cases and materials.
- For temperature calculation we have to turn on the energy equation.
- Provide Boundary conditions.
- Initialize the solution.
- We can also create surface monitors for plotting different graphs.
- Calculate the solution by providing number of iteration.

• The graph between pressures versus dynamic pressure is plotted in steady turbulent flow.

3.4.5 Solver setup and Solution

After the meshing is completed the model is imported to FLUENT software and firstly the mesh and mesh quality were checked and if the meshing is not good then error will be shown and simulation will not be access further.

The governing equation-

The governing equation of computational fluid dynamics (CFD) is known as Navier-Stokes equations. The Navier-Stokes equations consist of conservation of mass, momentum, energy, species etc. equations. The governing equations are following-

Conservation equation of mass

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho.V) = 0$$

Conservation equation of momentum

$$\frac{\partial \rho V}{\partial t} + \nabla.(\rho.VV) = -\nabla p + \nabla.\bar{\bar{\tau}} + \rho g$$

Turbulent model equation

The *k-ε* turbulent model is used for this experiment. Where *k* is the turbulent kinetic energy and *ε* is turbulent dissipation energy, the governing equation for this are-

The turbulent kinetic energy *k*, is given by-

$$\frac{\boldsymbol{\partial}}{\boldsymbol{\partial t}}(\boldsymbol{\rho}.\boldsymbol{k}) + \frac{\boldsymbol{\partial}}{\boldsymbol{\partial x_i}}(\boldsymbol{\rho k u_i}) = \frac{\boldsymbol{\partial}}{\boldsymbol{\partial x_j}}\left[\left(\boldsymbol{\mu} + \frac{\boldsymbol{\mu_t}}{\boldsymbol{\sigma_k}}\right)\frac{\boldsymbol{\partial k}}{\boldsymbol{\partial x_j}}\right] + \mathbf{P_k} + \mathbf{P_b} - \boldsymbol{\rho\varepsilon} - \mathbf{Y_M} + \mathbf{S_k}$$

Turbulent dissipation rate ε is given by

$$\frac{\partial}{\partial t}(\rho.\varepsilon)+\frac{\partial}{\partial x_i}(\rho\varepsilon u_i)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right]+C_{1\varepsilon}\frac{\epsilon}{k}(P_k+C_{3\varepsilon}P_b)-C_{2\varepsilon\rho}\frac{\epsilon^2}{k}+S_E$$

Production of K

P_k represent the generation or production of turbulent kinetic energy due to mean velocity gradient and calculated

$$P_k=-\rho u_i u_j C_\mu \frac{k^2}{\varepsilon}$$

$$P_k=\mu_t S^2$$

$$P_k=\sqrt{(2}S_{ij}S_{ij})$$

Modelling turbulent viscosity-

μ_t is the turbulent viscosity and calculated as

$$\mu_t=\rho C_\mu \frac{k^2}{\varepsilon}$$

The values of constant are

$$C_{1\varepsilon}=1.44$$
$$C_{2\varepsilon}=1.92$$
$$C_\mu=0.009$$
$$\sigma_k=1.0$$
$$\sigma_\varepsilon=1.3$$

For the two phase flow VOF model is used and the governing equation for that is –
The tracking of the interfaces between the phases is accomplished by the solution of a continuity equation for the volume fraction of one or more of the phases. For the q^{th} phase, the governing equation is

$$\frac{1}{\rho_q}[\frac{\partial}{\partial t}(\alpha_q\rho_q) + \nabla.(\alpha_q\rho_q\vec{v}_q) = S_{\alpha q} + \sum_{p=1}^{n}(\dot{m}_{pq} - \dot{m}_{qp})]$$

Where

$\dot{m}_{pq}$ Is the mass transfer from phase P to Q,

$\dot{m}_{qp}$ is the mass transfer from phase Q to P and

$S_{\alpha q}$ Is the source term

The equation will only be solved for more than one phase if only single phase is present then governing equation is

$$\sum_{q=1}^{n}\alpha_q = 1$$

3.5 Solution

After applying the boundary condition the different cases are run in both the steady and transient condition.

3.5.1 Residual Plot

The residual plots are used for judging convergence of the solution. Fig 10. shows the variations of residuals with respect to iterations.

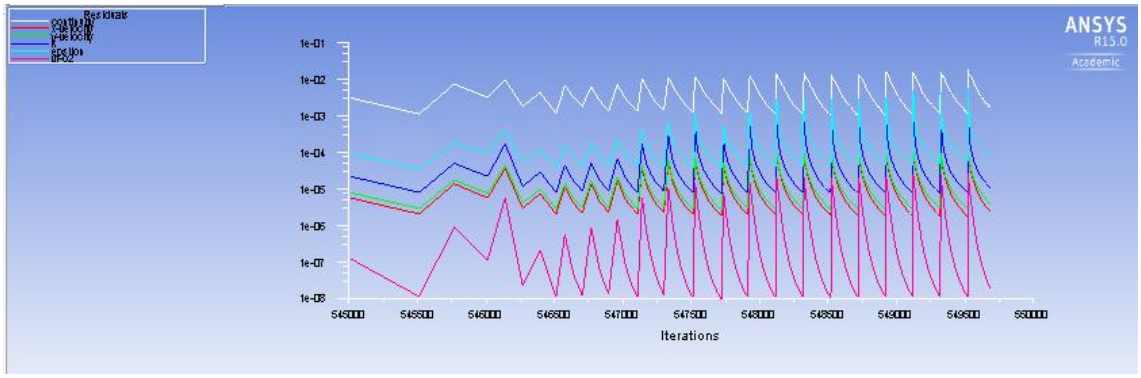


Fig10. Plot between residual and number of iterations.

The time step size used for iterations is 0.01 and the number of timesteps are 30000.

Smaller the time step size,more accurate the result would be.

3.6 Input Details of thermodynamic modelling

Basic oxygen steel making process is simulated through thermodynamic modelling and results of developed model are discussed here. Total blowing time taken for modelling is around 16 minutes with the time-step of 1 minute. Initial input parameters for case I are derived from Cicutti et al. (2000). The reason for taking data from the work of Cicutti et al. (2000) to check model performance is that they have reported the composition of slag and metal for different stages of blowing period to determine the evolved slag weight and composition with blowing time. Furthermore, they also calculated the foaming capacity of slags at the different blowing stages. Input for Other cases (i.e. Case 2, Case 3, Case 4) is taken from typical plant data.

		Case 1	Case 2	Case3	Case 4
HOT METAL	Mass in tons	170	150	155	150
	Carbon (wt. %)	4.48	5.02	4.16	5.01
	Manganese (wt. %)	0.56	0.3	0.4	0.4
	Silicon (wt. %)	0.65	0.59	0.8	0.6
	Sulphur (wt. %)	0.011	0.037	0.0035	0.0035
	Phosphorous (wt. %)	0.12	0.096	0.11	0.11
SCRAP	Mass in tons	30	20	15	20
	Carbon (wt. %)	0.11	0.11	0.11	0.11
	Manganese (wt. %)	0.36	0.36	0.36	0.36
	Silicon (wt. %)	0.021	0.021	0.021	0.021
	Sulphur (wt. %)	0.022	0.022	0.022	0.022
DOLOMITE	Mass(in tons)	2.8	4	2.8	2.8
	MgO	40.5	40.5	40.5	40.5
	CaO	58	58	58	58
	SiO_2	0.85	0.85	0.85	0.85
	Sulphur	0.022	0.25	0.25	0.25
LIME	Mass	7.4	9.5	7.4	7.4
	CaO	93.5	93.5	93.5	93.5
	SiO_2	6.5	6.5	6.5	6.5
	Sulphur	0	0	0	0
INITIAL TEMPERA-TURE		1623	1688	1606	1580
BLOWING TIME(minutes)		16	15.19	16	16
OXYGEN FLOW RATE (Nm3/min)		620	620	620	620
IRON ORE INPUT(tons)		1.9	1.9	1.9	1.9

Table 2.Input parameters

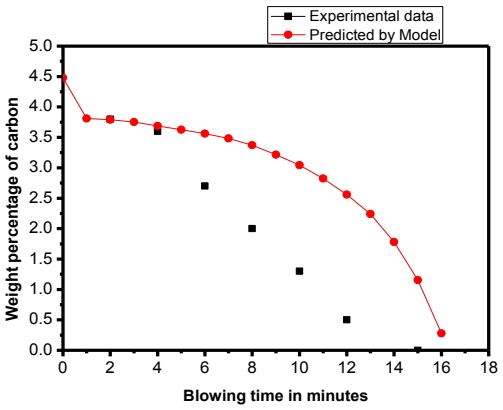
Chapter4: Results and discussion

The predicted variation of C, Si, Mn and P by this model and some available experimental results are shown in the following figures for different cases.

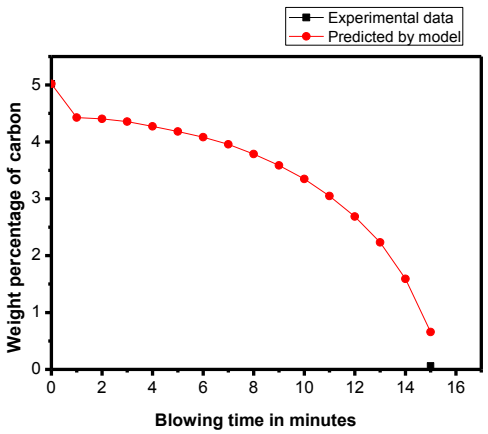
4.1 Plot of Decarburisation

Variation in carbon weight percent with time is given in Figure 4 for various cases. The final carbon content we obtained is around 0.2 to 0.3% for the first case which is close to the experimental data reported by Cicutti et al. Decarburisation process is simulated in two stages, first in oxygen driven model and second in slag driven model. In oxygen driven model, it is assumed that oxygen directly reacts with carbon in the bath to convert into CO and CO_2 (which escapes into the atmosphere) and secondly in the slag driven model, where FeO from slag reacts with carbon in bath to oxidise it. The final bath carbon weight percentage from the typical plant data is compared with the values predicted by our model in case 2 and 3. The final obtained results are in close agreement with our predicted values of the model. But the deviation in the obtained results may be due to assumption of constant oxygen efficiency which is generally not the case in real plant experiments.

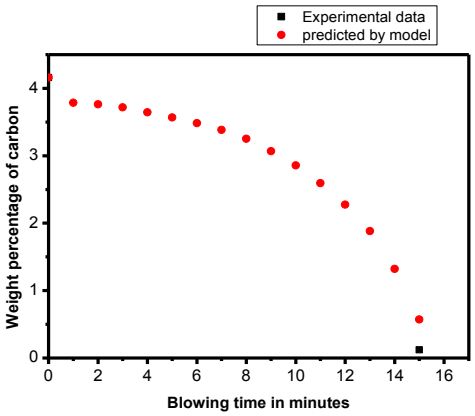
Case 1



Case 2



Case3



Case 4

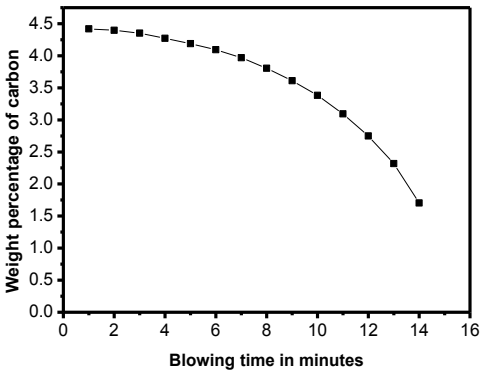


Table 3: Plots of decarburisations for different cases.

4.2 Plot for removal of silicon and manganese.

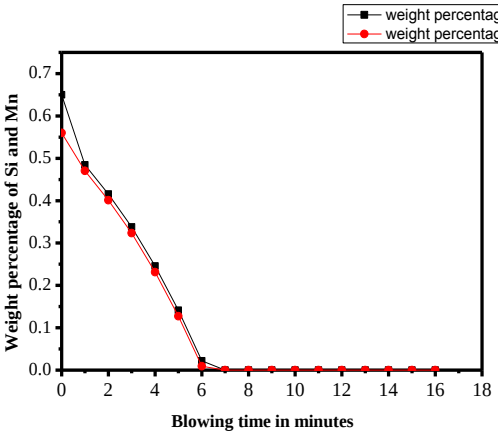
The removal of silicon takes place rapidly in first few minutes, but as temperature increases direct de-siliconisation decreases and indirect de-siliconisation takes place in the slag metal interface (Blanco and Diaz, 1993) . Fig 5 shows the variation of Si and Mn with the blowing time for different cases. It can be inferred from the curves, that de-siliconisation completes within 4-6 minutes of blowing period. According to Rao et.al.1996, silicon is removed as per two reactions in early phase of blow itself.

$$[Si] + 2[O] \rightarrow (SiO_2) \quad (16)$$

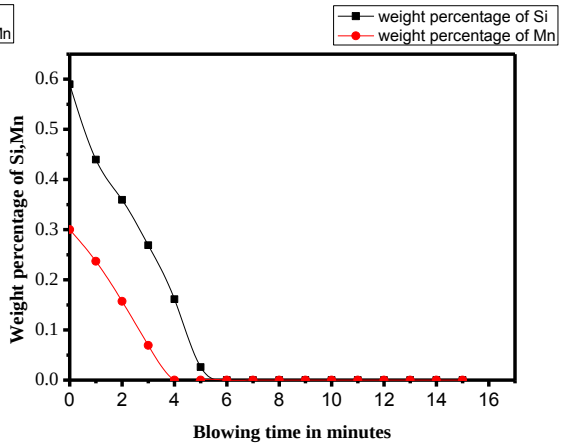
$$[Si] + (FeO) \rightarrow (SiO_2) + 2Fe \quad (17)$$

As per their assumption, Silicon is dropped till the bath silicon reaches an equilibrium level or till that time when the slag layer of specified thickness is formed. And after the formation of slag layer, generation of droplets starts which help in further oxidation of silicon (Rao et.al. 1996). As per the results of our model Si reacts with lime to form $CaO.SiO_2$ to form part of slag. As slag starts forming after the second minute, FeO from the slag reacts with Si to again form SiO_2.Our model has attempted to predict de-siliconisation also quite accurately, as de-siliconisation is modelled in three stages- oxygen driven, slag driven and droplet generation. Each part of model helps in refining of steel.

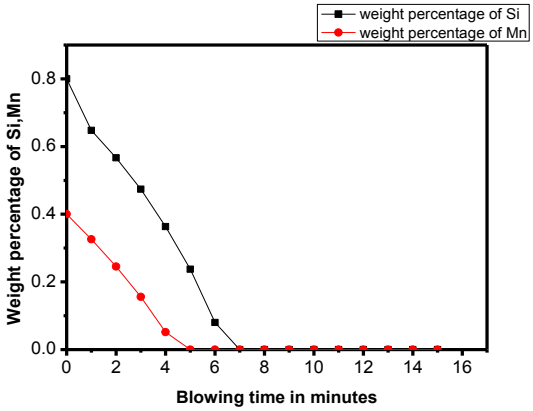
Case 1



Case 2



Case3



Case 4

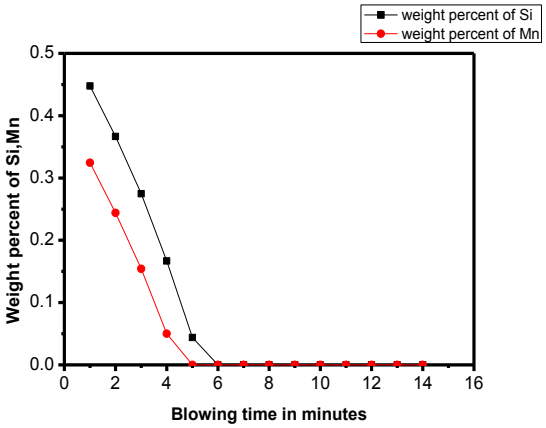


Table 4: Plots of removal of Si and Mn for different cases

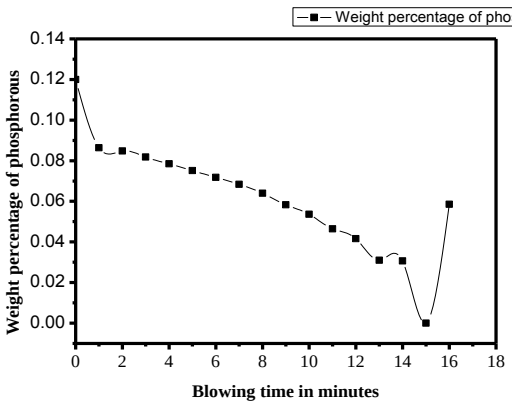
Removal of Mn is favoured by oxygen blowing rate and as per our model results, Mn gets completely removed within 7-8 minute of blowing period. The accuracy of results of Mn removal as derived from our model shows that the prediction of our three part model is quite reasonable. Mn is also removed in three stages- blown oxygen driven, slag driven and droplet generation. Each part of model helps in refining of steel. Sarkar et .al, 2015 have modelled the process dynamics by dividing the LD convertor into three separate continuous stirred tank reactors. Oxidation reactions are assumed to be primarily taking

place at the interface between the slag and the metal phases in the emulsion. And the mass transfer of FeO in the slag phase are assumed to be rate controlling. However they have not modelled the initial part of the blow before the formation of emulsion. The results of his work are in variance with our results as predicted by our model.

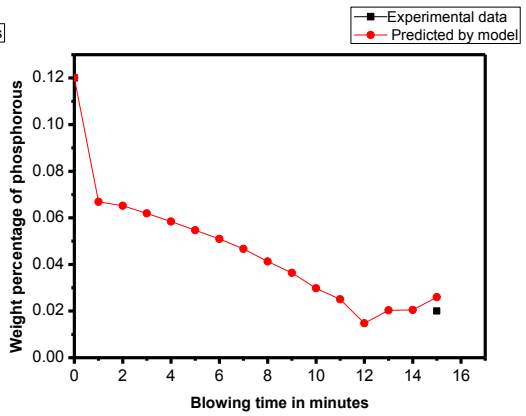
4.3 Plot for phosphorous removal

Ikeda et al. (1982) have studied the relationships among the metal oxidation, the decarburization and the dephosphorization in stainless and carbon steel refining. They have found out that for de-phosphorization of carbon steel refining with slag of optimum iron oxide content and refining at low temperature are favourable. Iso et al. (1987) have studied the possibility of blowing control based on exhaust gas data. They have found out that phosphorus and manganese contents of steel and the total iron content of slag at blow end can be controlled by controlling the O_2 level. And this can be used as an effective parameter to represent the progress of the reaction. (Iso et al.1987). But none of the models till date have not been able to model the phosphorous content of bath and the parameters on which phosphorous content in bath depends upon. Our model has attempted to give the exact parameters on which phosphorous content in the bath depends. Fig. 6 shows the variation of phosphorous with respect to blowing time. And for case 2 and case 3, a comparison has been showed with the end point results of a typical plant data. Phosphorous removal is favoured in low temperature .The reversion of phosphorous is captured in our model and shows how phosphorous reversion is strongly dependent on temperature as Gibbs free energy of phosphorous oxidation is function of temperature and gives positive value at high temperature.

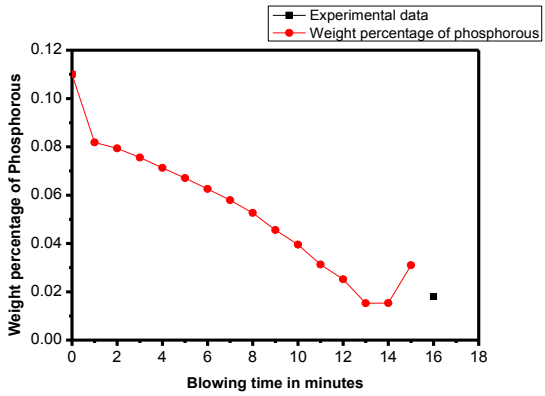
Case 1



Case 2



Case3



Case 4

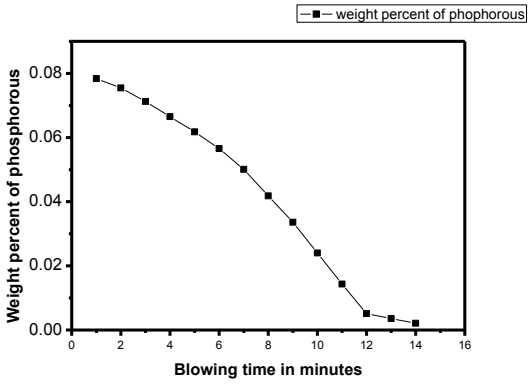
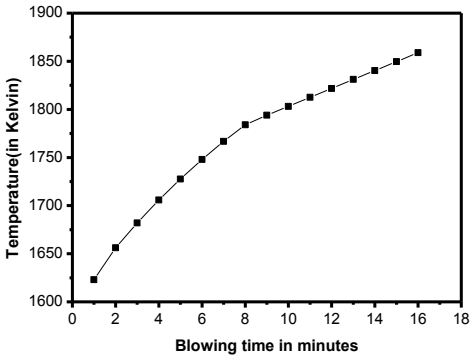


Table 5. Plots of dephosphorisation for different cases.

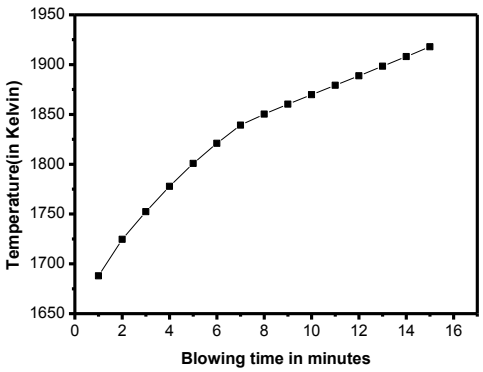
The bath temperature as predicted by the model is plotted against the blowing time in Fig 7 for different cases. The final temperatures as obtained by the model are 1576.638 ^{o}C, 1644.944 ^{o}C, 1594.101 ^{o}C, 1573.807 ^{o}C for the input values 1350 ^{o}C, 1415 ^{o}C, 1333 ^{o}C, and 1307 ^{o}C for the four different cases respectively. The dynamic models developed so far for predicting bath composition are based on a very crude and unrealistic assumption

like temperature to be linearly varying with time. The model presented here captures the varying temperature in the bath by considering it as a function of enthalpy and heat capacity. Each mole of reactant is taken into account for updation of temperature. As the bath temperature increases, variation in Gibbs free energy comes into play which changes the whole thermodynamics of bath process, by deciding the dominance of each reaction in the bath, giving insight about the weight of each element remaining in bath to predict bath composition.

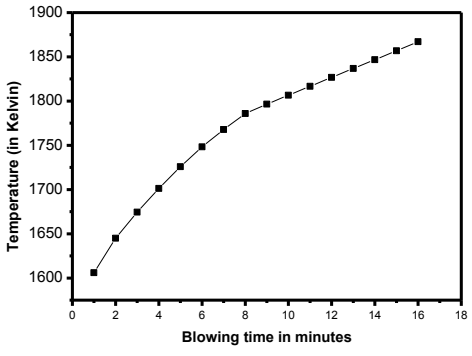
Case 1



Case 2



Case 3



Case 4

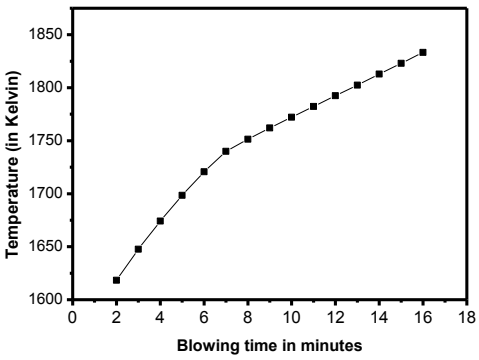


Table.6. Variation of bath temperature with respect to blowing time

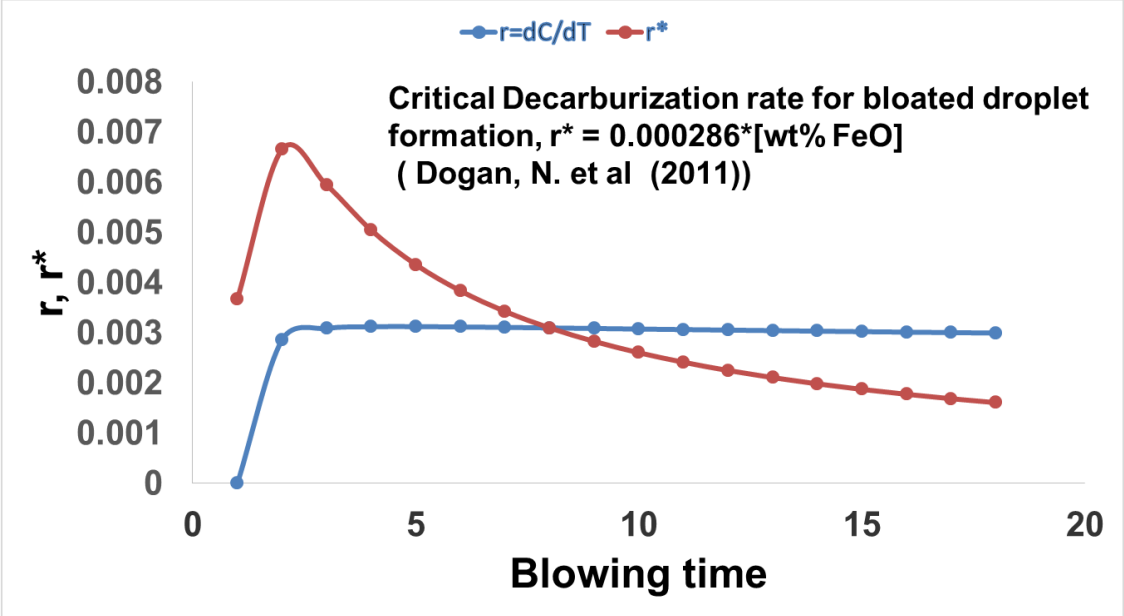


Figure 11: Variation of decarburisation rate and critical decarburisation rate with blowing time

Dogan et al. (2011) have used the equation for threshold decarburization rate (given by Molloseau and Fruehan, 2002) to give the residence time of their "ballistic motion model" to predict the residence time of their bloated droplets.

r_c * = 2.86*10^- 4 × (mass% FeO)

As the decarburisation rate crosses the threshold decarburisation limit bloating of droplets starts. The literal meaning of bloat is to make or become swollen. Bloating is the starting point before the slag foaminess starts. This gives the prediction of slopping time. It takes about 8 min for the droplet to bloat. As the metal droplets bloat, its interfacial surface area increases which in turn increases the reaction kinetics of the bath. This in turn increase the decarburisation rate .therefore bloating basically synergises the decarburisation rate, leading to more of bloating and subsequently the foaminess of the slag. After 8 minutes, it just takes 24 sec more for the slopping to start and this result is also confirmed by the CFD results.

4.4 Results from CFD analysis

After providing boundary condition and initializing the solution we run the different turbulent cases.

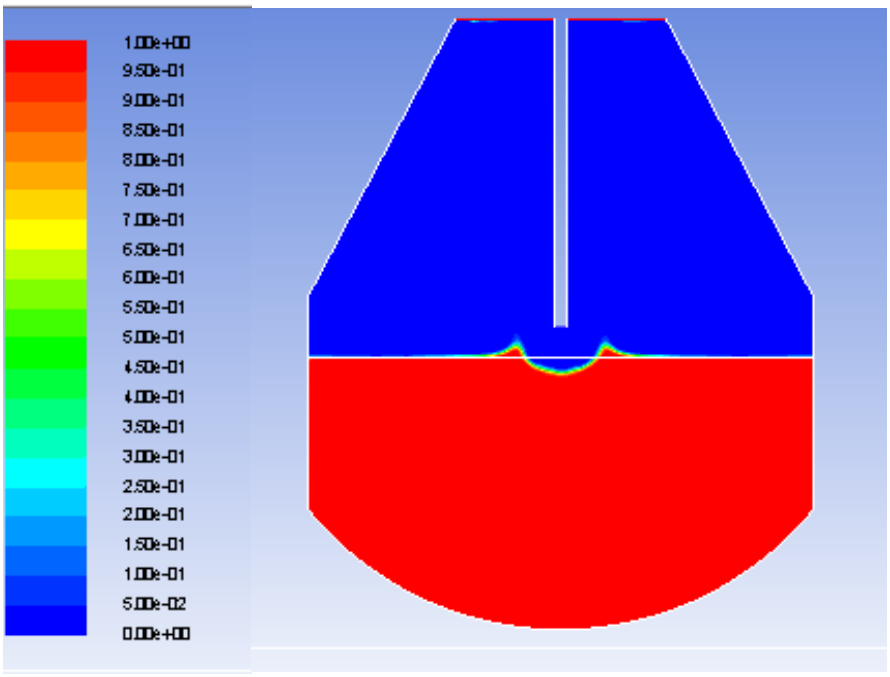


Fig 12. Contours of volume fraction of metal slag mixture (80% hot metal and 20 % slag) After 1.1 s

Contours of volume fraction of slag mixture consisting of 80% hot metal and 20% slag after 1.1 sec are shown in Fig.12.Here the variation of volume fraction is shown with difference in colour. Blue colour represents zero volume fraction of hot metal, or in simple terms it the absence of hot metal or presence of air in the converter. After 1.1 sec, a slight dimpling effect can be seen on the hot metal surface as a result of high speed oxygen jet purged on the bath surface by the purged .this figure represents the bath surface and fluid flow behaviour after 1.1 sec of blowing time.

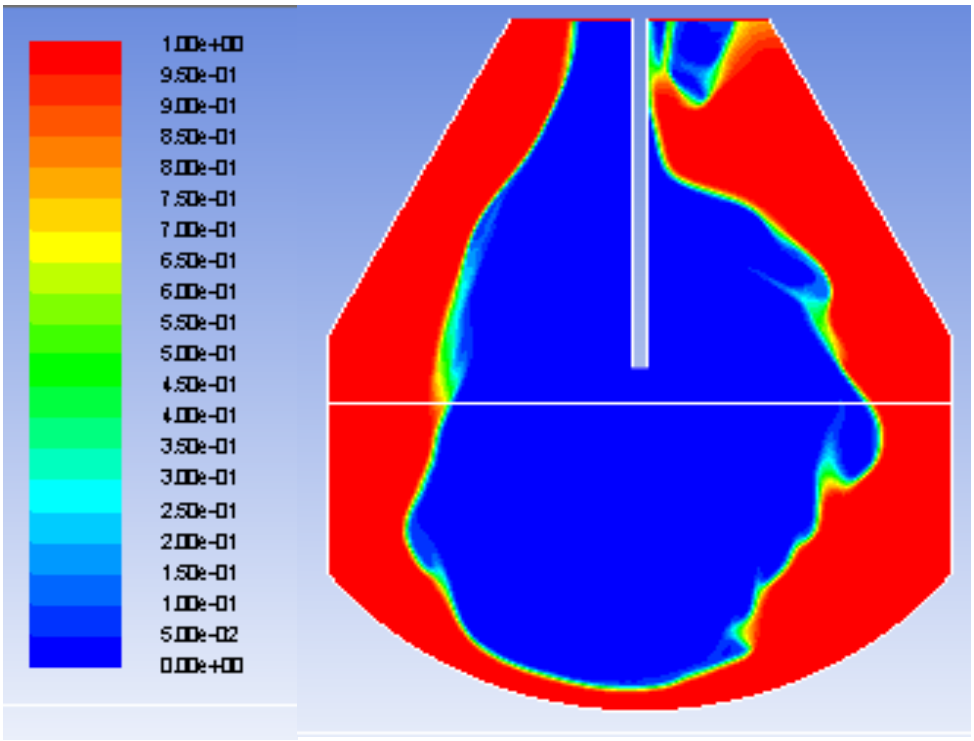


Fig13.Contours of volume fraction of metal slag mixture (80% hot metal and 20 % slag) after 24 sec

Figure 13. shows the contours of volume fraction of metal slag mixture after 24 sec. The phenomena of slopping can be seen here. After 24 sec hot metal starts escaping out of the converter. The turbulence created by oxygen jet has replaced the space of hot metal by oxygen. Around 8 min 24 sec, slag becomes foamy enough to show the slopping phenomena.

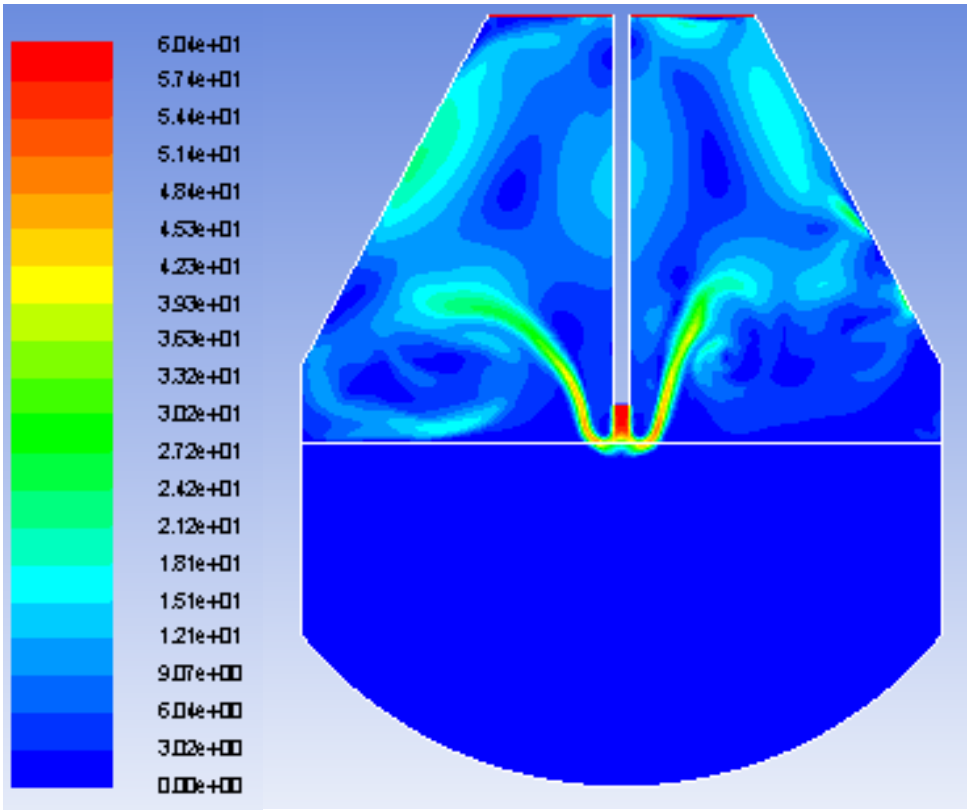


Fig 14.Contours of velocity magnitude after 1.1 sec

Fig 14 show the contours of velocity magnitude after 1.1 sec. the colour variation shown the variation of min to maximum values of velocity. The velocity is maximum at the outlet of lance and gets distributed as the oxygen jet reaches the bath surface and splashes with the hot metal. This figure represents the variation of velocity in the LD converter after 1.1 sec of blowing time.

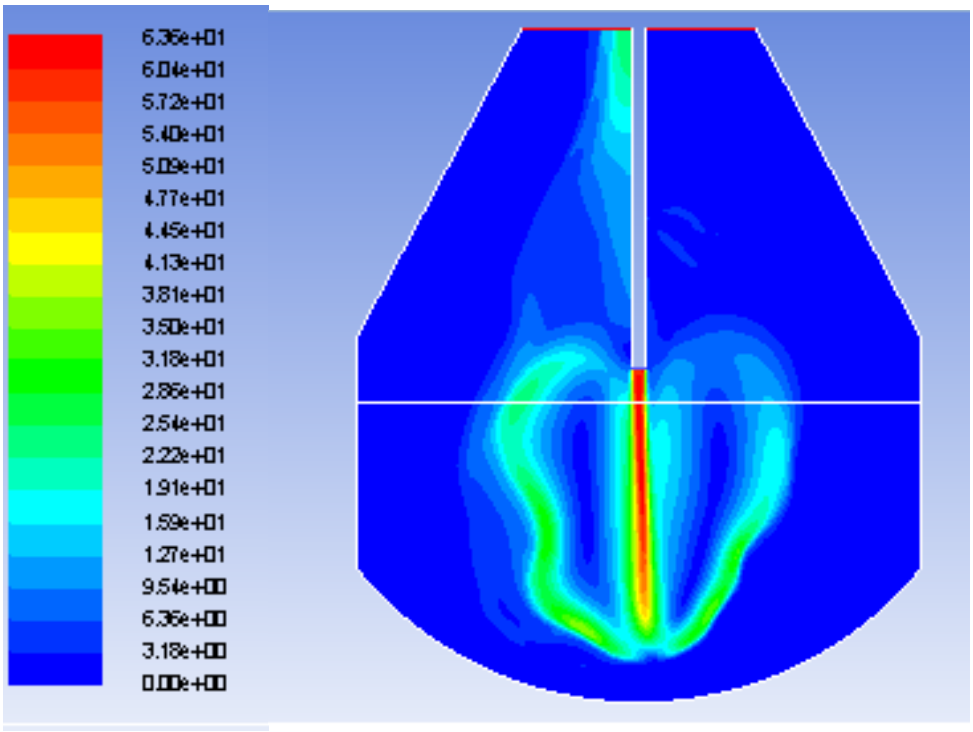


Fig 15.Contours of velocity magnitude after 24 sec

Figure 15 represents after 24 sec. One important point to be noted here is that the distribution of velocity is not uniform on both the sides of the lance we have taken vibration of lance into account by taking differential gradient of mesh in both the sides of the lance.

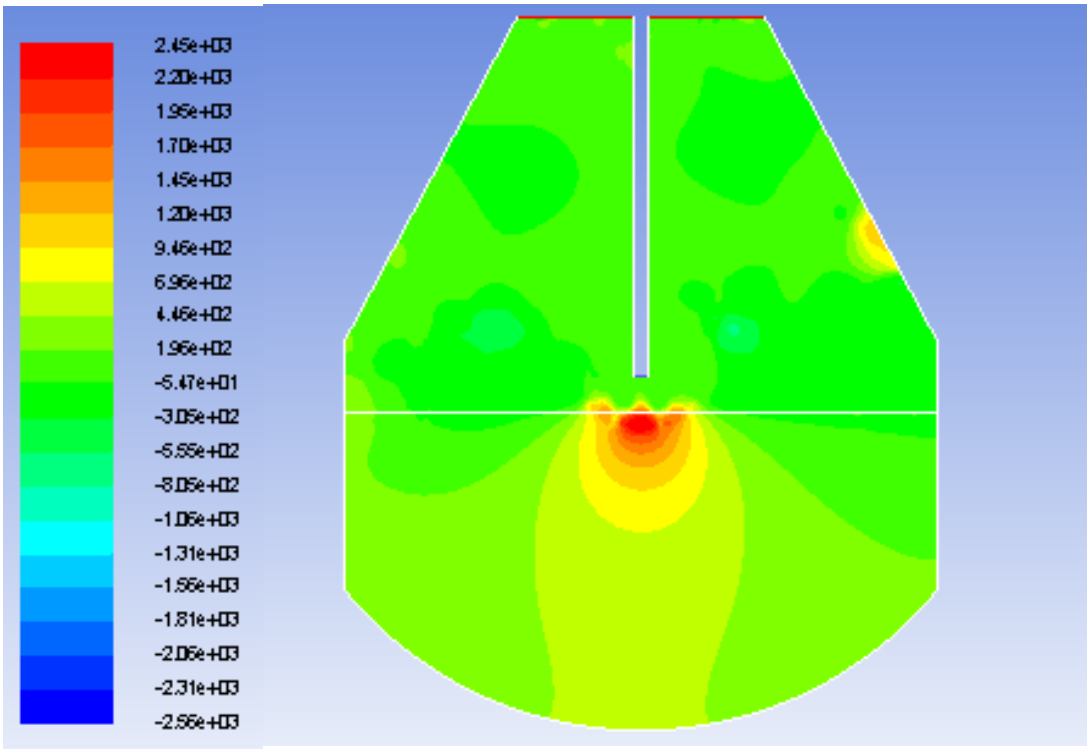


Fig 16.Contours of dynamic pressure after 1.1 sec

Figure 16 shows the variation of dynamic pressure in the LD converter after 1.1sec of the blow time. There is increase in dynamic pressure just below the lance due to hitting of oxygen jet with the bath surface. There is a visible increase in dynamic pressure at the side of the wall of the converter on the right side due to presence of tap hole on the right hand side of converter.

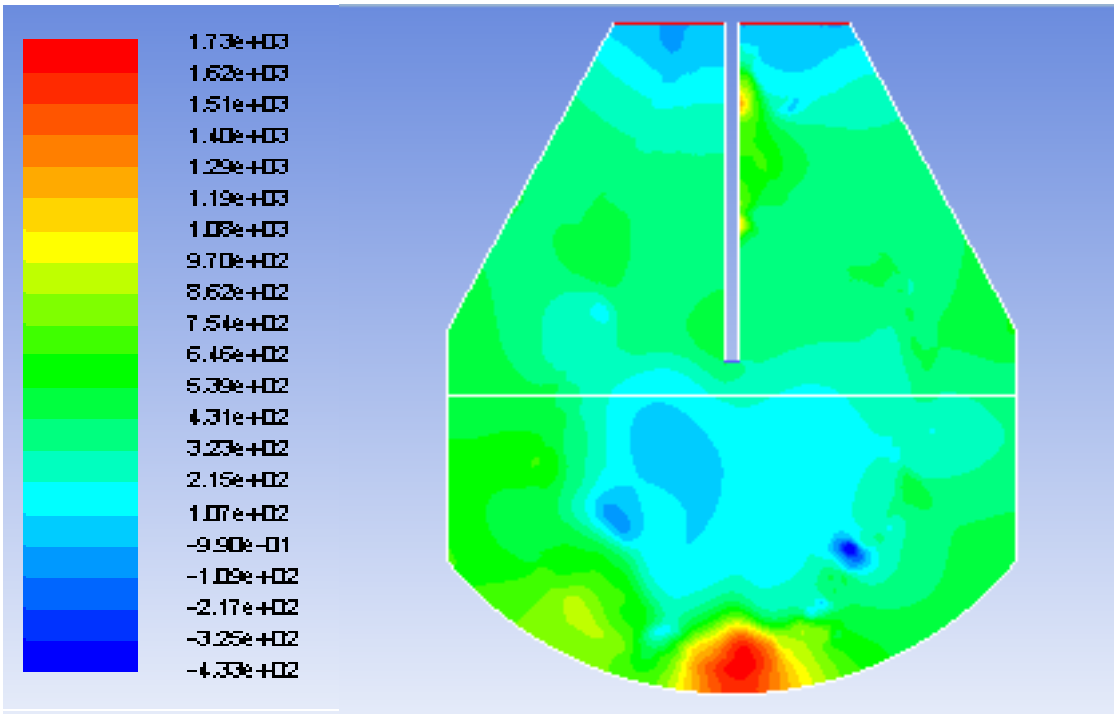


Fig 17.Contours of dynamic pressure after 24 sec

Fig 17 shows the variation of dynamic pressure after 24 sec in the LD converter. It is visible in the figure that the dynamic pressure is highest on the bottom surface of the LD converter. And it is a general trend that while making the LD converter refractory lining is made thicker on the bottom side as the highest amount of erosion is occurs there. This fact is also validated by our results of dynamic pressure after 24 seconds.

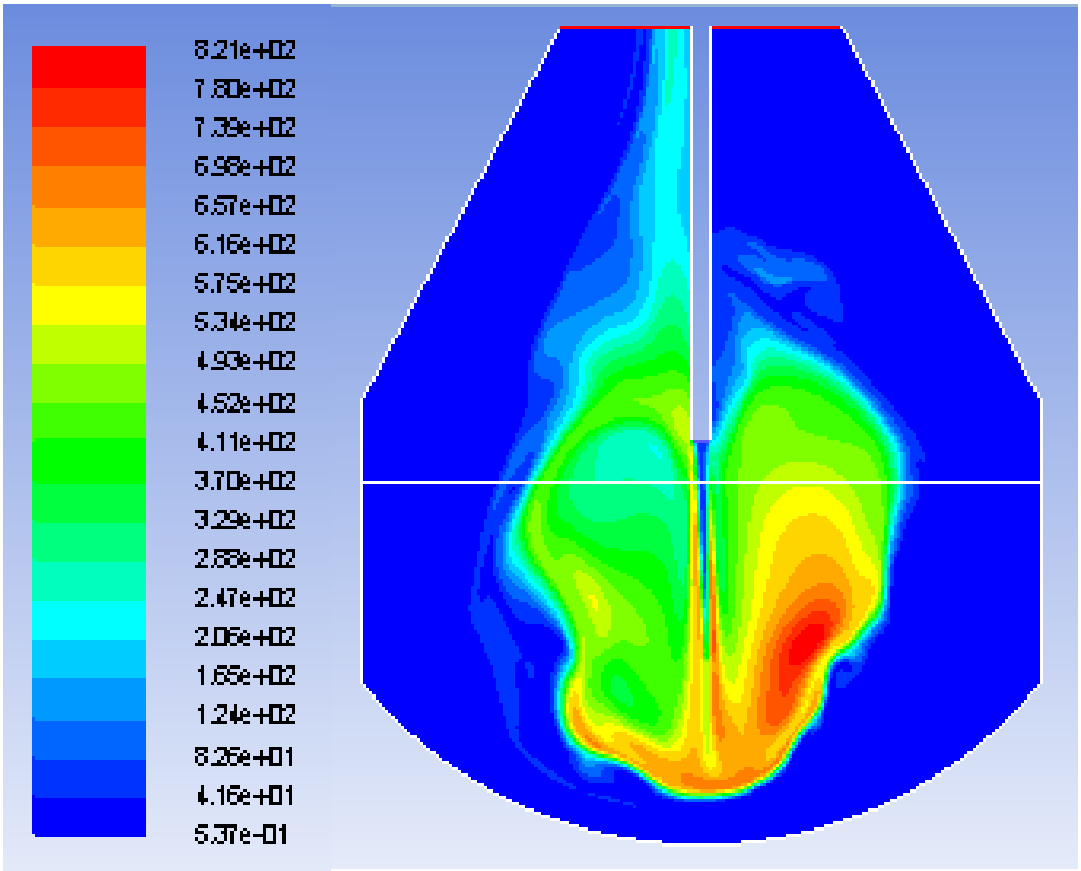


Fig 18.Contours of turbulent intensity after 24 sec

Figure 18. shows the variation of turbulent intensity with the blowing time after 24 second in the LD converter. Turbulent intensity is highest in the middle of the bath containing hot metal and slag.

Chapter 5: Conclusion

A dynamic process model for basic oxygen steel making process has been developed based on thermodynamic criteria of feasibility and extent of occurrence of possible reactions of basic oxygen furnace. The prediction of bath composition and temperature for every minute of blowing duration is objective of this work. Variation of temperature with the blowing time is modeled by considering it a function of enthalpy and heat capacity. Prediction of slopping initiation time for particular blowing condition based on correlation with model predicted decarburization rate and critical decarburization rate for bloating of metal droplet is found to be good agreement with plant data. Based on calculated decarburization rate prediction of slopping starting time is around 8 min 24 sec for the specific conditions and used input data. Temperature based modeling of de-phosphorisation process is attempted with some success as phosphorous reversion phenomenon is captured by our model. The predicted results of this model are observed in good agreement with experimental results. This work can be extended to obtain insights about the process happening inside the bath as it gives sequence of removal of impurities and the possible parameters on which removal of impurities depends upon like oxygen flow rate, initial temperature of the bath ,Gibbs free energy ,droplet generation, iron ore, flux quantity. In addition to that, the developed model can be coupled with computational fluid dynamic simulation for predicting slopping or spitting phenomenon of basic oxygen furnace.

Chapter 6: Future Scope

Our model gives the details of hot metal composition for every minute. If this detail is coupled with the bath viscosity and other fluid flow parameters at all the position inside basic oxygen steel making furnace, we can generate another model which will give better understanding of bath kinetics and the process. This work can be extended to a sequel development of different esoteric and effective models, which will ultimately contribute in achieving a quantum jump for automation of steel industry.

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