Fifth International Conference on CFD in the Process Industries
CSIRO, Melbourne, Australia
13-15 December 2006

COMPUTATIONAL FLUID DYNAMICS SIMULATION OF PYROMETALLURGICAL PROCESSES

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ABSTRACT

High temperature processing of raw materials in metals production and recycling often involves complex multi-phase fluid flow and heterogeneous chemical reactions at various scales. A good understanding of the process physics and chemistry is crucial for process operation and process development. Computational fluid dynamics (CFD) has become a very useful simulation tool to improve process understanding and development. At the same time industrial processes challenge the CFD development in many aspects with its complex transport phenomena in large-scale reactors with locally small-scale physics and chemistry. The current paper discusses the applications of CFD to a number of high temperature metallurgical and materials processing applications. The focus is on the special efforts for the development and implementations of sub-models with process-dependent characteristics: melting of aluminium scrap, an ironmaking blast furnace hearth, a submerged arc furnace for phosphorus production, waste combustion in a rotary kiln, and heat treatment furnaces.

INTRODUCTION

Metallurgical processes involve the extraction of metals from different types of ores or from a variety of metal scrap, e.g. from iron ore to hot metal, from hot metal to steel; from copper concentrates to pure copper; from aluminium scrap to pure aluminium or its alloys, to name a few. The processes involve various types of materials flow in solids, liquids, gases, and their mixtures, from one part of the equipment to another, and from one equipment to another. Metallurgical processes are normally complicated due to its multi-phase, high temperature, and highly reactive nature. The complex phenomena of flow, heat and mass transport play very important roles in reaction kinetics and overall reactor performance.

CFD has been found useful in studying various metallurgical processes, and various aspects of a specific process. It can be used for (1) insight understanding of an existing process, (2) modification and optimization of the operation and design in an existing process, and (3) new process development. CFD modelling of the fluid flow in metals processing such as gas-stirring in ladle metallurgy and continuous casting of steel is the most widely studied unit operations in process metallurgy. Gas and particle flow and heat transfer as well as chemical reactions are more recently modeled with CFD for various smelting processes, such as copper and nickel flash smelting, blast furnace ironmaking HIsmelt and Sirosmelt for iron and non-ferrous smelting, Hall-Héroult Cell for aluminium production, cyclone smelting, etc. The use of CFD has also been found in cleaning and energy recovery of metallurgical off-gases such as cyclones and waste-heat boilers. In hydrometallurgical processes, CFD codes have been used to model stirring tanks for mineral leaching, thickeners for liquid-residual separation, and tank-houses for electro-refining.

On the other hand, the metallurgical processes are challenging various aspects of CFD modelling. A lot of phenomena have not yet been properly described or incorporated into the general CFD framework. For example, magneto-hydrodynamics (MHD) finds a lot of applications in metallurgical and materials processing operations, and accurate representation of reactive particulate flows. However, many new developments are taking place in CFD world, and two interesting examples worthwhile mentioning are the coupling of fluid – solid structure interactions and combination of CFD with DEM (Discrete Element Method) for multi-phase particulate flows.

Many comprehensive books and review articles are available for the application of CFD in process metallurgy (Review articles: Schwarz, 1991, 1994, 1996, 2001; Mukhopadhyay et al. 2004; Johansen, 1996; Szekely, 1989, 1990, 1991, 1994; Evans, 1997; Guthrie, 1991. Monographs in transport phenomena in metallurgical and materials processing: Szekely and Themelis, 1971; Szekely, 1979, Szekely, Evans and Brimacobe, 1989; Themelis, 1995). Several international symposia dedicated to computational modelling in particular use of CFD in minerals, metals and materials processing industries have been organized. Examples are the series of international conferences focusing on CFD application in process industries organized by CSIRO since 1997 (Schwarz et al., 1997, 1999; Witt and Schwarz 2003; Johansen and Page, 2005). Other examples include the symposia organized by TMS: Fluid Flow phenomena in Metals Processing (El-Kaddah et al., 1999), Computational Modelling of Materials, Minerals and Metals Processing (Cross et al., 2001), and Multiphase Phenomena and CFD Modelling and Simulation in Materials Processes (Nastac and Li, 2004).

At Delft University of Technology (TU Delft) in the Netherlands, various research and education activities have been conducted for metallurgical processes since late 1990s.

Firstly, introduction and use of CFD in metallurgical process simulation has been an integrated part of education in MSc. program for the students of raw materials technology, and a number of case studies have been conducted by the students in the course of transport phenomena in metallurgical processes. Secondly, use of CFD in the research projects both at MSc. study and PhD study has been practiced in a broad area of materials processing and metallurgical processes. The projects include typical pyrometallurgical processes (ironmaking blast furnace, and submerged arc furnace), metals recycling (aluminium scrap melting and refining) and thermal waste processing, as well as heat treatment furnaces. This paper will give an overview on the various examples of using CFD in high temperature raw materials processing.

MELTING OF ALUMINIUM SCRAP

Melting and refining of aluminium scraps are often made in rotary furnaces in Europe. In the rotary furnace, the feed is a complex combination of various aluminium scrap with different sizes, shapes and contaminations. Efficient melting of the scrap in the molten phase is a critical issue in the secondary aluminium industry. This example illustrates the coupling of fuel combustion model with a user developed melting model of metallic scrap by using a commercial CFD code CFX 5.

To study the scrap melting behaviour, a furnace model has been developed based on a CFD framework, and coupled with user developed aluminium melting sub-model (Zhou, 2005; Zhou et al., 2006). The furnace model consists of a gas region with turbulent flow and combustion as well as radiative heat transfer in the upper part of the furnace, and a solid – liquid region of salt and aluminium metal in the lower part of the furnace. The aluminium melting model was developed for a single particle and multi-sized particle groups in the molten salt and aluminium melt based on the experimental study and heat transfer theory in a population balance approach. In the melting model, salt shell formation on the metal solids and its re-melting, and subsequent solid aluminium melting were included.

For the CFD framework, the standard k-ε model was applied in most of the current simulations. The full buoyancy model was selected for the gas phase, and Eddy Dissipation Model (EDM) was used for the combustion of the natural gas with oxygen. For the scrap melting process, heat transfer from the gas zone through the gas – scrap interface is the key for the scrap melting process and radiation plays a dominant role. Several radiation models including P-1, Discrete Transfer Method (DTM) and Monte Carlo Model (MCM) were tested and their effect on melting was studied. DTM has been chosen in most of the simulations in this research because of its reasonable accuracy, robustness and less computing time.

To represent the distributed nature of the feed, aluminium scrap were classified into several groups depending on the size of the scrap, and the melting sub-model was subsequently modified from a single aluminium particle to the multi-particle system. Aluminium melting behaviour was calculated with the exchange of information between the melting sub-model and the CFD combustion space. Heat sink due to scrap melting was calculated and fed back to the CFD combustion space model. Gas flow and temperature distribution in the top combustion space of CFD model were used to calculate the scrap melting rate in the sub-model.
Figure 1 shows the simulated changing history of particle size distribution for an initial Weibull size distribution. It indicates that melting takes place appreciably after between 4200 and 4800 seconds, and it also proves that the complete melting time will be at least 3.5 hours (12600 seconds) in this case. Figure 2 illustrates the energy distribution of the scrap melting process. It is obvious that the fuel efficiency (energy used directly for scrap heating and melting) accounts for 50 – 60%, the energy lost to the off-gas is as high as 40%, and the wall heat loss is about 5%.

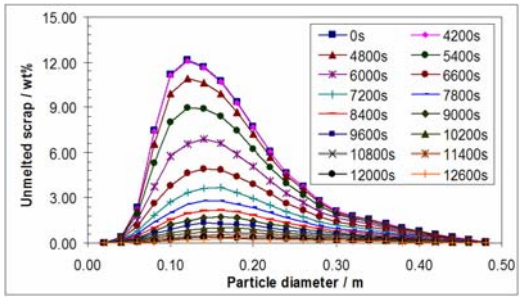


Figure 1: Simulated changing history of the Weibull size distribution of the feed.

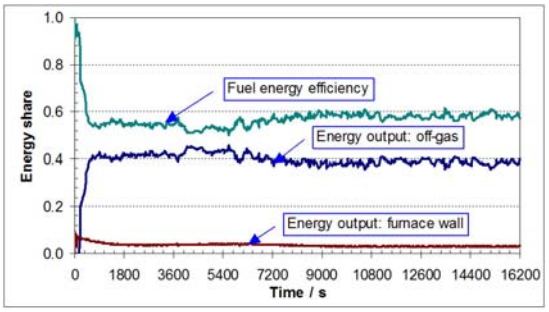


Figure 2: Overall energy flows through inlet, outlet and furnace walls.

In practice, the salt ratio in the feed is a critical factor in processing of the aluminium scrap. A lower salt ratio in the feed is favoured to increase the furnace productivity, to lower the processing cost (e.g. salt slag with impurities must be processed and re-used), the material cost (e.g. salt flux including additives such as cryolite) and the energy cost (natural gas and oxygen) as is confirmed in this study, as well as to reduce the environmental impact. The effects on heat transfer due to the insulation of the salt shell formed on the scrap particle and the insulation of the top salt layer have been found significant, and this also suggests a lower salt to scrap ratio.

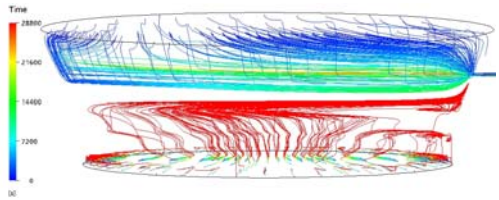
HOT METAL FLOW THROUGH THE COKE-BED OF A BLAST FURNACE HEARTH

In the ironmaking blast furnace, the metallic iron is produced from the reduction of iron ores with coke. The packed coke bed in the lower part of the blast furnace, namely the hearth, dissolves slowly in a pool of liquid iron that is tapped regularly. The coke particles in the hearth exhibit a size distribution in time and space, and thus lead to non-uniform porosity distribution in the hearth. This

causes the flow of molten metal through the coke-bed to be irregular and non-uniform, bringing about channeling in the coke bed and detrimental effect on the refractory lining life of the hearth.

The current example illustrates the use of CFD in simulating heterogeneous and slowly dissolving packed bed of coke particles. To include the changing properties of the packed bed, a special porosity model is developed based on population balance modeling to track the local changes in size distribution and bed porosity during dissolution of coke particles. The CFD flow model established with a general-purpose code CFX 5 (now ANSYS-CFX) is coupled with the porosity model, and incorporates both the buoyancy force from density difference caused by temperature difference and by carbon concentration difference of the liquid iron (Post et al., 2003, 2005).

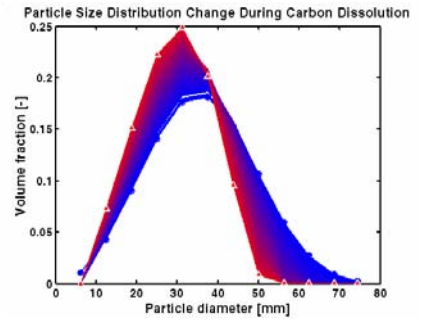
Figure 3 shows the predicted flow pattern and carbon dissolution through the population balance model coupled with the flow model. Figure 4 shows the porosity changes in the coke-bed for two different particle size distributions. Experiments with packed beds made up of dissolving spheres, have been setup to evaluate the bed porosity, and to develop a dissolution model. Distributed coke properties determine the distribution of local bed porosity, the flow behaviour of hot metal and liquid slag, the dissolution behaviour of coke particles and refractory erosion both because of local flow behaviour. The bed porosity model, dissolution model and CFD model enabled different initial coke size distributions, the use of more inert versus more reactive coke types, and the use of a mix of different coke types to be predicted. All scenarios result in specific hot metal flow behaviour in the hearth, which results in different hearth wall refractory erosion behaviour.



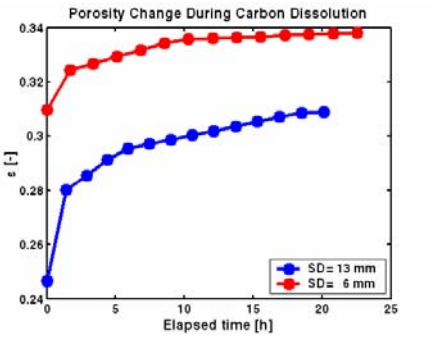
(a) timeline distribution

(b) carbon concentration

Figure 3: CFD predictions of molten iron flow and carbon dissolution in the blast furnace hearth.



(a). Change in particle size distribution: blue circle (o): starting PSD, red triangle (Δ): ending PSD).



(b) Change in coke bed porosity (ε): two different particle sizes

Figure 4: Change in particle size distribution and coke bed porosity (ε) during dissolution to the hot metal.

PHOSPHORUS PRODUCTION IN A SUBMERGED ARC FURNACE

Elemental phosphorus is usually produced with a submerged arc furnace (SAF). The reduction rate, phosphorus recovery and energy consumption are the primary concerns for the economic production of phosphorus. The complex transport phenomena within the SAF involve the phosphorus and CO gas flow, heat transfer among phases and gas – solid reduction reactions in a slowly descending packed bed. Ore mineralogy, flux and coke properties, mixing conditions, bed strength and porosity are important parameters in the performance of the furnace. A process model based on CFD (Fluent 6.1) and reaction kinetics has been developed to describe product gas generation and flow as well as energy distribution inside the furnace (Adema, 2005; Scheepers et al., 2006). Empirical modelling based on large sets of industrial data is currently developed with the use of multiple regression analysis techniques utilized in linear analysis and in non-linear modeling.

The porous media model with Ergun's equation is used to calculate the resistance to gas flow through the packed bed. The heating and melting of the solid in the bed while moving down the furnace is modelled with a user defined sub-model. The sub-model defines an energy sink dependent on the specific heat (C_p), bed velocity and temperature gradient. The P-1 radiation model in combination with an effective thermal conductivity developed in this study is used to simulate radiative heat transfer in the packed bed of the furnace. Turbulence in the gas flow was simulated with standard k-ε model. Heat

source of 3 sub-volumes under the 3 electrodes are used to represent the electric arcs. Electric and arc heating have not been simulated in this study.

In this study, defining the mass source in the gas phase is a challenge. In the furnace, the only mass source in the gas phase arises from the product of the gas – solid reduction reaction of the phosphate minerals, which takes place within the whole volume of the packed bed (mainly in the high temperature zone in the lower part of the furnace). This cannot be defined as fixed mass source at inlet boundaries. Definition of gas phase heat source is accomplished through a user defined scalar to represent P_2O_5 concentration (kg/m^3) moving down with the burden flux velocity. The decrease of the scalar was calculated using a temperature dependent reaction rate from the high temperature experiments. The P_2O_5 decrease rate ($kg/m^3 \cdot s$) is used to calculate the gaseous product generation and the reaction energy sink.

Figure 5 illustrates the simulated temperature distribution in the furnace. In the arc zones beneath the 3 electrodes, a maximum temperature of 3800 K was calculated (the dark zone below the electrode above 2200 K). Figure 6 shows the calculated concentration change of P_2O_5 in the feed due to reduction reaction. It can be seen that the P_2O_5 concentration drops quickly in the middle of the packed bed, and the volume between upper red zone (no reaction yet) and the lower blue zone (completely reduced) denotes the reaction zone.

Validation of temperature distribution within the furnace

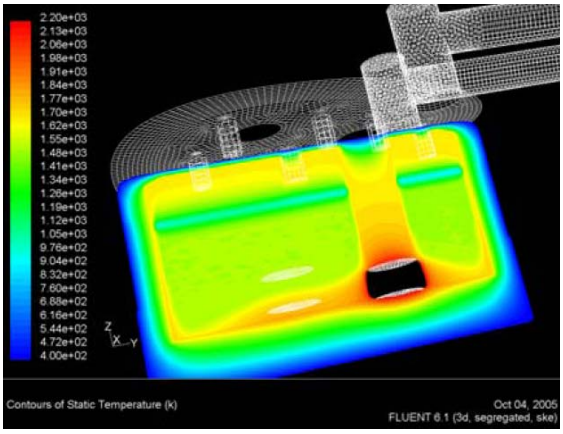


Figure 5: Predicted temperature distribution across one

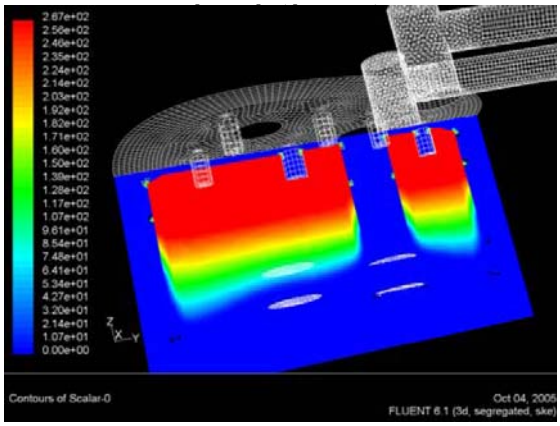


Figure 6: Predicted the distribution of P_2O_5 concentration (user-defined scalar) as it is consumed by the reaction.

refractory lining was conducted according to the embedded thermocouple measurements, and reasonable agreement has been reached at least for the lining zone (Scheepers et al., 2006). Further model development and fine tuning of model parameters are on the way. Different type of phosphate ores are under investigation for the kinetic parameters, which will be tested in the developed CFD model for the overall reduction behavior in the furnace, namely the P_2O_5 loss to the slag and specific energy consumption.

HAZARDOUS WASTE COMBUSTION

Processing of hazardous waste in a rotary kiln incinerator is a complex process. Since hazardous waste has often very complicated chemical compositions and physical forms, the transport phenomena within the incinerator are not well understood, and the incineration process expects large uncertainties in process chemistry and is difficult for emission control. For better understanding of the incineration process, various transport phenomena taking place in the rotary kiln will be discussed and analyzed in this case. To get more quantitative understanding, process simulation was conducted by using CFD to characterize gas flow and mixing, temperature and species distribution caused by waste combustion in the incinerator (Yang et al., 2003, 2005). To include all the waste streams in a single CFD model is difficult task, and how to define the different waste streams with different calorific values and chemical compositions is a challenge to the CFD modeling.

In this study, hazardous waste in various forms is firstly converted to a hydrocarbon-based virtual fuel mixture based on an overall mass and energy balance. Afterwards two gas streams of fuel-rich and fuel-lean were defined according to the requirement of the CFD program. By various proportion of fuel-rich and fuel lean streams, all waste inlet streams (waste and air) can be defined for the right heating value and chemical compositions. The combustion of the simplified waste fuels was then simulated with CFD combustion models. Figure 7 shows the concept of the artificial fuel definition step. Through this step, the poorly defined hazardous waste with various forms, chemical composition

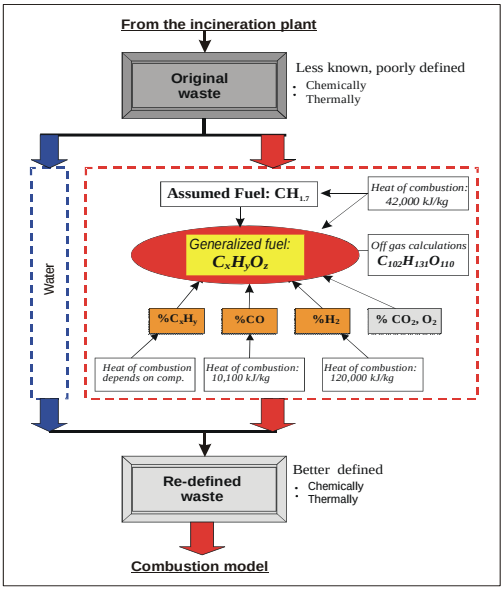


Figure 7: Concept of artificial fuel definition for the hazardous waste incineration plant.

and heating values are modeled as well defined virtual fuel mixed with combustion air and other inert gases (water vapor, carbon dioxide and nitrogen).

The simulation of the subsequent fuel combustion process was carried out with Phoenics 3.5. In the simulation, only the gas phase behavior is considered, and the waste gasification and vaporization were assumed to take place rapidly upon entering the kiln. Standard k-ε model was used for modeling gas turbulence. The 7-gas combustion model was used for gas-phase combustion and heat transfer. With the 7-gas combustion model, the overall thermal behavior could be estimated, and the species distribution could be predicted as well, such as fuel (C_3H_4-based in this model), oxidant (O_2), intermediate and final combustion products (CO, H_2, CO_2, H_2O), and the inert component of nitrogen (N_2).

The distribution of temperature and chemical species is broadly investigated under various operating conditions. The predicted temperature distribution has been validated with the available measurement data from an operating rotary kiln waste incinerator, and reasonable agreement between the predicted and measured data has been reached, as is illustrated in Figure 8.

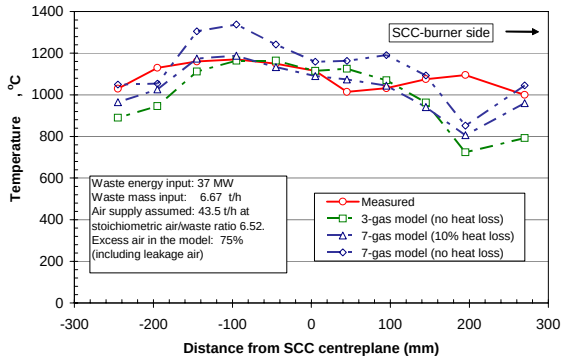


Figure 8: Temperature profile crossing view-ports of the rotary kiln incinerator.

HEAT TREATMENT FURNACES

Simulation of a Continuous Steel Reheat Furnace

Steel reheat furnaces are used to treat the steel slabs in hot rolling mill. The temperature distribution and homogeneity inside the slabs are critical for the hot rolling process. To predict temperature distribution, the gas flow and heat transfer were simulated with the CFD package Phoenics 3.2, using low-Reynolds-number turbulence models in combination with higher-order convection schemes and a radiation model (Yang et al., 2004). The transient heating of slabs is simulated with a moving slab technique, which allows the individual slabs to be heated up while moving along the furnace. The individual slab movement and its temperature evolution can be tracked (Langrangian frame of reference), and the temperature distribution for all the slabs passing through the furnace can be monitored as well (Eulerian frame of reference). The simulation confirmed that both temperature profiles (Langrangian and Eulerian frames of reference) coincide in the pseudo-steady state operation.

Simulation of a Mobile Heat Treatment Furnace

In the following example, a mobile heat treatment furnace was simulated by using CFD to investigate thermal performance of the furnace and the heating process of the metal pieces (Yang et al., 2005). The furnace is used to heat treat dredging pumps and impellers to obtain the required microstructure and mechanical properties through stress relief, annealing, hardening and tempering. Since the temperature evolution inside the metal piece cannot be tracked in practice, CFD simulation provides a useful tool to predict the temperature evolution within the metal during the heat treatment. The current CFD model (Phoenics 3.5) consists of turbulent combustion, thermal radiation, and conjugate heat transfer. Temperature measurement was carried out to provide thermal boundary conditions and calibrate model parameters. An overall energy balance indicted a relatively low energy efficiency of the furnace (about 20-25% on average over the whole heat treatment period). To improve the energy efficiency design changes were made with the model. Reducing the amount of excess air will save a lot of energy and the cost in production. Heating of the furnace by means of radiation plates proved to be an interesting alternative.

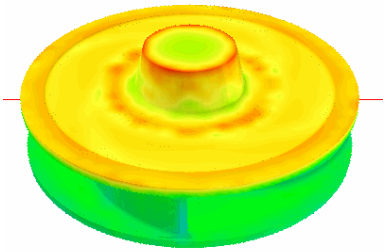


Figure 9: Predicted temperature distribution on the surface of the impeller at the end of heat treatment operation (970 – 1050°C).

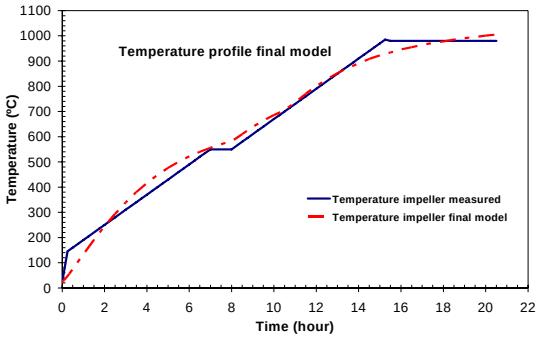


Figure 10: Comparison of the impeller surface temperature profile: measurements vs. CFD prediction.

Figure 9 shows the predicted temperature distribution on the surface of the impeller at the end of heating operation. Figure 10 shows the predicted temperature profile in comparison with the preset temperature profile for process control according to the temperature profile measured on the surface of the impeller. To simulate different stages of the heat treatment operation, the global combustion model was applied in different time period with varying fuel supply and excess air fractions. After fine tuning the

various combustion parameters, the heating curve of the metal can be very well simulated (see Figure 10).

CONCLUDING REMARKS

High temperature processing of raw materials, in particular pyrometallurgical processes to extract and refine metals from primary resources – ores and secondary resources – metals scrap, involve complex multi-phase flow of materials (solids, liquids and gases) and energy, and are complicated by the simultaneous chemical reactions and transport of species. In order to better understand the process insights and to improve the process performance, CFD has proved to be a very convenient and useful tool in the simulation of the complex and coupled transport phenomena in industrial-scale reactors. The CFD framework can incorporate most chemical and physical phenomena simultaneously taking place together with the transport of momentum, energy and chemical species, as have been illustrated in the simulation examples in the paper.

It is believed that along with the rapid increase in the computing power and significant development of multi-physics models, complicated industrial processes involved with flow and transport of mass, momentum, energy, and chemical species in multi-phase and high temperature reactive systems could be simulated more accurately and CFD will become a very powerful engineering and design tool.

ACKNOWLEDGMENTS

The authors are grateful for the various funding organizations in the Netherlands for the research projects described in this paper: E.E.T. (Economy, Ecology and Technology) program, Senter-Novem, Corus Group plc, Thermphos International B.V. and AVR.

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