

1D COMBINED FLOW AND THERMODYNAMIC MODELLING OF A LEAD BLAST FURNACE

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ABSTRACT

A lead blast furnace is a complex metallurgical reactor. With mathematical modelling, using information from laboratory scale experiments, operational data and information obtained from physical modelling, the contribution of heat and mass transfer, thermodynamics and kinetics can be combined in one single package that allows to evaluate the effect of the different key contributors to the process.

In this paper, a combined 1D flow, thermodynamic and kinetics model for a lead blast furnace is presented. The stack, where the temperature is too low to consider equilibration, is described using 1D flow and kinetics models. The bosh and the hearth, where equilibrium is more readily attained, are modelled using the thermodynamic programming library ChemApp®.

The model is tested for a simplified blast furnace charge. Future developments are discussed.

NOMENCLATURE

\tilde{G}	[kg.s ⁻¹]	mass flow rate [kg/s]
S	[kg.s ⁻¹]	source term
c	[J.kg ⁻¹ .K ⁻¹]	heat capacity
T	[K]	temperature
h_{ij}	[W.m ⁻²]	heat transfer coefficient between phase i and j
A_{ij}	[m ²]	heat transfer surface between phase i and j
f_{ij}	[]	fraction of the reaction heat of reaction j absorbed by/withdrawn from phase i
Q	[W]	reaction heat
a_i	[]	fraction reacted according to reaction i
$E_{a,i}$	[J]	activation energy of reaction i
R	[J.mol ⁻¹ .K ⁻¹]	universal gas constant
p_i	[]	relative partial pressure of component i
P_i	[]	relative equilibrium saturation pressure of component i
k_1	[m.s ⁻¹]	reaction rate constant for reaction 1
k_2	[]	reaction rate constant for reaction 2
k_3	[]	reaction rate constant for reaction 3
t	[s]	reaction time
d	[m]	diameter of reacting grain
ΔG_r^0	[J.mol ⁻¹]	standard Gibbs free energy of reaction
K	[]	equilibrium constant of reaction
α	[]	relaxation parameter
[]		solid state
{ }		liquid state
()		gas state

INTRODUCTION

The blast furnace is a counter-current reactor. Solid materials, consisting of sinter and coke, are fed at the top of the furnace. Blast air is injected at the bottom of the furnace. The oxygen in the blast air reacts with the coke in the solid charge to form mainly CO-gas and heat. The heat is used to smelt the charge. The liquid oxides are reduced by the coke in the hearth (direct reduction). The CO-gas ascends in the furnace and reduces part of the oxides in the solid charge in a solid-gas reaction (indirect reduction).

MODEL DESCRIPTION

Overview

The blast furnace can be divided in three parts as shown in Figure 1: the stack, the bosh and the hearth (Hussain and Morris (1989)). In the stack, the upper part of the furnace, temperatures are not believed to be high enough for thermodynamic equilibrium to be reached. In this part of the furnace reaction rates are calculated using experimental rate equations. In the bosh and the hearth of the furnace, temperatures can reach 1200°C and more. Here the assumption of thermodynamic equilibrium is reasonable.

Three phases are considered: a gas phase, a liquid phase and a solid phase. For each phase a temperature and mass flow rate profile is calculated. Within each phase different constituting components are considered.

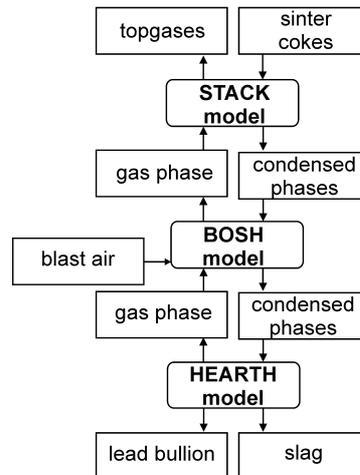


Figure 1: Schematic diagram of the parts of the model

Grid and boundary conditions

The model is one-dimensional. The furnace is divided into cells as presented in Figure 2. The arrows in Figure 2 indicate the location of the tuyeres through which the blast air is injected.

Since the solid charge is fed through the top of the furnace, the boundary conditions for the flow and the heat transfer equations for the condensed phases and components are set at the top. For the gas phase, two boundary conditions are set: (1) there is no gas flow through the bottom of the furnace, and (2) there is an ingoing gas flow of blast air through the bottom of the cell indicated by the arrows in Figure 2.

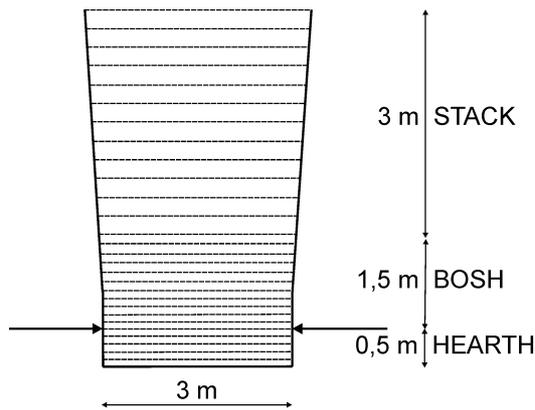


Figure 2: Division of the blast furnace into computational cells

Flow calculations

The mass flow rates of the different phases and of the components of each phase are calculated by solving the continuity equation, integrated using the finite volume technique:

$$\vec{G}_{in} + S = \vec{G}_{out} \quad (1)$$

This equation can be solved for each phase and for each phase constituent. For the flow of the condensed components a boundary condition is imposed at the top of the furnace. For the gas flow a boundary condition is imposed in the cell where the blast air enters the system, and a zero flow boundary condition is imposed at the bottom of the hearth.

Heat transfer calculations

Three phases are considered in the model, each with its own temperature field. In the shaft, these temperatures are calculated by solving the energy equation for each phase in each cell:

$$\left(\vec{G}_k c_k T_k\right)_{out} - \left(\vec{G}_k c_k T_k\right)_{in} = \sum_{\substack{j=1 \\ j \neq k}}^3 h_{kj} A_{kj} (T_j - T_k) + \sum_i f_{ki} Q_i \quad (2)$$

The necessary heat capacity data is obtained from FactSage©. For the heat transfer coefficients and heat

exchanging surfaces, correlations can be found in Incropera and DeWitt (2002), Niu et al. (1996) and Mackey and Warner (1972).

The temperatures of the phases in the bosh and the hearth result from the reaction calculations and will be discussed in that section.

Calculation of chemical reactions

The calculation method of the chemical reactions occurring in the furnace is specific for each of the three parts of the furnace. In the stack, experimental reaction rate relations are used (e.g. Habashi (1980)). However in a first stage the model is tested using dummy values for the rate constants.

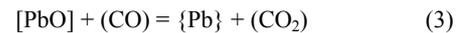
In the bosh and the hearth, thermodynamic equilibrium is calculated.

Reactions in the stack

Since the charge is simplified, only a restricted number of reactions are considered.

Indirect reduction of lead oxide with CO

The CO-gas formed in the bosh and the hearth ascends through the furnace and partially reduces the solid lead oxide in the stack according to the following reaction:

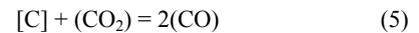


For this reaction a shrinking core reaction rate relation is used to calculate the amount of PbO reduced in each cell of the stack:

$$1 - (1 - a_1)^{1/3} = \frac{\exp\left(-\frac{E_{a,1}}{RT}\right) p_{\text{CO}} k_1 t}{d} \quad (4)$$

Boudouard reaction

The coke in the charge can react with the ascending CO₂ to form CO according to the so-called 'solution loss' reaction:



The empirical relation used to calculate the amount that reacts or forms is:

$$a_2 = k_2 \left(\frac{p_{\text{CO}_2} - p_{\text{CO}}^2}{K} \right) \exp\left(-\frac{E_{a,2}}{RT}\right) \quad (6)$$

where

$$K = \frac{p_{\text{CO}}^2}{p_{\text{CO}_2}} = \exp\left(-\frac{\Delta G^0}{RT}\right) \quad (7)$$

and

$$\Delta G_r^0 = 40,887 - 41.801T \quad (8)$$

Condensation of lead vapour

The lead vapour which is formed in the bosh can condense in the colder stack:

$$(Pb) = \{Pb\} \quad (9)$$

The experimental reaction rate relation is:

$$a_3 = k_3(p_{Pb} - P_{Pb}) \quad (10)$$

Reactions in the bosh

This part of the furnace is assumed to be in thermodynamic equilibrium. In each cell the equilibrium amounts and temperature are calculated from the incoming condensed components from the top and the incoming gas components from the bottom, as shown in Figure 3. The results of the calculation are the amounts of the components at equilibrium and the equilibrium temperature. These calculations are performed with the programming library ChemApp®.

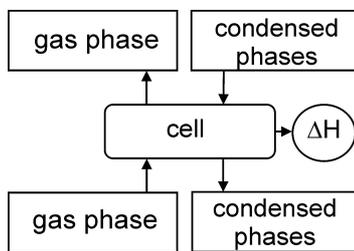


Figure 3: Schematic of the calculation principle in the bosh and the hearth

The source terms needed for the flow calculation are determined for each component as the difference between the stream out of the cell and the stream into the cell of that component.

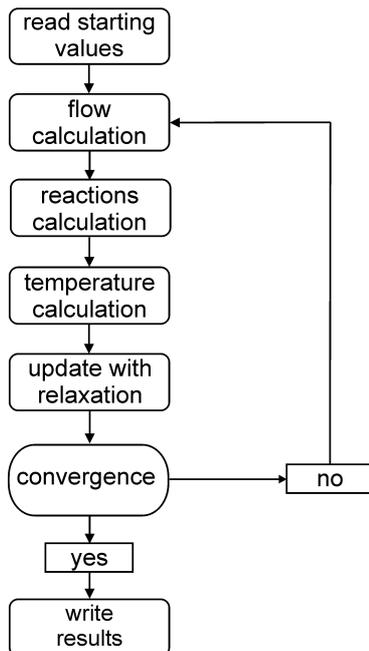


Figure 4: Numerical calculation scheme

Reactions in the hearth

The hearth is the part of the furnace below the tuyeres. It is assumed that no blast air enters this part. So the input into this region is a stream of condensed components. It is however possible that some gases form in this region due to reaction between the remaining coke and the oxides in the slag phase. So a stream of gases out of the hearth is accounted for in the model.

Numerical implementation

To assure numerical stability a relaxation mechanism has been implemented. The new values of quantities such as mass flow rates or temperatures calculated in each iteration step are not used as such as input values for the next step. Only a fraction of this new solution is added to the corresponding fraction of the old solution:

$$X_{new} = (1 - \alpha)X_{old} + \alpha X_{newcalculated}$$

The sequence of calculation is summarised in Figure 4.

RESULTS

Testing conditions

In this first stage of the research the model is tested for a simplified blast furnace charge. The ratio blast air to solid charge and the ratio coke to sinter are taken from Cowperthwaite et al. (1980). The heat losses are estimated to obtain a realistic tapping temperature. It is not possible to use the heat losses of a real furnace because of the limited charge. Therefore the losses are varied to target the experimental tapping temperature of 1200°C.

Grid

The furnace is divided into the three submodels as indicated in Figure 2. The stack is divided into 15 cells, the bosh into 10 cells and the hearth into 5 cells.

Charge

The charge consists of solid PbO and C. The blast air contains N₂ and O₂. The mass rates are indicated in Tables 1 and 2.

Table 1: Composition of sinter (T = 156°C)

sinter	mass flow rate (kg/s)
PbO	3.85
C	0.61

Table 2: Composition of blast air (T = 40°C)

blast air	mass flow rate (kg/s)
N ₂	1.83
O ₂	0.58

Temperature profile

The temperature profile calculated with the model using the stated testing conditions is depicted in Figure 5. For

the interpretation of this figure and the following figures it is important to bear in mind that condensed components flow from top to bottom of the furnace, while gases flow in the opposite direction.

The blast air enters the furnace at a height of 4.5 m below the stock line. The oxygen in the blast air reacts with the coke in the charge to form mainly CO. This is an exothermic reaction, so a peak value of the temperature, as indicated in Figure 5, can be expected. The gas ascends in the furnace, hereby heating the solid charge that is descending through the furnace. Therefore the gas temperature drops from bottom to top and the temperature of the condensed phases increases from top to bottom.

Once the condensed phases have passed the tuyeres some heat is lost to the water-cooled hearth walls and the temperature decreases to a tapping temperature of about 1200°C.

The transition from the stack model to the bosh model is in this calculation quite sharp because of the change in reaction rate calculations. Further work is needed to correct this.

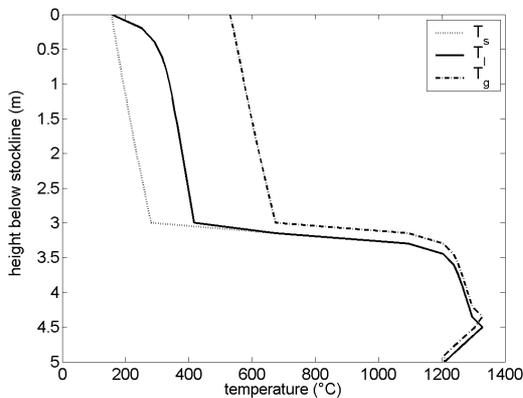


Figure 5: Temperature profiles of the different phases

Pb balance

In Figure 6 the mass flow rate of the lead containing components is presented. Lead oxide enters the furnace through the top. In the stack the PbO reacts with the ascending CO to form Pb and CO₂. In the bosh the remaining solid PbO is reduced to liquid lead and lead vapour. This vapour ascends and condenses in the higher regions of the furnace. This mechanism of lead evaporation and condensation is believed to be an important factor in the heat balancing of the furnace. This mechanism is visible in Figure 6. Not all of the PbO is reduced to liquid Pb. Some of the PbO melts and is tapped at the bottom as slag.

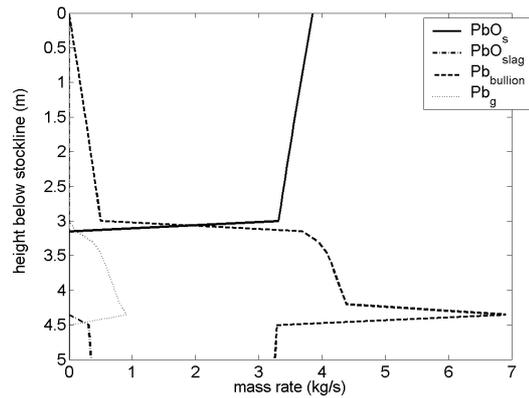


Figure 6: Mass flow rate profiles of the lead containing components

C-balance

In Figure 7 the mass flow rate profiles of the carbon containing components is presented. Carbon is charged as coke at the top of the furnace. In the shaft this carbon reacts with CO₂ to form CO through the Boudouard reaction. In the bosh most of the lead oxide is reduced, partially through direct reduction with the coke, which explains the drop of the mass flow rate of coke, and partially through indirect reduction with CO, which explains the drop in CO flow rate and the rise in CO₂ flow rate. At tuyere level, the remainder of the coke reacts with the oxygen in the blast air to form CO and CO₂.

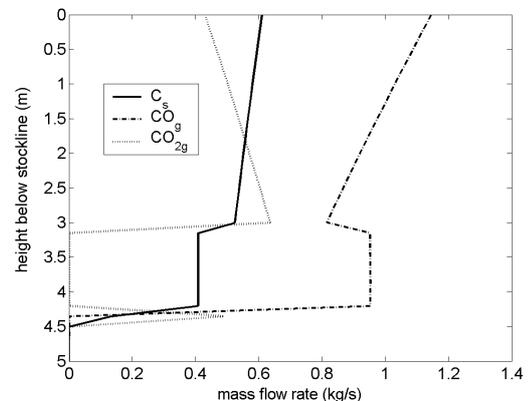


Figure 7: Mass flow rate profiles of the carbon containing components

Variation of coke to sinter ratio

In this calculation the amount of coke charged into the furnace is varied. The effect on the flow rate of bullion and slag at the bottom of the furnace is depicted in Figure 8. As can be expected, the amount of lead lost to the slag decreases as the amount of coke charged into the furnace increases. The conditions in the bosh are more reducing in that case.

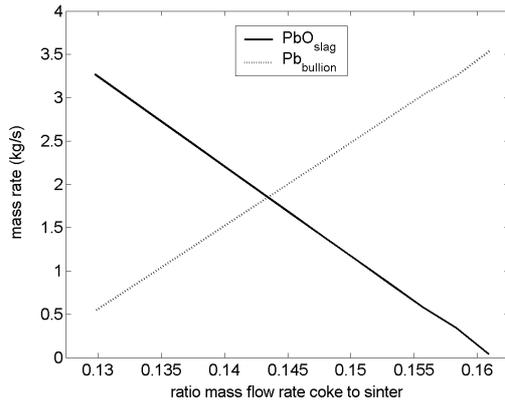


Figure 8: Effect of the variation of the coke to sinter ratio on the amount of lead lost to the slag

DISCUSSION

The model has been tested for a simplified charge. The results give only a rough indication of some of the main processes in the blast furnace which have been identified experimentally: the burning of coke with oxygen gas from the blast air and the associated temperature rise, the recirculating behaviour of Pb, the fact that the gases heat the solid charge in their way up the furnace.

The model can be used for some trend studies as shown above with the effect of the coke to sinter ratio on the lead losses to the slag.

The calculated profiles are quite sharp because of the simplified charge used. Most of the components, like PbO, O₂ and C, react almost completely in the furnace. The reactions and phase changes occur over a very limited temperature range. In a real blast furnace charge however, some components react more slowly or do not react at all and this has for example a smoothening effect on the temperature profile.

The transition from the stack model to the bosh model is also quite sharp. The calculation principles for both zones are very different. In the stack kinetic rate relations are used, while in the bosh and the hearth equilibrium is calculated. Further research is needed to smoothen the transition between these two concepts.

Although the charge is simplified, the calculation time is considerable (20 to 30 minutes for a relative error of 10^{-11} on a Pentium 4 2.4GHz processor with 512Mb RAM). This is mainly due to the minimization routine of the ChemApp© package. It can be expected that for a realistic charge calculation times will be even greater. A first estimate from trials would be 80 hours.

FUTURE RESEARCH POSSIBILITIES

This model is in its first stage of development. A first logical improvement is to expand the model for a real blast furnace charge.

Secondly the model can be extended by dividing the stack zone into two regions: one at the top of the furnace in which no reactions are incorporated and only heat transfer is allowed, and below that a zone with the same principles of the stack zone in this model. The bosh zone could also be divided into a top zone where only smelting of the solid charge is allowed, and below that the bosh zone as it is implemented in this model.

This model is one-dimensional. An extension to two or even three dimensions may be an interesting step. For each of the stated extensions of the model, a compromise has to be made between detail in the results and calculation time. Adding components and complexity undoubtable will increase the calculation time substantially.

CONCLUSION

The model presented in this paper simulates the main processes in the lead blast furnace. Although still in development, the model is able to deliver a qualitative view of the temperature distribution and the mass flow in the blast furnace. In the future the model will be tested for a realistic blast furnace charge in order to obtain more insight in the working of the lead blast furnace.

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