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OBJECT-ORIENTED MODEL OF A FERROMANGANESE FURNACE

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ABSTRACT

Process modelling is often a large and time consuming task. It is therefore an advantage to divide the process model into smaller sub-models which are easier to handle. Object-oriented methodology has the possibility of modularize the process model in a structured manner. The methodology makes it possible to model parts of a process without being concerned with the inner conditions of neighbouring parts, as long as the interface between the parts is preserved. In this paper, the method is applied on a mass-balance model of a ferromanganese furnace.

INTRODUCTION

One of the major difficulties in operating electric ferromanganese furnaces today is the lack of information on the inner furnace conditions. Furnace operation will improve if critical process variables can be computed or estimated on-line, since the operators and metallurgists then will be able to take better decisions on how to run the furnace.

The existing process knowledge is represented in different types of models, ranging from stringent mathematical models to rather vague assumptions on which direction the process variables seem to go in certain situations. In this paper, focus will be made on first principles modelling of mass transport and reactions.

The purpose of the model is to 1) increase the understanding of the dynamics of the furnace, 2) on a longer term basis, use the model in improved furnace control and 3) investigate a technique that makes it possible to easily change parts of the model and apply different model representations within the same framework. The first two points are obviously important in order to improve the furnace performance. Simulations on a good model can predict the furnace conditions some hours or days ahead. The operators may, hence, intervene at an early stage to prevent bad furnace conditions. The third point is important for efficient process modelling. By efficient is meant the ability to easily change the model, e.g. by including new chemical substances or changing thermodynamic properties. We believe that our model approach, object-oriented methodology, facilitates this.

This paper is organized as follows. The next section describes the modular, object-oriented concept used in the modelling. In the third section the process is modelled using first principles knowledge. In section four some simulations are presented. Finally, concluding remarks are given.

THE OBJECT-ORIENTED METHODOLOGY

The model is implemented using the object oriented programming language (OOPL) C++ [1]. In ordinary programming languages the data structure and the operations that work on the data structure are only loosely connected. In OOPL, however, the data structure and the operations are incorporated in discrete objects. Two important characterizations of the objects are [2]:

- *Classification*, which means that objects with the same data structure and operations are grouped into a class. A data structure or an operation that is local to a class, i.e. objects of other classes have no interest of knowing it, may be hidden or *encapsulated* inside the class.
- *Inheritance*. A class can be defined very generally (e.g. vehicle), and then specialized classes may be created using the general class as a basis (e.g. bicycle, ship, aircraft). The specialized classes will then *inherit* the data structure and the operations of the general class.

The two items listed above imply that 1) programming code may be reused in a much larger extent than ordinary programming languages support, 2) the inner representation of an object may be hidden for other objects, and 3) an object may be specialized if necessary.

An OOPL enables us to develop a model that consists of a number of modules, connected through well-defined interfaces. This is an advantage in the modelling process, where, typically, the structure of the process is known, but the content of each part needs to be modified. The representation of a subprocess inside a module may be hidden from the surrounding modules as long as the interface between the modules is well defined.

This concept is shown in figure 1. The figure shows two furnace zones, a transport module that defines the transport of solids, liquids and gas between the two zones. Since the model is a dynamic model, a numerical integrator (equation solver) is necessary to integrate the differential equations. The zones containing differential equations that should be solved, need an interface toward the numerical integrator module.

The system shown in figure 1 is a simplified example of the model to be presented in the next section. Carbon (C) and manganese oxide (MnO_x) enters the zone from above, while CO-gas enters from below. In the zone, there is one reaction, denoted GR (meaning gas reduction) in the figure. MnO_x and CO-gas are consumed in the reaction, and MnO and CO_2-gas are produced. CO- and CO_2-gas leave at the top of the zone. Carbon passes the zone without reacting. MnO continues to the next zone. Between the zones, there is a transport calculation module. In this module the flow rates of materials and gas between the zones are calculated. In the direct reduction zone, there are four species; MnO and C entering from the above zone, and Mn and CO-gas which are produced in the zone. Some C and MnO will pass through the zone. The direct reduction zone has one reaction, denoted DR in the figure.

The amount of each of the species is given by an ordinary differential equation:

$$\frac{dN_x}{dt} = F_{x,in} - F_{x,out} + r_x V \qquad (1)$$

where

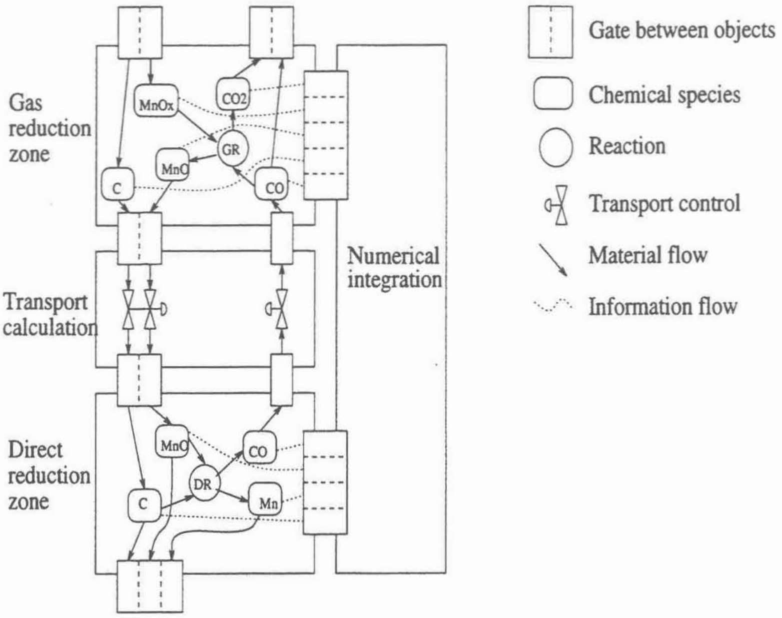

FIG. 1: Modules in the dynamic model of the furnace

N_x	the amount of species x in the zone
$F_{x,in}$	molar flow of x into the zone
$F_{x,out}$	molar flow of x out of the zone
r_x	the amount of x generated in the reaction
V	volume of the zone

These equations must be (numerically) integrated, and the result of the integration returned to the species inside each zone. This is illustrated by the dotted lines in the figure.

Suppose we want to study the effect of the Boudouard-reaction in the gas reduction zone. This reaction is easily put into the gas reduction zone, and connected to the species taking part in the reaction; C, CO and CO_2. The other zones, and the interfaces toward other zones are unaffected. This is an example of how a part of the object-oriented model is changed, without interfering with the rest of the model. When a simulation is run on the modified model, it will naturally behave differently from the original one.

Likewise, when new chemical species are added, no change is needed if a substance is added in one of the zones. If a species is supposed to flow from one zone to another, the transport calculations between the zones need to be modified.

An advantage of the modelling technique chosen here is that the model is generically hybrid, in the sense that the contents of each zone are of little importance as long as the interfaces to the other modules are preserved. Another advantage is that the modularity makes it easy to visualize the objects and the connections between them . This facilitates communication between people in the discussion of the model.

DYNAMIC FIRST PRINCIPLES MASS-BALANCE MODEL

In this section a dynamic mass-balance model of an electrical ferromanganese furnace is developed. Figure 2 illustrates how the furnace may be divided into zones, in which different phenomena take place. In the upper parts of the charge, water evaporates, and the ore is partly reduced. In higher temperature ranges, deeper down in the furnace, the reduction of the ore in the solid state continues. In the hearth of the furnace the ore melts and reacts directly with carbon to form metal. At the bottom, slag and metal are tapped from a slag/metal zone. In the following, the most important chemical species and the mechanisms in and between the suggested zones will be modelled.

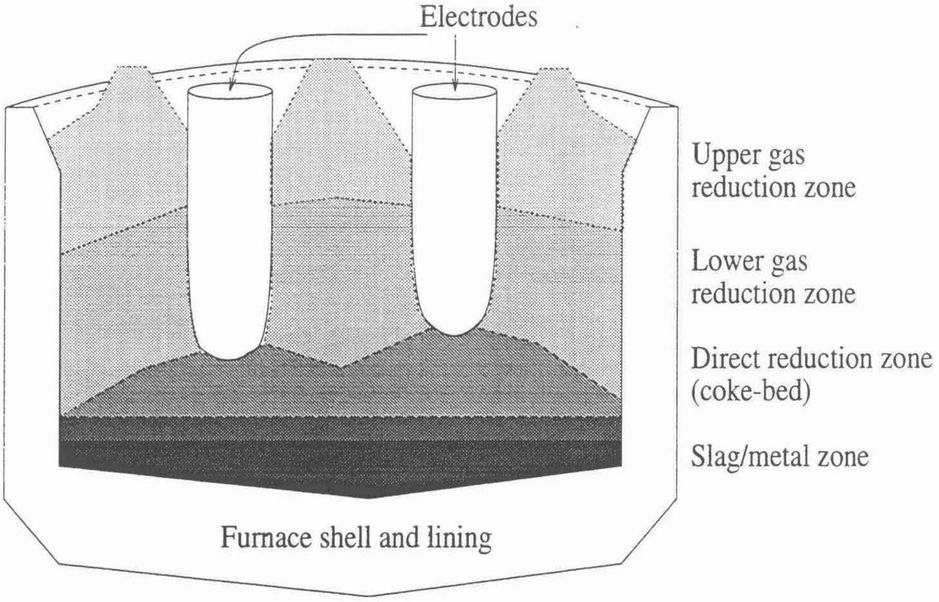

FIG. 2: A sketch of the zone division in the furnace

REACTIONS

The following species and reactions are considered in the model [3, 4]: (Approximate temperature ranges are given in brackets)

- Upper gas reduction zone ($400 - 700°C$)

$$3MnO_{2(s)} + 2CO_{(g)} \rightarrow Mn_3O_{4(s)} + 2CO_{2(g)} \tag{2}$$

$$3Mn_2O_{3(s)} + CO_{(g)} \rightarrow 2Mn_3O_{4(s)} + CO_{2(g)} \tag{3}$$

The oxygen rich manganese ores are assumed to react with rising $CO_{(g)}$ to form $Mn_3O_{4(s)}$. It is assumed that oxygen from a spontaneous dissociation from $MnO_{2(s)}$ will react with $CO_{(g)}$ to form $CO_{2(g)}$.

$$Fe_2O_{3(s)} + CO_{(g)} \rightarrow 2FeO_{(s)} + CO_{2(g)} \tag{4}$$

All the iron(III)oxide is assumed to be reduced by $CO_{(g)}$ to iron(II)oxide. The iron(II/III)-oxide (Fe_3O_4) is omitted as it is an intermediate product which will increase the number of components in the model, without influencing the overall model.

$$H_2O_{(l)} \rightarrow H_2O_{(g)} \tag{5}$$

Water entering the furnace with the raw materials will partly evaporate.

- Lower gas reduction zone ($700 - 1200°C$)

$$Mn_3O_{4(s)} + CO_{(g)} \rightarrow 3MnO_{(s)} + CO_{2(g)} \tag{6}$$

$$FeO_{(s)} + CO_{(g)} \rightarrow Fe_{(s)} + CO_{2(g)} \tag{7}$$

The manganese oxide, $Mn_3O_{4(s)}$, is assumed to be reduced by $CO_{(g)}$ to $MnO_{(s)}$. Iron(II)oxide is also reduced to metallic iron.

$$CaCO_{3(s)} \rightarrow CaO_{(s)} + CO_{2(g)} \tag{8}$$

$$MgCO_{3(s)} \rightarrow MgO_{(s)} + CO_{2(g)} \tag{9}$$

$$MnCO_{3(s)} \rightarrow MnO_{(s)} + CO_{2(g)} \tag{10}$$

These three carbonates are important ingredients in the raw materials, and are thus included in the model. When the ore is heated, these carbonates will decompose.

$$H_2O_{(g)} + CO_{(g)} \rightleftharpoons H_{2(g)} + CO_{2(g)} \tag{11}$$

Some of the water is assumed to react with $CO_{(g)}$, and form hydrogen-gas and $CO_{2(g)}$. The Boudouard-reaction is assumed to be important in this temperature range:

$$C_{(s)} + CO_{2(g)} \rightarrow 2CO_{(g)} \tag{12}$$

- Direct reduction zone ($1200 - 1500°C$)

  $$MnO_{(l)} + C_{(s)} \rightarrow Mn_{(l)} + CO_{(g)} \tag{13}$$

  Manganese oxide is reduced directly by carbon, forming metalling iron and manganese, and $CO_{(g)}$ which will rise to the upper parts of the furnace and contribute to the prereduction of the ores.

  $$SiO_{2(l)} + 2C_{(s)} \rightarrow Si_{(l)} + 2CO_{(g)} \tag{14}$$

  Small amounts of silicon is produced as well.

- Melted slag/metal zone ($1300 - 1400°C$)

  $$2MnO_{(l)} + Si_{(l)} \rightleftharpoons 2Mn_{(l)} + SiO_{2(l)} \tag{15}$$

  In the slag/metal zone, this reaction is assumed to take place.

The kinetics of the reactions are assumed to be given by the equation [5, 6]

$$r = f(\cdot)ke^{-E/RT} \tag{16}$$

where

E	is the activation energy
k	is the frequency factor
$f(\cdot)$	is the rate law

All the reactions, except reactions 11 and 15, are assumed to be irreversible.

The above list considers the major reactions assumed to take place in an electric ferromanganese furnace. Not all the reactions are elementary reactions, but the result of two or more such mechanisms. An example of this is the dissociation of oxygen from $MnO_{2(s)}$ in the upper zone. The oxygen then reacts with $CO_{(g)}$ to form $CO_{2(g)}$.

Some potentially important reactions are omitted, such as possible circulation of alkalis in the furnace [7]. Note also that the model considers pure compounds, and not complex minerals as found in the ores. It is emphasized that the model is kept at a relatively simple level. This is necessary in order to be able to operate and understand the model. The structure of the model, however, makes it relatively easy to include species and reactions at a later point, if necessary.

SPECIES

The species considered in the model are listed in table 1. In addition to the species that take part in the reactions, aluminium oxide (Al_2O_3), which is a major slag component, is also included in the model. Other species like sulphur, phosphorus, barium oxide, potassium oxide, etc. are not included in the model at this stage.

TABLE 1: Chemical compounds in the model

Compound name	Formula	To be found mainly in/as
Aluminium oxide	Al_2O_3	Raw material, slag
Carbon	C	Raw material, reducing agent, metal
Carbon monoxide	CO	Reducing agent, flue gas
Carbon dioxide	CO_2	Flue gas
Calcium carbonate	$CaCO_3$	Raw material
Calcium oxide	CaO	Slag
Iron	Fe	Metal
Iron(II)oxide	FeO	Intermediate product
Iron(III)oxide	Fe_2O_3	Raw material
Hydrogen	H_2	Flue gas
Water	H_2O	Raw material, flue gas
Magnesium carbonate	$MgCO_3$	Raw material
Magnesium oxide	MgO	Raw material, slag
Manganese	Mn	Metal
Manganese carbonate	$MnCO_3$	Raw material
Manganese(II)oxide	MnO	Slag, intermediate product
Manganese(II/III)oxide	Mn_3O_4	Intermediate product
Manganese(III)oxide	Mn_2O_3	Raw material, intermediate product
Manganese(IV)oxide	MnO_2	Raw material
Silicon	Si	Metal
Silicon oxide	SiO_2	Raw material, slag

ZONE DIVISION

As the reactions indicate, the furnace is divided into four zones. The model is shown schematically in figure 3. Three boundary zones are included. The raw material zone provides the furnace with raw materials, while the flue gas zone and the tap zone accumulates produced gases and slag/metal respectively.

In each zone there is a number of species, which is a subset of the species listed in table 1. In addition, the reactions that concern the particular zone is defined inside the zone.

In the two gas reduction zones, all species, except water and the gases CO, CO_2 and H_2, are assumed to be solid. In the direct reduction zone, only carbon is solid. The rest of the species are assumed to be in liquid or gas phase. In the melted slag/metal zone, all species, except the $CO_{(g)}$, are assumed to be liquid. The coke-bed is, for simplicity, assumed to be formed as a cylinder.

The zones are assumed to be isothermal, and since no energy balance is included, assumed also to have constant temperature over time. The model is unidimensional in vertical direction, and contains thus no information on variations in other directions.

TRANSPORT BETWEEN THE ZONES

Solid/liquid transport

The transport of solids and liquids inside the furnace is assumed to be determined by two factors; 1) tapping and 2) volume change due to the reactions taking place in the zones.

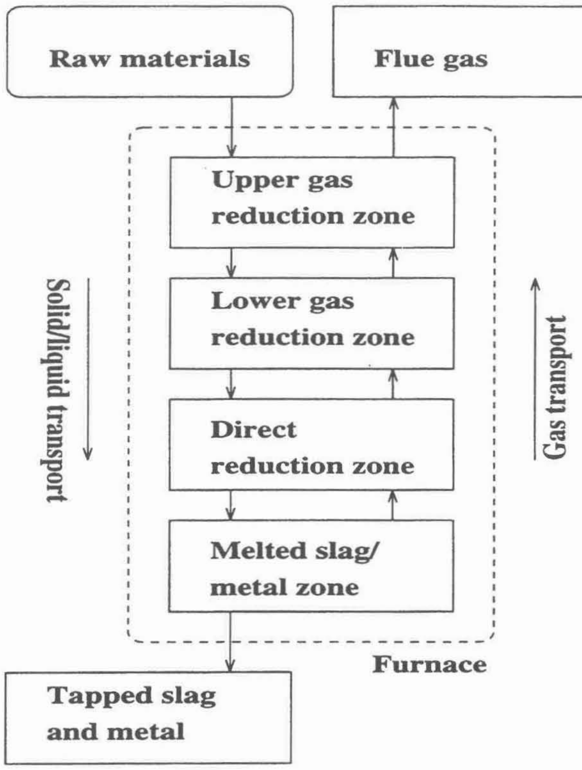

FIG. 3: The zone division of the furnace model

- **The two upper zones** (the prereduction zones) of the furnace are assumed to have a constant volume. The solid volumetric flow into the zone is then defined as:

$$q_{s,in} = \frac{1}{T_s}(V_{s,avail} - V_s) + q_{s,out} - q_{s,rea} \tag{17}$$

where

V_s	volume of the solid and liquid material in the zone
$V_{s,avail}$	volume available for solid and liquid material in the zone
T_s	time constant, solid transport
$q_{s,out}$	volumetric rate of material out of the zone
$q_{s,rea}$	volumetric rate of material formed due to reactions

The molar flow of component j is given by:

$$F_{j,in} = \frac{\rho_j}{M_j}\frac{V_{j,over,f}}{V_{over,f}} q_{s,in} \tag{18}$$

where

ρ_j	density of the component
M_j	atomic weight of the component
$V_{j,over,f}$	volume of the component in the above zone
$V_{over,f}$	total volume of solid and liquid material in the above zone

- The liquid flow out of the **direct reduction zone** (coke-bed) is assumed to be a function of the density and viscosity of the slag and metal passing through the coke-bed, the pressure drop over the zone, coke particle size, etc. For simplicity it is assumed constant. In a full model, Ergun's formula [6] could be applied to calculate a flow through the coke-bed. The height of the direct reduction zone depends on the amount of coke in the zone. The flow of material into the zone is given by equation 17.
- The flow out of the slag/metal zone is given by the tapping of the furnace.

Carbon saturation in the metal

The carbon saturation in the metal limits the transport of carbon between the direct reduction zone (i.e. the coke-bed) and the melted slag/metal zone. The metal is assumed to be carbon saturated. The content of carbon in the metal depends on the temperature, the manganese content and the silicon content, following the relation [8]:

$$(\mathrm{wgt\%C}) = 1.34 + 0.00254T + 0.0265(\mathrm{wgt\%Mn}) - 0.34(\mathrm{wgt\%Si}) \tag{19}$$

where T is the temperature in Celsius. The relation is valid for a silicon content of less than 10% and a Mn/Fe-ratio of 4. However, for metals with very low silicon content, as is the case in ferromanganese, the relation is valid also for a Mn/Fe-ratio less than 4.

Gas transport

The gas transport is driven by the gas pressure in the zones. If the total gas pressure in a zone exceeds 101kPa (1atm), gas is assumed to leave the zone. The following assumptions are made:

- The gas-fraction of each zone is constant
- All gases are assumed to be ideal.
- The gas pressure is held at one atmosphere in all the zones

The gas flow out of a zone is assumed to be:

$$F_{g,out} = -\frac{1}{T_g}(P_{ref} - P_g) + F_{g,in} + F_{g,rea} \tag{20}$$

where

$F_{g,out}$	total flow of moles out of the zone
$F_{g,in}$	total flow of moles into the zone
$F_{g,rea}$	total number of moles of gas reacted per time unit
T_g	time constant, gas transport
P_{ref}	wanted pressure in the zone (1 atm)
P_g	actual pressure in the zone

The amount of component j (in moles), allowed to flow out of the zone is given by:

$$F_{j,g,out} = p_j F_{g,out} \tag{21}$$

where

$F_{j,g,out}$	flow (in moles) of compound j out of the zone
p_j	partial pressure of compound j in the zone

SIMULATION EXAMPLE

The model presented in the previous sections is used to simulate different types of furnace conditions. The input to the model is the charge mix composition and the tapping procedure. The model output is the concentration of all the species listed in table 1 in each of the zones and the varying heights of the direct reduction zone and the slag/metal zone. In the following simulations, the change in the reduction of MnO due to an increased amount of carbon in the charge mix will be studied.

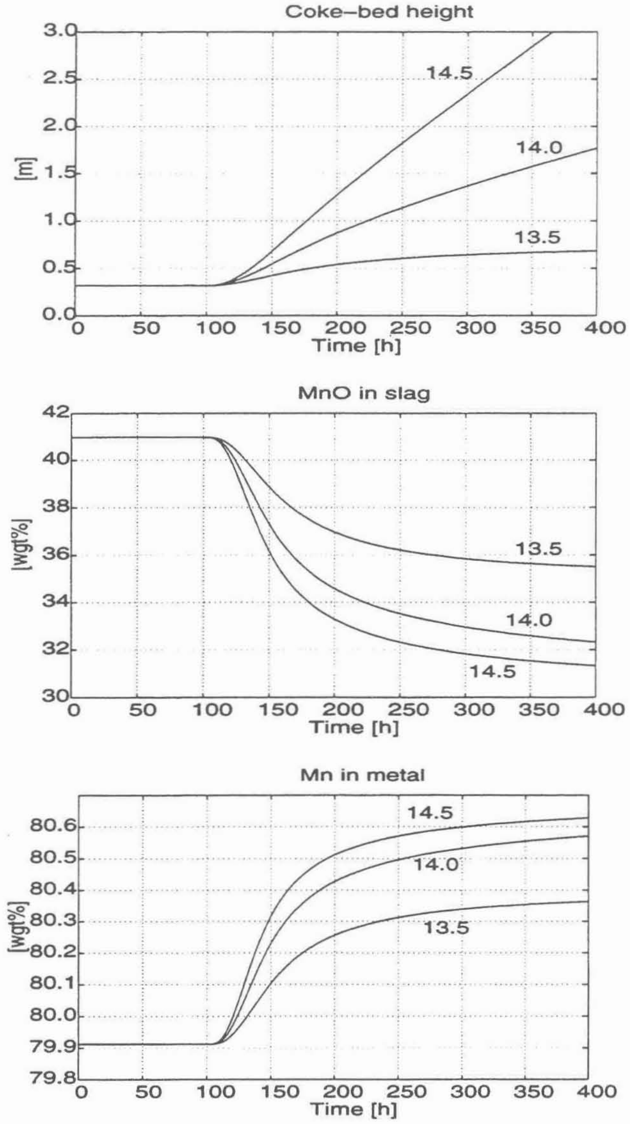

FIG. 4: Simulation of changes in the coke-bed height, the concentration of MnO in the slag and the concentration of Mn in the metal, due to increased carbon content in the charge mix

CARBON CHANGE IN CHARGE MIX

Figure 4 shows how the model reacts to a step change in the amount of carbon from 13.0wgt% of the mix, to 13.5wgt%, 14.0wgt% and 14.5wgt% at time 100 hours. There is some transport delay from the top of the furnace to the coke-bed and the melted zone. Then the increased amount of carbon will force more MnO to react and form Mn, until the situation is stabilized at another level. The rate law of reaction 13 is assumed to be proportional to the available surface of the coke in the coke-bed, and proportional to the deviation of the MnO-concentration from equilibrium. In this case equilibrium is assumed to be at 30wgt% MnO.

The figure shows that as the amount of coke in the coke-bad increases, the reduction of MnO is increased. As the process approaches equilibrium, however, the concentration potential is reduced, and a build-up of coke takes place.

In these simulations it is assumed that the temperature is kept constant within each zone. Since the reduction of MnO is an endothermic reaction, the average temperature of the coke-bed will decrease as the coke-bed increases. Then the MnO-reduction will slow down, and an even worse build-up of coke than demonstrated here will occur.

The thermodynamic data used in the simulations are taken from [9] (Manganese compounds and carbonates) and [10].

CONCLUSION

An object-oriented model for a ferromanganese furnace has been developed. The use of object-oriented methodology is particularly useful when 1) the process consists of several process units (see for instance [11]), 2) parts of the model is under development or is often changed. The model presented in this paper is an example of the latter.

The model gives some insight to the dynamics of the furnace and may be used to test hypothesis on relations between transport mechanisms and reaction kinetics. When energy balances are included in the model, an overall furnace behaviour may be simulated.

The object-oriented methodology has proven to be an efficient way of modelling, not only plants containing a large number of components, but also on large unit processes which may be divided in subprocesses or zones. The OOPL also support the reuse of programming code.

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