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DIRECT REDUCED IRON

Technology and Economics of Production and Use

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CHAPTER 13

Computer Modeling and Analysis of Processes for the Production and Use of DRI

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The computer is indispensable for research, design and operation of metallurgical processes. This chapter is concerned with the use of commercially-available computer software to develop DRI process models and the use of such models in process analysis. The first part of this chapter introduces the basic concepts of model development. The second part of the chapter illustrates the use of software for making simple process calculations. The third part of the chapter describes how more complex processes are modeled with commercially available software.

INTRODUCTION

Technical Factors

Process modeling using computers has become commonplace with the availability of low-cost computer hardware, an increase in the number of computer-trained engineers and the advent of process simulation software. The application of such programs has proven to be successful in three areas: (1) the design of new processes and flow sheets; (2) increasing the efficiency of plant operations by demonstrating the effects of process alternatives and expediting the decision-making process; and (3) operator guidance and training. The greatest benefit comes when effort in all three areas is integrated.

Process simulation is a problem-solving technique whereby mathematical equations are used to describe the mechanisms of processing operations. Given accurate data, solving these equations rigorously will give accurate predictions of the outcome of the process. The general principles involving process simulation are described in a number of chemical and metallurgical engineering texts. Basically, every system must obey the laws of conservation of mass and energy, but these laws alone are seldom adequate to completely specify a system. Most systems

have a number of restrictions, conditions, and subsidiary relationships that must also be satisfied, and under ideal conditions the number of stream variables minus the number of restrictions will equal zero (i.e., there are no degrees of freedom).

Commonly the mathematical equations are not rigorous and data may be missing, so most models do not give exact quantitative results. Still, semi-quantitative or even qualitative results may be useful in making decisions concerning alternative operations.

Process simulation can be used to:

1. develop new process technology,
2. evaluate alternative flow sheets,
3. evaluate research and pilot plant data,
4. perform feasibility studies,
5. scale up design calculations,
6. train plant operators,
7. analyze actual plant performance,
8. study process control schemes, and automate and run plants.

Some of the advantages and benefits of process simulation are:

1. It is less costly in time and money to simulate a proposed process than to conduct research or operate a pilot plant. Simulations reduce the test program by permitting identification of key parameters early in the development stage, and guiding the most efficient collection of data.
2. Hazardous and high cost processes can be experimented with cheaply and at a lower risk to the environment.
3. The engineer is required to develop a detailed understanding of the process using consistent design criteria.

In the second example the inlet gas temperature was varied from 890 to 950 K while keeping all other reactor parameters constant at the basis case condition described above. This simulates a situation where the reactor is initially operating at the basis case whereupon the inlet gas temperature changes. This causes the equilibrium reactor temperature to vary over a much smaller temperature range; in this case, 854–870 K. The results of the two extremes are shown in Table X. A close inspection of these results shows why a 60° increase in inlet gas temperature caused only a 16° increase in reactor temperature—as the reactor temperature increases, the equilibrium gas contains less CH_4 , CO_2 and H_2O , thus the overall process becomes more endothermic as the reactor temperature increases.

In the last example the reactor pressure was varied between 2.25 and 7 atm while keeping all other reactor parameters constant at the basis case conditions described earlier. This simulates a situation where the reactor is initially operating at the basis case, then the reactor pressure changes. Going from 2.25 to 7 atm caused the equilibrium reactor temperature to vary between 846 and 890 K. Details of the two extremes are shown in Table XI. An inspection of these results shows why a threefold increase in reactor pressure caused a 44° increase in reactor temperature—as the reactor pressure increases the equilibrium gas contains more CH_4 and H_2O , thus the overall process becomes less endothermic as the reactor pressure increases.

These three examples show how a program capable of making simultaneous equilibrium and heat balance calculations can give important insight into how various process parameters affect the conditions of a reactor. The EQS4WIN program was particularly useful because of its unique ability to allow the equilibrium temperature to be a dependent variable, solved by the program. The information gained in this type of study is very valuable in putting together more complex reactor or flow sheet models using other software designed for that purpose. In fact, the information gained from the simulations performed here was used as a basis for developing a control model for a conceptual iron carbide production process involving four reactors. This is covered in the next section.

REACTOR MODELING

So far, the discussion of modeling has been restricted to single unit operations involving fairly simple chemistry. This section will deal with combinations of two or three unit operations, that is, two or more reactors or processes taking place in one reactor that has two or more zones. The first example uses the Pyrosim program to model the production and melting of DRI. The second example uses the spreadsheet program Excel to model a control strategy for the production of iron carbide (Fe_3C). ← 1st part

Reduction and Melting of DRI

DRI is conventionally produced as a scrap substitute for EAF steelmaking or for enriching the feed to a blast furnace. The value of DRI produced by a coal-based process for EAF feed could be less than that for a gas-based DRI because of the additional gangue and sulfur content. One way to overcome this drawback while producing a premier material is to melt the DRI in an electric furnace immediately upon discharge from the reduction furnace to form an iron-carbon alloy (1–2% C). This liquid metal can be used in an adjacent EAF steelmaking operation or cast and shipped.^{3,4} In this example the Pyrosim program was used to model the production of DRI by a coal-based rotary kiln followed by melting the DRI in an electric furnace. The process was simulated by using three stages in the flow sheet. All thermodynamic data for Pyrosim come from the accompanying database program Thermo.

The reduction of iron ore in a rotary kiln has been discussed in the chapter on Direct Reduction Processes. The rotary kiln is characterized by extreme composition and temperature gradients along its length, and it is therefore difficult to model such a process realistically as a single unit operation. A common way to handle the difficulty is to divide the reactor into zones whose boundaries are more conceptual than physical. The kiln is divided into two zones, one for preheating the charge and devolatilizing the coal and the other for reduction to iron (DRI) and discharge. The gas and solid phases flow countercurrently, a circumstance that adds complexity to a

Table X—Effect of Inlet Gas Temperature on Reactor Temperature and Conditions

Inlet Gas T	Reactor T	% CH_4	% H_2	% H_2O	%CO	% CO_2	$\log(p\text{O}_2)$	Atm $\log(p\text{O}_2)$	$\log(\eta)$
890 K	854 K	50.8	32.4	10.1	3.6	3.3	-25.55	-25.58	+0.39
950 K	870 K	48.7	34.6	8.0	4.5	3.2	-25.15	-25.15	+0.42

Table XI—Effect of Reactor Pressure on Reactor Temperature and Conditions

Reactor P	Reactor T	% CH_4	% H_2	% H_2O	%CO	% CO_2	$\log(p\text{O}_2)$	Atm $\log(p\text{O}_2)$	$\log(\eta)$
2.25 atm	846 K	49.2	34.2	9.3	4.1	3.4	-25.98	-25.88	+0.44
7.0 atm	890 K	51.4	31.1	10.9	3.5	3.0	-24.21	-24.15	+0.32

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process model. The division into two zones is arbitrary, and although more zones may improve the model accuracy, two zones are probably adequate in this case where detailed operating information is lacking.

The rotary kiln was modeled by specifying certain information for each zone. First, the temperature for each stream entering and leaving each zone was set as was the composition of each solid species. Next, the CO/CO₂ and H₂/H₂O ratios in the *prereduction zone* gas were set and the ore was specified as being reduced to Fe₃O₄. Similar gas ratios were specified for the *reduction zone* as was the degree of metallization. In effect, this is equivalent to writing reactions for the main chemistry occurring in each zone and assigning an "extent of completion" factor for each reaction. Obviously the adequacy of this approach depends on the amount and reliability of data obtained from an operating plant. Where data were lacking, reasonable assumptions were made or the parameters were left as unknowns to be solved by the computer model. Once the zones were correctly specified, Pyrosim completed the mass balance, and also calculated a heat balance.

The EAF melting of DRI is a steady-state process in which the DRI is fed continually into the furnace as the charge meltdown occurs. Most of the FeO in the DRI is reduced by residual carbon in the charge to produce CO. Sulfur and phosphorus partition favorably to the slag. The DRI melting operation was modeled differently than was the rotary kiln. One of the advantages of Pyrosim is its ability to employ two different types of approaches in a single multi-reactor model. The EAF was assumed to be an equilibrium reactor, which is reasonable since mass transfer and kinetics are relatively fast between liquids and

gases near 1600°C. The elements or species making up each of the three phases (gas, slag and metal) must be specified, as well as the temperature and pressure. Pyrosim has a free energy minimization routine which calculates the amount and composition of each phase. Then a heat balance is performed to determine the amount of electrical energy required. The distribution of S and P between slag and metal can be simulated by assuming appropriate activity coefficients for these elements, but these elements were not tracked in this example.

A flow sheet and equipment sketch for the process is shown in Figure 9. Typical data on the operating characteristics of a rotary kiln were obtained from published and private sources.⁵⁶ Ore, flux and coal are charged into the prereduction zone where the coal is devolatilized, the flux calcined and partial reduction of the hematite occurs. The solids temperature increases to 1050°C in this zone. Air is introduced to partially burn the coal volatile matter and CO coming in from the reduction zone. The combustion of these gases provides the necessary energy to heat the charge and carry out the chemical reactions of oxide reduction and flux calcination. The amount of air introduced into the prereduction zone was adjusted until the zone showed a small surplus of heat judged adequate for heat loss. A summary of product composition and weight is shown in Table XII.

The solid product of the prereduction zone is a mixture of coal char, calcined flux, coal ash, ore gangue and iron oxide (mostly magnetite). This product passes into the reduction zone where it is heated to 1100°C and magnetite is carbothermally reduced. Equation 1 gives the chemistry for a similar process. This reaction is strongly endothermic. Heat is provided by burning some of

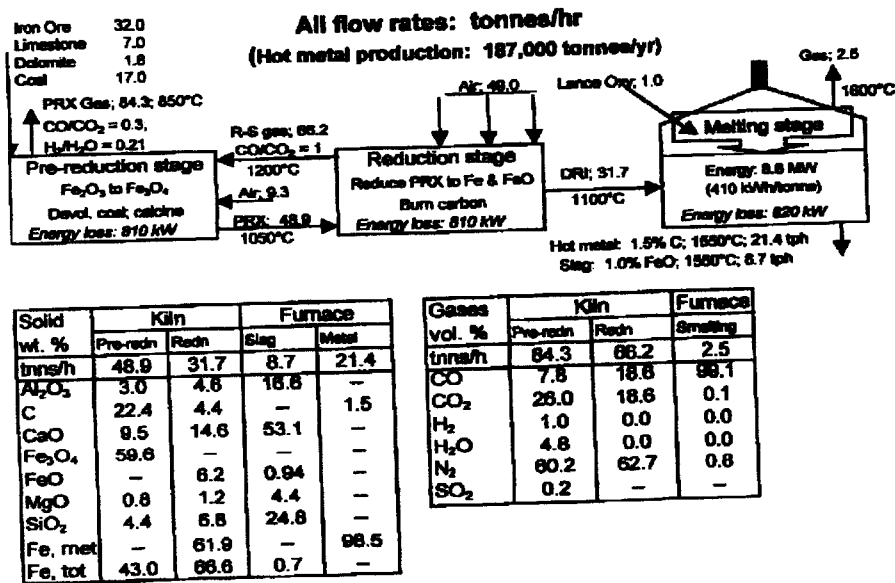


Fig. 9 - Sketch of rotary kiln - EAF melting furnace flow sheet modeled by Pyrosim.

the residual coal char and using air to burn some of the CO evolved during reduction. The amount of coal char and air were adjusted manually until there was an overall small surplus of heat in this zone to allow for losses. The coal ash is assumed to be captured by the DRI solids.

The DRI contains some unreduced wüstite and residual coal char and is fed directly to an EAF and melted. The DRI temperature was assumed to drop from 1100 to 1000°C in transit to the EAF. Various simulations were made to show the effect of cooling the DRI to different temperatures before it entered the EAF. During melting most of the wüstite is reduced by the residual char. The remaining carbon partly dissolves in the metal and part is oxidized by injected oxygen. Oxygen is added to the EAF not only to burn the carbon down to the specified tap amount, but also to ensure good mixing in the bath and to provide additional heat. The main source of heat is still electrical energy.

The kiln was modeled using the "empirical reaction" mode, in which the extent of possible reactions is set by the user according to published operating data and the model assumptions. The user may set various operating parameters, such as the CO/CO₂ and H₂/H₂O ratio in the gas, the wüstite to metallic iron ratio in the product and other specifications sufficient to close the mass and heat balance. The rigor imposed by forcing the closure of the heat and mass balance allows the program to calculate operating details not given by the published reports. Also, once the model is set up and running the user can change some of the assumptions made in the beginning and see which of them has the greatest effect on the results. This sort of "sensitivity analysis" provides insight into which operating parameters have the greatest effect.

The EAF melter was modeled using the "equilibrium reactor" mode in which all phases reach equilibrium and solution phases are assumed in general to be ideal. However, the user does have the option for specifying a fixed value of an activity coefficient for solution species so that the slag/metal distribution of an element like sulfur can be approximated with some degree of accuracy. In the present case, the emphasis was mainly on the heat and mass balance which is virtually independent of small changes in melt composition. The distribution of S and P between metal and slag was not tracked in this example.

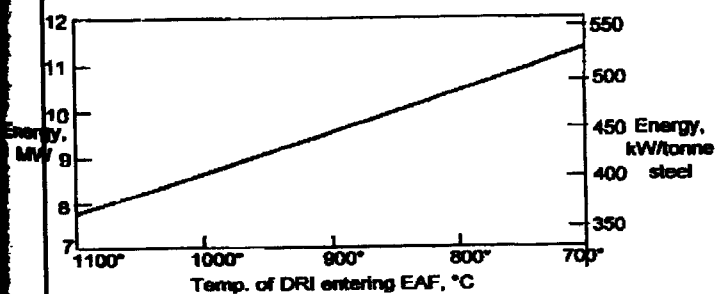


Fig. 10 - Effect of DRI temperature on hourly energy requirement in EAF.

Table XII - Product Data for Rotary Kiln - EAF Melting Furnace Modeled by Pyrosim

Solid wt%	Kiln		Furnace	
	Pre-redn	Redn	Slag	Metal
tonne/h	48.9	31.7	8.7	21.4
Al ₂ O ₃	3.0	4.6	16.6	-
C	22.4	4.4	-	1.5
CaO	9.5	14.6	53.1	-
Fe ₂ O ₄	59.6	-	-	-
FeO	-	6.2	0.94	-
MgO	0.8	1.2	4.4	-
SiO ₂	4.4	6.8	24.8	-
Fe, met	-	61.9	-	98.5
Fe, tot	43.0	66.6	0.7	0.8

Gases vol%	Kiln		Furnace
	Pre-redn	Redn	Smelting
tonne/h	84.3	66.2	2.5
CO	7.8	18.8	99.1
CO ₂	26.0	18.6	0.1
H ₂	1.0	0.0	0.0
H ₂ O	4.8	0.0	0.0
N ₂	60.2	62.7	0.8
SO ₂	0.2	-	-

The sensible heat in the hot DRI into the EAF contributes substantially to the energy required by the EAF. Pyrosim was used to calculate the effect of DRI charge temperature on rate of energy consumption in the EAF to melt the DRI, and the result is shown in Figure 10. A drop in DRI temperature from 1000 to 700°C caused the specific energy requirement to go from 410 to 530 kWh/tonne hot metal. These results show a clear advantage in energy saving by hot charging DRI to the EAF.

Pyrosim is limited to four reactors in series, has other limitations on specifying how reactor products are split and cannot incorporate controllers on streams and reactors (Appendix A). Even with these limitations it is an excellent tool for gaining insight into appropriate processes and understanding the principles involved in putting together a model.

Process Control in the Production of Iron Carbide

Iron carbide (Fe₃C; cementite) is a potentially advantageous scrap substitute for EAF steelmaking because of its stability and carbon content. Iron oxide is reduced and carburized in one or more fluidized beds at elevated pressures and temperatures in the vicinity of 600°C.

The fundamentals of the formation of Fe₃C in a single reactor were described in connection with the EQS4WIN model. This section describes the use of a spreadsheet (Excel) to develop a multi-reactor model for iron carbide production with emphasis on developing a process control strategy. To minimize complexity only the major unit operations are included in the model.