JONES, R. Computer simulation of pyrometallurgical processes. APCOM 87. Proceedings of the Twentieth International Symposium on the Application of Computers and Mathematics in the Mineral Industries. Volume 2: *Metallurgy*. Johannesburg, SAIMM, 1987. pp. 265 – 279.

Computer Simulation of Pyrometallurgical Processes

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A knowledge of the steady-state mass and energy requirements of a particular process is essential to a determination of the economic feasibility of that process. A predictive simulation technique can be of great value in this respect.

A versatile computer program based on a fundamental thermodynamic approach has been developed for the prediction of process requirements. The equilibrium composition of a multiphase system is determined by the technique of free-energy minimization. Energy-balance calculations are performed using the appropriate thermodynamic data for the chemical species present in the composite materials used. All models for the process units under consideration are written in modular form, the output being calculated from the input and the specified operating conditions.

The computer program is written in such a way that it can be used easily by anyone familiar with the processes involved, even though he may have no previous experience with a program of this type. The program is structured so as to facilitate the varying of one parameter without any alteration to the others, thus simplifying the investigation of the effects of any parameters considered to be important.

The program has the advantage of being able to compare existing and new processes on the same basis, namely from the ores to the molten metal.

Introduction

Pyrometallurgical operations are essentially concerned with the high-temperature processing of materials. These processes can be extremely complex, involving reactions between gas, solids, liquid slag, and liquid metal. These four streams, singly or in combination, are sufficient to characterize the products from most pyrometallurgical processes of interest.

Pyrometallurgical processes must be evaluated at many stages during their development and design, and when operating changes are introduced. Because experimental work in pyrometallurgy is expensive, a system should be characterized as thoroughly as possible before experimental work is undertaken. Computer simulation allows the requirements of a particular process to be determined quickly and reliably.

The essential problem involves the development of a technique that will allow the prediction of the outcome of a particular process under specified operating conditions. To this end, a computer program, *PYROSIM*, was developed by the author to calculate predictive steady-state mass and energy balances for a wide variety of processes. Since many different raw materials must be taken into account, the program is very flexible in this

regard.

Simulations must be simple to perform and directly applicable if they are to be used successfully.

The *PYROSIM* computer program

The simulator is based on the description of the process units and streams involved in a flowsheet. The state of any stream is completely specified by the vector of flowrates of each chemical species together with the temperature and pressure. A complete specification of the plant can be obtained by including the operating conditions of each process unit. These conditions include the operating temperature, pressure, and the energy losses from the unit. In addition, it is necessary to specify whether the process is temperature-controlled or energy-controlled.

Any process unit has a number of feed streams, each at its own particular temperature. From the chemical analysis of the feed streams, the number of moles of each chemical species is calculated. It is often necessary to treat minerals as ideal mixtures of chemical compounds, since thermodynamic data are not readily available for minerals as such.

The appropriate thermodynamic constants (the standard enthalpy and entropy of formation, and Cp coefficients) are then assigned to each of the chemical species so that the partial molal enthalpy of each component can be calculated at the stream temperature. In general, the partial molal enthalpy is a function of temperature, pressure, and composition. The effect of composition on the enthalpies of individual components is small in most cases; there is also very little data available on the variation in enthalpy with composition. The effects of composition on enthalpy are therefore ignored, which is equivalent to the treatment of the process streams as ideal solutions. Except for gases under high pressure, the dependence of enthalpy on pressure is small. (If deemed important, the effect can be allowed for by the use of equations of state or reduced property correlations.) In this field of interest, the enthalpy is assumed to depend solely on temperature. The enthalpy of each pure compound is calculated relative to the elements in their standard state at 25^0C and 1 atm. The total enthalpy of a stream is taken to be equal to the sum of the enthalpies of all the compounds in the stream.

The total number of moles of each of the chemical species entering a particular unit is then placed in a vector of feed species. In this way, an indefinite number of feed streams (limited, of course, by available memory) containing material of any composition and at any temperature can be accommodated. The unit model is then applied to the feed vector. The model is essentially a mapping of the elements in the chemical species of the feed vector onto vectors of the species in the resulting gas, solids, slag, and metal streams. The enthalpy of these resulting streams is then calculated as described above.

The energy requirement of a process

is calculated as the difference between the enthalpy of the products and that of the feed streams. The specified losses of energy from the process unit are then added to this amount to give the energy requirement of the process unit. In this way, the enthalpy calculation can be performed independently of any specific reaction path.

Some or all of the products (gas, solids, slag, and metal) from the first unit then become part of the feed to the next unit. The fraction of each of the product streams entering the next unit can be independently specified.

For a recycle stream, one of the streams within the recycle loop must be estimated. In this way, the loop is 'torn' open, and the calculations can be done as already explained. Some form of iteration is then applied to the calculation of the 'tear' stream until convergence is attained. The topology of most pyrometallurgical flowsheets is fairly simple, and iteration by direct substitution is adequate. It should be noted that there is a complicating feature in the calculation of a recycle loop. The models describing some units use the technique of free-energy minimization, which is discussed below. This technique is applied to a specific set of compounds and elements. If any of the specified elements is absent, the calculation breaks down. If an element is present only in the recycle stream, this stream cannot be assigned a value of zero at any stage in the iterative calculations. To overcome this difficulty, an approach is used in which an intermediate stream is estimated on the basis of the feed to the previous unit.

The *PYROSIM* program achieves its generality by obtaining all the required information from a number of data files. These files cover the names of the process units, the thermodynamic data for the chemical species under consideration, the stoichiometry of the compounds, the chemical analyses of the feed materials, and the specifications of the chemical species present in each phase at equilibrium. All these files are managed by the program, and data can be added, deleted, edited, or listed. Thus, the program is kept independent of any particular process route.

Process models

The models of individual process units that are to be included in the program must have a standard form, since the output from a unit must be calculated from the input to that unit and the specified operating conditions.

The following features need to be borne in mind when a model for a process unit is set up.

It is assumed that the amount, composition, and temperature of the feed materials entering the unit are known. The operating pressure and the energy losses must be specified in all cases. The temperature is specified for process units where an external energy source is present. Otherwise, the process is said to be energy-controlled and the temperature is determined by the program. The

temperature is calculated, by trial and error, to be such that the difference between the enthalpy of the products and that of the feed is equal to the loss of energy from the unit.

The model must simulate real operation as closely as possible. The user is required to specify only what he is free to specify in practice. For example, one can specify the ratio of the materials in the feed but not the composition of the metal. The amounts and compositions of the product streams (gas, solids, slag, and metal) are calculated from the feed materials and the operating conditions. Any additional parameters of interest can also be calculated at this stage. For example, it is useful to report the calculated liquidus temperature of the slag for an electric-arc furnace model.

As discussed above, all that is required of a process model is that it maps the elements in the feed vector onto the species in the vectors of gas, solid, slag, and metal products.

No process model should be regarded as being absolutely definitive. Through a process of interaction with the users of the simulation, there will hopefully be a steady evolution of improved process models.

Models may be empirical, specific, general, kinetic, or equilibrium. Of course, the ideal to which every simulation aspires is to be able to predict the outcome of any process. For this reason, much effort was expended to provide a technique for the prediction of the distribution of the elements in the various chemical species in the product streams. The models that are most generally applicable are those based on a fundamentally sound description of the process being simulated. A technique has been made available that will provide a model based on the description of the chemical equilibrium of a multiphase system.

Technique of free-energy minimization

Pyrometallurgical processes take place at high temperatures. For this reason, the attainment of equilibrium in many processes is not prevented by kinetic limitations. However, a general method for the prediction of the composition of an isothermal multiphase system at equilibrium is required.

Problems relating to the chemical equilibrium of a system involving several chemical species are notoriously intractable, requiring the solution of many simultaneous non-linear equations. However, such problems can be reduced to the minimization of the Gibbs free energy of the system, which is the fundamental description of chemical equilibrium. In general, there is an infinite number of ways in which non-negative mole numbers can be assigned to the possible product compounds such that the chemical reactions involving the specified reactants will be balanced. At a specified temperature and pressure, the most stable products (the desired solution to the problem) are those associated with the lowest free energy.

The Gibbs free energy of the

multiphase multicomponent system is given by

$$G = \sum_i \sum_p n_i^p \mu_i^p \quad [1]$$

where n_i^p = number of moles of species i in phase p

μ_i^p = chemical potential of species i in phase p

The chemical potential is given by

$$\mu_i^p = \mu_i^0 + RT \ln a_i^p \quad [2]$$

where μ_i^0 = reference chemical potential for species i

a_i^p = activity of species i in phase p

It is convenient to set $\mu_i^0 = 0$ for all elements in their standard states. Then

$$\mu_i^0 = \Delta G_{fi}^0 \quad [3]$$

where ΔG_{fi}^0 = Gibbs free energy of formation of species i at the process temperature

The gas phase is assumed to behave ideally and in the gas phase $a_i^p = x_i^p P$ where x_i^p is the mole fraction of species i in the (gas) phase p. Condensed phases are non-ideal, so that $a_i^p = \gamma_i^p x_i^p$ where γ_i^p is the activity coefficient of species i in the (condensed) phase p.

Each element is conserved in the process, so that

$$\sum_i \sum_p a_{ij} n_i^p = b_j \ (j = 1,2, \ldots, l) \quad [4]$$

where a_{ij} = number of atoms of element j in species i

b_j = number of moles of element j in the feed

l = total number of elements

This minimization problem has the free energy of the system (equation 1) as the objective function, and the number of moles of each of the chemical species in each phase as the variables. The constraints that apply are those of mass conservation for each element present in the system, as well as those of non-negativity of the number of moles of each species present. The equality constraints can be taken care of by the use of the technique of undetermined Lagrange multipliers.

Eriksson[1] has devised a method for free-energy minimization which uses a truncated Taylor series expansion of the non-linear equations around successive estimates of the solution to provide a system of linear equations to be solved within each iteration. Further details on the derivation of the equations, and on the techniques involved in their solution, have been given elsewhere.[1-6] The starting estimate of the number of moles of each of the chemical species present in each phase is arbitrary, and a starting point of one mole of each is used.

The number of equations to be solved is equal to the number of elements plus the number of phases. A number of possible compounds may therefore be included in the description of the equilibrium system, since the program will be able to show which compounds will not form to any appreciable extent.

A number of corrections are applied to the calculations to ensure that all the solutions will be positive and to eliminate compounds that are present only in negligible

quantities, since their inclusion would unduly slow down convergence of the system of equations.

The linear equations that must be solved in each iteration are often somewhat ill-conditioned, i.e. they form a matrix with a very small determinant. These systems can still be solved accurately using only single-precision arithmetic if the matrix is first scaled before being solved by Gaussian elimination with partial pivoting. The scaling is done by the multiplication or division of each row by a factor of 10 until the largest element in each row has a value between 1 and 10. The scaling is done in this way, rather than by the reduction of the largest element in each row to unity, to avoid the introduction of any roundoff error during the scaling process.

The technique has been applied to a wide variety of systems and has been found to be extremely reliable and stable over a wide range of conditions.

The most useful application of the technique has been to the simulation of electric-arc furnaces where, as a fairly good approximation, it can be said that the temperature and pressure of the tapped products are approximately uniform. Here the assumption of isothermal equilibrium is reasonably accurate.

If an accurate list of chemical species present at equilibrium is specified, the technique allows very good estimates for the equilibrium products to be generated, even if the system is treated as consisting of ideal solutions. Treatment of the systems as non-ideal would obviously provide more accurate results, but there is a paucity of data on activity coefficients in the complex systems of interest. A sensible approach involves the treatment of the solutions as ideal in the first place, followed possibly by the inclusion of activity coefficients. Provision has been made for these to be added to the program if they become available at a later stage.

The specification of the chemical species present at equilibrium is very simple. A list of all species of interest is displayed by the program, and the user then indicates the species that are expected to be present in each phase at equilibrium.

Figure 1 shows a typical screen layout for the specification of a slag phase. Once the list of species has been specified, the matrix of equations is automatically set up by the program. Thus the user is spared the error-fraught tedium of doing this manually.

Thermodynamic data

Because the program relies heavily on thermodynamic data for its predictions and for the energy

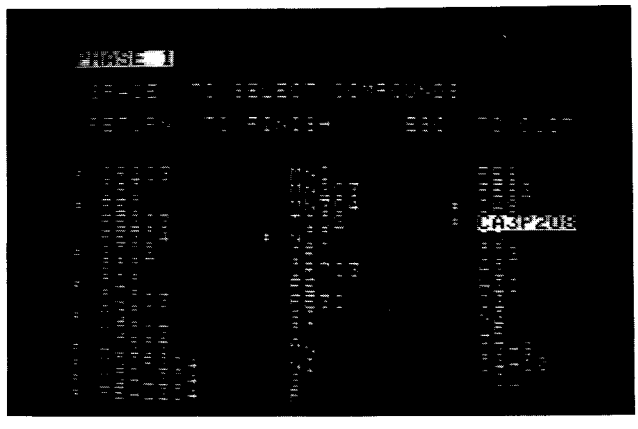

FIGURE 1. Screen layout during the specification of the chemical species present in a slag phase

COMPOUND.DATA

CP (J/K/MOL) = C1 + 1E-3*C2*T(K) + 1E5*C3*T(K)^-2 + 1E-6*C4*T(K)^2

HO (J/MOL) = Standard Enthalpy of Formation at 298K, 1 atm

SO (J/K/MOL) = Standard Entropy of Formation at 298K, 1 atm

COMPOUND	MW	PHASE	TEMP (K)	HO(J)	SO(J/K)	C1	C2	C3	C4
CR2O3	151.99	1	298 - 1800	-1129680	81.170	119.370	9.205	-15.648	0.000
FEO	71.85	1	298 - 1650	-272044	60.752	50.802	8.615	-3.310	0.000
		2	1650 - 3687	-261069	55.413	68.199	0.000	0.000	0.000
CR	52.00	1	298 - 1000	0	23.640	17.715	22.966	-0.377	-9.033
		2	1000 - 2130	4051	32.681	18.067	15.531	-16.698	0.000
		3	2130 - 2945	11758	18.065	39.330	0.000	0.000	0.000
		4	2945 - 3100	378631	154.528	30.786	0.000	0.000	0.000
FE	55.85	1	298 - 800	0	27.280	28.175	-7.318	-2.895	25.041
		2	800 - 1000	-52991	-111.337	-263.454	255.810	619.232	0.000
		3	1000 - 1042	157699	354.770	-641.905	696.339	0.000	0.000
		4	1042 - 1060	-529453	-1036.133	1946.255	-1787.497	0.000	0.000
		5	1060 - 1184	-418215	-979.395	-561.932	334.143	2912.114	0.000
		6	1184 - 1665	8260	35.959	23.991	8.360	0.000	0.000
		7	1665 - 1809	6144	33.243	24.635	9.904	0.000	0.000
		8	1809 - 3135	3401	17.276	46.024	0.000	0.000	0.000
		9	3135 - 3600	406766	173.396	27.062	0.000	0.000	0.000

TABLE 1. Sample of thermodynamic data for chemical species

calculations, it is imperative to obtain the best available data. For all chemical species of interest, therefore, data have been obtained from McGill University's F*A*C*T thermodynamic database[7] in Montreal, Canada, via a computer satellite link.

Examples of the data used by the program are given for only a few species in Table 1.

Programming considerations

Experience has shown that simulation programs will be used only if they are able to produce results that are easy to interpret and that can be obtained from a limited amount of readily available data. It is necessary for the program to simulate real operation as closely as possible. In this way, it is easily seen what the outcome of any experimental work is likely to be, and the effects of any changes to an existing process are easily determined.

Furthermore, the program must be easy to use. It needs to be forgiving when the user makes a mistake and must always recover from errors. When data are requested from the user, it must be made abundantly clear exactly what is required. Default values should be provided to save the unnecessary input of standard data. The program should also retain data from the previous run of the simulator and allow the user to modify this, instead of having to enter all the data every time a simulation is run. This approach makes it easy for the user to perform a number of comparative studies involving the alteration of only one variable at a time.

The program is divided into conceptually separate modules, each

of which can be individually tested and debugged. This makes the program far easier to read. Further development of a program in which this structure has been implemented is also far easier.

In line with the latest trends in process-simulation software, the computer program was written for a microcomputer. There is a distinct shift towards the use of personal computers for process simulation wherever possible. Although personal computers operate more slowly and have less memory available than mainframes, they have the important advantage of being more accessible to the user.

It is essential for the program to be accessible to as many people as possible, since this is the best way to ensure a steady evolution of improved process models.

Examples

The PYROSIM program was originally developed for the simulation of stainless-steel production routes, but has also been successfully applied to the production of ferrochromium, chromium carbide, vanadium, and niobium, to the calcination of limestone, and to the removal of sulphur from coal. Three examples are presented to demonstrate the versatility of the PYROSIM simulator.

Example 1: The manufacture of ferrochromium

Ferrochromium is conventionally produced in a submerged-arc furnace, from chromite, a source of carbon (typically coal), and some fluxes. Subsequently, the metal and the slag are separated and cooled.

The results of a simulation of ferrochromium production are shown in Addendum I. The small difference between the calculated slag composition and that obtained in industrial practice is ascribed to the fact that isothermal equilibrium is not truly obtained in this particular operation.

The reactions taking place in the furnace are extremely complex, and the solution of the resultant chemical equilibria is virtually impossible without the use of a computer program using the technique of free-energy minimization. This typical problem involves the presence of 3 phases, 27 chemical species, and 12 elements. The presence of the following chemical species is allowed for in the specification of the species present at equilibrium:

GAS CO, CO_2, H_2, H_2O, N_2

SLAG Cr_2O_3, FeO, SiO_2, CaO, MgO, Al_2O_3, $MgCr_2O_4$, $MgAl_2O_4$, $FeCr_2O_4$, CaS, $Ca_3P_2O_8$

METAL Cr, Cr_3C_2, Cr_7C_3, $CrSi$, Fe, Fe_3C, Si, SiC, C, FeS, P.

The furnace model must be able to select, from a number of sets, the appropriate set of equilibrium species, depending on the elements present. For example, H_2, H_2O, and N_2 would be left out of the gas specification if there were no sources of hydrogen and nitrogen in the feed materials.

The inclusion of the spinel-forming double oxides in the slag phase and the carbides in the metal phase increases the accuracy of the model. The distribution between the slag and the metal of the impurities sulphur and phosphorus is currently modelled on the assumption that CaS and

$Ca_3P_2O_8$ are present in the slag and FeS and P are present in the metal. The equilibrium of this complex, multiphase, multireaction system is readily solved by the program.

The use of a completely arbitrary starting estimate for the number of moles of each substance present required 13 iterations to solve the system of equations to an accuracy of more than five decimal places. This ensured that an isolated minimum had been found.

The program can be used to devise recipes of various raw materials to produce a particular grade of ferrochromium. The generation of recipes, a design process, is carried out by repeated simulations, each of which uses a better estimate of the process requirements than the previous one, until the desired specifications are met. Slag properties can be calculated at the same time.

Detailed studies can be made of the effects of particular changes to the process. For example, the user may wish to investigate the effect of varying only the coal addition to the process on the degree of reduction of the various oxides. Such studies are extremely difficult to carry out experimentally, since it is difficult to keep all the other variables constant while one parameter is varied. Such investigations may be useful in industry as well as in undergraduate education.

Example 2: Production of semi-stainless steel

Stainless steel is conventionally produced in three stages. First, high-carbon ferrochromium is produced in a submerged-arc furnace, as described in example 1. The metal and slag are then cooled and separated, and the ferrochromium is melted in an open-arc furnace together with a source of iron, other alloying additions such as nickel, and fluxes. A refining stage is then carried out to lower the level of carbon in the alloy and to remove impurities.

Addendum II shows the results of a simulation of the first and second stages, resulting in the production of semi-stainless steel.

Example 3: Drying and pre-heating of the furnace charge

In the production of ferrochromium, the requirements of electrical energy can be reduced by the use of the furnace off-gas to dry and preheat at least part of the furnace charge.

Addendum III shows the results of such a process. It can be seen that a saving of 15% of the electrical energy requirements can be expected, relative to the case of no drying and preheating.

Conclusions

The *PYROSIM* program can simulate the production of a number of materials by a variety of different process routes. Similar processes can then be compared on the basis of the costs of raw materials and the consumption of electrical energy.

The technique of free-energy minimization is a very valuable one for the solution of problems relating to chemical equilibrium. Eriksson's method[1] is robust and reliable. When this technique is placed within a framework that allows for the simple

specification of mineral feeds and calculates energy requirements, the potential of this approach is more fully realized.

The simulator exhibited good convergence for all the flowsheets investigated.

The availability of a computer program for the simulation of pyrometallurgical processes should be of value to everyone concerned with the comparison of process routes. A great deal of time and effort can be saved by the use of such a program.

Acknowledgements

This paper is published by permission of the Council for Mineral Technology. This work was done in partial fulfilment of the requirements of the MSc degree from the Department of Metallurgy and Materials Engineering of the University of the Witwatersrand.

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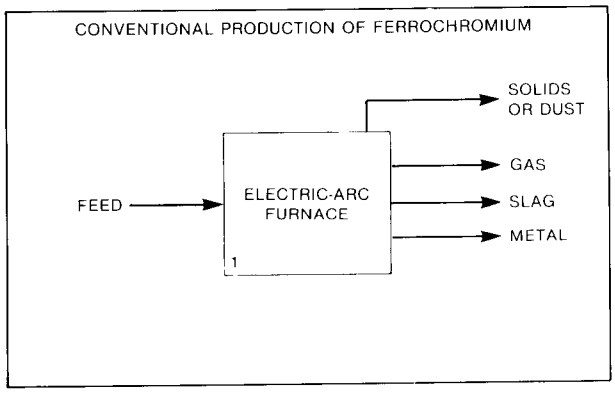
7. Thermfact, 447 Berwick Avenue, Mont-Royal, Quebec, Canada H3R 1Z8.

Addendum I: Simulation of a process for the production of ferrochromium

MASS

	FLOW (KG/HR)	TEMP. (DEG.C)
FEED 1		
CHROMITE	520.0	25
QUARTZITE	90.0	25
LIMESTONE	115.0	25
COAL	210.0	25
PRODUCTS 1		
GAS	340.0	1700
SLAG	308.2	1700
METAL	287.2	1700



OPERATION

UNIT 1

OPERATING TEMPERATURE = 1700 DEG.C
OPERATING PRESSURE = 1 ATM
SLAG LIQUIDUS TEMPERATURE = 1620 DEG.C
SLAG BASICITY = 1.2
EFFECTIVE SLAG CR2O3=.1 FEO=.1 SIO2=32.5 CAO=18.9 MGO=20.8 AL2O3=26.3 CR/FE=.7
EFFECTIVE METAL CR=57.4 FE=33.5 SI=2.08 C=7 S=.001 P=.005

ENERGY

UNIT 1 REQUIRES 1130 KWH (4050 MJ) PER HOUR OF OPERATION, INCLUDING A RATE OF ENERGY LOSS OF 100 KW
THIS IS 3920 KWH PER TON OF METAL PRODUCED IN THIS UNIT

ANALYSES

(MASS %)

	CR2O3	CRO	FEO	FE2O3	FE3O4	SIO2	SIO	CAO	CACO3	MGO	MGCO3	AL2O3	MGCR2O4	MGAL2O4
FEED 1														
CHROMITE	46.300	0.000	20.000	4.000	0.000	1.100	0.000	0.200	0.000	11.500	0.000	14.500	0.000	0.000
QUARTZITE	0.000	0.000	0.500	0.000	0.000	99.500	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	4.200	0.000	0.000	92.070	3.280	0.000	0.450	0.000	0.000
COAL	0.311	0.000	0.420	0.000	0.000	6.086	0.000	0.303	0.000	0.236	0.000	2.440	0.000	0.000
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SLAG	0.006	0.000	0.131	0.000	0.000	32.482	0.000	18.867	0.000	13.280	0.000	7.361	0.123	26.425
METAL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

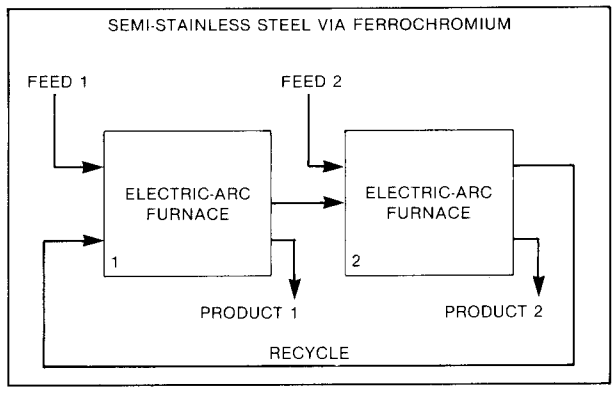
	MNO	MN2O3	MN3O4	TIO2	NIO	CR	CR3C2	CR7C3	CRSI	FE	FE3C	SI	SIC	C
FEED 1														
CHROMITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
QUARTZITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
COAL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	57.000
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SLAG	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METAL	0.000	0.000	0.000	0.000	0.000	13.720	27.107	19.352	4.026	29.915	3.800	0.262	0.581	1.232

	NI	S	P	FES	CAS	CA3P2O8	CO	CO2	H2	H2O	O2	N2	AR	VOL.
FEED 1														
CHROMITE	0.000	0.010	0.017	0.000	0.000	0.000	0.000	0.000	0.000	2.400	0.000	0.000	0.000	0.000
QUARTZITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
COAL	0.000	0.560	0.090	0.000	0.000	0.000	0.000	0.000	0.000	2.900	0.000	0.000	0.000	29.744
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	96.143	0.042	1.289	0.016	0.000	2.511	0.000	0.000
SLAG	0.000	0.000	0.000	0.000	0.895	0.429	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METAL	0.000	0.000	0.005	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Addendum II: Simulation of a conventional process for the production of a semi-stainless steel

MASS

	FLOW (KG/HR)	TEMP. (DEG.C)
FEED 1		
CHROMITE	520.0	25
QUARTZITE	90.0	25
LIMESTONE	115.0	25
COAL	210.0	25
PRODUCTS 1		
GAS	340.0	1700
SLAG	308.2	1700
TO NEXT UNIT		
METAL	287.2	25
FEED 2		
CHROMITE	85.0	25
NICKEL	66.0	25
QUARTZITE	35.0	25
LIMESTONE	65.0	25
STEEL SCRAP	632.0	25
PRODUCTS 2		
GAS	42.9	1650
SLAG	128.0	1650
METAL	999.3	1650



OPERATION

UNIT 1

OPERATING TEMPERATURE = 1700 DEG.C
OPERATING PRESSURE = 1 ATM
SLAG LIQUIDUS TEMPERATURE = 1620 DEG.C
SLAG BASICITY = 1.2
EFFECTIVE SLAG CR2O3=.1 FEO=.1 SIO2=32.5 CAO=18.9 MGO=20.8 AL2O3=26.3 CR/FE=.7
EFFECTIVE METAL CR=57.4 FE=33.5 SI=2.08 C=7 S=.001 P=.005

UNIT 2

OPERATING TEMPERATURE = 1650 DEG.C
OPERATING PRESSURE = 1 ATM
SLAG LIQUIDUS TEMPERATURE = 1338 DEG.C
SLAG BASICITY = .8
EFFECTIVE SLAG CR2O3=10.7 FEO=1.2 SIO2=41.9 CAO=25.2 MGO=9.3 AL2O3=9.9 CR/FE=7.8
EFFECTIVE METAL CR=18.3 FE=74 NI=6.6 SI=.05 C=1.1 S=.004 P=0

ENERGY

UNIT 1 REQUIRES 1130 KWH (4050 MJ) PER HOUR OF OPERATION, INCLUDING A RATE OF ENERGY LOSS OF 100 KW
THIS IS 3920 KWH PER TON OF METAL PRODUCED IN THIS UNIT

UNIT 2 REQUIRES 586 KWH (2110 MJ) PER HOUR OF OPERATION, INCLUDING A RATE OF ENERGY LOSS OF 50 KW
THIS IS 587 KWH PER TON OF METAL PRODUCED IN THIS UNIT

ANALYSES

(MASS %)

	CR2O3	CRO	FEO	FE2O3	FE3O4	SIO2	SIO	CAO	CACO3	MGO	MGCO3	AL2O3	MGCR2O4	MGAL2O4
FEED 1														
CHROMITE	46.300	0.000	20.000	4.000	0.000	1.100	0.000	0.200	0.000	11.500	0.000	14.500	0.000	0.000
QUARTZITE	0.000	0.000	0.500	0.000	0.000	99.500	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	4.200	0.000	0.000	92.070	3.280	0.000	0.450	0.000	0.000
COAL	0.311	0.000	0.420	0.000	0.000	6.086	0.000	0.303	0.000	0.236	0.000	2.440	0.000	0.000
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SLAG	0.006	0.000	0.131	0.000	0.000	32.482	0.000	18.867	0.000	13.280	0.000	7.361	0.123	26.425
TO NEXT UNIT														
METAL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FEED 2														
CHROMITE	46.300	0.000	20.000	4.000	0.000	1.100	0.000	0.200	0.000	11.500	0.000	14.500	0.000	0.000
NICKEL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
QUARTZITE	0.000	0.000	0.500	0.000	0.000	99.500	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	4.200	0.000	0.000	92.070	3.280	0.000	0.450	0.000	0.000
STEEL SCRAP	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PRODUCTS 2														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SLAG	1.513	0.000	1.202	0.000	0.000	41.868	0.000	25.199	0.000	4.910	0.000	4.913	11.626	6.896
METAL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

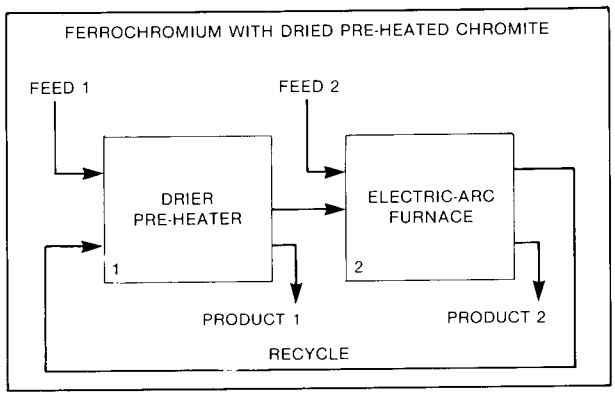
	MNO	MN2O3	MN3O4	TIO2	NIO	CR	CR3C2	CR7C3	CRSI	FE	FE3C	SI	SIC	C
FEED 1														
CHROMITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
QUARTZITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
COAL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	57.000
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SLAG	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TO NEXT UNIT														
METAL	0.000	0.000	0.000	0.000	0.000	13.720	27.107	19.352	4.026	29.915	3.800	0.262	0.581	1.232
FEED 2														
CHROMITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
NICKEL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
QUARTZITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
STEEL SCRAP	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	99.510	0.000	0.250	0.000	0.150
PRODUCTS 2														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SLAG	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METAL	0.000	0.000	0.000	0.000	0.000	16.554	1.709	0.172	0.109	68.793	5.575	0.007	0.005	0.460

	NI	S	P	FES	CAS	CA3P2O8	CO	CO2	H2	H2O	O2	N2	AR	VOL.
FEED 1														
CHROMITE	0.000	0.010	0.017	0.000	0.000	0.000	0.000	0.000	0.000	2.400	0.000	0.000	0.000	0.000
QUARTZITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
COAL	0.000	0.560	0.090	0.000	0.000	0.000	0.000	0.000	0.000	2.900	0.000	0.000	0.000	29.744
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	96.143	0.042	1.289	0.016	0.000	2.511	0.000	0.000
SLAG	0.000	0.000	0.000	0.000	0.895	0.429	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TO NEXT UNIT														
METAL	0.000	0.000	0.005	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FEED 2														
CHROMITE	0.000	0.010	0.017	0.000	0.000	0.000	0.000	0.000	0.000	2.400	0.000	0.000	0.000	0.000
NICKEL	100.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
QUARTZITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
STEEL SCRAP	0.000	0.050	0.050	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PRODUCTS 2														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	94.999	0.251	0.000	4.751	0.000	0.000	0.000	0.000
SLAG	0.000	0.000	0.000	0.000	0.506	1.344	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METAL	6.604	0.000	0.000	0.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Addendum III: Simulation of a process for the production of ferrochromium, in which the off-gas is used to dry and pre-heat the furnace charge

MASS

	FLOW (KG/HR)	TEMP. (DEG.C)
FEED 1		
CHROMITE	520.0	25
OFF GAS	329.5	1500
PRODUCTS 1		
GAS	342.0	666
TO NEXT UNIT		
SOLIDS OR DUST	507.7	666
FEED 2		
QUARTZITE	90.0	25
LIMESTONE	115.0	25
COAL	210.0	25
PRODUCTS 2		
GAS	329.5	1700
SLAG	296.9	1700
METAL	296.4	1700



OPERATION

UNIT 1

OPERATING TEMPERATURE = 670 DEG.C
OPERATING PRESSURE = 1 ATM

UNIT 2

OPERATING TEMPERATURE = 1700 DEG.C
OPERATING PRESSURE = 1 ATM
SLAG LIQUIDUS TEMPERATURE = 1647 DEG.C
SLAG BASICITY = 1.4
EFFECTIVE SLAG CR2O3=0 FEO=.1 SIO2=30.1 CAO=19.6 MGO=21.6 AL2O3=27.3 CR/FE=.3
EFFECTIVE METAL CR=55.7 FE=32.5 SI=3.72 C=8.1 S=0 P=.01

ENERGY

UNIT 1: ENERGY CONTROLLED PROCESS WITH A RATE OF ENERGY LOSS OF 10 KW

UNIT 2 REQUIRES 1030 KWH (3710 MJ) PER HOUR OF OPERATION, INCLUDING A RATE OF ENERGY LOSS OF 100 KW
THIS IS 3470 KWH PER TON OF METAL PRODUCED IN THIS UNIT

ANALYSES
(MASS %)

	CR2O3	CRO	FEO	FE2O3	FE3O4	SIO2	SIO	CAO	CACO3	MGO	MGCO3	AL2O3	MGCR2O4	MGAL2O4
FEED 1														
CHROMITE	46.300	0.000	20.000	4.000	0.000	1.100	0.000	0.200	0.000	11.500	0.000	14.500	0.000	0.000
OFF GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TO NEXT UNIT														
SOLIDS OR DUST	47.425	0.000	20.486	4.097	0.000	1.127	0.000	0.205	0.000	11.780	0.000	14.852	0.000	0.000
FEED 2														
QUARTZITE	0.000	0.000	0.500	0.000	0.000	99.500	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	4.200	0.000	0.000	92.070	3.280	0.000	0.450	0.000	0.000
COAL	0.311	0.000	0.420	0.000	0.000	6.086	0.000	0.303	0.000	0.236	0.000	2.440	0.000	0.000
PRODUCTS 2														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SLAG	0.002	0.000	0.086	0.000	0.000	30.070	0.000	19.597	0.000	13.722	0.000	7.435	0.032	27.711
METAL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

	MNO	MN2O3	MN3O4	TIO2	NIO	CR	CR3C2	CR7C3	CRSI	FE	FE3C	SI	SIC	C
FEED 1														
CHROMITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
OFF GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
TO NEXT UNIT														
SOLIDS OR DUST	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FEED 2														
QUARTZITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
COAL	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	57.000
PRODUCTS 2														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
SLAG	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METAL	0.000	0.000	0.000	0.000	0.000	11.658	31.594	13.978	6.079	28.456	4.291	0.489	1.571	1.874

	NI	S	P	FES	CAS	CA3P2O8	CO	CO2	H2	H2O	O2	N2	AR	VOL.
FEED 1														
CHROMITE	0.000	0.010	0.017	0.000	0.000	0.000	0.000	0.000	0.000	2.400	0.000	0.000	0.000	0.000
OFF GAS	0.000	0.000	0.000	0.000	0.000	0.000	96.465	0.030	0.906	0.008	0.000	2.591	0.000	0.000
PRODUCTS 1														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	92.945	0.029	0.873	3.657	0.000	2.496	0.000	0.000
TO NEXT UNIT														
SOLIDS OR DUST	0.000	0.010	0.017	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
FEED 2														
QUARTZITE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
LIMESTONE	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
COAL	0.000	0.560	0.090	0.000	0.000	0.000	0.000	0.000	0.000	2.900	0.000	0.000	0.000	29.744
PRODUCTS 2														
GAS	0.000	0.000	0.000	0.000	0.000	0.000	96.465	0.030	0.906	0.008	0.000	2.591	0.000	0.000
SLAG	0.000	0.000	0.000	0.000	0.930	0.417	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
METAL	0.000	0.000	0.010	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000