Learning and Teaching using Process Modeling and Simulation

Xiaowei Pan

Department of Metallurgy, University of Johannesburg, PO Box 17011 Doornfontein, 2028 Johannesburg, South Africa, phone: +27 11 559 6371; fax: +27 11 559 6194 ; e-mail: xpan@uj.ac.za

ABSTRACT

Depending on the way of teaching, teachers can make enormous difference in the quality of learning and teaching at university. This paper covers how to use process modelling and process simulation to help students to understand some of the complex industrious processes easier and better. Many industrial processes, such as the production of ferroalloy, are extremely complicated and often those processes are interacted and involve many physicochemical reactions that mostly happen simultaneously. In this paper, application of simulation to learning and teaching of ferroalloy production subject is presented. It is observed that students are more likely to infuse the knowledge they learnt into the current subject they are studying, if process simulation is integrated into the subject with direct tie-ins of examples of what-if scenario that are linked to the real process and have real meaning of improvement. Other issues relevant to simulation are discussed, including process suitability for simulation, development of a simulation model, classes of simulation, advantages and disadvantages of process simulation.

Keywords: learning, teaching, process simulation, ferrochrome production

1. INTRODUCTION

Ferrochrome production is one of the subjects lectured at the Department of Metallurgy, University of Johannesburg. Ferrochrome, an alloy used to make stainless steel and especial steels, is mainly produced by carbothermic reduction of chromite ore in a submerged arc furnace or in a DC plasma furnace. The raw material, consisting of chromite ores, fluxes and reductants, are batched and mixed before being fed into the furnaces. In the furnace, the chromite ore (consisting mainly of iron oxides, chromium oxide, magnesium oxide, and aluminum oxide) are reduced with carbon to for the alloy. The reduction is highly endothermic and the production process is energy-intensive, and consumes approximately 3,300-3,800kWh per ton of metal produced. The energy is generally supplied in the form of electrical energy through carbon electrodes.

As MgO and Al2O3 are oxides with high liquidus temperature, fluxes like limestone, dolomite and quartz are loaded to form liquid slag phase so that it can be tapped out of the furnace. Alloy and slag are tapped through the taphole into ladles in a cascade arrangement, with the alloy being trapped in the first ladle, and the slag overflowing to the next ladles or into a pit, see in Figure 1.

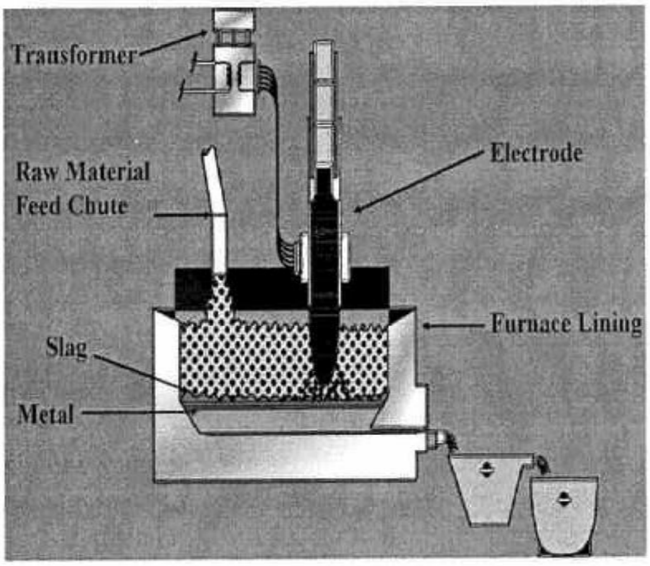


Fig. 1. Schematic representation of a submerged arc furnace used to produce ferrochrome, including furnace, raw material, slag, metal, electrode, tap-hole and ladles.

South Africa, with about 80% of world chromite ore reserves, is one of the major producers of ferrochrome, and its production accounts for about 34% of the total production in the world. With an increased challenge from other major producers, such as China and India, the ferrochrome producers in South Africa are exploring options to reduce the production cost.

The cost of electricity accounts for about 35-40% of total production cost. Due to the shortage of power supply in South Africa, the cost of electricity has more than doubled since 2008, and a plan has been tabled to increase the electricity price by 16% every year from 2013 to 2018.

With a sharp increase in electricity cost, it is imperative to look for any alternatives that can use less electricity. A simulation of ferrochrome production, with no doubt, can be used to investigate various alternatives in a virtual environment, including the effect of various chromite ores on the electrical energy consumption [1]. Relevant work used to develop a simulation for ferrochrome production has been done and can be found [2-4].

To help students to apply the principles to the production processes, particularly to understand the pragmatic challenges facing the industry, simulation makes the learning easier and faster in the classroom.

2. PROCESS MODELLING AND SIMULATION

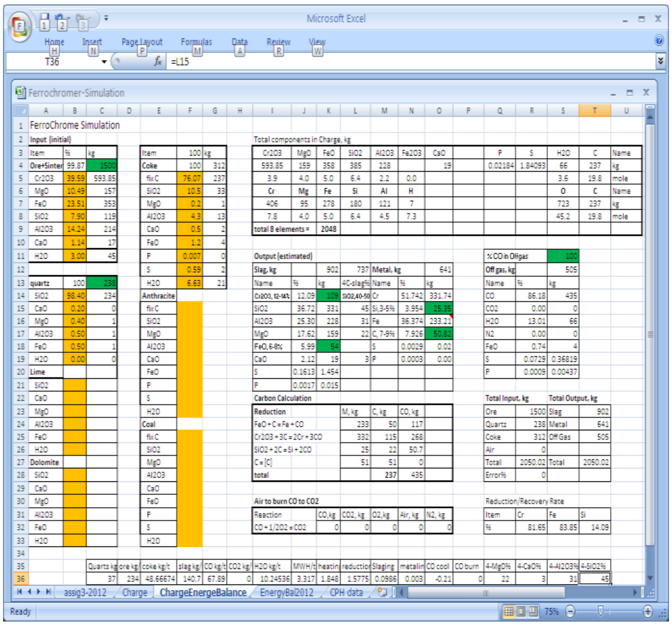
Process modeling in general is the process of producing a model which is a presentation of the process of interest. A process model is similar to but simpler than the process it represents. The main purpose of a model is to enable us to understand, analyze and predict the effect of changes to the process. A process model intended for a simulation study can be classified as a first principle model or knowledge-base model. The first principle model is developed using mathematics conjunction with science like physics and chemistry. When a process is very complex and is ill-understood, the process cannot be simplified in any kind of mathematics. With enough experience or experiments, a large amount of data can be used to generate a knowledge-based model, using techniques like fuzzy logic, decision tree, and neural networks.

On the one hand, a process model should be a close approximation to the real process and incorporate most of its salient features and functions, including, process inputs, outputs and disturbances. On the other hand, a process model should not be so complex that it is impossible to understand and experiment with it. A good model is a judicious tradeoff between realism and simplicity. It is quoted that “All models are bad, it maters how useful they are” from a presentation by X. Pan and B. Livneh [5]. It is accentuated well that a model is a good one only if it is useful.

3. SIMULATION OF FERROCHROME PRODUCTION

An excel-based simulation called Ferroalloy Simulation (Ferroalloy-Sim), is developed and used to help learners to understand the effect of different chromite ores on the electricity consumption used to produce high carbon ferrochrome in submerged are furnace (HCFeCr) [1].

The Ferroalloy Simulation is developed using the principles of mass balance and energy balance incorporated with operational conditions. The interface can be seen in Fig. 2. The simulation requires three inputs and generates the results of charge recipe, mass and composition for slag, metal, and off gas, with the energy consumption associated with the production process.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U
1	FerroChrome Simulation																				
2	Input (initial)								Total components in Charge, kg												
3	Item	%	kg		Item	100	kg		Cr2O3	MgO	FeO	SiO2	Al2O3	Fe2O3	CaO		P	S	H2O	C	Name
4	Ore+Sinter	99.87	1500		Coke	100	312		593.85	159	358	385	228		19		0.02184	1.84093	66	237	kg
5	Cr2O3	39.59	593.85		fix C	76.07	237		3.9	4.0	5.0	6.4	2.2	0.0					3.6	19.8	mole
6	MgO	10.49	157		SiO2	10.5	33		Cr	Mg	Fe	Si	Al	H					O	C	Name
7	FeO	23.51	353		MgO	0.2	1		406	95	278	180	121	7					723	237	kg
8	SiO2	7.90	119		Al2O3	4.3	13		7.8	4.0	5.0	6.4	4.5	7.3					45.2	19.8	mole
9	Al2O3	14.24	214		CaO	0.5	2		total 8 elements =		2048										
10	CaO	1.14	17		FeO	1.2	4														
11	H2O	3.00	45		P	0.007	0		Output (estimated)								% CO in Offgas		100		
12					S	0.59	2		Slag, kg		902	737	Metal, kg		641		Off gas, kg		505		
13	quartz	100	238		H2O	6.63	21		Name	%	kg	4C-slag%	Name	%	kg		Name	%	kg		
14	SiO2	98.40	234		Anthracite				Cr2O3, 12-14%	12.09	109	SiO2,40-50	Cr	51.742	331.74		CO	86.18	435		
15	CaO	0.20	0		fix C				SiO2	36.72	331	45	Si,3-5%	3.954	25.35		CO2	0.00	0		
16	MgO	0.40	1		SiO2				Al2O3	25.30	228	31	Fe	36.374	233.21		H2O	13.01	66		
17	Al2O3	0.50	1		MgO				MgO	17.62	159	22	C, 7-9%	7.926	50.82		N2	0.00	0		
18	FeO	0.50	1		Al2O3				FeO, 6-8%	5.99	54		S	0.0029	0.02		FeO	0.74	4		
19	H2O	0.00	0		CaO				CaO	2.12	19	3	P	0.0003	0.00		S	0.0729	0.36819		
20	Lime				FeO				S	0.1613	1.454						P	0.0009	0.00437		
21	SiO2				P				P	0.0017	0.015										
22	CaO				S				Carbon Calculation								Total Input, kg		Total Output, kg		
23	MgO				H2O				Reduction			M, kg	C, kg	CO, kg			Ore	1500	Slag	902	
24	Al2O3				Coal				FeO + C = Fe + CO			233	50	117			Quartz	238	Metal	641	
25	FeO				fix C				Cr2O3 + 3C = 2Cr + 3CO			332	115	268			Coke	312	Off Gas	505	
26	H2O				SiO2				SiO2 + 2C = Si + 2CO			25	22	50.7			Air	0			
27	Dolomite				MgO				C = [C]			51	51	0			Total	2050.02	Total	2050.02	
28	SiO2				Al2O3				total				237	435			Error%	0			
29	CaO				CaO																
30	MgO				FeO				Air to burn CO to CO2								Reduction/Recovery Rate				
31	Al2O3				P				Reaction	CO,kg	CO2, kg	O2,kg	Air, kg	N2, kg			Item	Cr	Fe	Si	
32	FeO				S				CO + 1/2O2 = CO2	0	0	0	0	0			%	81.65	83.85	14.09	
33	H2O				H2O																
34																					
35			Quarts kg	ore kg/	coke kg/t	slag kg/	CO kg/t	CO2 kg/	H2O kg/t	MWH/t	heating	reductio	Slaging	metalin	CO cool	CO burn	4-MgO%	4-CaO%	4-Al2O3%	4-SiO2%	
36			37	234	48.66674	140.7	67.89	0	10.24536	3.317	1.848	1.5775	0.0986	0.003	-0.21	0	22	3	31	45	

Fig. 2. Ferroalloy simulation used to calculate charge recipe and electricity consumption for ferrochrome production in a submerged arc furnace

Lumpy chromite ores produced in six different locations of the Bushveld Igneous Complex in South Africa are used. Quartzite is added as flux, and coke is used as reductant. The names of different chromite ores produced in South Africa are listed in Table I with other process parameters used to produce one ton of ferrochrome.

Based on the production of ferrochrome in South Africa, the following conditions are used as major smelting parameters:

- 6% FeO in slag
- 12% Cr2O3 in slag
- 45% SiO2 in the 3-component slag of SiO2-MgO-Al2O3
- 8% carbon in metal
- 4% silicon in metal
- Slag temperature 1700 ^{0}C
- Metal temperature 1600 ^{0}C

ore names	ore kg/t	quartzite kg/t	coke kg/t	slag kg/t	CO kg/t	MWH/t
Steelpoort	2202.02	455.73	490.86	1350.10	684.61	3.33
Lannex	2265.62	413.24	488.43	1369.81	680.29	3.31
Elandsdrift	2338.73	371.27	486.67	1405.82	678.95	3.32
Mooinooi	2339.57	372.90	487.49	1423.85	678.63	3.33
Millsell	2460.79	338.00	489.06	1563.55	679.01	3.41
Tweefontein	3196.63	164.69	483.11	2017.23	670.50	3.63

Table 1. Major smelting parameters used to produce one ton of hcfecr in saf using different lump ores

4. SIMULATION RESULT

4.1. Smelting Parameters

The main parameters used to produce high carbon ferrochrome in a submerged arc furnace are selected and listed in Table I, including raw material consumption, energy consumption, mass of metal, slag and offgas. They are expressed in terms of kilogram per ton of produced metal (kg/t):

- Ore consumption, ore-kg/t
- Flux, quartzite consumption, quartzite-kg/t
- Reductant, coke consumption, coke-kg/t

- Electric energy consumption, MWh/t
- Metal produced, t
- Slag produced, slag-kg/t
- Offgas produced, offgas-kg/t

4.2. Composition of SA Chromite Lumpy Ores

The selected chromite lumpy ores contain mainly Cr2O3, FeO, SiO2, MgO, Al2O3 and small amount of CaO. The range of chemical composition is 29-43% Cr2O3, 20-24% FeO, 4-20% SiO2, 11-17% MgO, 10-14% Al2O3, 1-2% CaO.

The contents of MgO, Al2O3 and CaO have small changes in all selected chromite ores, particularly CaO with a range of only 1-2%. The major changes of the chromite ores appear in the contents of SiO2, Cr2O3 and FeO. The content of SiO2% increases from 4% of Steelpoort ore to 19% of Tweefontein ore, and the contents of Cr2O3%, FeO% decreases from 43 to 38, and 24 to 23 respectively, as shown in Fig. 3. The total content of Cr2O3 and FeO decreases from 67% to 50%, from Steelpoort ore to Tweefontein ore.

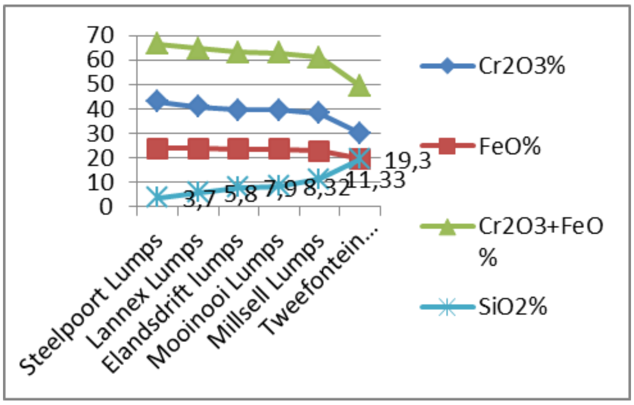


Fig. 3. Chemical composition of chromite lumpy ores, with increase in SiO2% and decrease in Cr and Fe oxides from Steelpoort ore to Tweefontein ore

4.3. Raw Material Consumption

The consumption of ores, flux quartzite, reductant coke, and the produced mass of slag and CO gas are shown in Fig. 4**,** with left axis in terms of kg per ton of metal (kg/t). The electric energy consumption is also shown in the same Figure with right axis in mega watt/hour per ton of metal (MWh/t).

When producing one ton of high-carbon ferrochrome in SAF, the Tweefontein lump ore has the highest ore consumption at 3200 kg/t, 22% and exceeds by more than 30% the consumption of Millsell and other ores. At the same time, the Tweefontein lump ore requires the lowest quartzite consumption at 160 kg/t. It is 205%-225% lower than the quartzite consumption comparing the ores of Millsell, Elandsdrift, and Mooinooi, and it is by 277%-251% lower when comparing the ore of Steelpoort and Lannex, see in Fig. 5.

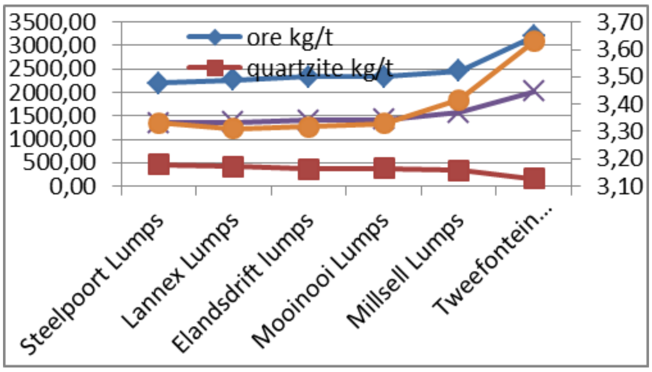


Fig. 4. Raw material consumption when producing one ton of high-carbon ferrochrome using different chromite lumpy ores of South Africa, with left axis for kg/t, and right axis for MWh/t

With the combination of high ore consumption and low quartzite consumptions when using lump ore from Tweefontein, the production process generates the most slag, about 2000 kg/t. it is 22% more than that of Millsell ore, and 29-33% more than the others.

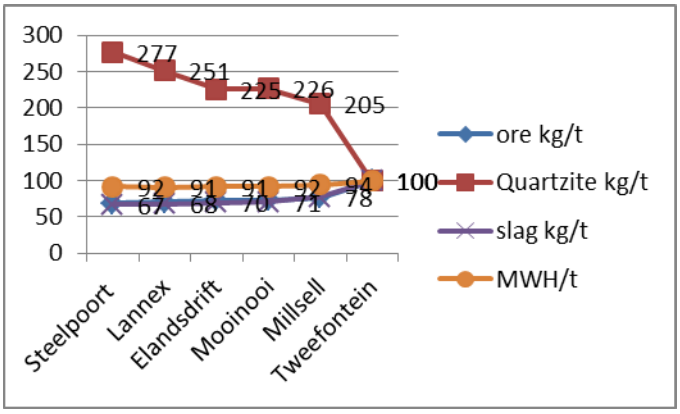


Fig. 5. Consumption of ore, quartzite, energy and production of slag when producing one ton of high carbon ferrochrome, compared with Tweefontein chromite lump ore

4.4. Electric Energy Consumption

The electric energy consumption ranges from 3.31 to 3.63 MWh per ton metal produced (MWh/t), when using the selected 6 different chromite lumpy ores. Tweefontein lumpy chromite ore requires the highest electric energy, with amount of 3.63 MWh/t, as shown in Fig. 7. Millsell lumpy ore requires the second highest energy at 3.41 MWh/t, and the rest of 4 chromite ores consumes similar amount of electric energy from 3.31 to 3.33 MWh/t.

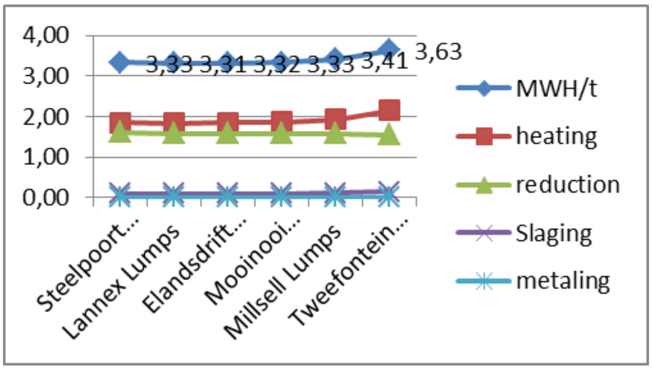


Fig. 6. Electric energy used for heating, reduction of oxides and forming of molten slag and metal when using different chromite lumpy ores produced in South Africa.

5. DISCUSSION OF PROCESS SIMULATION

5.1. Processes applicable for modelling and simulation

In general, whenever there is a process that can be modelled and that requires analysis, and carries out what-if experiment, process simulation is the right tool of choice, particularly for those processes with the following features:

- It is impossible or extremely expensive to measure or observe the processes, e.g., the changes of raw materials and the effects on the production of ferroalloy.
- Process models can be formulated but analytic solutions are either impossible or too complicated with large queuing models.
- It is impossible or extremely expensive to validate the mathematical model describing the processes, e.g., due to insufficient data.

5.2. Development of a simulation model

A process model used for simulation consists of the following components:

- Process entities
- Process input

- Process output
- Functional relationships

In the simulation of ferroalloy production, for instance, the ferroalloy production processes are the process entities, the process input includes raw materials, energy, equipment, charge recipe, etc. The process output includes the product of ferroalloy, slag, and off gas. The functional relationships consist of all mathematic equations, including mass balance of all chemical reactions, enthalpy changes of all materials in the inputs and outputs during the processes of heating, chemical reaction and cooling. The sequences of production and some limits of the operation associated with ferroalloy smelting are part of the functional relationships.

Modeling is arguably the most critical part of a simulation study. Indeed, a simulation study can be only as good as the simulation model (L Sevgi, 2006)[6]. The development of a simulation model comprises the following steps:

1. Identify the problem within a concerned process.
2. Define overall objective of the study with a set of performance measures, as quantitative criteria.
3. Collect and pre-process real process data.
4. Develop a process model using a simulation software.
5. Validate the model using real process data.
6. Document model for feature use and improvement.
7. Select appropriate conditions and conduct what-if scenario simulations.
8. Interpret and present the results
9. Make recommendations for future actions

5.3. Classes of simulations

Simulation helps us to create a virtual system of a real process or a system, with human in the process loop. The simulation is made to perform as if it were the real process. The more advanced version of simulation allows the human to interface with the virtual mockup operating in a realistic simulation environment. There are three classes of model-based simulations, namely virtual simulation, constructive and live simulations:

- Virtual simulations represent systems both physically and electronically.
- Constructive simulations represents a system and its deployment, including computer-aided design/manufacturing (CAD/M)
- Live simulations are simulated operations with real operators and real equipment, such as initial production run, operational tests.

5.4. Advantages and pitfalls of process simulation

It is no doubt that process simulations have become one of the most used techniques to help identify and improve processes both for manufacturing industries and business operations. When used judiciously, a simulation can have the following benefits:

- Obtain a better understanding of the process by developing the process model and observing the system operation in detail.
- Test hypotheses about the process for feasibility.
- Study the effects of certain variables of the process through what-if scenario experiments without disrupting the real process.
- Experiment with new or unknown situations to explore any feasible ways to improve the process.
- Identify the bottlenecks in the processes, and find the most effective variables to eliminate the bottlenecks.
- Use a systems' approach to problem solving based on process analysis and re-designs.

Process simulation can be a time consuming and complex exercise, starting from model development through input-output analysis to the involvement of process experts and decision makers in the entire process. The following is a check list of pitfalls to guard against:

- Unclear objective.
- Selecting wrong performance measures.
- Process model is too complex or too simple.
- Invalid process model.
- Clashing of two independent process models with contradictory results.
- Erroneous assumptions of the process.
- Bugs in the simulation system.

5.5. Integration of simulation with learning and teaching

Researches have been done on the way in which simulation technology is used in a classroom. As stated by the office of technology assessment [7], it is becoming increasingly clear that simulation technology, in and of itself, does not directly change teaching or learning. Rather, the critical element is how the technology is incorporated into instruction.

It is observed that students are more likely to infuse the knowledge they learnt into the current subject they are studying, if process simulation is integrated into the subject with direct tie-ins and examples of what-if scenario that are linked to the process and have real meaning of improvement. Without the integration of the simulation into a subject, students perceive simulation as a separate computer-based subject, unassociated with the context of the real processes. Consequently the contents and the concepts of the subject are often left fragmented in the learner's mind.

Integration of simulation into subjects requires teachers to alter their teaching processes, no longer being the sole distributor of information and knowledge. It is from the teacher's perspective to include the use of the simulation technology to fit into the overall contents of a subject, whether there are transitions before and after the learning activity with the rest of instruction, and the extent to which simulation use is not a separate activity from other instructional contents.

6. CONCLUSION

Whereas the usage of computer simulation, particularly in engineering, began over half century ago, only the last past 2 decades or so have simulation theory and technology made a dramatic impact across the engineering fields, mainly due to the remarkable developments in the computer and computational science including both hardware and software. In this paper, application of simulation to learning and teaching of ferroalloy production subject is presented. Simulation can provide most needed exercises in the classroom, whereas they are not possible due to the complexity of the processes and the long time to carry out the required mathematic calculations. Using simulation, students can understand the processes of production better through the linkage of the subject to the real processes of production. It is observed that students are more likely to infuse the knowledge they learnt into the current subject they are studying, if process simulation is integrated into the subject with direct tie-ins and examples of what-if scenario that are linked to the real process and have real meaning of improvement. Other issues relevant to process simulation are discussed, such as process suitability for simulation, development of a simulation model, classes of simulation, advantages and disadvantages of process simulation.

REFERENCE

[1] X. Pan, South African lumpy chromite ores on ferrochrome production, International Journal of Research in Engineering and Technology (IJRET), ISSN 2277-4378, Vol.2, No. 3, 2013, pp. 112-116

[2] M.H Farjadi and J. Azari, "Effect of chromite ore quality on ferrochrome production efficiency", INFACON X, Cape Town, 2004 pp. 103-107

[3] L. Hu, "Selection of chromite ores in HC FeCr production", Ferroalloys, No6, 1990, pp. 21-28

[4] O. Naiker and T. Riley, "Xstrata Alloys in Profile", Southern African Pyrometallurgy 2006, Johannesburg, pp297-305

[5] B Livneh, X Pan, Neural networks to predict and control pyro-metallurgical processes, Proceedings of Heavy Mineral Conference, South African Institute of Mining and Metallurgy, Johannesburg, 1997, pp. 231-236

[6] L Sevgi, Modeling and simulation concepts in engineering education: virtual tools, Turk J Elec Engin, Vol. 14, No. 1, 2006, pp. 113-116

[7] Office of technology assessment (OTA). (1995), Teacher and technology: making the connection. Washington, DC: US Government Printing Office.