Mass Balance Calculations in Copper Flash Smelting by Means of Genetic Algorithms

V.M. Sanchez-Corrales, J.A. Valera-Gonzalez, P. Flores-Perez, and M. Perez-Tello

This paper presents mass balance calculations using genetic algorithms for copper smelting in an Outokumpu flash furnace. Based on the elemental composition of the copper concentrates being fed to the reactor, the mineralogical composition of the concentrate mixture is adjusted by means of genetic algorithms. The macroscopic mass balance equations for the species entering and leaving the furnace are solved and the compositions and flow rates of matte, slag, and the off-gas stream are computed. Good agreement between the predicted and plant data was obtained in terms of matte and slag flow rates, matte grade, and copper, iron, magnetite, and silica contents in the slag. Predictions are more suitable and faster to obtain with this method than a conventional method in which the mineralogical composition of the feed is not adjusted. Future applications of the formulation are discussed.

INTRODUCTION

The Outokumpu flash furnace is widely used for smelting copper sulfide concentrates.[1,2] By taking advantage of the exothermic reactions involved, a nearly complete autogenous smelting system is established. Industrial results[1,2] indicate that an autogenous operation can be obtained under conditions that lead to a matte grade of 60–65% using an oxidizing gas stream containing 45–80 vol.% oxygen.

A common practice in industry consists of blending two or more copper concentrates to make up the feed to the flash smelting furnace. To establish the appropriate operating conditions in the furnace for concentrate mixtures of varying composition, mass and energy balance calculations must be performed on a regular basis.

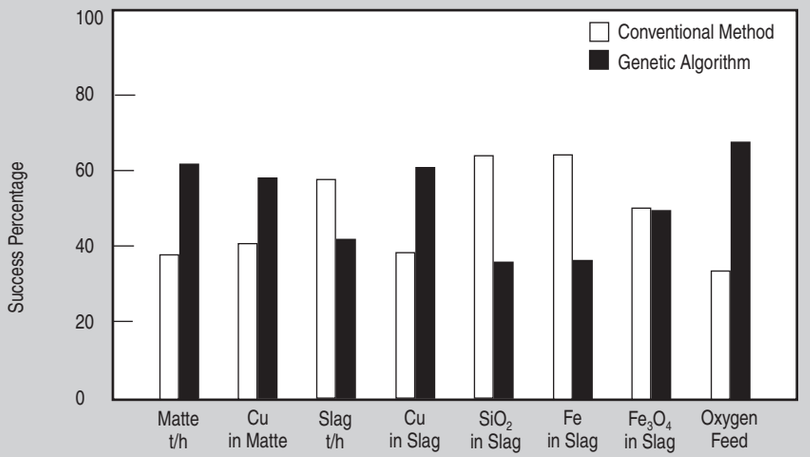

Figure 1. The success percentage for the conventional method and the genetic algorithm-based method for several mass balance calculation terms.

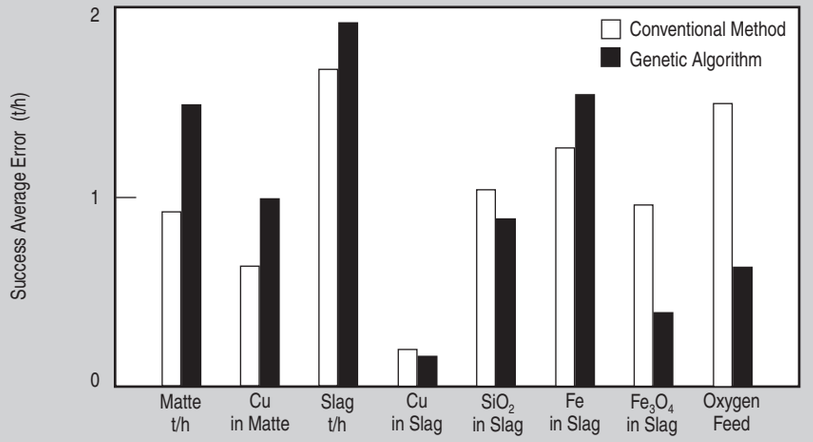

Figure 2. The average absolute error for the conventional method and the genetic algorithm-based method considering the successful cases for each method.

Typically, mass balance calculations are based upon the current elemental analysis of the concentrates blend being fed to the reactor. During this process, a trial-and-error procedure is followed until the computed mineralogical composition of each concentrate closely matches its elemental analysis. This method strongly relies on the process engineer's experience. In addition, it is time consuming, and, as the number of blending streams increases, the problem may become intractable even for experienced engineers. This paper describes the application of genetic algorithms (GA) to improve the accuracy of the mass balance calculations currently performed in modern copper flash smelters.

Genetic algorithm is a generalized term to represent a family of numerical methods built upon the fundamental laws of biological evolution. These methods have shown to be particularly useful in the analysis of numerical problems with no unique solution.[3] They have been extensively used as optimization techniques[4] in a number of engineering processes such as steelmaking, polymer production, design of pharmaceutical formulations, hydrocyclone design and performance, preparation of concrete mixtures, and cathodic protection.[5–10]

The genetic algorithm method used in this work takes into consideration the raw elemental analysis of the concentrates and computes the corresponding mineralogical composition of the feed. Such a composition is further used in the mass balance equations to predict the amounts and compositions of matte, slag, and the off-gas stream. See the sidebar for methodology details.

RESULTS AND DISCUSSION

Mass balance results for both methods were compared with actual smelter data corresponding to 38 days of operation. In every case, different mixing ratios of Cananea and La Caridad copper concentrates were used to make up the feed. The results concerning the production rate and composition of both matte and slag, as well as the SO_2 content in the off-gas stream, are considered here for discussion. A successful calculation was attributed to the method that more closely matched the plant results. A comparison of the two methods in terms of success percentage in predicting several mass

METHODOLOGY

Mass balance calculations for the flash smelting of copper concentrate mixtures were performed using two different methods and the results compared with plant data from the Mexicana de Cobre copper flash smelter in La Caridad, Mexico. Typical mineralogical compositions of the feedstocks to the flash smelting furnace are shown in Table A. Two copper concentrates, Cananea and La Caridad, are the main components of the feed. Compositions of flux, recycle wastes, and recycle dust are also included.

The chemical reactions considered in the mass balance equations were selected from the literature.[1,2] Thermodynamic data for the chemical reactions were obtained from both METSIM[11] and HSC[12] databases. The chemical reactions are listed in Table B in the order of increasing values of the standard Gibbs free energy at 1,200°C. The fractional conversions of the chemical reactions as well as the species distribution ratios in matte, slag, and off-gas stream were specified based on the experience of La Caridad smelter operators.

In the conventional method (CM), the basis for the calculations was the elemental analysis of the mixtures of Cananea and La Caridad concentrates. In the second method, the mineralogical composition of the mixture was computed by means of genetic algorithm (GA) prior to solving the mass balance equations.

The GA used in this work is classified as an auto-adaptive genetic algorithm[13] and its overall strategy is shown in Figure A. Details of the algorithm can be found in Reference 14. The initial population is generated by randomly selecting a set of mineralogical compositions which are denoted as individuals of the population. Multiple crossover, repeated mutation, and function minimization at the evaluation step were used. A performance function, also called fitness condition, was defined as follows:

$$f_c = \lambda_1 \varepsilon_1 + \lambda_2 \varepsilon_2 \qquad (A)$$

In Equation A, ε_1 is the primary error computed from the following expression:

$$\varepsilon_1 = \sqrt{\sum_{i=1}^{n_e} \left(\omega_{ie} - \omega_{ic}\right)^2} \qquad (B)$$

in which ω_{ic} and ω_{ie} represent, respectively, the computed and experimental values of the mass fraction of the i-th element, and the summation is over the total number of elements in the feed, n_e.

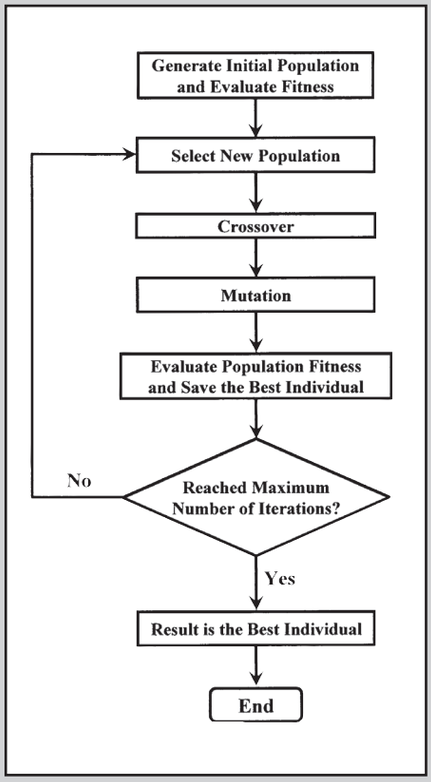

Figure A. The overall strategy of the genetic algorithm used in this work to adjust the mineralogical composition of the feed.

Similarly, the secondary error ε_2 was computed from:

$$\varepsilon_2 = \sqrt{\sum_{j=1}^{n_s} \left(\varpi_{je} - \varpi_{jc}\right)^2} \qquad (C)$$

In Equation C, symbols ϖ_{jc} and ϖ_{je} represent, respectively, the computed and experimental values of the mass fraction of the j-th species, and the summation is over the total number of species in the feed, n_s. Symbols λ_1 and λ_2 in Equation A are weighting factors that indicate the relative contributions of the primary and secondary errors ε_1 and ε_2 to the total value of the fitness condition f_c.

From a numerical standpoint, the goal of the GA is to compute the numerical values of ω_{ic} and ω_{jc} such that the fitness condition f_c is a minimum. The parameters used in this study were as follows: population size = 100 individuals; crossover probability = 0.5–0.9; mutation probability = 0.05–0.5; crossover repetition = 1–20; mutation repetition = 1–20; $\lambda_1 = 2$, and $\lambda_2 = 1$. Since the actual elemental analysis is involved in the primary error, it was given a higher weighting factor. The computing cycle was finished after 1,000 iterations.

Table A. Typical Mineralogical Composition of the Feedstocks to La Caridad Flash Smelting Furnace (% by Weight)

Species No.	Symbol	Concentrate Feed		Flux	Recycle Waste	Recycle Dust	
		La Caridad	Cananea			Flash Smelting Furnace	Electrostatic Precipitator
1	FeAsS	0	0.74	0	0	0	0
2	As_2S_3	0.84	0	0	0	0	0.67
3	Sb_2S_3	0.15	0.03	0	0.10	0	0.11
4	Bi_2S_3	0.04	0.02	0	0.04	0.33	0.04
5	ZnS	1.28	0.49	0	0.56	1.18	0.91
6	PbS	0.03	0.06	0	0.40	0	0.03
7	$CuFeS_2$	30.50	33.22	0	0	14.79	31.61
8	FeS_2	33.80	40.29	0	0	0	26.70
9	CuS	8.50	8.01	0	0	0	6.10
10	Cu_2S	17.00	4.22	0	45.00	13.36	15.91
11	CuO	0	1.00	0.03	0	0	0
12	SiO_2	3.57	4.44	95.00	0	24.92	12.12
13	Al_2O_3	4.29	6.98	3.40	0	4.77	4.87
14	Fe_3O_4	0	0.50	0	15.50	11.65	0.24
15	FeO	0	0	1.52	0	0	0
16	FeS	0	0	0	10.00	0.77	0.38
17	As_2S_2	0	0	0	0.10	0	0
18	Cu	0	0	0	0	0	0.01
19	Cu_2O	0	0	0	0	0.01	0
20	$CuSO_4$	0	0	0	0	26.25	0
21	As_2O_3	0	0	0.01	0	1.52	0
22	Sb_2O_3	0	0	0.01	0	0.28	0
23	Bi_2O_3	0	0	0.01	0	0	0
24	ZnO	0	0	0.01	0	0	0.01
25	PbO	0	0	0.01	0	0.17	0
26	Fe_2SiO_4	0	0	0	28.30	0	0.29
	Total	**100**	**100**	**100**	**100**	**100**	**100**

Table B. Chemical Reactions Considered in the Mass Balance Calculations of the Flash Smelting Furnace

Reaction No.	Chemical Reaction	ΔG^0_{1200}, kJ/mol
1	$As_2S_3\ (s) + 9/2\ O_2\ (g) \rightarrow As_2O_3\ (l) + 3\ SO_2\ (g)$	–1,097.7
2	$Sb_2S_3\ (s) + 9/2\ O_2\ (g) \rightarrow Sb_2O_3\ (l) + 3\ SO_2\ (g)$	–1,095.2
3	$As_2S_3\ (s) + 9/2\ O_2\ (g) \rightarrow 1/2\ As_4O_6\ (g) + 3\ SO_2\ (g)$	–1,086.0
4	$Sb_2S_3\ (s) + 9/2\ O_2\ (g) \rightarrow 1/2\ Sb_4O_6\ (g) + 3\ SO_2\ (g)$	–1,082.1
5	$Bi_2S_3\ (s) + 9/2\ O_2\ (g) \rightarrow Bi_2O_3\ (l) + 3\ SO_2\ (g)$	–958.0
6	$2\ CuSO_4\ (s) + 3\ FeS_2\ (s) \rightarrow Cu_2S\ (l) + 3\ FeS\ (l) + 4\ SO_2\ (g)$	–889.9
7	$FeAsS\ (s) + 9/4\ O_2\ (g) \rightarrow 1/2\ As_2O_3\ (l) + FeO\ (l) + SO_2\ (g)$	–516.2
8	$FeAsS\ (s) + 9/4\ O_2\ (g) \rightarrow 1/4\ As_4O_6\ (g) + FeO(l) + SO_2\ (g)$	–510.4
9	$FeS\ (s) + 3/2\ O_2\ (g) \rightarrow FeO\ (l) + SO_2\ (g)$	–352.4
10	$ZnS\ (s) + 3/2\ O_2\ (g) \rightarrow ZnO\ (l) + SO_2\ (g)$	–330.0
11	$FeS_2\ (s) + O_2\ (g) \rightarrow FeS\ (l) + SO_2\ (g)$	–316.4
12	$PbS\ (s) + 3/2\ O_2\ (g) \rightarrow PbO\ (l) + SO_2\ (g)$	–299.9
13	$As_2S_3\ (s) + O_2\ (g) \rightarrow As_2S_2\ (l) + SO_2\ (g)$	–253.5
14	$CuS\ (s) + 1/2\ O_2\ (g) \rightarrow 1/2\ Cu_2S\ (l) + 1/2\ SO_2\ (g)$	–163.0
15	$CuFeS_2\ (s) + 1/2\ O_2\ (g) \rightarrow 1/2\ Cu_2S\ (l) + FeS\ (l) + 1/2\ SO_2\ (g)$	–121.1
16	$FeAsS\ (s) + 1/2\ O_2\ (g) \rightarrow 1/2\ As_2S_2\ (l) + FeO\ (l)$	–94.1
17	$FeO\ (s) + 1/6\ O_2\ (g) \rightarrow 1/3\ Fe_3O_4\ (l)$	–49.1
18	$Cu\ (s) + 1/4\ O_2\ (g) \rightarrow 1/2\ Cu_2O\ (l)$	–29.8
19	$FeO\ (s) + SiO_2\ (s) \rightarrow FeO \cdot SiO_2\ (l)$	–9.6

balance calculations is presented in Figure 1.

The GA method provided better predictions for the matte production rate, copper content in the matte, copper content in the slag, and oxygen feed in approximately 60% of the total events. On the other hand, the conventional method provided better predictions for the slag production rate, silica content in slag, and iron content in slag in about 60% of the total events. Both methods showed similar predictions for the magnetite content in the slag.

The average error for the events in which a given method provided the best prediction was calculated. The comparison of the average error associated with the GA and conventional method calculations, in t/h, is presented in Figure 2. In all instances, the error was less than 2 t/h. For the matte production rate, copper content in matte, slag production rate, and iron content in slag, the conventional method showed lower values of the average error than the GA method. On the other hand, the GA method presented a lower success average error in the calculations concerning the silica content in the slag, magnetite content in the slag, and the oxygen feed. The average error in the calculation of copper content in the slag was similar for both methods and it was the lowest error value, approximately 0.2 t/h.

The average error considering the total number of events was also calculated. A comparison of the results, expressed in t/h, for the various mass balance calculation terms is presented in Figure 3. The GA method presented significantly lower errors for the matte production rate and the oxygen feed predictions. No significant difference was observed for both methods' predictions of copper, silica, iron, and magnetite content in the slag. Finally, the conventional method predictions of copper content in matte and the slag production rate are better than those of the GA method.

Calculations concerning the SO_2 content in the flash furnace off-gas stream are presented in Figure 4 in terms of SO_2 vol.%. The calculated smallest, average, and largest values for both methods are compared with the reported average plant data. The smallest and average values of both methods closely match the actual plant average value of approximately 35%. Whereas in general the predictions

shown in Figure 4 are reasonable, the largest predicted values by both methods are close to 48%, which significantly differ from the plant data. Further improvements in the algorithm should be devoted to minimize this error.

CONCLUSION

The GA method used in this work proved suitable for mass balance calculations in the flash smelting of copper concentrate blends of varying compositions. Since both matte and slag compositions are important variables in setting up the control strategies for flash smelting, these results indicate that a combination of the two methods could be used as a tool for the control and optimization of the flash-furnace operation.

The application of the GA method in this work refers to the processing of a mixture of two copper concentrates. However, its use can be extended for the treatment of more complex blends made up of any number of components. This aspect was considered in the selection of parameters for the autoadaptive GA.

Because of the practical difficulty in assessing the actual mineralogical composition for the daily flash furnace feed, the adjusted mineralogical composition computed with this method could help improve both mass and energy balance calculations needed for the thermal control of the furnace. In addition, this approach could be applied in other unit operations in a smelter complex, such as the matte-converting step.

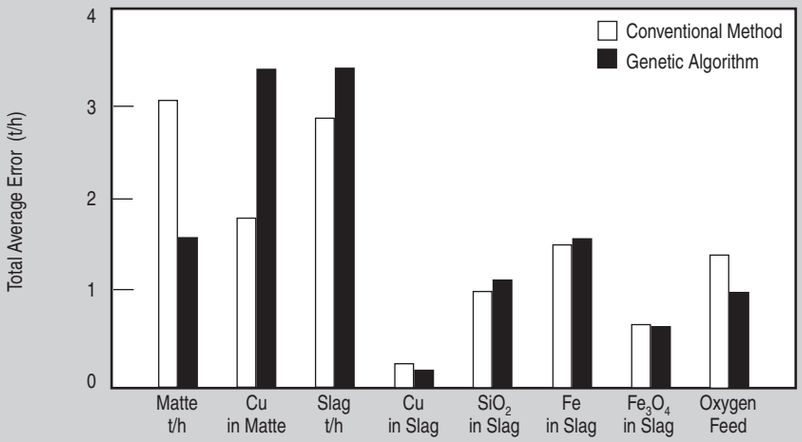

Figure 3. The average absolute error for the conventional method and the genetic algorithm-based method considering all the plant cases studied.

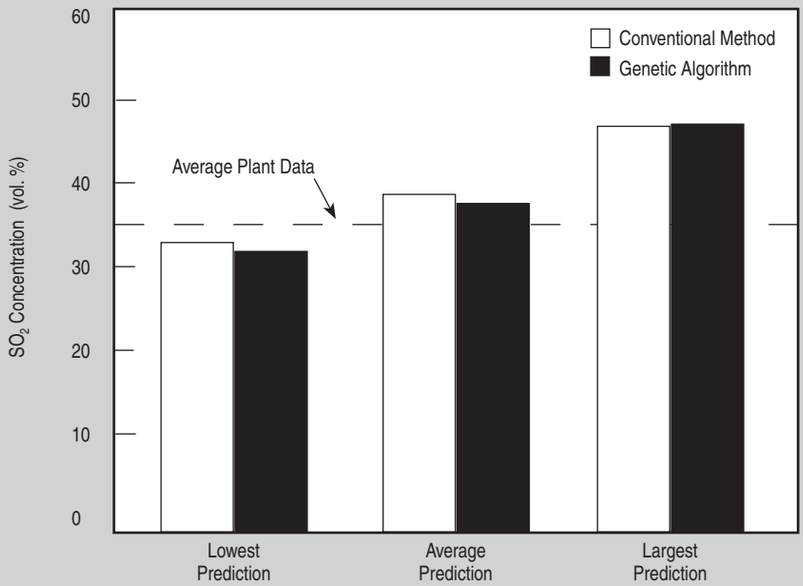

Figure 4. The lowest, average, and largest predicted values of SO_2 concentration in the off-gas stream of the flash smelting furnace using the two methods tested in this work. The average plant data is shown for comparison.

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