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Dynamic modelling of molten slag-matte interactions in an industrial flash smelting furnace settler

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Abstract— Depleting copper resources and advancing technologies have challenged industries to develop more viable, adaptable and cost efficient processes using also secondary raw materials in copper production. This study is targeting to that goal by dynamic modelling of flow and heat transfer coupled with chemical kinetics in an industrial scale flash smelting furnace settler using commercial CFD software ANSYS Fluent. First, different physical phenomena occurring inside the settler, for example, settling and separation of the matte/slag phases, and heat transfer between slag/matte phases and settler walls are studied. Secondly, reaction kinetics between matte and slag, and between slag/matte and settler walls, and impurity element distribution will be studied. This would also include phase changes phenomena due to these reactions and the flow of the reaction gases inside the settler. Settling of polydispersed droplets, their coagulation, breakage, and WEEE particle behavior are further targets of the modelling work.

Keywords— *Flash Smelting Settler; Matte droplets settling; Copper losses.*

1. Introduction

Pyrometallurgy is a widespread process which is used to extract copper from the copper ore. In recent times, material industries are looking for alternative raw materials. Moreover, due to technological advancements relatively low grade ores are being used which required updating of several process parameters for an optimized process [1]. In this regard several raw materials have been tried with the original raw material, for example, waste electrical and electronic equipment (WEEE) scrap. This research aims to study the effect of recent technological advancements and change in raw materials on the copper flash smelting process for supporting process parameters' update. The flash smelting furnace and raw material feeding system was previously modelled with good effects in several studies [2-8], however, there is still scope in the modelling of the settler part. There are many phenomena that occur inside the settler, for example, slag/matte reactions, slag/matte interactions, and matte droplets settling process. Several studies were conducted related to matte droplets settling through the slag phase, for example, effects of matte droplet diameter on the settling process and losses of matte droplets during slag tapping [9-16]. However, these studies were mainly conducted for steady state conditions and effects of droplet size on matte droplets settling rates remains to be studied quantitatively using transient cases.

The effect of matte droplets size on copper losses was examined in a study conducted by Xia et al. [17] for a continuous matte and slag tapping system. They concluded that copper losses are inversely proportional to the matte droplet size i.e. copper losses decrease with increasing copper matte droplets size and vice versa. Moreover, they concluded that the position of the tapping hole and rate of tapping also affect the copper losses. Low tapping rates are suitable for lower copper losses and the slag tapping hole should be at least 10-15 cm higher than the interfacial layer between the slag and matte phases otherwise during slag tapping some fraction of the matte phase will also be tapped out with the slag phase [17]. Moreover, various other phenomena such as higher turbulence at the inlet, matte slag velocity distribution, and impingement effect of higher velocity droplets on striking the matte slag mixture in the settler were studied in recent years [18, 19]. They concluded that matte-slag mixture falling from the flash smelting furnace is concentrated at the center of the inlet instead of covering the complete inlet surface. They introduced new in-house module to properly define the matte slag velocity and mass flow distribution [18, 19]. This study is a stepping stone for further studies considering different phenomenon occurring in a flash smelting process, for example, coalescence of matte droplets and chemical reactions between matte/slag phases. Moreover, it is an extension to the previous studies conducted on matte droplets settling in a flash smelting settler and considers the effects of matte droplets size on the settling rates and copper losses quantitatively considering transient case. In this study Eulerian model was used

to study the settling of matte droplets in the slag phase and quantitative values of the settling rates cannot be obtained solely with the Eulerian model. Discrete phase model (DPM) is required in combination with the Eulerian model to track the droplets and to calculate the quantitative values of the matte droplets settling rates. Therefore, comparison of the settling rates obtained from numerical modelling, and the settling rates obtained from Hadamard Rybczynski equation (presented in Equation 1.1) are included in the future targets. For this study settling rates for different droplets are compared using volume fraction contours at different time intervals. Another important fact is that the Stokes law presented in Equation 1.2 cannot be directly used for calculating the settling velocities of the matte droplets, because it defines terminal velocities of solids settling through a fluid and to use it for bubbles or liquid droplets, it requires the viscosity correction factor. Findings from this work would help in developing a settler with continuous tapping instead of intermittent tapping. The Commercial Computational Fluid Dynamics software package ANSYS Fluent version 18.1 was used for this study.

$$|W_m| = \frac{1}{6} g \frac{(\rho_m - \rho_s)}{\mu_s} D^2 \frac{(\mu_m + \mu_s)}{2\mu_s + 3\mu_m} \quad \text{Equation 1.1}$$

$$|V_0| = \frac{1}{8} g \frac{\rho_m - \rho_s}{\mu_s} D^2 \quad \text{Equation 1.2}$$

2. Background theory

2.1. Computational Fluid Dynamics

Computational Fluid Dynamics is a combination of several conservation laws (mass, momentum, energy), empirical equations (to account for turbulence effects), and multiphase, and discrete phase models (to account for phase interactions, mass transfer, interfacial layer, and particle tracking). It uses different solution algorithms to solve different processes numerically. In general, it consists of preprocessing, solving, and post processing. During preprocessing a physical model is created and discretized which is solved numerically using suitable solution algorithms and then results are analyzed during the post processing. The above-mentioned conservation laws, and empirical equations are combined in the form of partial differential equations generally known as Navier-Stokes equations and are defined for each discretized volume. The Navier-Stokes equations are further converted into algebraic equations for each variable defined in the domain (velocity, pressure and volume fractions etc.) These algebraic equations are then solved numerically to obtain the optimized results. Equation 2.1 and Equation 2.2 represents the Navier-Stokes equation defined in each control volume and its space discretization for each face surrounding that particular control volume respectively. [20, 21]

$$\int \frac{\partial p \phi}{\partial t} dV + \oint p \phi \vec{v} \cdot d\vec{A} = \oint \Gamma_\phi \nabla \phi d\vec{A} + \int S_\phi dV \quad \text{Equation 2.1}$$

$$\frac{\partial p \phi}{\partial t} V + \sum_f^{N_{faces}} p_f \phi_f \vec{v}_f \cdot \vec{A}_f = \sum_f^{N_{faces}} \Gamma_\phi \nabla \phi_f \cdot \vec{A}_f + S_\phi V \quad \text{Equation 2.2}$$

3. NUMERICAL MODELLING

3.1. Calculation domain and Discretization

An industrial scale Flash Smelting Settler with slightly curved bottom is considered for the computational domain. The dimensions of the settler are listed in Table 3.1 and shown in Fig. 3.1. The physical domain was discretized into 1 million volume elements/cells for the numerical computations.

3.1.2. Governing equations and models

In this study an Eulerian-Eulerian two phase model was used for the computational fluid dynamics study. An Eulerian model is advantageous when the dispersed phase has a higher concentration, and it accounts for the interaction, penetration and mass transfer between the phases. Moreover, it solves the volume fraction equation for each phase separately [21, 22]. Matte and slag phases were considered for all three cases. These cases are explained in the section 3.1.3. Table 3.2 shows the physical properties of the matte and slag.

Table 3.1. Settler dimensions

Settler		Dimensions/ Radius (m)	Position on x,y,z coordinates (m)
Length (along z axis)		18	
Width (along x axis)		6	
Height (along y axis)	Centre line	0.87	
	In Sides	0.70	
Slag tap hole		0.045	0.55, 0.35, 18
Matte tap hole		0.045	0.55, -0.1, 0
Slag/matte Inlet		2.25	0, 0, 3.75

Table3. 2. Materials and Physical Properties. [17]

Materials /phases	Physical Properties				Diameter μm		
	Density kg/m^3	Viscosity $\text{kg/m} \cdot \text{s}$	Specific Heat $\text{J/kg} \cdot \text{K}$	Thermal Conductivity $\text{W/m} \cdot \text{K}$	Case1	Case2	Case3
Slag	3150	0.45	1100	6	Continuous phase		
Matte	5100	0.04	850	15	100	300	500

Figure 3.1. Calculation domain

For the Turbulence modelling, $K-\varepsilon$ two equations mixture model is suitable when an Eulerian-Eulerian model is used. The $K-\varepsilon$ two equations mixture model is robust, simple and gives optimal performance regarding computational cost and accuracy. Therefore, for this settler modelling $K-\varepsilon$ two equations mixture model was used as a turbulence model. [21, 22] For Fluid-Fluid exchange coefficient symmetric model was used which is shown in Equation 3.1. This model is suitable when secondary phase becomes the primary phase in one of the region in the physical domain, for example, in this case matte phase after settling down at the bottom of the settler will become the primary phase in that region.

$$K_{sm} = \frac{\alpha_s(\alpha_s\rho_s + \alpha_m\rho_m)f}{\Gamma_{sm}} \quad \text{Equation 3.1}$$

Where, f is the drag function and was determined by Equation 3.2 using Schiller and Naumann law, α_s and α_m are volume fraction of slag and matte respectively, ρ_s and ρ_m are densities of slag and matte, Γ_{sm} is the particulate relaxation time

$$f = \frac{C_D Re}{24} \quad \text{Equation 3.2}$$

Where, C_D is the drag coefficient, and Re Reynolds number.

Matte dispersed-phase interfacial area concentration within the slag can either be calculated using the transport equation or by the simple algebraic equation using a specified droplet diameter [21]. Advantage for using transport equation is that the coalescence or breakup models as a source term can be used using different coalescence and breakup models present in the ANSYS Fluent 18.1 version, for example, Hibiki-Ishii, Yao-Morel etc. [21]. In addition to that user defined models can also be added. For this study interfacial area concentration was calculated with a simple algebraic equation, Equation 3.3. Therefore, interfacial tension between matte and slag phases was not considered during the numerical calculations. However, a future aim of this study is to account for the coalescence

and breakup of the droplets using transport equation and in that case interfacial tension between matte and slag phases will be considered.

$$A_i = \frac{6\alpha_m(1-\alpha_m)}{d_m} \quad \text{Equation 3.3}$$

Where, A_i is the matte dispersed-phase interfacial area concentration within the slag, α_m is volume fraction of continuous matte phase. Equation 3.3 is derived from surface to volume ratio for a spherical droplet. Complimentary volume fraction of the continuous phase ($1 - \alpha_m$) is introduced in the equation to ensure that when α_m approaches 1 interfacial area concentration approaches zero. [21]

3.1.3. Boundary Conditions and Solution Algorithms

Three different cases based on homogeneous matte droplet diameters (used as a dispersed phase) are studied. Case 1 is studied considering 100 μm diameter, case 2 was studied for 300 μm diameter, and case 3 was studied for 500 μm diameter matte droplets. For the slag/matte mixture (from the flash furnace) inlet, a velocity boundary condition was used. The complete domain was initialized with the slag phase and the inlet velocities for the mixture were calculated from the mass flow inlet. Mass flow inlet values were obtained from [17] which used an industrial scale flash smelting furnace setup with 60% matte grade. Flow at the inlet corresponds to the plug flow. Mass flow rates and thermal boundary conditions used in this study are shown in Table 3.3. Mass flow rates and inlet velocities are coupled and fixed for the inlet of the settler for each case. Change in mass flow rate or inlet velocities will have a substantial effect on the settling rates and copper/matte loss. Since for both intermittent and continuous tapping systems, higher inlet velocities or mass flow rates means the settler will fill up quickly and therefore there will be less time for the settling process. In addition to that higher flow current across the settler due to higher inlet velocity will affect the settling velocity and also will carry the droplets to the slag outlet. Pressure Outlet boundary condition was used for the slag outlet so that the loss of matte droplets through the slag outlet can be studied. As the complete domain was initialized with the slag phase, matte phase was not present in the settler at the start of the simulation and, therefore, it was allowed to accumulate in the settler and it was not extracted from the matte outlet. Consequently, for this study zero outflow was set for the matte outlet boundary.

Table 3.3. Mass flow rates and thermal boundary conditions.

Boundaries	Temperature ($^{\circ}\text{C}$)	Mass flow rate (kg/s)		Velocity (m/s)
		Slag	Matte	
Inlet	1603	19.44	29.18	0.0007481
Bottom wall	1373			
Side walls	1420			

The second order upwind discretization method was used to solve the algebraic conservation equation for the momentum, and for volume fraction calculation the HRIC scheme was used. Pressure velocity coupling was achieved with the SIMPLE algorithm.

4. Results and Discussions

Settling of matte phase through the slag phase is determined for different matte droplet diameters. Diameters normally averages 300 μm in an industrial flash smelting settler process with matte droplet diameter ranging from 100 μm to 500 μm [17]. Small size droplets have lower settling velocities, therefore results in loss of matte droplets during the slag phase tapping [17]. This is also depicted in the results presented for the three different droplets cases considered for this study. Simulation results presented here depicts two phenomena; loss of matte droplets during slag tapping at different time intervals and for different droplet size, settling rates for each droplet size are compared using volume fraction contours at different time intervals. Copper losses in different flash smelting furnaces are quantified in various references. Some values for copper losses from the literature are mentioned here as references to compare the results for the three cases considered in this study. Copper losses for different matte grades in industrial flash smelting furnaces were presented by [19]. For 60 % matte grade copper/matte loss in the Luanshya Smelter (Reverberatory

Furnace) was approximately 1%, and for same grade matte in Outokumpu flash smelting furnace it was around 1.3%. Similarly results presented in [20] revealed that copper losses in Flash smelting furnace are around 1.1%. Furthermore, in Table 4.1 more references are provided for the copper losses in Outotec and Inco flash smelting furnaces [21]

Table 4.1. Copper losses (% Cu in slag) in various furnaces [21]

Outotec FS: Hibi Kyodo Smelting Co. Tamano, Japan	Outotec FS: Sumitomo Toyo, Japan	Outotec FS: Rio Tinto Kennecott, USA	Inco Flash Smelting
0.74	1	0.5 – 4	1 – 2

4.1. Case1: Settling of 100 μm matte droplets through slag phase

In Figure 4.1 volume fraction contours for 100 μm matte droplets at different time intervals are presented. A vertical plane (YZ-axis) at the center of the settler ($X=0.5\text{m}$) is used for showing the volume fraction contours. At the start of the simulation the whole domain was initialized with slag phase and slag/matte mixture from the flash smelting furnace reaction shaft was entered from the inlet. Lighter slag phase from the incoming mixture will stay at the top layer and the heavier matte droplets will start descending through the slag phase. Since the settling process of 100 μm matte droplets is substantially slow, most matte droplets will, therefore, remain suspended in the slag phase and will be carried away with slag phase through the slag outlet. This is also depicted in Figure 4.1 for various time intervals as volume fraction of the matte droplets at the bottom of the settler is very low. These results suggest that there are higher chances of matte (copper) losses, if higher fraction of 100 μm or smaller size matte droplets are present in the incoming mixture from the flash smelting furnace.

Figure 4.1. Volume fraction contours for 100 μm diameter matte droplets at different time intervals.

4.2. Case2: Settling of 300 μm matte droplets through slag phase

Figure 4.2 shows the volume fraction contours for 300 μm matte droplets at various time intervals. After 10 minutes, thin layer of matte droplets can be seen and this layer starts to grow with time and thicker layers can be observed at higher time intervals as increment in volume fraction of matte can be observed with time at the bottom of the settler. One more interesting conclusion from these contours is that this layer of matte droplets is thicker at the sides of the

inlet or away from the inlet. It may be because of higher turbulence near the inlet as compared to the sides of the inlet or away from the inlet. Second reason is that as the droplets move away from the inlet towards the slag outlet they have more time to settle down. Comparing Figures 4.1 and 4.2, it can be concluded that 300 μm matte droplets settle faster than 100 μm droplets.

Figure 4.2. Volume fraction contours for 300 μm diameter matte droplets at different time intervals

4.3. Case3: Settling of 500 μm matte droplets through slag phase

Figure 4.3. Volume fraction contours for 500 μm diameter matte droplets at different time intervals.

Volume fraction contours for 500 μm matte droplets at different time intervals are presented in Figure 4.3. From these contours it can be concluded that settling process is a lot faster for 500 μm matte droplets as compared to the 100 μm , and 300 μm matte droplets. This is visible as a thicker layer of matte phase at the bottom of the settler. Secondly, volume fraction of suspended droplets in the slag layer is lower because of higher settling rates which suggest that less copper losses will occur for 500 μm droplets as compared to 100 μm and 300 μm droplets.

4.4. Comparison of settling velocities and copper losses with literature

Matte droplets in the continuous slag phase remain suspended either due to higher viscosity of slag, formation of Fe_3O_4 crystallization structure, gas carrying some of the small droplets from the matte phase, or lower diameter of matte droplets, as it is concluded by [17, 25, 26] that small matte droplets of size 100 μm remain suspended in the slag phase. In the above three cases effects of matte droplets' size was solely consider to study the settling phenomena. However, there are other parameters which also affect the settling process, for example, droplet breaking and coalescence, and inertial forces. A study conducted by [27] mentioned that the inertial forces have a negative effect on the liquid droplets collision efficiency when droplet size is small; however, the effect is reversed when droplet size is increased. Therefore, large liquid droplets have higher chances of coalescence as compared to smaller ones. This is one of the reasons of lower copper losses in a settler with larger matte droplets. To compare the settling rates and efficiency of the three cases, the copper/matte loss % was calculated. The results are presented in Table 4.2. These results are in agreement with the previous results as shown in the form of volume fraction contours which reveal that copper/matte loss % is higher in the following order: 100 μm > 300 μm > 500 μm . Copper losses presented in Table 4.2 are higher than the literature values [28-30]. This is because in normal flash smelting process intermittent slag tapping is used; however, in this study, tapping was continuous. There could be various reasons for higher copper losses in the continuous tapping system: settling time is not enough, flow current moving across the settler towards the slag outlet may disturb the settling rate. Moreover, there are some parameters, for example, droplet coalescence is not considered in this study which can play a significant role in matte droplet settling. Tapping velocity also effects the loss of copper by increasing the zone of copper droplets entrainment to the slag-outlet [31]. In this study, tapping velocity was high around 2.55 m/s and low tapping velocity is recommended to reduce the affecting zone for the entrained droplets around the slag-outlet [31]. This might be one of the reason that the copper losses were higher than the literature values.

Table 4.2. Copper losses for various droplets diameter

Miscellaneous	Time (min)	Matte Mass Flow (kg/s)		
		100 μm	300 μm	500 μm
Slag Outlet	5	0.00	0.00	0.00
	10	1.01	0.65	0.12
	15	2.26	1.71	0.70
	20	3.45	2.51	1.13
	25	4.52	3.30	1.42
	30	5.53	4.01	1.61
	35	6.50	4.67	1.76
	40	7.40	5.23	1.86
	Avg. Matte mass flow through slag outlet (kg/s)	3.84	2.76	1.07
Copper/matte loss (%)		13.15	9.46	3.68

5. Conclusions

The transient behavior of copper matte droplets in a flash smelting furnace settler was modeled by the CFD software ANSYS Fluent. This is the first report of the research programme and only the settling of the droplets was included in addition to the continuous flow of the slag, which simulated continuous tapping of the slag. As expected, the bigger droplets settled faster than the smaller ones. The settling velocity of the small droplets was too low compared to the slag flow through the settler, which resulted in higher copper losses than those reported in literature from industrial

operations. It can be concluded based on the results of this study that matte droplets coalesce during settling and, thus, form bigger drops that descend faster.

In the next phase of the project, droplet coalesce and breakup will be added to the model for more realistic simulation. Finally, chemical reaction kinetics and rate equations from ongoing experimental research will be added as user-defined-functions (UDF), in order to have a realistic CFD model of the settler part of the flash smelting furnace.

The full settler geometry and time dependent simulation was found to be very heavy computing task that was not possible to do with personal computer. Including more phenomena and introducing UDFs in the model will increase the computing power need still further.

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