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Fluid Dynamic Modelling of the Operational System of Capture of Gases for the Copper Mattes Conversion Process

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In this paper studied the momentum, heat and mass transfer of a flow of gases coming from the process into a Peirce-Smith converter. This flow is captured by a primary and secondary hood type side gate. The flow regimen inside both hoods is turbulent. The simulation of the system was solved using k-ε model. Metallurgical gases into the converter, rich in SO_2, reach very high temperatures, which should be captured by both hoods, which are in charge of first cooling step with the help of the ambient air, by which a mixture model is contemplated for the SO_2 and N_2 gases.
Simulation delivered velocity, pressure, temperature and concentration profiles. From these results it is possible to determine the average values into the two hoods, resulting in an average velocity of 11.4 and 3.6 m/s inside of the primary and secondary hood respectively, identifying the area of leak in the floodgate of the primary hood. The average temperature at which SO_2 gases occur is approximately 1200 °C which ascend and cool to come into contact with the flow that enters the secondary hood with a temperature of 20° C, reaching an output average temperature of 640° C. The highest concentration of SO_2 is produced inside the converter, reaching a value of 1.155 mol/m³.

1. Introduction

In Chile, the process for producing copper from sulphide ores consists of four stages: processing, flotation, smelting and electrorefining. Within this whole system, the stage has always caused the greatest environmental problems has been the copper smelting of sulphide ores. This problem comes from the nature of its operation: the mineral chalcopyrite ($CuFeS_2$) to be melted, generated as products: copper matte, composed of Cu_2S and FeS, together with SO_2 gas. Then, the matte must be transferred to the converting furnace, where blister copper (99% Cu) is obtained. As seen in Figure 1a, due to the mode of operation of this process (discontinuous or "batch") the presence of fugitive gases is inevitable when the matte is being charging in the conversion process. For this reason, to prevent escape of SO_2 into the atmosphere, secondary hoods have been implemented for off-gas capture as shows in Figure 1b.

Figure 1: Fugitive gases from the matte charging of conversion process (a) and CPS converters equipped with secondary hood (b).

To study the operation of gas capture system, it is necessary to analyse the behaviour of four parameters: velocity, pressure, temperature and concentration. The main function of this system is the capture of SO_2 gases generated from the matte oxidation. Velocity, pressure and flow determine the hood capacity suction. The temperature and concentration are essential because they determine how sulphur is present, which can be as SO_2 or SO_3 according to reaction Eq(1).

$$SO_2 + \frac{1}{2}O_2 = SO_3 \quad (1)$$

At high temperatures (around 1200°C), it is favoured production of SO_2 and O_2, and as decreases, the system will tend to produce SO_3. This gas should be avoided, since contact water vapor, producing the phenomenon known as acid mist (Davenport and King, 2005), according to equation Eq(2).

$$SO_3 + H_2O = H_2SO_4 \quad (2)$$

The objective of the gas capture system is the efficient capture of SO_2 gas.
Leaving the hood, the off-gas must be cooled from 650°C to 350°C, to eliminate the presence of fine-grained particles into the electrostatic precipitator. If the temperature is below the above-mentioned, reaction Eq(1) tends to produce SO_3, which can generate the presence of sulfuric acid, according to reaction Eq(2). This would result in corrosion of the walls of the electrostatic precipitator, which would force to stop the processes.
In this paper, we will be studied the four variables mentioned above on a primary and secondary Peirce-Smith converter capture system gases using the modelling and simulation program Comsol Multiphysics 4.3 version.

2. Theoretical Basis

2.1 Momentum Transfer Equation

The objective of the momentum transfer equations is the determination of the velocity field and pressure to which it is subjected fluid flow, either liquid or gaseous, in a work domain. In this particular study, it becomes more important, since this model the fluid dynamics will determine heat and mass transport by convection. The momentum transport will be represented by the Navier-Stokes equations. The Navier - Stokes are mathematical expressions that describe the motion of viscous and incompressible fluids, and related basic transport phenomena of mass and momentum. They show that the dynamic behaviour of the fluid is governed by the conservation of mass or continuity equation, and the conservation of momentum or momentum (COMSOL Multiphysics 4.3, 2013). The Navier - Stokes is expressed according to the Eq(3).

$$\frac{\partial u}{\partial t} - \nabla \cdot \eta(\nabla u + (\nabla u)^T) + \rho u \cdot \nabla u + \nabla p = F \quad (3)$$

And the continuity equation is defined by the equation Eq(4).

$$\nabla \cdot u = 0 \quad (4)$$

Eq(3) includes the following quantities: ρ is the density kg/m³, η is the viscosity Pa·s, u is the velocity vector m/s, p is pressure Pa, F is the volume force vector N/m³. These equations can also be extrapolated to turbulent flow simulations. An alternative to simplify this problem is to consider the average equations, using the statistical regularity. For incompressible fluids, the velocity component is determined as follows Eq(5).

$$u_i = \bar{u}_i + u_i' \quad (5)$$

Where u_i is the velocity field over a given time interval, $\bar{u}_i$ is the average time component and u'_i is a component which fluctuates. Then, the Navier - Stokes modified is written as Eq(6) and continuity as Eq(7).

$$\rho\frac{\partial U}{\partial t} - \nabla \cdot \eta(\nabla U + (\nabla U)^T) + \rho U \cdot \nabla U + \nabla\overline{(\rho u' \otimes u')} + \nabla p = \mathrm{F} \quad (6)$$

$$\nabla \cdot \mathrm{U} = 0 \quad (7)$$

Where U is the average velocity and $\overline{u' \otimes u'}$ is the term which represents the interaction between the velocity fluctuations, and is called Reynolds stress tensor. The only difference from the original Navier-Stokes equation is the insertion of Reynolds stress tensor, which is considered as the contribution of turbulent fluctuations in the flow of convective momentum. Finally, is required a closure scheme, which is to impose assumptions to simulate the flow completely. A well-known and recurrent scheme closure is the k-ε model, consisting of two additional transport equations solved: the turbulence kinetic energy, k, and the dissipation rate of turbulence energy, ε. Momentum transport is quantified using Eq(8).

$$\overline{u'\otimes u'} = -\nu_T \cdot (\nabla U + (\nabla U)^T) \tag{8}$$

With Eq (9).

$$\nu_T = \frac{\eta_T}{\rho} = C_\mu \frac{k^2}{\varepsilon} \tag{9}$$

Where ν_T is the turbulent kinematic viscosity, η_T the dynamic viscosity turbulent and C_μ is a constant model with a value of 0.09. This closes the system resulting in the following equations for the conservation of momentum Eq(10) and continuity).

$$\rho \frac{\partial U}{\partial t} - \nabla \cdot (\eta + \eta_T)(\nabla U + (\nabla U)^T) + \rho U \cdot \nabla U + \nabla p = F \tag{10}$$

2.2 Heat transfer equation

The off-gas temperature gases is the parameter that determines the conditions that must have each component of the capture gases system, the concentration of SO_2 and SO_3 gases, according to Eq(1), in addition to the proper functioning of the gas system capture.
It is defined as heat transfer to the movement energy due to the temperature difference. The heat transfer mechanisms are: conduction, convection and radiation.
Heat conduction takes place through different mechanisms in different media. Theoretically, in a gas it is performed through collisions of molecules; a fluid through oscillations of each molecule in a "cage" formed by its closest neighbors; in metals mainly by electrons that carry heat and in other solids by molecular motion, in crystals takes the form of vibrations in the network known as photons. Typically for heat conduction, the flow is proportional to the temperature gradient. Heat transfer is represented by Eq(11).

$$\rho C_p u \nabla T = \nabla (k \nabla T) + Q \tag{11}$$

Eq(11) includes the following quantities: $\rho C_p u \nabla T$ is heat flux by convection, $\nabla(k\nabla T)$ is the heat flux by conduction, Q is the heat source, k is the thermal conductivity and C_p is the specific heat capacity at constant pressure.

2.3 Mass transfer equation

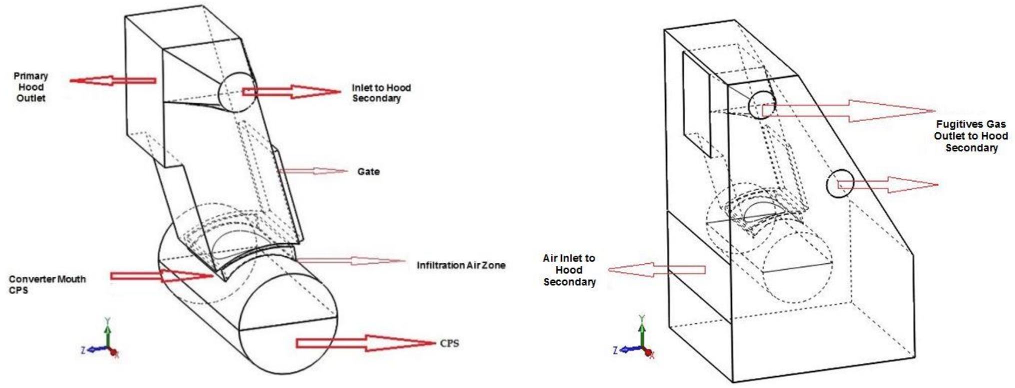
The SO_2 concentration in the off-gases inside the hood is the parameter that determines the economic feasibility of the recovery process gases. If this component is diluted in the off-gases, the sulfuric acid plant requires too much energy to carry out the reaction Eq(2). For this reason, should be controlled the ratio SO_2/N_2 inside the hood. Analogously to heat transport, the equation that defining the mass transports is Eq(12).

$$u \nabla c_i = \nabla (D_i \nabla c_i) + R_i \tag{12}$$

Eq(12) includes the following quantities: $u\nabla c_i$ is mass flux by convection, $\nabla(D_i \nabla c_i)$ is the mass flux by diffusion, c_i is the concentration of the specie I, D_i denotes the diffusion coefficient, R_i is a reaction rate expression for the specie i and u is the velocity vector.
The three coupled equations form the study that modelled the off-gas capture system in the stage conversion.

3. System Modelation

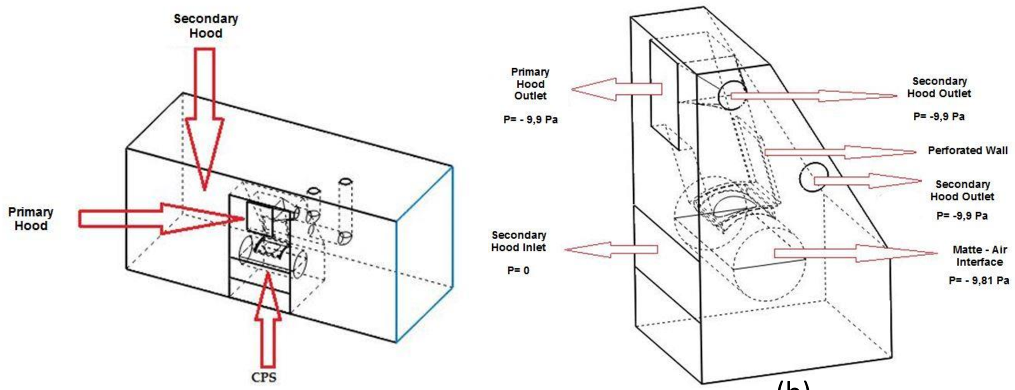
The geometries used in the modelling can be seen in the figures presented below. In Figure 2a appears the Peirce Smith converter coupled to the primary hood through the converter mouth. Through this last can escape fugitive gases from the conversion reactions, those which will be captured by the secondary hood (Safe, Matson and Deakin, 2002). This also included the presence of a gate, used for recycling of anode copper scrap, which aims to regulate the working temperature (Biswas and Davenport, 1994). As the gate closure is not hermetic, there may be presence of fugitive gases through it. In Figure 2b you can see the secondary hood geometry. In addition it can be seen that the secondary hood has geometry such that it covers entire the converter and primary hood, so to capture all the fugitive gases.



(a) (b)

Figure 2: Geometry of the primary hood and Peirce – Smith converter (a) and of the secondary hood (b).

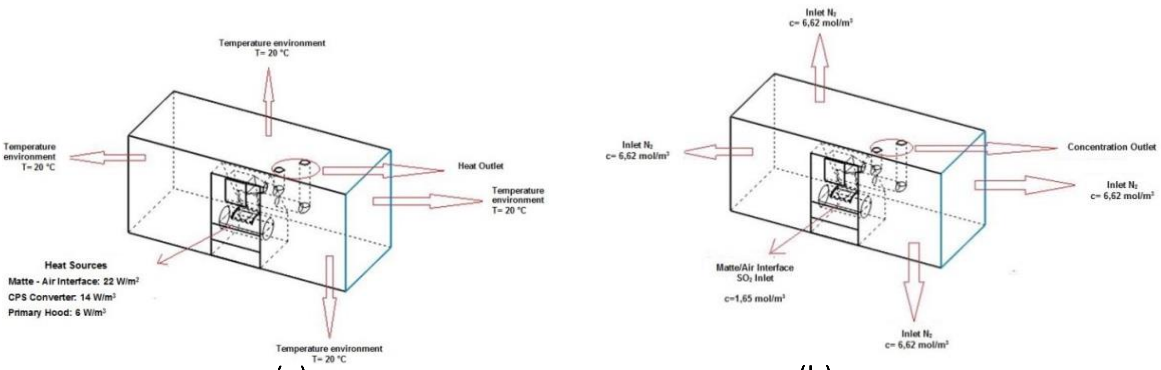
The entire system, which includes infiltration, can be seen in Figure 3a. Fluid dynamic boundary conditions used for the system are shown in Figure 3b. Note that, for the movement of gases, it is common to use a suction pressure to allow its flow into the processing steps (Safen and Stevens, 2000).



(a) (b)

Figure 3: Complete view system modelling (a) and boundary conditions for gas flow modelling.

The boundary conditions for heat transfer are shown in Figure 4a, and the boundary conditions for mass transfer are shown in Figure 4b (Pérez et al, 2016).



(a) (b)

Figure 4: Boundary conditions for heat (a) and mass (b) transfer modelling.

Conditions which cause high temperature conversion process and that are responsible for its operation autogenously are the exothermic reactions of slag – forming stage Eq(13) (Aguilera et al, 2014).

$$FeS + 3/2O_2 = FeO + SO_2, \qquad \Delta H^0 = -462{,}411\ [kJ/mol] \tag{13}$$

And then the copper – forming stage Eq(14).

$$Cu_2S + O_2 = 2Cu + SO_2, \qquad \Delta H^0 = -217{,}317\ [kJ/mol] \tag{14}$$

The effect of both reactions inside the converter and primary hood were quantified as source terms, equivalent in this case to: 22 W/m², 14 W/m³ for matte - air interface, and 6 W/m³ for the converter - primary hood interface. The walls were considered as resistive walls, that is to say, a small fraction of heat is lost through them, and its value is 0.002 m²K/W.
The values of the boundary conditions for SO_2 generated are obtained from the reactions Eq(13) and Eq(14).

4. Results

In Figure 5 it can be seen the velocity field of the off-gas from the Peirce-Smith converter (a) and the pressure profile inside the hood (b).

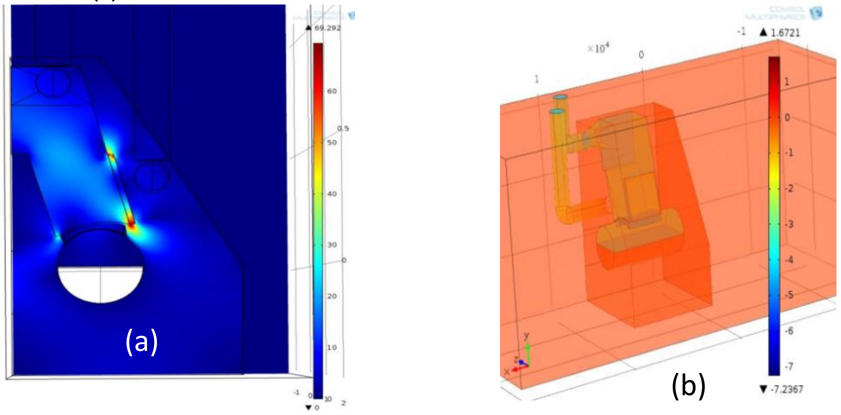


Figure 5: Velocity profile inside the gas collection system, side view (a) and Pressure profiles (Pa) inside the gas collection system, complete view in 3D (b).

From Figure 5a, it can be seen the importance of the presence of the secondary hood. Even if the charging of matte to the furnace was perfect, there will always be a flow of gas escaping through the gate by which copper scrap is added to regulate the temperature of the converter. Although volumes are small, they must be caught in accordance with environmental legislation.
As is known, the most common driving force for the transport of any type of fluid is the pressure difference. It can be seen that inside the gas collection system, the lowest pressure is in the outlet of the secondary hood, reaching a value of -4.5 Pa, guaranteeing the suction of the gases generated.
Figure 6a presents the profile of temperatures (°C) inside the hood, side view (a) and Figure 6b presents the SO_2 concentration profile (mol/m³) inside the hood, side view.

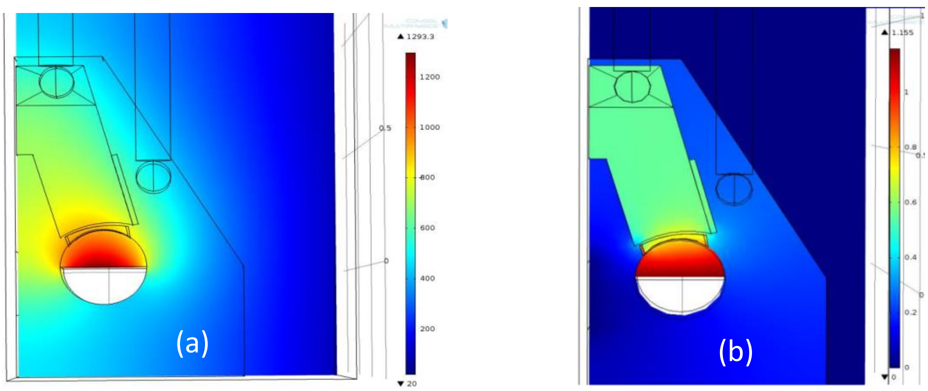


Figure 6: Temperature profile (°C) inside the gas collection system, side view (a), and the SO_2 concentration profile (mol/m³) inside the hood, side view (b).

In the Figure 6a it can be seen that the temperature of the conversion process is given by the oxidation reactions of FeS and Cu_2S, besides regulating the temperature by recycling scrap copper. Within the parameters used in the copper smelter, the temperature of the gases inside the gas capture system should be between 1,200 and 600 ° C, so that it can pass through the electrostatic precipitator without damaging its structure. It can be considered that the proposed capture system operates within the required ranges that do not harm the process areas.
In the Figure 6b it can be seen that the airflow through the primary hood is capable of capturing the highest concentration of SO_2 coming from the conversion. However, the existing opening between the mouth of the converter and primary hood occurs the greatest loss of SO_2 from this system. This is based on the fact that the mouth of the converter has a concentration of 0.7 mol/m³, while the hood has 0.6 mol/ m³ of SO_2. Inside the secondary hood, the SO_2 concentration is about 0.3 mol/m³.
These concentrations allow that the SO_2 treatment can perform economically profitable, because if the gases captured by the secondary hood were more diluted, the process would have a marginal energy cost associated very high.

5. Conclusions

Secondary hood design was modelled by a stationary analysis using COMSOL Multiphysics.
Turbulence model k-ε is suitable for modelling the flow of gases inside the primary and secondary hood.
It was determined the velocity profile inside the primary and secondary hood.
Due to the turbulent flow inside the primary hood and fugitive gases existing in the gate, this area causes a constant escape of SO_2, with an average value of 0.27 mol/m³.
It was determined the temperature profile inside the hood.
The average temperature in the melting bath reaches a value of 1,200°C, which is consistent with the theoretical values.
The temperature inside the primary hood decreases by the action of infiltrated air and the gases leave the hood with an average temperature of 640°C.
It was determined the SO_2 concentration profile inside the primary and secondary hood.
The highest concentration of SO_2 was found inside the converter with an average value of 1.155 mol/m³, and N_2 was found in the environment, at the entrance of the secondary hood and into the converter with a value of 4.634 mol/m³.
The average concentration of SO_2 reached inside the primary hood corresponds to 0.55 mol/m³.
Nearby to the gate inside the secondary hood have an average concentration of 0.27 mol/m³ of SO_2, demonstrating that exists in this zone fugitive gas capture.

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