Temperature modelling in a furnace

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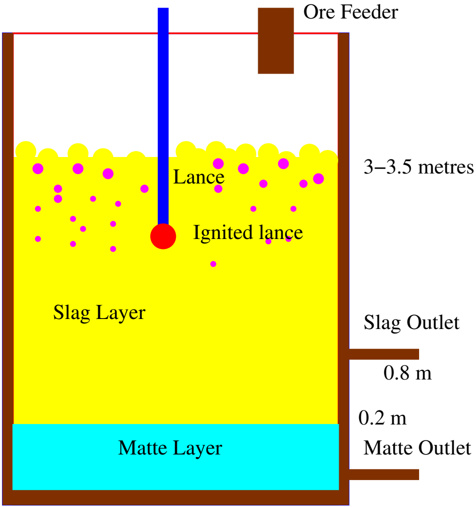
Outline

Study Group

- The smelting of Platinum group metals (PGM) is conducted in a violently disturbed, high temperature container fueled by coal and oxygen.
- The furnace is very difficult to examine while in operation due to the excessive temperatures and dangerous environment.
- The group was requested to present some possible models for the process and the temperature in the furnace during operation.
- An issue of primary concern is stability. Eruptions can occur causing very dangerous conditions and hampering production.
- An improvement in understanding of the process is also desirable.



Main features of the furnace

The Process

- Ore is placed in the furnace and heated to high temperature with a **lance** that inputs air, coal and oxygen.
- This ignites the coal, generating heat, and the air assists in stirring of the mixture.
- At higher temperatures free metals, after melting, settle into the **matte** layer at the base.
- Remaining material stays in the **slag** layer at the top.
- In the ore, rock and "platinum group metals" (PGM) exist in a ratio of $9:1$ approximately.
- Slag and matte layers are **tapped** at different times from different heights to extract the product and waste and to keep the process stable.
- The tapping process can lead to rapid changes in height and hence volume, potentially causing a heating imbalance and potential overheating or cooling.

Important features

- The extracted metals are approximately 8 times more dense than “rock” - the matte layer will be extremely stable.
- A considerable amount of gas is generated during the process. Mainly Sulphur Dioxide but also other oxides and sulphides of metals (Cu, Pl, Ca....)
- This large amount of gas causes significant bubbling of the surface of the slag.
- The surface of the slag layer exhibits significant splashing and turbulence. This is regarded as a desirable feature of the process and there is an *optimal splashing*.
- The matte layer appears to be relatively thin ($\approx 20cm$) and motionless, the slag cycles from $3.5 - 1$m in depth. This leads to significant changes in the heat balance in a short time.

Potential Problems

- Mismatch between heat input from the lance and heat absorption; - overheating or overcooling (especially during tapping)
- Variable feed quality of coal - the heat input requirement for conversion changes
- The human operator may misjudge the furnace state - furnace responses time delays, error in lance height
- The chemical reactions at the end of the lance may experience **thermal runaway** if it gets too hot - like milk suddenly foaming out of a pan when boiling. This may be exacerbated if the layer thins and the heat from the lance can not escape. Due to the exponential dependence on temperature in Arrhenius chemical kinetics.

The Chemistry

- Carbon burns producing heat and CO, CO_2
- CO strips off oxygen from the oxides and sulphides (endothermic). Noxious gases SO_2, CO … are released.
- Further reduction occurs (at higher temperature) releasing the metals. Typically:

$$C + O_2 \rightarrow CO_2, \quad CO_2 + C \rightarrow 2CO$$

$$Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$$

$$CaO + SiO_2 \rightarrow CaSiO_3$$

$CaSiO_3$ floats to the surface.

Thermodynamics: theory and practice

Theoretical Framework:
Gibbs free energy minimisation determines the final state (ie combination of compounds at a particular temperature). It is assumed the transient times between states are small (microseconds).

In Practice:

The initial composition is ‘unknown’.

Lab Work:

A small sample is heated and changes in composition with associated heat input required recorded.

The CFD Calculations (slag):
Assume thermodynamic equilibrium at the local temperature everywhere.

Global Gas Production Model

- Aim to determine changes in the gas content in the slag layer (bubbles etc) associated with changes in lance input and tapping of matte/slag.
- The thought is that if the volume fraction of gas exceeds a critical value then a bubble flow/churn flow transition will result; more splashing.
- Try to avoid detailed dynamics (momentum exchange etc), treating the slag as being uniform in temperature $T(t)$ and composition. The gas temperature and liquid temperature are assumed to be the same.

The Equations

Let α be the volume fraction of gas, $(1-\alpha)$ is occupied by liquid/solid. V_0 the volume of the slag (assumed fixed for the steady state situation).

Gas Conservation:

$$\frac{d}{dt}[V_0\rho_g\alpha] = L_g(t) + R_g(t) - S_g(t)$$

$L_g(t)$ lance gas input, $R_g(t)$ production rate of gas due to feed conversion, and $S_g(t)$ is the loss through the surface..

Liquid Conservation:

$$\frac{d}{dt}[V_0\rho_l(1-\alpha)] = L_l(t) - R_g(t) - S_l(t)$$

Energy Conservation:

$$\frac{d}{dt}[V_0(\rho_g\alpha c_g T + \rho_l(1-\alpha)c_l T)] = H_{comb} - (H_{conv} + H_{lost})$$

Scaling, Expected Result

- Scaling will enable us to order the importance of various terms and reduce the system.
- The important time scales will be identified.
- Equilibrium point identified and classified.

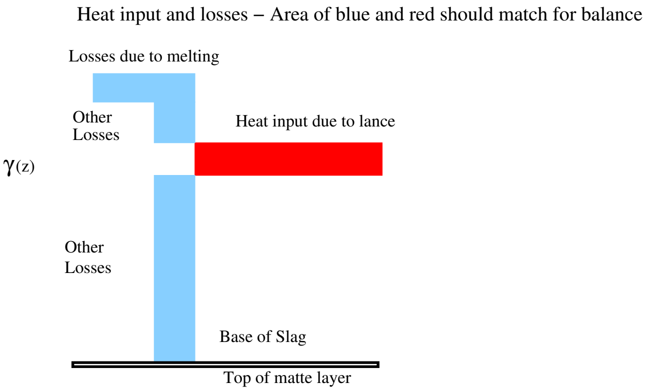
One dimensional Model

- Assume the variation is mainly in the vertical direction (not necessarily valid).
- There is a lot of **turbulence** $\Rightarrow$ rapid diffusion - α_{Turb} is a turbulent diffusion coefficient.
- Assume that only the slag layer matters - all else as boundary conditions
- Lance, chemical processes and losses modeled by heat loss/ gain terms

$$\alpha_{Turb} T_{zz} - \alpha_{Mol} T = \gamma(z),$$

where:
α_{Turb} is turbulent diffusion (mixing)
α_{Mol} is molecular diffusion in side wall (loss through sides)
$\gamma(z)$ is heat loss gain internally, via lance (input) and chemistry (loss)

One-dimensional model



Heat Loss/Gain function

Define a heat loss/gain function that corresponds to the near-surface melting, lance injection and general chemical background absorption.

$$\begin{aligned}\gamma(z) = \gamma_1 &- (\gamma_1 + \gamma_2)\mathcal{U}(z - L_1)\\ &+ (\gamma_1 + \gamma_2)\mathcal{U}(z - L_2)\\ &- (-\gamma_1 + \gamma_3)\mathcal{U}(z - L_3)\end{aligned}$$

where $\mathcal{U}$ is the Heaviside step function,
L_1 is the height at the bottom of the lance (region of influence),
L_2 is the height of the top of the lance (region of influence), and
L_3 is the height at which the melting of the ore has been "completed",
γ_1 is losses due to chemistry,
γ_2 is heat input from the lance,
γ_3 is losses due to melting of the ore.

Laplace Transform Solution

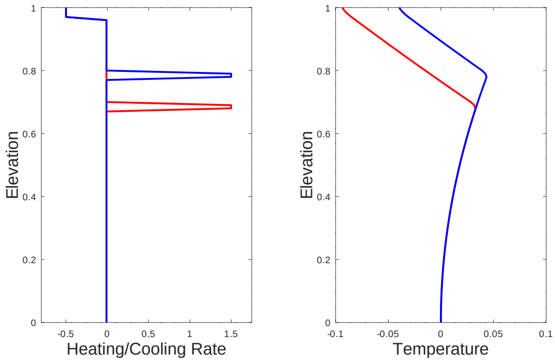
$$(s^2-\lambda^2)\hat{T} - sT(0) - T'(0)$$
$$= \frac{1}{s\alpha_{Turb}}\left(-\gamma_1 - (\gamma_1+\gamma_2)e^{-L_1 s} - (-\gamma_1+\gamma_2)e^{-L_2 s} - (-\gamma_1+\gamma_3)e^{-L_3 s}\right)$$

where $\hat{T}$ is the transform of T, i.e. $\hat{T}(s) = \mathcal{L}\{T(z)\}$ giving

$$\begin{aligned} T(z) = &-\left(\frac{\gamma_1}{\alpha_{Mol}}\right)(\cosh(\lambda z)-1) \\ &+\left(\frac{\gamma_1+\gamma_2}{\alpha_{Mol}}\right)\mathcal{U}(z-L_1)(\cosh(\lambda(z-L_1))-1) \\ &-\left(\frac{\gamma_1+\gamma_2}{\alpha_{Mol}}\right)\mathcal{U}(z-L_2)(\cosh(\lambda(z-L_2))-1) \\ &-\left(\frac{-\gamma_1+\gamma_3}{\alpha_{Mol}}\right)\mathcal{U}(z-L_3)(\cosh(\lambda(z-L_3))-1) \\ &+T(0)\cosh\lambda z + \frac{T'(0)}{\lambda}\sinh\lambda z \end{aligned}$$

where $\lambda = \sqrt{\alpha_{Mol}/\alpha_{Turb}}$.

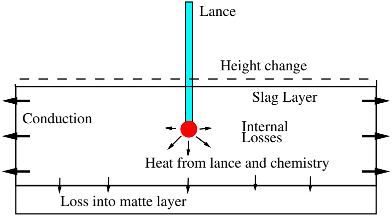
Preliminary Calculations for turbulent diffusion, 1D model



- Temperature(z) - lance height $H_L = 0.7$ (red) and $H_L = 0.8$ (blue).
- The region above the lance is "cooler" when the lance is lower.
- Hottest point always at level of the lance - diffuses up and down.
- Cooler above due to energy used for melting ore.

Well-mixed model

- Indications are that there is very violent mixing of the slag layer - which is quite shallow
- Suggests a zero-dimensional "heat-balance" model might be useful
- Heat input from the lance, losses through chemical reactions, phase changes, conduction through the boundaries, bubbling out the top must all add up to zero in **equilibrium operation**
- Could be used to determine the changes in heat balance if the layer depth changes - and requirements for adjusting lance inputs, e.g. during tapping of slag.



Thermal Runaway

- The furnace is mainly driven by heat resulting from the gas injected by the lance reacting with the slag.
- Aim to predict the onset of foaming (as in boiling milk) in which the bubbly region suddenly expands.
- Literature [1], suggests that milk boils over if the gas creation at the walls of the container suffers a sudden increase in temperature.
- The same may happen in the furnace at slag/gas interfaces, probably near the tip of the lance. [2]
- It takes place over very short time and length scales so might regard the slag/gas as a bubbly continuum with the possibility of thermal runaway occurring at the hottest point, whose location will be crucial for the control of foaming.

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[1] e.g. An experimental study of the pool boiling of milk by M.Kumar, O.Prakash, K.S.Kasana, Heat Transfer-Asian research, Vol 40,p159 (2011)

[2] For Arrhenius reactions such temperatures jumps can be predicted by the mathematical theory of thermal runaway. see Buckmaster and Ludford, Theory of laminar Flames, CUP 1982.

Next steps and closing remarks

- The slag region is actually short and fat, so a horizontal, axisymmetric model may be more appropriate.
- Consider the influence of bubbling and churn of gases, and conditions for thermal runaway.
- Consider the terms in the zero-dimensional heat balance, including the effect of level changes in tapping.
- Recommend more frequent but smaller tapping of slag to maintain a more consistent process.
- Less variation in slag level $\Rightarrow$ less adjustment of lance height, coal/oxygen feed etc.
- More detailed information (data) will be required to identify what instabilities matter. Discuss how some of the missing information can be collected in the plant.