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# PROBLEM 1: MATHEMATICAL SIMULATION OF A GLASS FURNACE

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## PROBLEM STATEMENT

To improve and control a process optimally, it is necessary to understand and measure the important parameters. This is no different for a glass melting furnace. The chemistry and physics is complex and interdependent. Furthermore, the very high temperatures employed make it very difficult to measure and see everything that is important. However, by making certain assumptions and simplifying it is possible to simulate the process using mathematical models. The accuracy of the simulation depends on the assumptions made and the models used.

It is fairly simple to model the glass flow using the three conservation laws:

- Continuity: —
- Momentum conservation: —
- Energy conservation: —

The general purpose CFD code Ansys Fluent® is implemented at PFG Building Glass to model the glass flows and the combustion space which solves the conservation equations and selected physical models.

The steps involved in solving a CDF problem are:

1. Define the modeling goals
2. Create the model geometry and mesh
3. Set up the solver and physical models
4. Compute and monitor the solution
5. Examine and save the results
6. Consider revisions to the numerical model parameters if necessary

The study group is asked to implement sub-models in step 3 above for the following two processes:

- The batch melting of glass
- The fining and refining process

The end goal is for the models to be implemented and tested in C or Ansys Fluent®.

## MODELING GOALS

1. Model the batch melting process
  - a. Options
  - b. Inputs: empirical constants defining chemical reaction rates, specie properties
  - c. Physical models: reaction rates, specie diffusivity, source terms
  - d. Assumptions
  - e. Computational domain boundaries
  - f. Boundary conditions
  - g. Mesh resolution

During the melting process, a blanket of foam (batch) made up of various chemical by-products forms on top of the molten glass (melt). The batch blanket is constantly melting into the melt. The task is to model the formation and evolution of this batch blanket and its interaction with the melt.

2. Model the fining and refining process
  - a. Options
  - b. Inputs: empirical constants defining chemical reaction rates, specie properties
  - c. Physical models: gas diffusion and bubble growth
  - d. Assumptions
  - e. Computational domain boundaries
  - f. Boundary conditions
  - g. Mesh resolution

During the melting process after the batch has melted, the temperature gets high enough for fining gases to be created by chemical reactions. These gases diffuse through the melt into existing bubbles in the melt. The task is to model this diffusion process and the evolution of these bubbles and their dependence and interdependence on temperature.

## THEORY

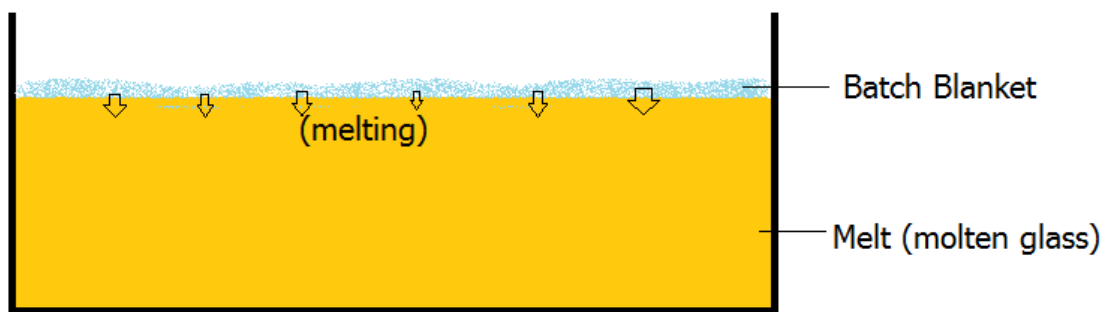
The glass-melt tank can be considered as a chemical reactor. In the first stage of the process, a large number of chemical reactions take place at different temperatures and in different phases. Most of the reactions happen in the vicinity of the batch blanket. After these fusion reactions, the glass melt contains incompletely dissolved sand grains, other refractory oxides, dissolved gasses and gas bubbles. The next stage in the melting process is the complete dissolution of the residual grains in the melt.

The freshly molten glass contains dissolved gasses, smaller gas inclusions, large bubbles and dissolved polyvalent ions present in a certain redox state which is determined by the amount of reducing or oxidizing components in the batch and the composition of the furnace atmosphere. At high temperatures, above a certain fining onset temperature level, the polyvalent ions are converted into a lower redox state and gasses such as oxygen or  $\text{SO}_2$  are generated in the melt. Owing to their low solubility, these fining gasses diffuse towards the bubbles already present in the melt. The composition of the bubbles then changes, and the original gas is diluted by the fining gasses. This causes the bubbles to grow and the initial equilibrium between the gasses in the bubble and the gasses dissolved in the melt is disturbed. Fining gasses and other dissolved gasses start diffusing into the growing seeds, driven by the difference in the equilibrium pressure of these gasses in the melt and the changing partial pressure in the bubble. The

growing bubble ascends to the glass-melt surface with a velocity proportional to the square of the diameter and proportional to the reciprocal value of the glass-melt viscosity.

The last stage of fining involves the slow cooling of the melt. The residual tiny bubbles that have not reached the glass-melt surface and the bubbles that have hardly grown can completely dissolve in the melt. This dissolution requires an increasing solubility as the melt cools down. Bubbles that contain gasses dissolving chemically in the melt can be re-absorbed because the solubility of these gasses in the melt will increase during temperature reduction. The dissolution rate of gasses and bubbles also depends on the diffusion coefficients of the gasses in the melt, and these values decrease with temperature reduction. This means that the dissolution of bubbles mainly takes place in a certain temperature range.

## BATCH MELTING



The coverage of the melt by a relatively cold batch blanket strongly influences the temperatures at the glass-melt surface. The temperature differences between the hot spot and locations underneath the batch blanket drive the free convection in a melting tank. This free convection influences the heat transfer processes, the residence time distribution and the mixing of the melt. The batch blanket consumes about 85% of the total energy needed for fusing the batch and temperature gradients in the blanket can be very high. It is important to predict the total energy consumption of the batch blanket, the temperature distribution, the batch blanket-glass melt interface temperature and the batch-blanket flow pattern. The mass transport of material from the batch blanket entering the glass-melt phase should be equal to the material molten in the batch blanket itself. The temperature at the interface batch blanket-glass melt, the length and thickness of the batch blanket and the local release of material from the batch blanket in to the glass-melt phase depends on:

- The heat transfer in the batch blanket itself,
- The kinetics of the fusion reactions in the batch blanket which depends mainly on the local temperature in the blanket,
- The flow pattern and movement of the batch blanket,
- The energy demand for chemical reactions

Heat is mainly transferred from the combustion space to the top of the blanket by radiation. The bottom side of the batch is heated by radiation and conduction of heat from the glass melt flowing underneath the batch blanket to the batch. The release of gasses at this hot batch-bottom side heats the inner parts of the batch blanket because dissociation gasses ascend through the batch. The penetration of heat into the batch material depends on the heat conductivity of the batch, the endothermic or exothermic

reactions and on the release of batch gasses. During these thermal processes in the batch blanket, the batch phases change due to chemical reactions and formation of liquid or gas phases. Composition and density are changed by disappearance of the original raw material, the formation of melts and by the changing batch porosity. The batch to melt conversion is built up by a series of sequential and parallel chemical reactions. The conversion rate is mainly limited by mass transfer and heat transfer. Therefore, the degree of batch to melt conversion is both dependent on the local temperature and on the temperature history of the glass batch. The energy balance for the batch blanket can be given by

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where  $\rho_b$  is the density of the glass batch,  $c_{p,b}$  is the heat capacity of the glass batch,  $\lambda_b$  is the effective heat conductivity,  $S$  is the net heat sink rate due to all chemical reactions,  $h$  is the heat transfer coefficient between the batch and enclosed gasses,  $f$  is the specific heat transfer area between the batch,  $T_g$  is the temperature of the gasses enclosed in the batch,  $T_b$  is the temperature of the glass batch and  $t$  is time. The last term can be neglected by incorporating it in  $\lambda_b$ .

In the simplest batch-blanket model, the melting rate  $q_{\text{melt}}$  is calculated by estimation rules such as

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where  $T_0$  is the melting onset temperature,  $A$ : melting starts at  $T=T_0$  and  $C$ : melting rate is doubled every  $C$  degrees.

## GAS BUBBLE BEHAVIOUR

After the fusion or dissolution of most batch components, the glass melt contains dissolved gasses and gas bubbles in sizes varying from 0.03mm up to several millimeters. The concentration of dissolved gasses in the fresh melt is relatively high. The most important gasses in the melt or in the gas bubbles are nitrogen, carbon dioxide, water vapor, oxygen, sulfur dioxide, argon and nitrogen oxide or carbon dioxide. The bubbles can be removed by two different processes: bubble ascension to the glass-melt surface, where the bubbles collapse, or complete absorption of the gasses by the melt.

The rising velocity of a bubble can be derived from Stoke's law:

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where  $v$  is the ascension velocity,  $R$  is the bubble radius,  $\rho$  is the density of the glass melt,  $g$  is gravity acceleration,  $\eta$  is the viscosity of the melt and  $c$  is a factor between 2/9 (rigid bubble surface) and 1/3 (mobile bubble surface).

The bubble ascension velocity is proportional to  $R^2$  and  $1/\eta$ . A small bubble hardly rises in the melt and the bubble neither grows nor shrinks when an equilibrium exists between the partial vapor pressures of the gasses in the bubble and the same gasses dissolved in the molten glass. There is then equilibrium for each gas species  $i$ :

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where  $L_i$  is the Henry solubility of gas  $i$  in the melt at 1 Pa vapor pressure,  $C_{gi}$  is the concentration of the dissolved gas  $i$  in the melt and  $p_i$  is the vapor pressure of gas  $i$  in equilibrium with the dissolved gas  $i$ .

The gas can dissolve chemically by reacting with the glass melt components or physically by occupying open sites in the melt structure. In general, the chemical solubility is orders of magnitude higher than the physical solubility. However, the chemical solubility is much more temperature dependent. Fining gasses such as  $SO_2$  and  $O_2$  dissolve chemically at low temperatures. A fining agent dissolved in the molten glass releases these gasses at increasing temperatures. Sulfates produce  $SO_2$  and  $O_2$  and polyvalent ions in the most oxidized state are reduced by temperature increments releasing  $O_2$ . A temperature increase in a melt containing fining agent increases the equilibrium pressure of the fining gasses, the equilibrium of the fining gas in the bubble and in the melt is disturbed and the fining gas diffuses into the bubbles. As a consequence, these bubbles grow and the original gasses in the bubble become diluted by the fining gas in the melt. This process disturbs the gas-melt phase equilibrium of the other gasses which now start diffusing into the growing bubbles as well. Bubble rise velocity accelerates therefore during the fining process. The bubble ascension rate increases with temperature and the glass melt is more readily stripped of the dissolved gasses.

The total bubble pressure is given by:

$$p_b = p_o + \rho H + \frac{2\sigma}{r}$$

Where  $p_o$  is the atmospheric pressure,  $\rho$  is the density of the melt,  $\sigma$  is the surface tension and  $H$  is the height of the melt above the bubble. The bubble pressure decreases as the bubble grows and rises in the melt. Above a certain temperature level, the total equilibrium pressure of the fining gasses may exceed the value total bubble pressure. The bubble then grows continuously because equilibrium between the dissolved gasses and the bubble cannot be reached. At this temperature level, the removal of gasses becomes very efficient and is called the fining onset temperature  $T_{onset}$ .

If the concentration of a dissolved gas is not in equilibrium with a bubble, an exchange of the gas takes place between the gas bubble and the melt. The bubble may grow or shrink by multi-gas species diffusion and can be described by the following relation:

$$\frac{dC_{bi}}{dt} = \frac{D_i}{r^2} (C_{si} - C_{bi}) - \frac{p_i}{R_g t} \left( \frac{C_{si}}{p_i} - \frac{C_{bi}}{p_i} \right)$$

where  $R_g$  is the gas constant,  $t$  is time,  $D_i$  is the diffusion coefficient of gas  $i$  in the molten,  $C_{si}$  is the concentration of gas  $i$  in the melt in equilibrium with the vapor pressure of gas  $i$  in the bubble

where  $L_i$  is the solubility of gas  $i$  in the molten glass,  $p_i$  is the partial vapor pressure of gas  $i$  in the bubble and  $p_{bi}$  is the partial pressure of gas  $i$  in the bubble.  $C_{si}$  is the concentration of gas  $i$  in the glass melt,  $Sh_i$  is the Sherwood number.

If, for most gasses,  $C_{si} > C_{bi}$ , then we have bubble growth. At high temperatures, the fining gas solubility in the melt decreased and the bubble starts growing. During cooling, the solubility of the fining gas increases

again and the value of  $C_{si}$  for the fining gas may become much smaller than  $C_{ij}$ . The slow-cooling stage of the melt to reabsorb gasses is called refining.

The calculation of gas exchange between the bubbles and the melt and bubble rise requires initial conditions:

- The initial bubble composition and size,
- The position of the bubble in the melt,
- The initial concentration level of dissolved gasses, and
- The concentration of the fining agent and the redox state

Very important in modeling bubble behavior in glass melts are the diffusion coefficients, the solubilities and the fining reaction equilibrium constants. These values often depend strongly on the temperature and the glass composition.

In a glass-melt tank, the bubbles follow a path from the position where these bubbles are formed to the outlet of the tank or the surface of the melt. This path differs from the glass-melt flow pattern due to buoyancy forces acting on the bubble. The concentration of dissolved gasses in the glass melt and the redox state are both location dependent.

The concentration change of a dissolved gas species  $i$  in the melt is determined by the convection and diffusion process:

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Where  $C_{si}$  is the local concentration of gas  $i$  on the melt,  $D_i$  is the diffusion coefficient,  $Q_i$  is the formation rate by chemical reaction and  $\mathbf{v}$  is the glass-melt velocity vector.