Mathematical modelling of alumina feeding

Attila Kovacs InFoMM CDT, Mathematical Institute, University of Oxford

Chris Breward, James Oliver and Andreas Münch (Oxford) Svenn Halvorsen and Ellen Nordgård-Hansen (Norce) Eirik Manger (Norsk Hydro)

ICIAM 2019

July 18, 2019

Hall-Héroult cell





Alumina feeding processes



3/14



Main question: How does the molten cryolite infiltrate and dissolve a porous alumina structure? Focus of talk is *Stage B*, raft problem.

Alumina feeding: raft problem





Alumina feeding: raft problem













For c(t) < y < H:

$$\frac{\partial T_3}{\partial t} = \frac{\partial^2 T_3}{\partial y^2},$$

At
$$y = c(t)$$
: $T_3 = 1 - \varepsilon$, $\psi \dot{c} = -Stk_{pf} \frac{\partial T_3}{\partial y}$,
At $y = 1$: $\frac{\partial T_3}{\partial y} = Nu(T - \theta_e)$





Δ

 $\partial \psi$

For b(t) < y < c(t):

$$egin{aligned} &\overline{\partial t} &= 0, \ &\overline{\partial t} &= 0, \ &\overline{\partial y} \left((1-\phi-\psi) u_2
ight) &= 0, \ &-\gamma rac{\mathcal{K}(\psi+\phi)}{(1-\phi-\psi)} \left(rac{\partial p_2}{\partial y} + eta
ight) &= u_2, \end{aligned}$$

At
$$y = b(t)$$
: $[p_i]_{-}^{+} = 0$, $u_1 - \frac{1 - \phi - \psi}{1 - \phi} u_2 = \psi \dot{b} \frac{1 - \rho}{1 - \phi}$,
At $y = c(t)$: $p_2 = -1$, $u_2 = \dot{c} \left(1 + \frac{\psi \rho}{1 - \phi - \psi} \right)$,



c(t)b(t)Н Infiltrated For 0 < y < b(t): $\frac{\partial T_1}{\partial t} + \frac{\partial}{\partial v} (q\phi_c u_1 T_1) = \alpha_{ip} \frac{\partial^2 T}{\partial v^2},$ $\frac{\partial}{\partial y}\left((1-\phi)u_1\right)=0,$ $\gamma \frac{-K(\phi)}{(1-\psi)} \left(\frac{\partial p_1}{\partial y} + \beta \right) = u_1,$ At v = 0: $T_1 = 1$, $p_1 = 0$. At y = b(t): $T_1 = 1 - \varepsilon$, $\psi \dot{b} = -Stk_{if} \frac{\partial T_1}{\partial y}$, $[p_i]^+_{-} = 0, \quad u_1 - \frac{1 - \phi - \psi}{1 - \phi} u_2 = \psi \dot{b} \frac{1 - \rho}{1 - \phi},$



Meaning and Symbol	Definition	Value
Infiltrating force (γ)	$KP/(\alpha_p\mu_c)$	10–200
Stefan number (St)	$\alpha_{fp}[T]c_f/L$	2.3
Newton cooling (Nu)	hH/k _p	3
Diffusivity ratio $(lpha_{\it ip}$)	α_i/α_p	2
Overheat ($arepsilon$)	T_c/T_m-1	0.015
Environment temperature ratio ($ heta$)	T_A/T_m	0.86
Conductivity ratio (<i>k_{if}</i>)	k _i /k _f	2.5
Conductivity ratio (<i>k_{pf}</i>)	k_p/k_f	0.5



Meaning and Symbol	Definition	Value
Infiltrating force (γ)	$KP/(\alpha_p\mu_c)$	10-200
Stefan number (St)	$\alpha_{fp}[T]c_f/L$	2.3
Newton cooling (Nu)	hH/k_p	3
Diffusivity ratio ($lpha_{\it ip}$)	α_i/α_p	2
Overheat (ε)	$T_c/T_m - 1$	0.015
Environment temperature ratio $(heta)$	T_A/T_m	0.86
Conductivity ratio (<i>k_{if}</i>)	k _i /k _f	2.5
Conductivity ratio (<i>k_{pf}</i>)	k_p/k_f	0.5



In this limit the infiltrated region does not exist, so only mushy region and uninfiltrated is important. For the uninfiltrated region we have

$$rac{\partial T_3}{\partial t} = rac{\partial^2 T_3}{\partial y^2}$$
 in $c(t) < y < 1$,

with boundary conditions,

 $T_3=1$ at y=c(t), $T_3=0$ at y=1

Small overheat ($\varepsilon \ll 1$) limit



In this limit the infiltrated region does not exist, so only mushy region and uninfiltrated is important. For the uninfiltrated region we have

$$rac{\partial T_3}{\partial t} = rac{\partial^2 T_3}{\partial y^2}$$
 in $c(t) < y < 1$,

with boundary conditions,

$$T_3=1$$
 at $y=c(t)$, $T_3=0$ at $y=1$

and for the mushy region we have (with suitable boundary conditions)

$$egin{aligned} &rac{\partial\psi}{\partial t}=0,\ &rac{\partial}{\partial y}\left((1-\phi-\psi)u_2
ight)=0,\ &-\gammarac{K(\psi+\phi)}{(1-\phi-\psi)}\left(rac{\partial p_2}{\partial y}+eta
ight)=u_2, \end{aligned}$$

Small overheat ($\varepsilon \ll 1$) limit



In this limit the infiltrated region does not exist, so only mushy region and uninfiltrated is important. For the uninfiltrated region we have

$$rac{\partial T_3}{\partial t} = rac{\partial^2 T_3}{\partial y^2}$$
 in $c(t) < y < 1$,

with boundary conditions,

$$T_3=1$$
 at $y=c(t)$, $T_3=0$ at $y=1$

fluid equations can be integrated in space and lumped into the boundary conditions giving

$$\psi = -\frac{\partial T_3}{\partial y} \frac{I}{\mathrm{St}}, \quad \dot{c} = \frac{1}{I}, \quad c(0) = 0$$

with introducing

$$I = \int_{0}^{c(t)} \frac{1}{\gamma K(\phi(x))} \, \mathrm{d}x$$
, $\dot{I} = \frac{1}{\gamma I K(\psi(c))}$, $I(0) = 0$

Small time asymptotics



- Expand $c = O(\sqrt{t})$ as $t \to 0^+$, so need small t asymptotics to initiate numerical solution, because 0 is singular.
- Seek similarity solution given

$$T \sim T(\eta), \quad c \sim 2\lambda_c \sqrt{t}, \quad I \sim 2\lambda_I \sqrt{t}$$

with $\eta = y/2\sqrt{t} = O(1)$ as $t \to 0^+$ and λ_c, λ_l to be determined from a system of nonlinear equations.



Similarity solutions for St = 1, $\gamma = 10$





For a parameter set two different solutions are possible: faster propagating with less freeze (

EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling

10/14

Numerical results (fast)



11/14

Stable propagation agrees with small-time solution, then clogs due to the boundary.

Numerical results (slow)



12/14

Unstable solution switches to the stable one in short time, then clogs due to the boundary.

Regime diagram for early time solutions





and the operating regime for the real system (dashed).



Conclusions:

- Developed a multiphase model for the infiltration of molten cryolite into a cold porous alumina
- Investigated the relevant small overheat $1-\theta \ll 1$ limit having a new type of Stefan condition coupling Darcy flow to heat equation
- Similarity solution at small times yields nonuniqueness with one stable solution and nonexistence
- Simulations show either clogging or full infiltration depending on the top boundary condition

Future work:

- What is the solution when there is nonexistence? (Different model)
- What are the next stages of the evolution?
- Refine physics (top boundary, pore size dependent capillary pressure, dropping LTE, composition effects)

Mathematical Institute