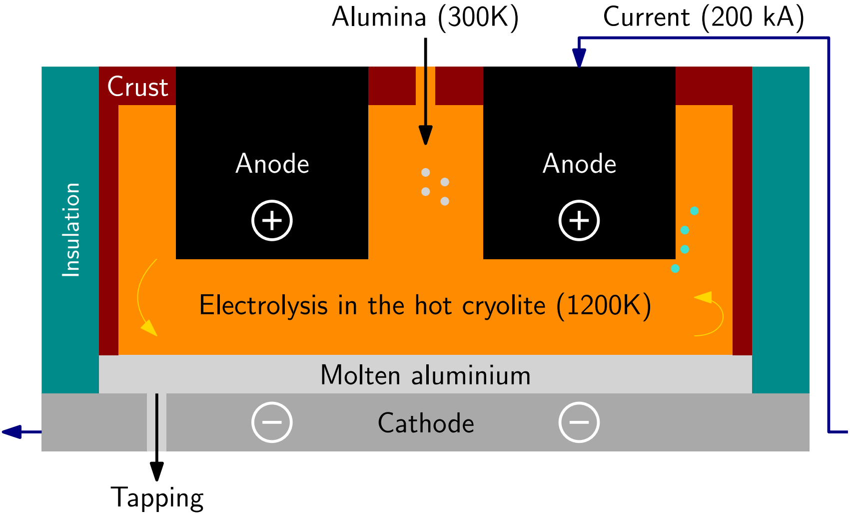
Mathematical modelling of alumina feeding

Attila Kovacs

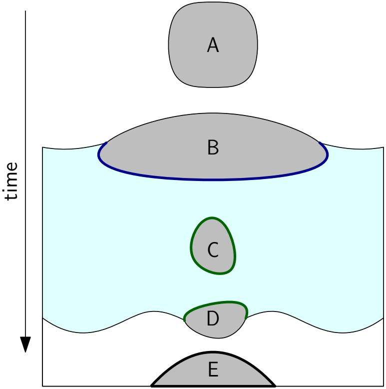
Chris Breward, James Oliver and Andreas Münch (Oxford)
Svenn Halvorsen and Ellen Nordgård-Hansen (Norce)
Eirik Manger (Norsk Hydro)

March 14, 2019

Hall-Héroult cell

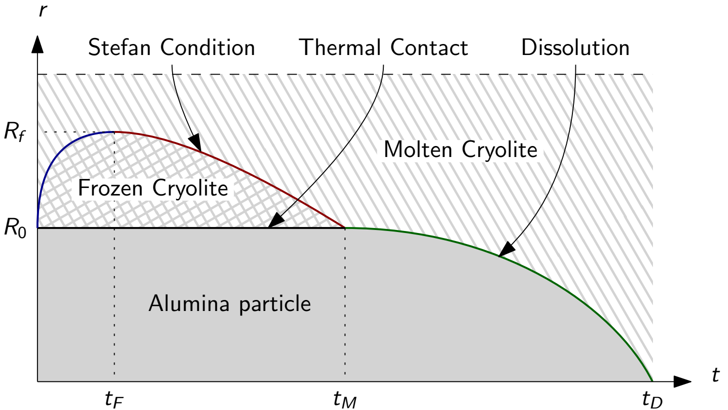


Alumina feeding processes



How does the molten cryolite infiltrate and dissolve a porous alumina structure?

Previous Analysis: Solid alumina particle

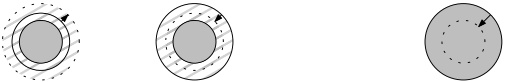


Freezing time | Melting time | Dissolution time

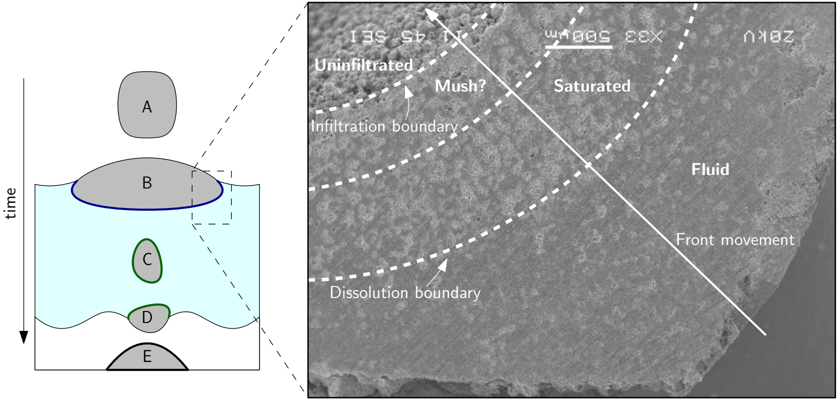
$$t_F \sim \frac{a^2 c_A \rho_A}{\pi^2 k_A}$$

$$t_M \sim \frac{a^2 c_A \rho_A (T_m - T_A)}{3 k_c (T_c - T_m)}$$

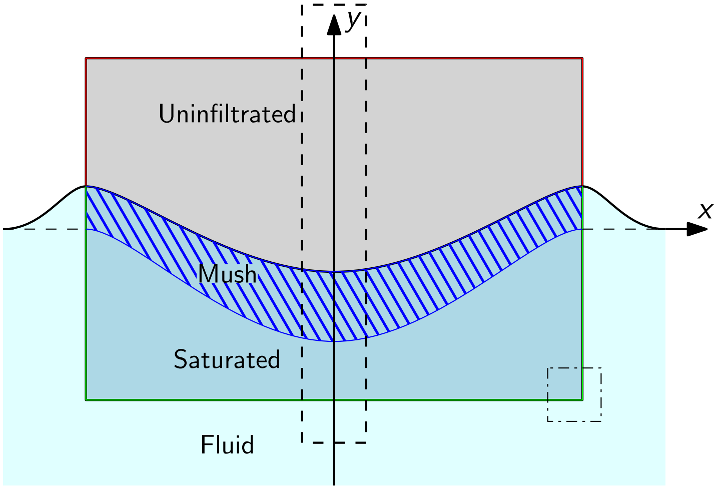
$$t_D \sim \frac{a^2 \rho_a (1 - C_s/\rho_c)}{2D(C_s - C_0)}$$



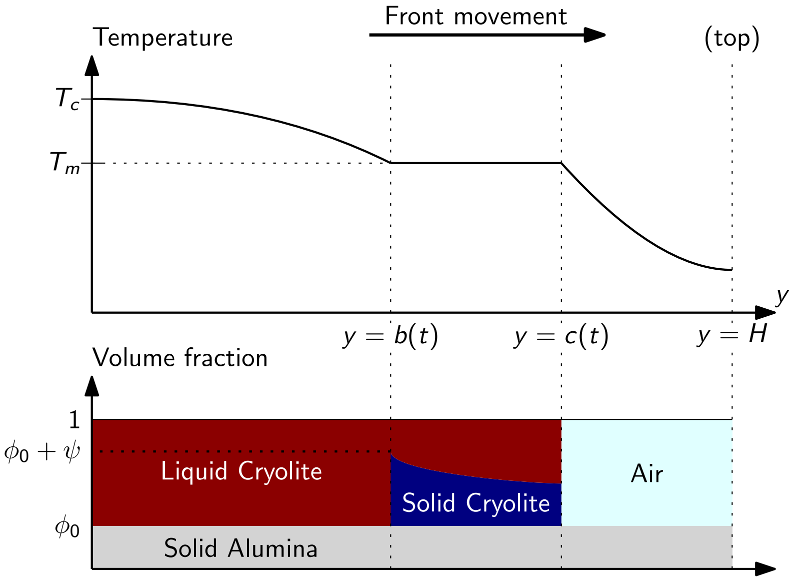
Alumina feeding: raft problem



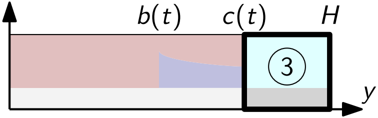
Alumina feeding: raft problem



1D Infiltration problem



1D Infiltration problem: uninfiltrated region



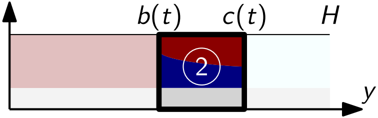
For $c(t) < y < H$:

$$\frac{\partial T_3}{\partial t} = \frac{k^*}{\rho_A c_A \phi} \frac{\partial^2 T_3}{\partial y^2}$$

$$\text{At} \quad y = c(t): \quad T_3 = T_m, \quad \rho_c \psi \dot{c} = -k_3 \frac{\partial T_3}{\partial y}$$

$$\text{At} \quad y = H: \quad k_3 \frac{\partial T_3}{\partial y} = h(T - T_e)$$

1D Infiltration problem: mushy region



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

$$\frac{\partial \psi}{\partial t} = 0$$

$$\frac{\partial}{\partial y}\left((1-\phi-\psi)u_2\right) = 0$$

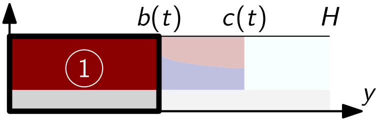
$$\frac{-K(\psi+\phi)}{\mu(1-\phi-\psi)}\left(\frac{\partial p_2}{\partial y} + \rho_c g\right) = u_2$$

At $\quad y = c(t): \quad p_2 = p_a - \dfrac{\sigma_c}{r_{pore}}, \quad u_2 = \dot{c}\left(1 + \dfrac{\psi\rho}{1-\phi-\psi}\right)$

At $\quad y = b(t): \quad [p_i] = 0, \quad u_1 - \dfrac{1-\phi-\psi}{1-\phi}u_2 = \psi\dot{b}\dfrac{1-\rho}{1-\phi}$

1D Infiltration problem: infiltrated region

InFoMM Industrially Focused Mathematical Modelling



For $0 < y < b(t)$:

$$\frac{\partial T_1}{\partial t} + \frac{\partial}{\partial y}\left(\frac{1-\phi}{a} u_1 T_1\right) = \frac{k_1}{a\rho_A c_A}\frac{\partial^2 T}{\partial y^2}$$

$$\frac{\partial}{\partial y}\left((1-\phi)u_1\right) = 0$$

$$\frac{-K(\phi)}{\mu(1-\psi)}\left(\frac{\partial p_1}{\partial y} + \rho_c g\right) = u_1$$

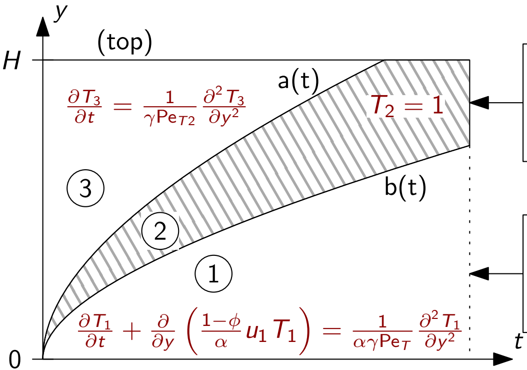
At $y = b(t)$: $T_1 = T_m$, $\rho_c \psi \dot{b} = -k_1 \frac{\partial T}{\partial y}$,

$[p_i] = 0$, $u_1 - \frac{1-\phi-\psi}{1-\phi} u_2 = \psi \dot{b} \frac{1-\rho}{1-\phi}$,

At $y = 0$: $T_1 = T_h$, $p_1 = \rho g H$

Full dimensionless problem

InFoMM Industrially Focused Mathematical Modelling



$$\frac{\partial \psi}{\partial t} = 0, \quad \frac{\partial}{\partial y}(\Phi u_2) = 0$$

$$u_2 = \frac{-K(\psi+\phi)}{1-\phi-\psi}\left(\frac{\partial p_2}{\partial y} + \beta\right)$$

$$\frac{\partial}{\partial y}\left((1-\phi)u_1\right) = 0$$

$$u_1 = \frac{-K(\phi)}{1-\phi}\left(\frac{\partial p_1}{\partial y} + \beta\right)$$

$y = 0$	$y = b(t)$	$y = c(t)$	$y = 1$
$T_1 = 1 + \varepsilon$	$T_i = 1$	$T_i = 1$	$\frac{\partial T_3}{\partial y} = \mathrm{Nu}(T_3 - \theta)$
$p_1 = 0$	$[p_i]_-^+ = 0$	$p_2 = -1$	
	$u_1 - \frac{\Phi}{1-\phi} u_2 = \psi \dot{b} \frac{1-\rho}{1-\phi}$	$u_2 = \dot{c}\left(1 + \frac{\psi\rho}{\Phi}\right)$	
	$\gamma\kappa\psi\dot{b} = -\frac{\partial T_1}{\partial y}$	$\gamma\psi\dot{c} = -\frac{\partial T_2}{\partial y}$	

Dimensionless parameters

Meaning	Symbol	Equation	Value
Infiltrating force	γ	$KP\tau/(\mu_c H^2)$	40–400
Newton cooling	Nu	hH/k^*	3
Condictivity ratio	κ	k^*/k_m	0.2
Thermal diffusivity	Pe_T	$H^2\rho_c c_c/(k_m\tau)$	1.3
Thermal diffusivity	Pe_{T2}	$\dfrac{H^2\rho_A c_A\phi}{\tau k_A\,(k_{air}/k_A)^{1-\phi}}$	1.77
Particle coldness	θ	T_A/T_m	0.246
Overheat	ε_T	$T_c/T_m - 1$	0.015
Density ratio	ρ	ρ_f/ρ_c	1.00966
Importance of gravity	β	$\rho_c gH/P$	0.01
Energy stored in phases	α	$\phi\frac{\rho_A c_A}{\rho_c c_c} + (1-\phi)$	0.81

Small time asymptotics

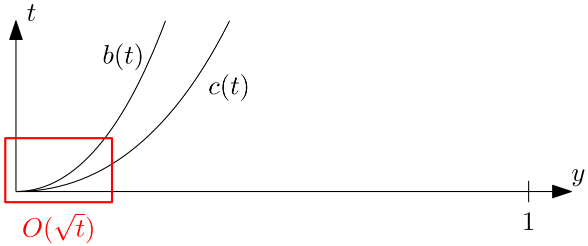
InFoMM
Industrially Focused Mathematical Modelling

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

$$T_i \sim f_i(\eta), \quad u_i \sim \frac{g_i(\eta)}{\sqrt{t}}, \quad p_i \sim h_i(\eta), \quad \psi \sim \psi_c,$$

$$b \sim 2\lambda_b\sqrt{t}, \quad c \sim 2\lambda_c\sqrt{t}$$

with $\eta = y/2\sqrt{t} = O(1)$ as $t \to 0^+$ and $\lambda_b, \lambda_c, \psi_c$ to be determined.



Transcendential system for $\lambda_b, \lambda_c, \psi_c$

$$K_2(\psi_c) = -2(\lambda_b - \lambda_c)g_2(1 - \phi - \psi_c) + \lambda_b g_1 (1 - \phi)\frac{K_2(\psi_c)}{K_1}$$

$$\gamma 2\kappa\psi_c\lambda_b = \frac{2\sqrt{\mathrm{Pe}_{T1}}\epsilon e^{-\mathrm{Pe}_{T1}(ag_1+\lambda_b)^2}}{\sqrt{\pi}\left(\mathrm{erf}\left(\sqrt{\mathrm{Pe}_{T1}}(ag_1 + \lambda_b)\right) - \mathrm{erf}\left(ag_1\sqrt{\mathrm{Pe}_{T1}}\right)\right)}$$

$$2\gamma\psi_c\lambda_c = -\frac{2(\theta - 1)\sqrt{\mathrm{Pe}_{T2}}e^{-\mathrm{Pe}_{T2}\lambda_c^2}}{\sqrt{\pi}\mathrm{erfc}\left(\lambda_c\sqrt{\mathrm{Pe}_{T2}}\right)}$$

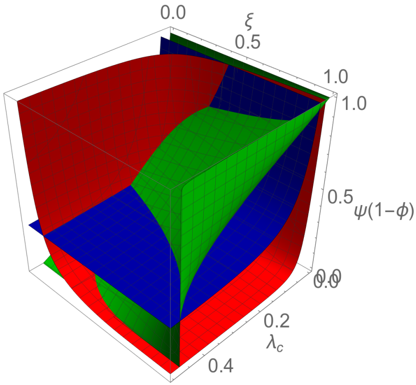
where g_1 and g_2 constants given by

$$g_1 = \lambda_c + \frac{(\lambda_c - \lambda_b)(\rho - 1)\psi_c}{1 - \phi}$$

$$g_2 = \lambda_c\left(1 + \frac{\psi_c\rho}{1 - \phi - \psi_c}\right)$$

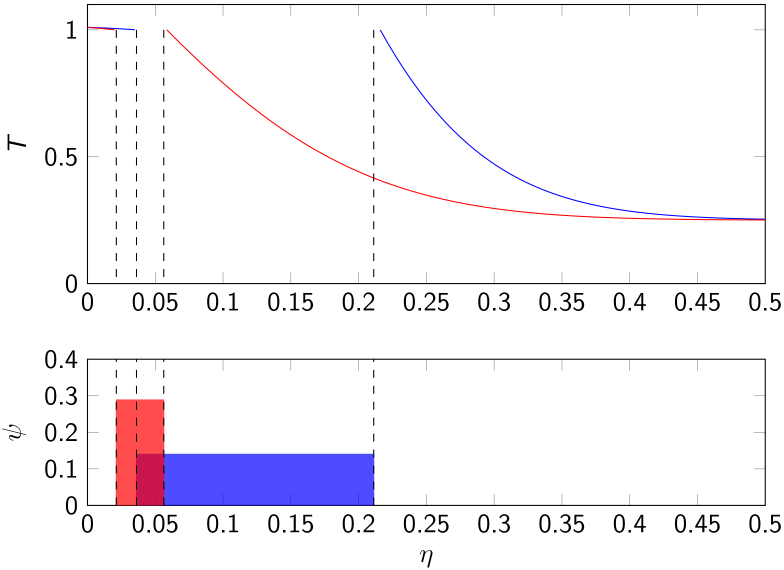
Constraint surfaces

Industrially Focused Mathematical Modelling



Two physical solutions with $\gamma = 200$ and $\mathrm{Pe}_{T2} = 1/7$.

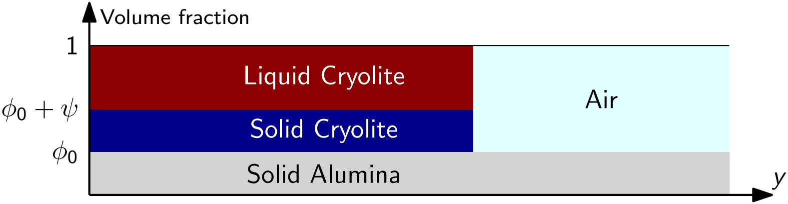
Similarity solution for $\gamma = 200$, $\mathrm{Pe}_{T2} = 0.14$



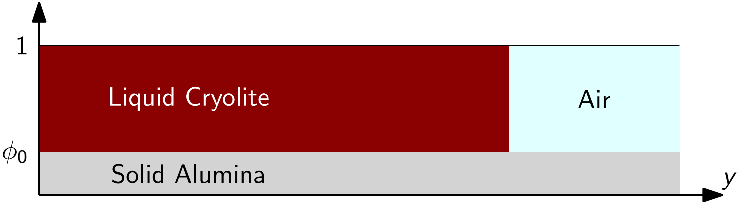
Sanity check: sublimits

InFoMM
Industrially Focused Mathematical Modelling

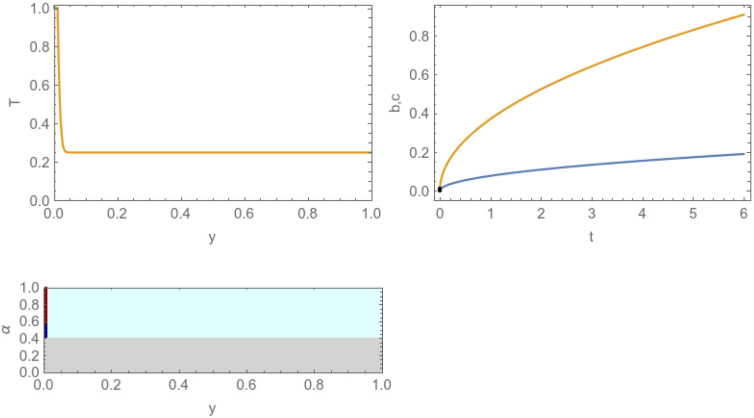
No heating ($\varepsilon = 0$, $\lambda_b = 0$)



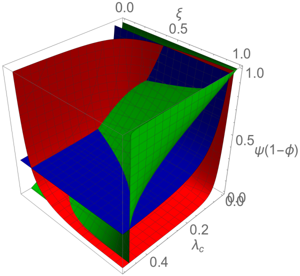
No cooling and heating (ε, $\theta = 1$)



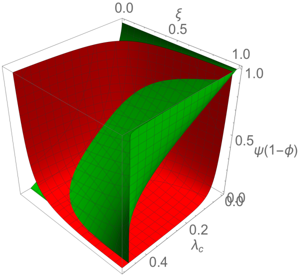
Comparison with numerical results



Nonexistence of Solutions



No physical solutions with $\gamma = 75$ and $\mathrm{Pe}_{T2} = 0.14$ due to no intersection in the physically admissible region.



No physical solutions with $\gamma = 75$ and $\mathrm{Pe}_{T2} = 1.7$ due to the Stefan condition (blue). $\psi > 1 - \phi$, meaning freezes more than the available fluid.

Conclusions and Future work

Conclusions:

- Developed a simple model for the infiltration of molten cryolite into a cold porous alumina structure (with phase change).
- Similarity solution at small times yields nonexistence and nonuniqueness.
- Preliminary numerical simulation suggest one solution is admissible while the other may blow up.

Future work:

- Characterise regions for similarity solution
- Investigate small time behaviour numerically: Alternatives to similarity solution?
- Are we missing physics e.g.
  - capillary pressure dependence on porosity
  - dropping local thermodynamical equilibrium
  - including composition effects