Production of Aluminium: Modeling, Analysis and Numerics

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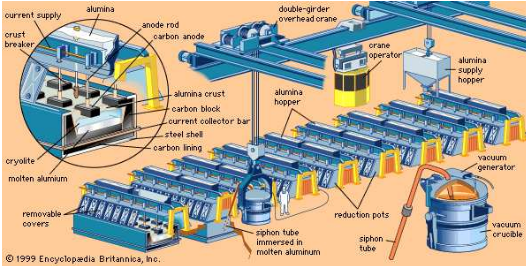
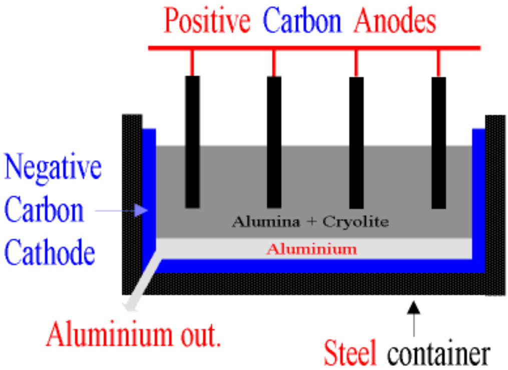
Contents

Part I: Modeling of Production of Aluminium

Motivation: Production of Aluminium

- electrolysis: reduce aluminium oxid to aluminium
- two non-miscible, conducting, incompressible fluids
- high temperatures & high currents: no experimental data
- industrial challenge: reduce electric power waste





- anod-metal distance: controlled movement of interface

... the industrial problem

- chem. reaction A: at surface of carbon anod

$$3\ O^{2-} + \frac{3}{2}\ C \rightarrow \frac{3}{2}\ CO_2(gas) + 6\ e^-$$

- chem. reaction B: at interface between the two fluids

$$Al_2O_3 + 6\ e^- \rightarrow 2\ Al^{3+} + 3\ O^{2-} + 6\ e^- \rightarrow 2\ Al + 3\ O^{2-}$$

- Global balance:

$$2\ Al_2O_3 + 3\ C \rightarrow 4\ Al + 3\ CO_2$$

- needed: $\approx 1000\ C^0$, high intensity of current
- "the higher intensity, the higher production"

- Goals/Problem: reduce power waste
  - reduce anod-metal distance: small distance between anod and surface of aluminium layer (‘a few centimeters’)
  - strong Lorentz forces: motion of the interface; instabilities
  - avoid short -circuits: no touching of fluid-fluid interface and anod
- Questions: how stabilize the position of the interface?
- Control parameter: height of anod, intensity of current, geometry
- experimental observations difficult to obtain

Modeling of the problem

- Physical phenomena and simplifying assumptions:
  - magnetohydrodynamics (MHD)
  - moving interface
  - electrochemistry (concentration of chemical species not homogeneous throughout liquids
  - three-phase flows (bubbles of carbon oxydes at surface of anods)
  - solidification process at boundaries
  - temperature effects (influence of physical parameters)

Continuum Model

- Maxwell equations coupled to multi-fluid Navier-Stokes equations

$$\partial_t \rho + \mathrm{div}(\rho \mathbf{u}) = 0,$$

$$\partial_t(\rho \mathbf{u}) + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u}) - \mathrm{div}\Big(2\eta \varepsilon(\mathbf{u})\Big) + \nabla p = \rho \mathbf{f} + \frac{1}{\mu}\, \mathbf{curl}\, \mathbf{B} \times \mathbf{B}$$

$$\mathrm{div}\, \mathbf{u} = 0 \qquad \mathrm{div}\, \mathbf{B} = 0$$

$$\partial_t \mathbf{B} + \mathbf{curl}\, \mathbf{E} = 0$$

$$-\partial_t(\varepsilon \mathbf{E}) + \mathbf{curl}\, \frac{\mathbf{B}}{\mu} = \mathbf{j} \quad \text{for} \qquad \mathbf{j} = \sigma(\mathbf{E} + \mathbf{u} \times \mathbf{B}),$$

- ρ density of fluids $\quad \boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$
  $\mathbf{B}$ magnetic field $\quad \sigma$ electric conductivity
  $\mathbf{j}$ electric current $\quad \eta$ viscosity
- Assumption: 'low frequency hypothesis': neglect $\partial_t(\varepsilon \mathbf{E})$.

$$\partial_t \mathbf{B} + \mathbf{curl}\Big(\frac{1}{\mu_0 \sigma}\ \mathbf{curl}\ \mathbf{B}\Big) = \mathbf{curl}(\mathbf{u} \times \mathbf{B}),$$
$$\mathrm{div}\ \mathbf{B} = 0$$

$$\Rightarrow \quad \partial_t\ \mathbf{B} + \mathbf{curl}\big(\tfrac{1}{\mu_0 \sigma}\ \mathbf{curl}\ \mathbf{B}\big) = \mathbf{curl}(\mathbf{u} \times \mathbf{B}), \quad \mathrm{div}\ \mathbf{B} = 0$$

- magnetic boundary conditions on $\partial\Omega$:

$$\mathbf{B} \cdot \mathbf{n} \quad , \qquad \mathbf{curl}\ \mathbf{B} \times \mathbf{n}$$

PART II: The one-fluid MHD equations – Analysis and Numerics

Analytical results/Numerical Strategies

- M. Sermange & R. Temam [1983]:
  - global weak solutions for $\Omega \subset \mathbb{R}^3$
  - local strong solutions for $\Omega \subset \mathbb{R}^3$
- Goal: Develop schemes that approximate weak solutions
- for simplicity here: only temporal discretization

- Scheme A: Let $n \geq 1$. Find $(\mathbf{u}^n, p^n, \mathbf{b}^n, r^n)$ such that

$$d_t \mathbf{u}^n - \Delta \mathbf{u}^n + (\mathbf{u}^{n-1} \cdot \nabla)\mathbf{u}^n + \frac{1}{2}(\mathrm{div}\ \mathbf{u}^{n-1})\mathbf{u}^n$$
$$+ \mathbf{b}^{n-1} \times \mathbf{curl}\ \mathbf{b}^n + \nabla p^n = \mathbf{g}^n$$
$$\mathrm{div}\ \mathbf{u}^n = 0 \qquad \mathrm{div}\ \mathbf{b}^n = 0$$
$$d_t \mathbf{b}^n + \mathbf{curl}(\mathbf{curl}\ \mathbf{b}^n) - \mathbf{curl}(\mathbf{u}^n \times \mathbf{b}^{n-1}) - \nabla r^n = 0$$

Numerical Strategies to solve one-fluid MHD equation

- discrete energy law: “multiply 1st eqn. by $\mathbf{u}^n$, and 3rd eqn. by $\mathbf{b}^n$”

$$\frac{1}{2}d_t\left[||\mathbf{u}^n||^2+||\mathbf{b}^n||^2\right]+\frac{k}{2}\left[||d_t\mathbf{u}^n||^2+||d_t\mathbf{b}^n||^2\right]$$
$$+||\nabla\mathbf{u}^n||^2+||\mathbf{curl}\ \mathbf{b}^n||^2=(\mathbf{g}^n,\mathbf{u}^n)$$

- Result [P.'08]: Subconvergence $(k, h \to 0)$ to weak solution of one-fluid MHD system

– drawback of scheme: system coupled

+/- iterative decoupling strategy: restrictive mesh-constraint $k \leq Ch^4$ needed for convergence

- Scheme B: decoupled scheme

$$d_t\mathbf{u}^n - \Delta\mathbf{u}^n + (\mathbf{u}^{n-1}\cdot\nabla)\mathbf{u}^n + \frac{1}{2}(\mathrm{div}\,\mathbf{u}^{n-1})\mathbf{u}^n + \mathbf{b}^{n-1}\times\mathbf{curl}\,\mathbf{b}^{n-1} - \nabla p^n = \mathbf{g}^n$$

$$d_t\mathbf{b}^n + \mathbf{curl}(\mathbf{curl}\,\mathbf{b}^n) - \mathbf{curl}(\mathbf{u}^{n-1}\times\mathbf{b}^{n-1}) - \nabla r^n = 0$$

- Property: A perturbed energy law holds *in a fully discrete setting*, for $k \le Ch^3$.
- Result [P. '08]: Subsequence convergence $(k, h \to 0)$ to weak solution of one-fluid MHD-system.

PART III: The two-fluid MHD equations – Analysis and Numerics

The Model

- Navier-Stokes with variable density and viscosity with Maxwell's equation

$$
\begin{aligned}
(\rho \mathbf{u})_t + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u}) - \mathrm{div}\big(\eta(\rho)\mathbf{D}(\mathbf{u})\big) &= -\nabla p + \mathbf{g} + \frac{1}{\bar{\mu}} \mathbf{curl}\, \mathbf{b} \times \mathbf{b}, \\
\mathrm{div}\, \mathbf{u} &= 0, \\
\rho_t + \mathrm{div}(\rho \mathbf{u}) &= 0, \\
\mathbf{b}_t + \frac{1}{\bar{\mu}} \mathbf{curl} \left(\frac{1}{\xi(\rho)} \mathbf{curl}\, \mathbf{b} \right) &= \mathbf{curl}(\mathbf{u} \times \mathbf{b}), \\
\mathrm{div}\, \mathbf{b} &= 0,
\end{aligned}
\tag{1}
$$

together with IC's & BC's

- Assumptions:
  1. $0 < \bar{\eta}_- \leq \eta \leq \bar{\eta}_+ \,, \qquad 0 < \bar{\xi}_- \leq \xi \leq \bar{\xi}_+ .$
  2. $$\rho_0 = \begin{cases} \overline{\rho}_1 > 0, & \text{constant on } \Omega_1, \\ \overline{\rho}_2 > 0, & \text{constant on } \Omega_2, \end{cases} \quad \text{with } \overline{\Omega}_1 \cup \overline{\Omega}_2 = \overline{\Omega}, \qquad \text{meas } (\Omega_i) > 0$$

- Properties:
  1. non-negativity, boundedness of ρ

$$\overline{\rho}_1 \leq \rho \leq \overline{\rho}_2 \qquad \text{in } \Omega_T$$

  2. energy law:

$$\frac{1}{2}\frac{d}{dt}\int_\Omega \left[\frac{\rho|\mathbf{u}|^2}{2} + \frac{|\mathbf{b}|^2}{\bar{\mu}}\right] dx + \int_\Omega \left[\eta(\rho)|\boldsymbol{\varepsilon}(\mathbf{u})|^2 + \frac{1}{\bar{\mu}^2\xi(\rho)}|\mathbf{curl}\,\mathbf{b}|^2\right] dx = \int_\Omega \rho\mathbf{g}\cdot\mathbf{u}\,dx$$

Analytical results

- weak formulation: For
  - $\Omega \subset \mathbb{R}^3$ polyhedral domain
  - $\mathbf{u}_0, \mathbf{b}_0 \in \mathbf{H} := \left\{ \boldsymbol{\xi} \in L^2(\Omega) : \mathrm{div}\boldsymbol{\xi} = \text{ weakly in } \Omega, \boldsymbol{\xi} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \right\}$
  - ρ_0 as above
  - $\mathbf{f} \in L^2(0, T; L^2)$

  exists a weak solution

  $\mathbf{u} \in L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{J})$

  $\mathbf{b} \in L^\infty(0, T; \mathbf{H}) \cap L^2(0, T; \mathbf{X})$

  $\rho \in L^\infty(\Omega_T) \cap C([0, T]; L^p)$ for all $p \geq 1$

  which satisfies an energy inequality.

... Tools employed

- general Galerkin method
- Aubin-Lions compactness result
- Compactness result by J. Di Perna & P.L. Lions ['89]: Solvability of

$$\rho_t + \mathrm{div}(\mathbf{u}\rho) = f \quad \text{in } \Omega_T, \quad \rho(0,\cdot) = \rho_0 \in L^\infty(\Omega) \qquad (2)$$

Let $\{\rho_k\}_{k\geq 0} \subset L^\infty(0,T;L^\infty(\Omega))$ solve

$$(\rho_k)_t + \mathrm{div}(\mathbf{u}_k\rho_k) + [\mathrm{div}\mathbf{u}_k]\rho_k = f_k \quad \text{in } \Omega_T$$
$$(\rho_k)(0,\cdot) = (\rho_k) \quad \text{in } \Omega$$

Assume:

(i) $\{\mathbf{u}_k\}_k \subset L^1\left(0,T;\mathbf{W}_0^{1,2}\right)$, and $\mathbf{u} \in L^1\left(0,T;\mathbf{W}_0^{1,2}\right)$, such that
$\mathbf{u}_k \to \mathbf{u}$ in $L^1\left(0,T;\mathbf{L}^2\right)$
$\mathrm{div}\mathbf{u}_k \to \mathrm{div}\mathbf{u}$ in $L^1\left(0,T;L^2\right)$

(ii) $f_k \to f$ in $L^1\left(0,T;L^2\right)$
$(\rho_k)_0 \to \rho_0$ in $L^2(\Omega)$

Then
$\rho_k \to \rho$ in $L^2\left(0,T;L^2\right)$
where $\rho : \Omega \to \mathbb{R}$ is unique solution of (2).

Problems to construct a convergent Finite Element Discretization

- Discrete Energy Law: In continuous setting: multiply
  (1_1) with $\mathbf{u}$
  (1_3) with $\frac{1}{2}|\mathbf{u}|^2$
  Observation: $\frac{1}{2}|\mathbf{u}|^2$ no admissible test function in FE-discretization
  Idea (N. Walkington ['07]): reformulation

$$(\rho\mathbf{u})_t + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) = \frac{1}{2}\Big\{\rho\mathbf{u}_t + [\rho\mathbf{u}\cdot\nabla]\mathbf{u} + (\rho\mathbf{u})_t + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u})\Big\}$$

- (uniform) positivity and L^∞- boundedness of discrete densities:
  Idea: M-matrix property of stiffness matrix related to

$$(d_t\rho^n, \chi)_h + (\mathbf{U}^n \cdot \nabla\rho^n, \chi) + \frac{1}{2}([\mathrm{div}\mathbf{U}^n]\rho^n, \chi) + \alpha h^\alpha (\nabla\rho^n, \nabla\chi) = 0$$

  Tools:
  - $\alpha > 0$: M–matrix properly gives $0 < \boldsymbol{\rho_1} \leq \rho^n \leq \boldsymbol{\rho_2} < \infty$
  - numerical integration
  - regularization term to NSE $\beta_2 h^{\beta_2}(\nabla d_t \mathbf{U}^n, \nabla \mathbf{W}^n) \qquad \beta_2 \geq 0$
- discrete version of compactness result by R. DiPerna & P.L. Lions: Idea (N. Walkington ['07])

Tool: to validate $\mathrm{div}\mathscr{U} \to \mathrm{div}\mathbf{u}$ in $L^1(0,T;L^2)$
we add the regularization term to NSE

$$\beta_1 k^{\beta_1} (\mathrm{div}\mathbf{U}^n, \mathrm{div}\mathbf{W}^n) \quad , \quad \beta_1 > 0$$

- a compactness result of J.L. Lions to control temporal changes of iterates: There exists $\kappa > 0$

$$\int_0^T \left[\rho_1 ||\mathscr{U}^+ - \mathscr{U}^-||^2 + ||\mathscr{B}^+ - \mathscr{B}^-||^2\right] ds \leq Ck^\kappa$$

  Tool:
  - inverse estimates
  - mesh-constraints: $F(k,h) \geq 0$
- Problems already experienced for one-fluid MHD equation: $\mathbf{H}(\mathbf{curl}), \mathbf{H}(\mathrm{div})$,
  Tool: discrete compactness result by F. Kikuchi ['89]

Result: A stable, convergent FE–based discretization

- Let $\{(\rho^n, \mathbf{U}^n, \mathbf{B}^n)\}$ be solution of FE –based fully discrete scheme
- L. Banas, A.P. ['08]: Let
  - $\mathscr{T}$ be strongly acute
  - $F(k, h; \alpha, \beta_1, \beta_2, d) \geq 0$ be valid
  - $\rho^0 \to \rho_0$ in L^2, $\quad (\mathbf{U}^0, \mathbf{B}^0) \rightharpoonup (\mathbf{u}_0, \mathbf{b}_0)$ in $[\mathbf{L}^2]^2$

  For $(k, h) \to 0$ exist a convergent subsequence, and $(\rho, \mathbf{u}, \mathbf{b})$, s.t.

$$\mathbf{U} \rightharpoonup \mathbf{u} \text{ in } L^\infty(0, T; \mathbf{L}^2), \mathscr{B} \rightharpoonup \mathbf{b} \text{ in } L^\infty(0, T; \mathbf{L}^2), \sigma \overset{*}{\rightharpoonup} \rho \text{ in } L^\infty(0, T; \mathbf{L}^\infty)$$

  Where $(\mathbf{u}, \mathbf{b}, \rho)$ is weak solution to (1).

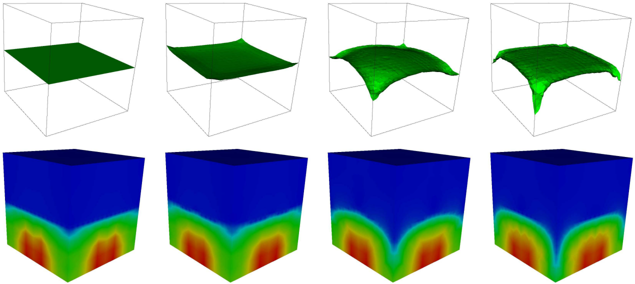
From Discretization to a fully practical Scheme

- Status:
  - + a convergent discretization of (1)
  - – a nonlinear algebraic problem
- Tool: A fixed point strategy for every $n \geq 1$
  - + linear, decoupled problems for $\{(\rho^{n,l}, \mathbf{u}^{n,l}, \mathbf{b}^{n,l})\}_{n,l}$
  - + a thresholding criterion
  - + contraction property for restrictive $F(k,h) \geq 0$
  - + perturbed discrete energy law, and
  - + uniform upper and lower l^∞–bounds for $\{\rho^{n,l}\}_{n,l}$

PART IV: Simulation of Aluminium Electrolysis

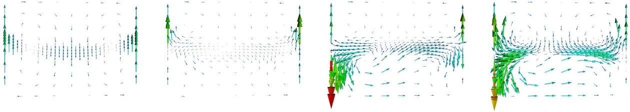
Aluminium Electrolysis – Two-Fluid MHD

- evolution of interface between two conducting fluids
  - top: lighter cryolite, bottom: heavier liquid aluminium

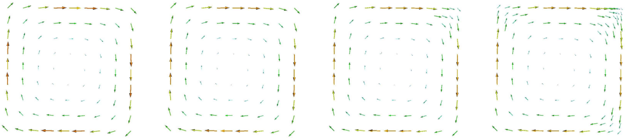


- magnitude of magnetic field

- 2D Velocity profile



- 2D Magnetic field profile



PART V: Summary

- Aluminium production: Two Fluid–MHD problem
- Goal/Problem: Develop convergent FE–based discretization such that computed iterates satisfy relevant properties
- Problems: Discrete energy law, upper and lower bounds for density, compactness result by R. DiPena & P.L. Lions
- Tools: reformulation, M–matrix property, numerical integration, regularization terms, mesh constraints

Thank you for your attention!