Simulation of liquid metal batteries

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29. June 2016

HELMHOLTZ GEMEINSCHAFT

LIMTECH Allianz

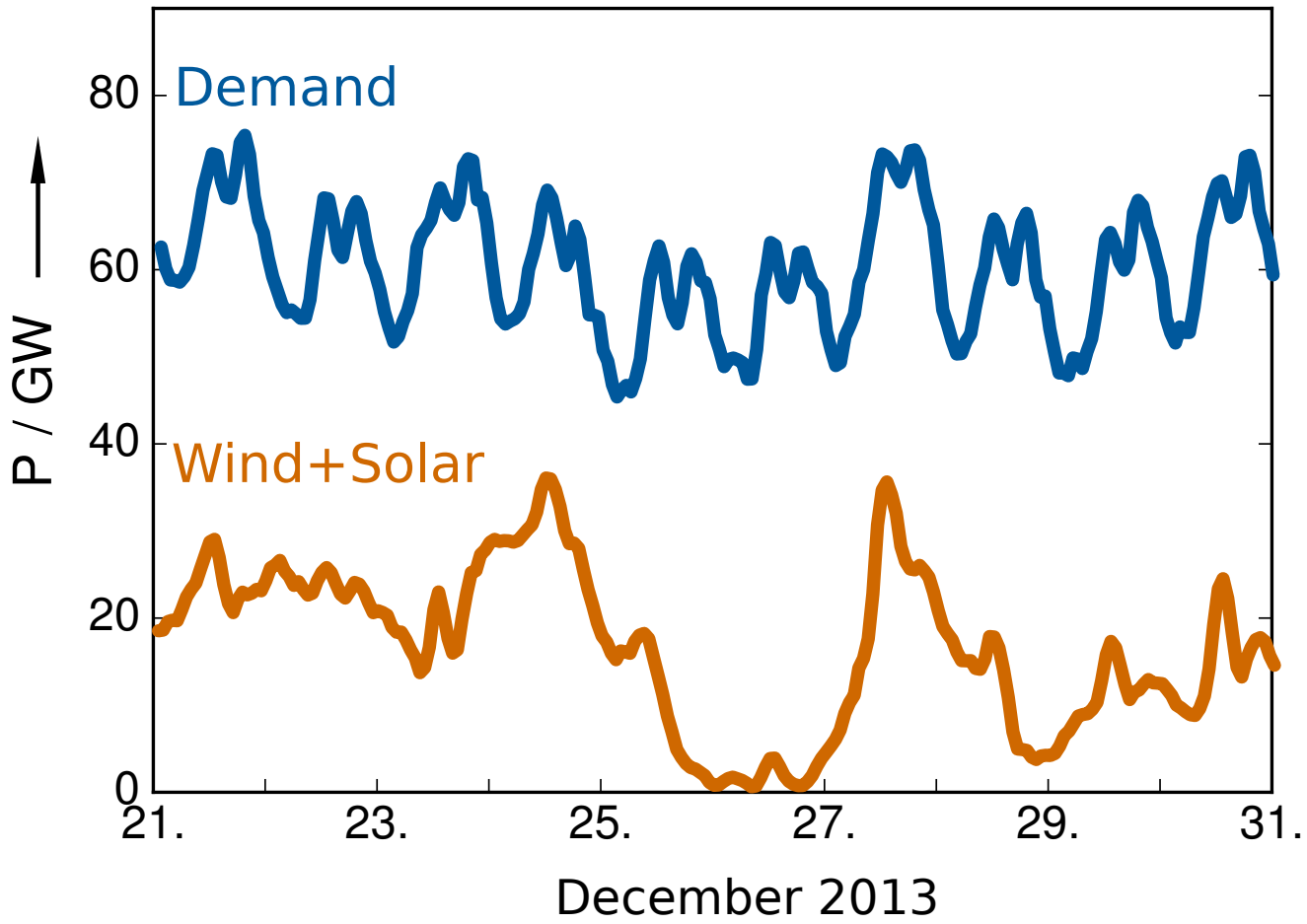
Limsi

DRESDEN concept

HZDR

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

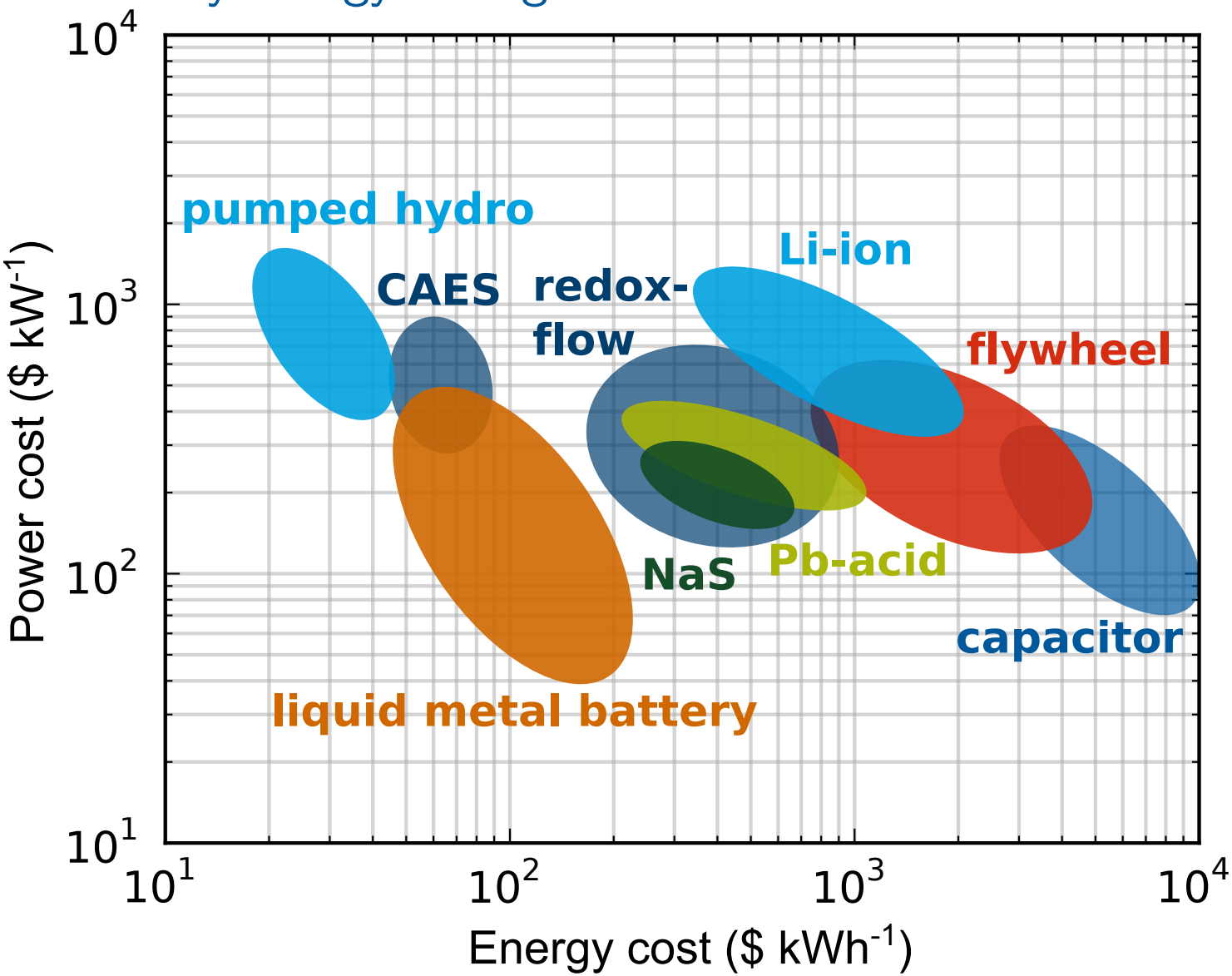
Motivation
Renewable energies



⇒ **Stationary storage** is **mandatory** for renewable energies

Motivation

Stationary energy storage



Kim et al. (2013) Chem. Rev.

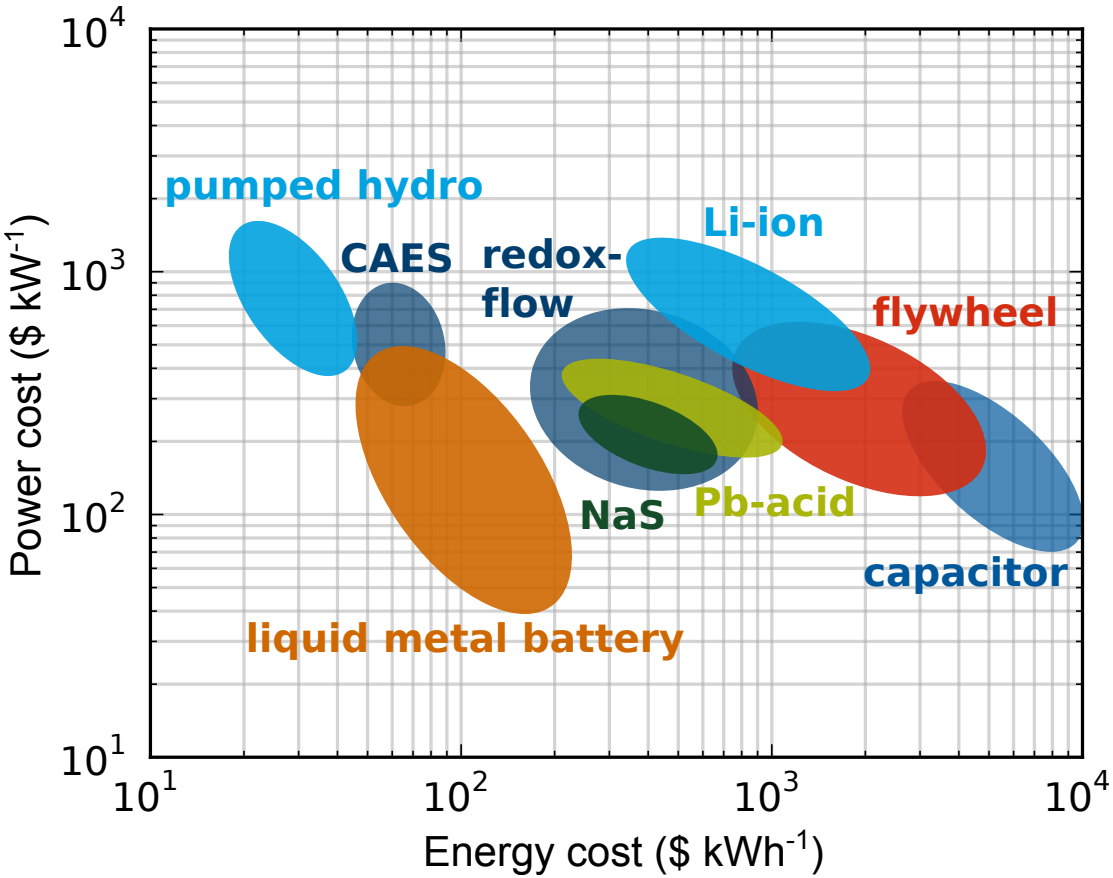
Motivation
Liquid metal battery

Pros

- simple construction
- cheap active materials
- high current densities (up to 13 A/cm^2)
- long life-time
- scalability

Cons:

- low cell voltage
- high temperature
- safety?



Kim et al. (2013) Chem. Rev.

Content

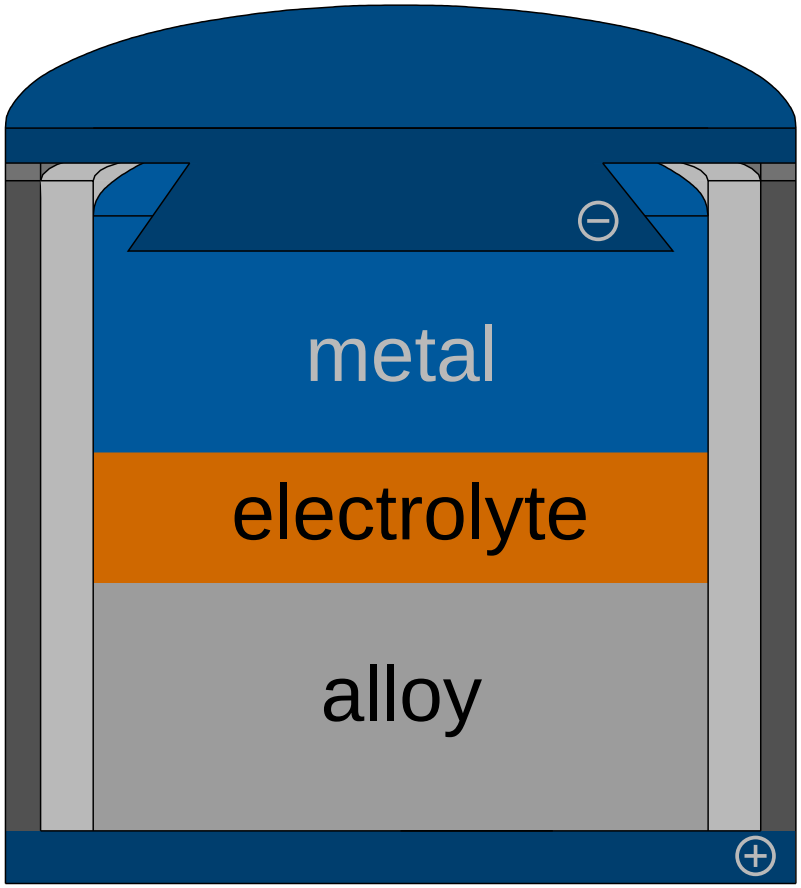
Liquid metal battery

- set-up
- operation
- fluid dynamics

Simulation

- Tayler instability
- electro-vortex flow
- interface instability

Liquid metal battery
Set-up and operation



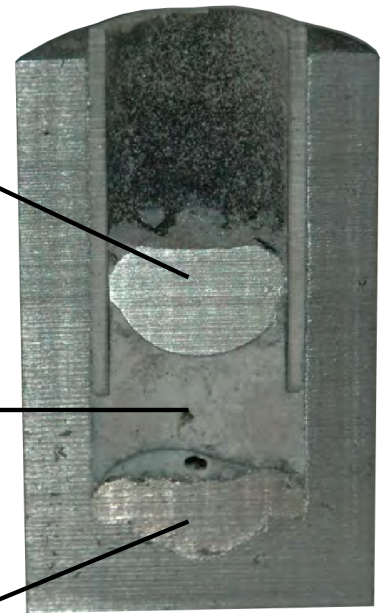
$Mg|MgCl_2\text{-}KCl\text{-}NaCl|Sb$

$T = 700°C$

$\rho = 1584\,kg/m^3$

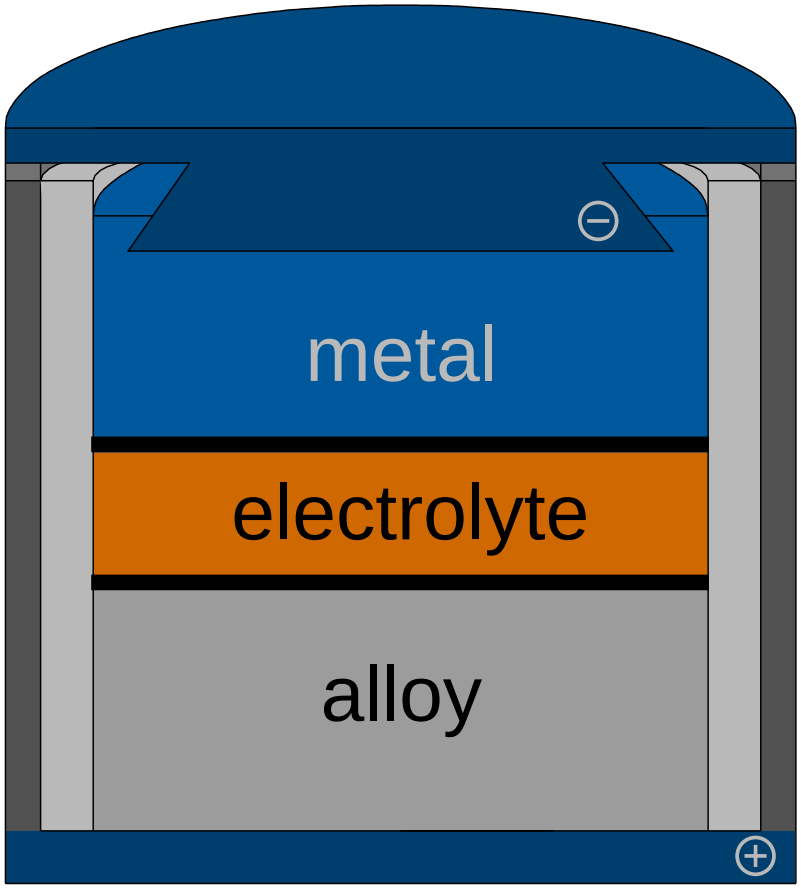
$\rho \approx 1670\,kg/m^3$

$\rho \approx 6530\,kg/m^3$



Sadoway (2011)

Liquid metal battery
Set-up and operation



$$\text{anode:} \quad \varphi_1 = \varphi_{01} + \frac{RT}{zF} \ln \frac{a_{Mg^{2+}}}{a_{Mg}}$$

$$\text{cathode:} \quad \varphi_2 = \varphi_{02} + \frac{RT}{zF} \ln \frac{a_{Mg^{2+}}}{a_{Mg(Sb)}}$$

$$Mg|MgCl_2\text{-}KCl\text{-}NaCl|Sb$$

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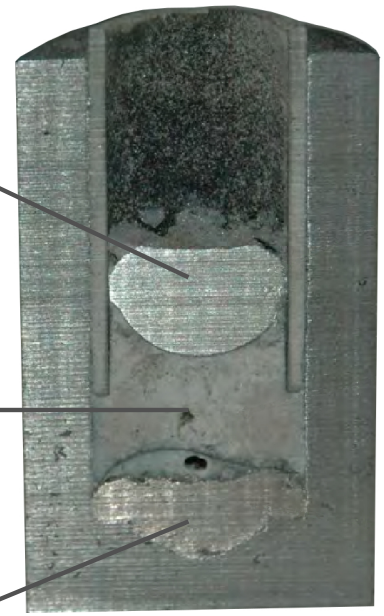
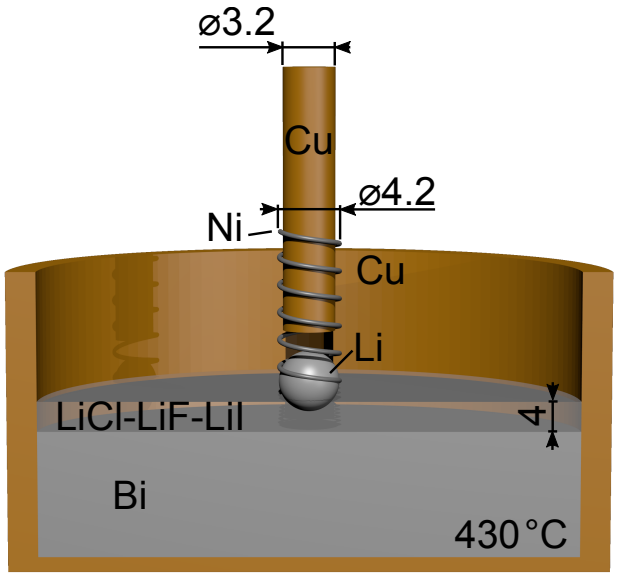


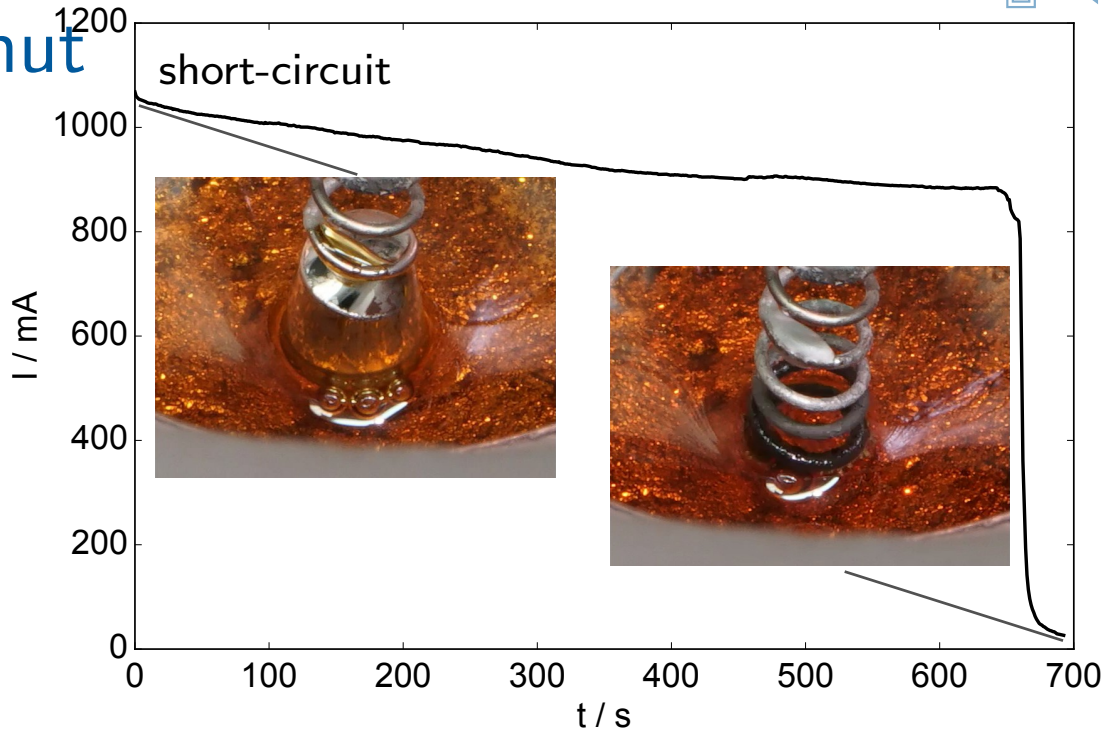
Sadoway (2011)

$$U = -\frac{RT}{zF} \ln a_{Mg(Sb)}$$

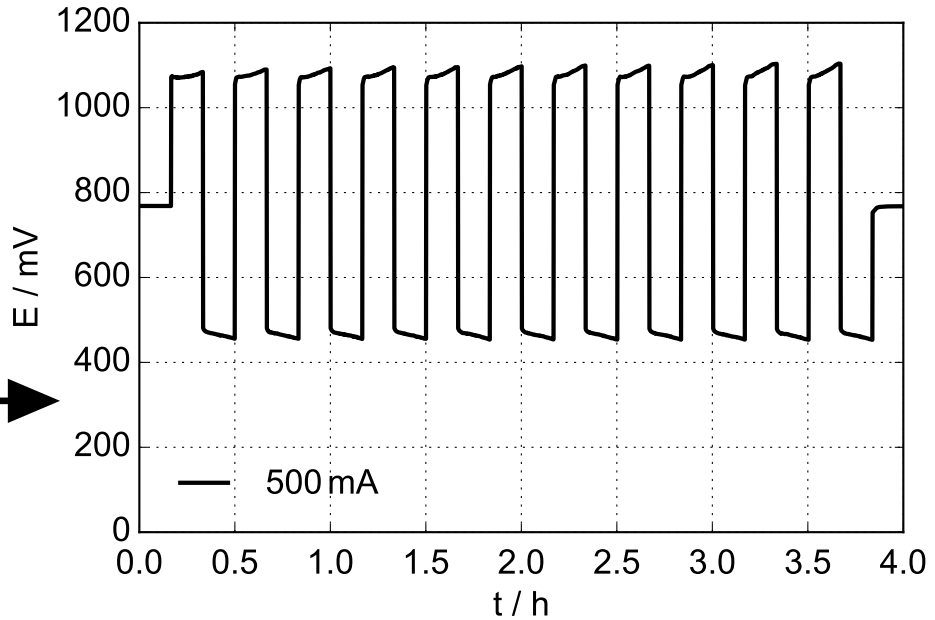
$\Rightarrow$ low cell voltage

Example: Lithium-Bismut



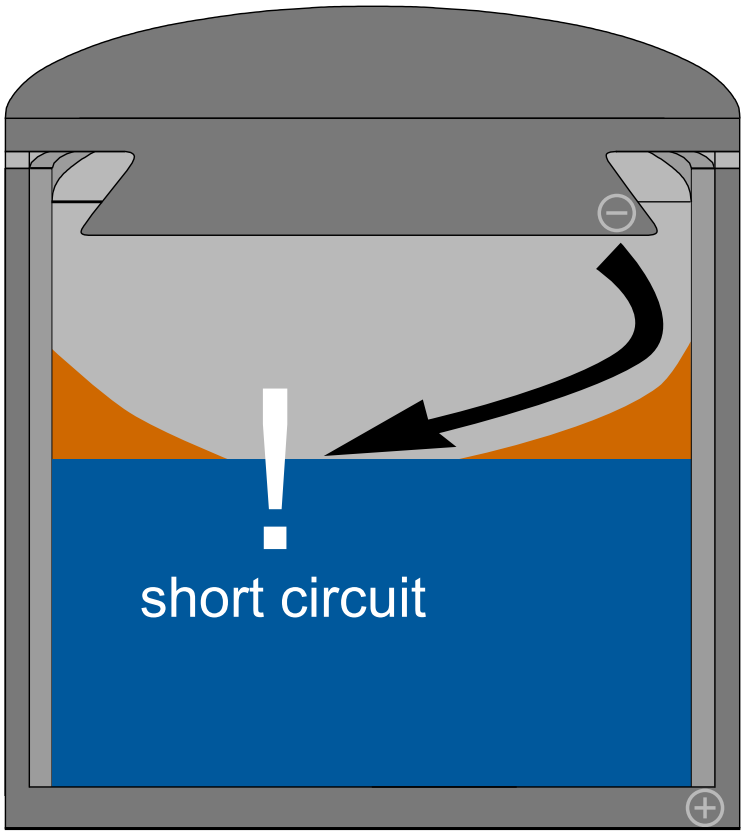


1 picture every 10 seconds



Liquid metal battery
Importance of fluid mechanics

① Safety

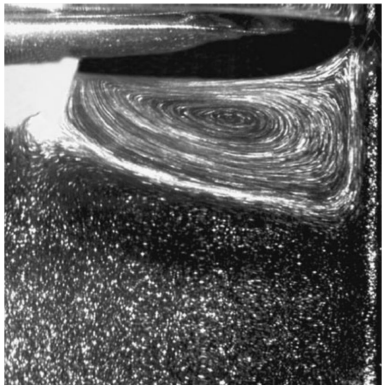


thin electrolyte; big cells

② Performance

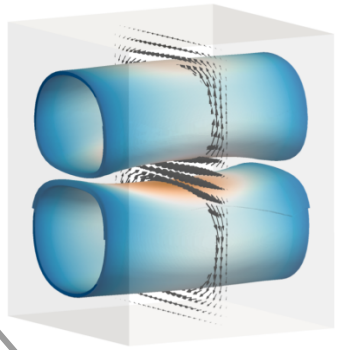
large currents

Liquid metal battery
from a fluid dynamics view

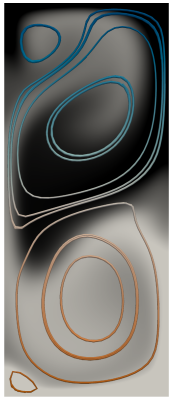


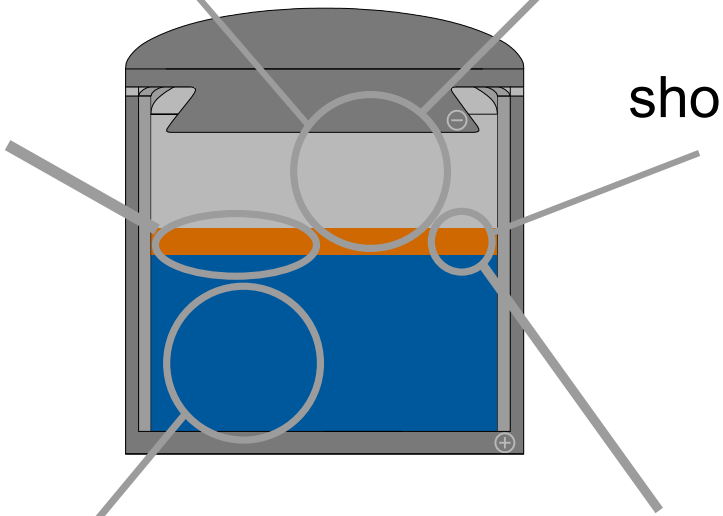
Marangoni convection

1.) Tayler instability

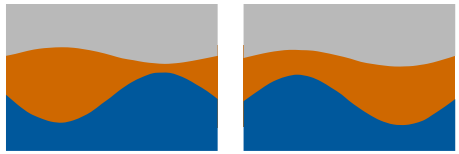


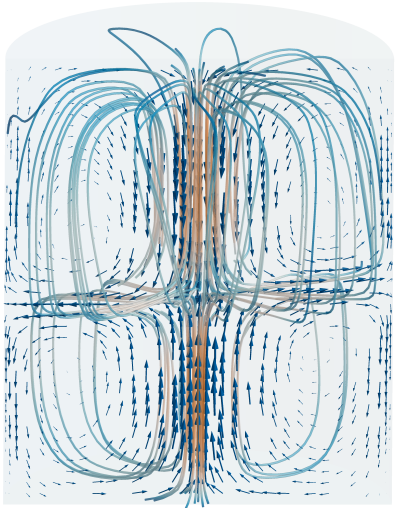
Rayleigh-Benard Konvektion





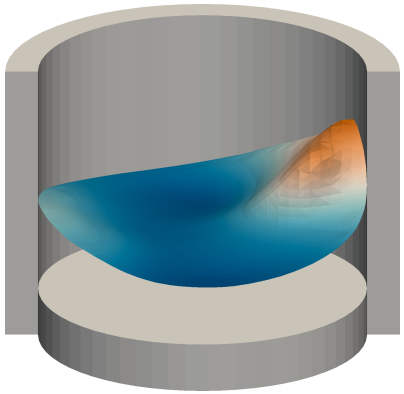
short wave instabilities





2.) electro-vortex flow

3.) long wave instabilities



Numerics

Navier-Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} = -\frac{\nabla p}{\rho} + \nu \Delta \mathbf{u} + \frac{\mathbf{f}_L}{\rho} \qquad \text{und} \qquad \nabla \cdot \mathbf{u} = 0$$

Lorentz force $\mathbf{f}_L = \mathbf{J} \times \mathbf{B} = (\mathbf{J}_0 + \mathbf{j}) \times (\mathbf{B}_0 + \mathbf{b})$

Numerics

Navier-Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} = -\frac{\nabla p}{\rho} + \nu \Delta \mathbf{u} + \frac{\mathbf{f}_\mathrm{L}}{\rho} \qquad \text{und} \qquad \nabla \cdot \mathbf{u} = 0$$

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Ohm $\mathbf{j} = \sigma\,(-\nabla \varphi + \mathbf{u} \times \mathbf{B})$

Kirchhoff $\nabla \cdot \mathbf{j} = 0$

$$\Bigg\} \quad \nabla^2 \varphi = \nabla \cdot (\mathbf{u} \times \mathbf{B})$$

Numerics

Navier-Stokes equation

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} = -\frac{\nabla p}{\rho} + \nu \Delta \mathbf{u} + \frac{\mathbf{f}_\mathrm{L}}{\rho} \qquad \text{und} \qquad \nabla \cdot \mathbf{u} = 0$$

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$$\Big\} \quad \nabla^2 \varphi = \nabla \cdot (\mathbf{u} \times \mathbf{B})$$

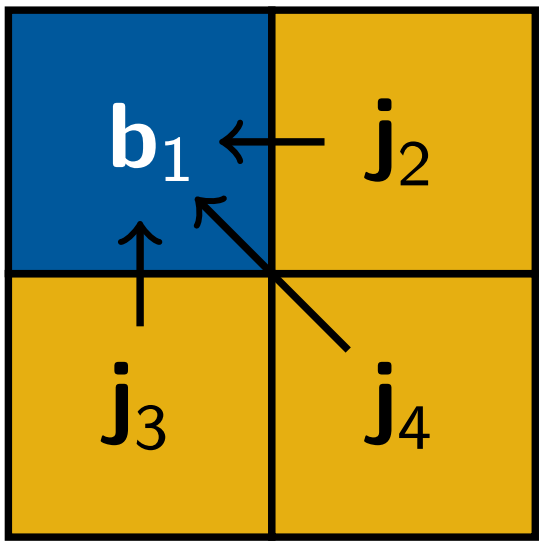
Ampère $\nabla \times \mathbf{b} = \mu_0 \mathbf{j}$

$$\rightarrow \mathbf{b}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int dV' \frac{\mathbf{j}(\mathbf{r}') \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} \text{ (Biot-Savart)}$$

$\Rightarrow$ strong current in fluid: **b** can not be neglected

Tayler-Instability
Numerics: Biot-Savart law

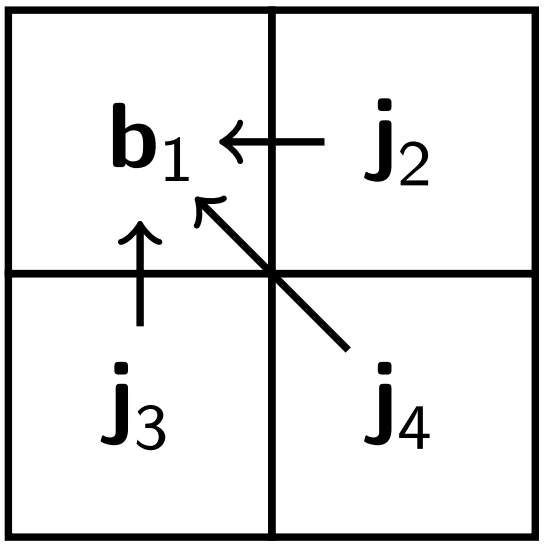
$$\mathbf{b} \sim \sum \frac{\mathbf{j} \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} V$$



$(\mathbf{r} - \mathbf{r}')$: distance of points

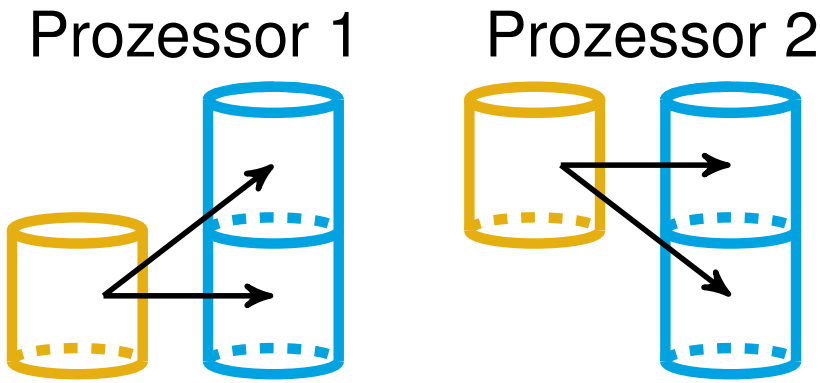
Tayler-Instability
Numerics: Biot-Savart law

$$\mathbf{b} \sim \sum \frac{\mathbf{j} \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} V$$



$(\mathbf{r} - \mathbf{r}')$: distance of points

MPI

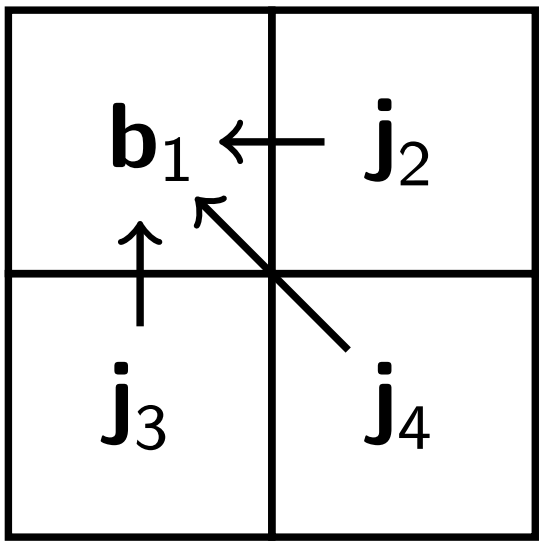


$\rightarrow$ local current induces field in all cells

$\rightarrow$ exchange and summation of field

Tayler-Instability
Numerics: Biot-Savart law

$$\mathbf{b} \sim \sum \frac{\mathbf{j} \times (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} V$$

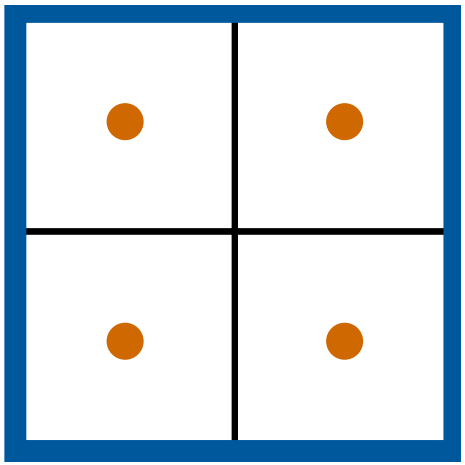


$(\mathbf{r} - \mathbf{r}')$: distance of points

Surface method

$\rightarrow$ Biot-Savart only at the surface
$\rightarrow$ Poisson equation in volume

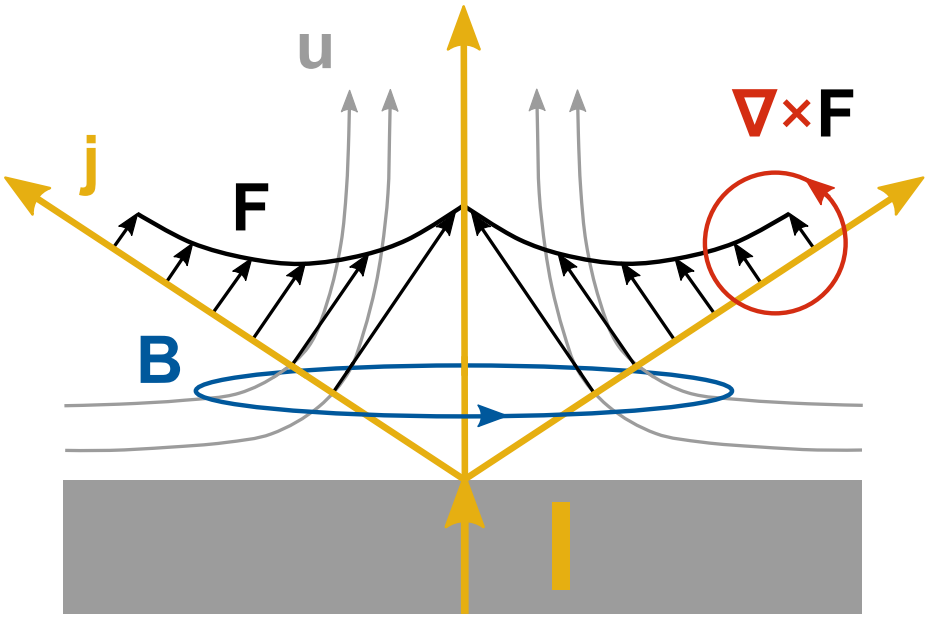
$$\frac{1}{\mu_0 \sigma} \Delta \mathbf{b} = -\nabla \times (\mathbf{u} \times \mathbf{b})$$



gain of speed: factor 10

Electro-vortex flow
Introduction

Point current source:

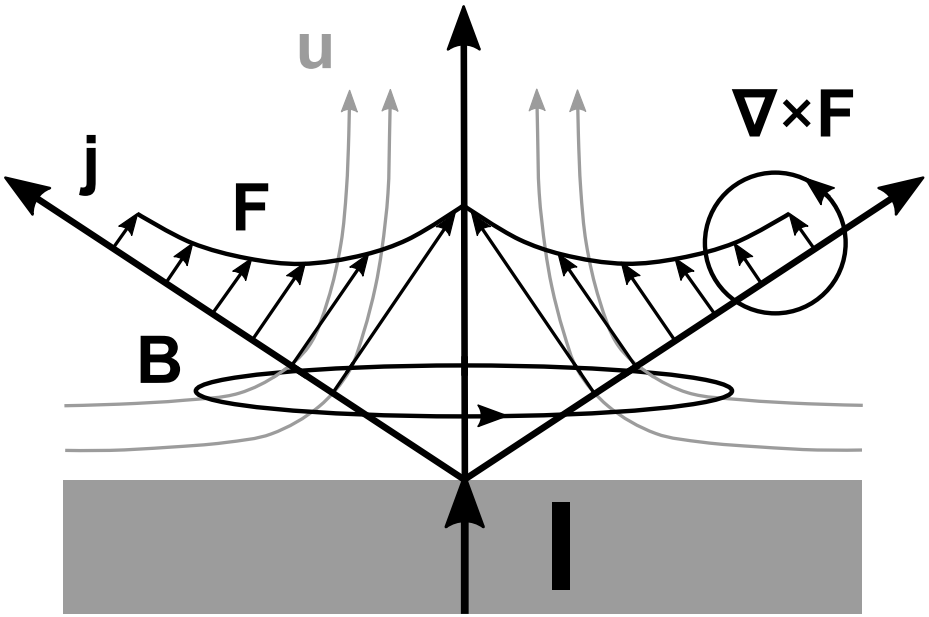


→ radial currents **j**

→ Lorentz force **rotational**

Electro-vortex flow
Introduction

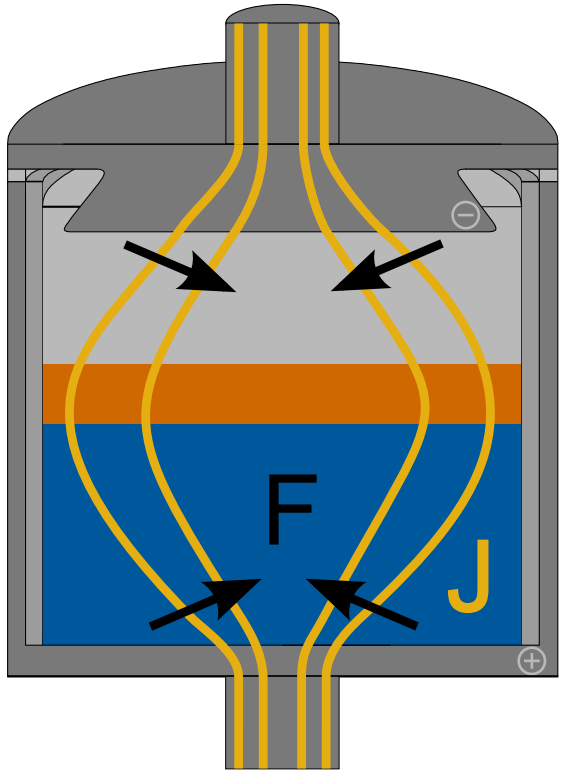
Point current source:



→ radial currents **j**

→ Lorentz force **rotational**

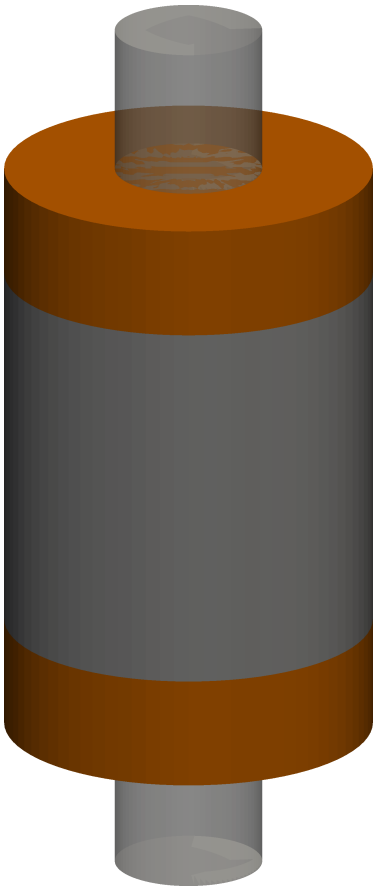
Liquid metal battery:



→ change in cross section

Electro-vortex flow

Numerical scheme



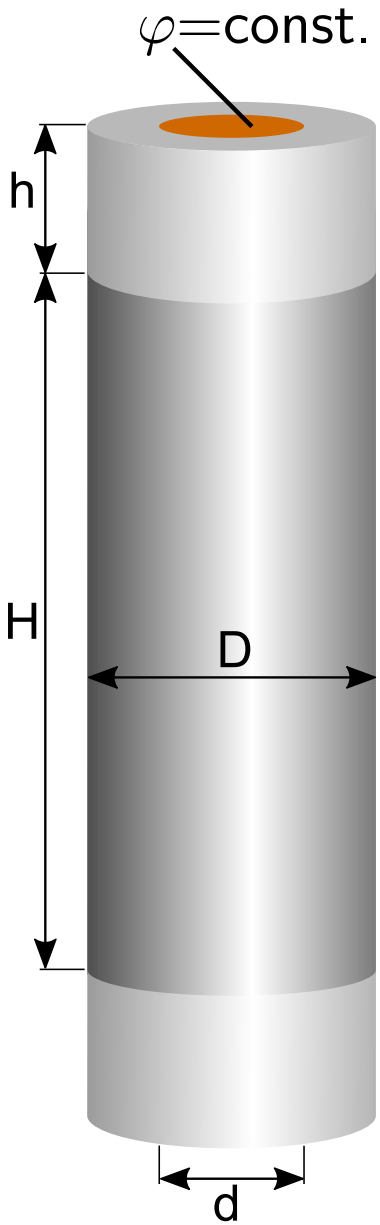
$\Delta P_0 = 0$ → $\mathbf{J}_0 = -\sigma \nabla P_0$ → Biot-Savart $(\mathbf{B}_0)$ → NSE → $\Delta\varphi = \nabla \cdot (\mathbf{u} \times \mathbf{B})$ → $\Delta\varphi_s = 0$ → $\mathbf{j} = \sigma(-\nabla\varphi + \mathbf{u} \times \mathbf{B})$ → Biot-Savart $(\mathbf{b})$ → $\mathbf{j}_s = -\sigma_s \nabla\varphi_s$ → Biot-Savart (update $\mathbf{b}$) → $\mathbf{f} = \mathbf{J} \times \mathbf{B}$ → $\Delta P_{0s} = 0$ → $\Delta P_0 = 0$

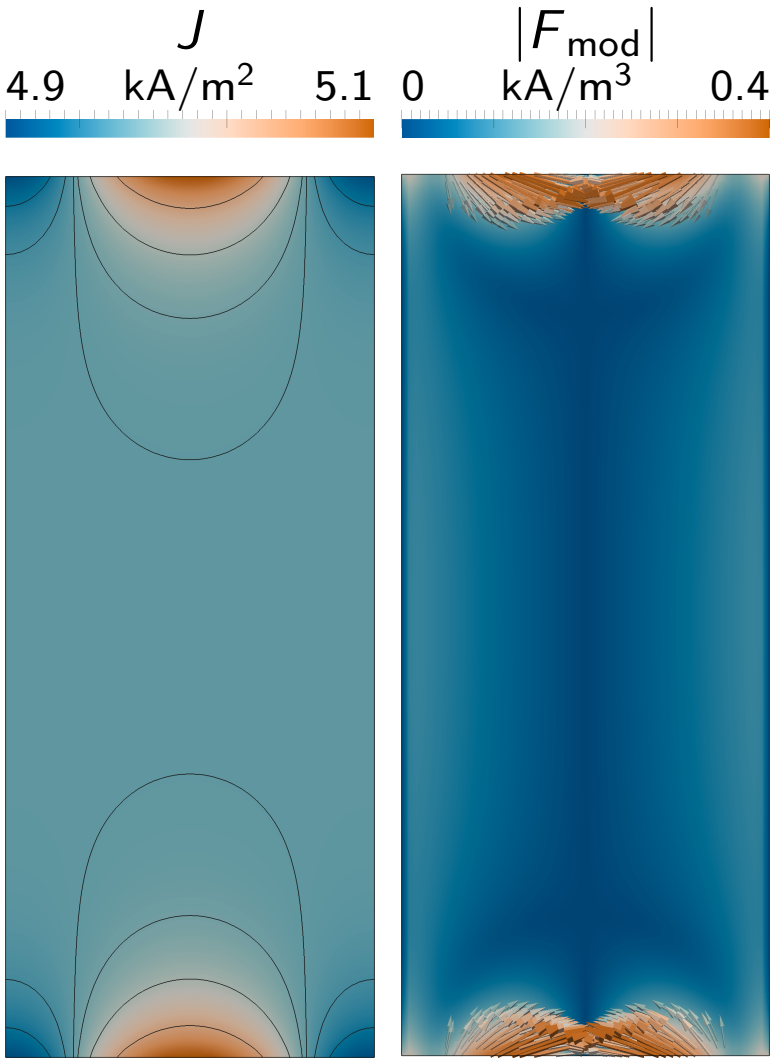
Boundary condition:

$\varphi_1 = \varphi_2$

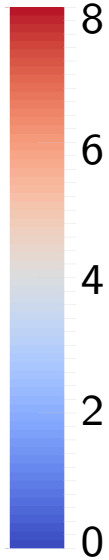
$\mathbf{j}_1 \cdot \mathbf{n}_1 = \mathbf{j}_2 \cdot \mathbf{n}_2$

Electro-vortex flow





d/D =0,5
H/D=2,4
h/D =0,5
D =1 m
I =3 kA
Na



Weber et al. Phys. Fluids (2015)

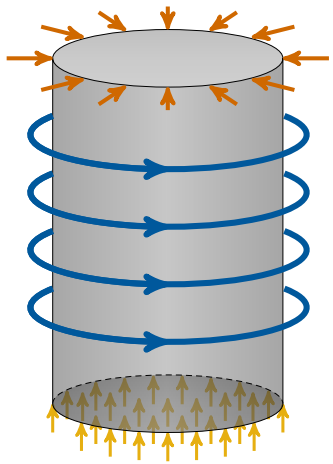
Tayler instability
Introduction

Brian James (2007)

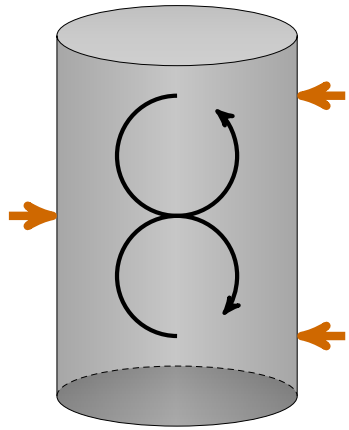
Lorentz force **F**

magnetic field **B**

current density **J**

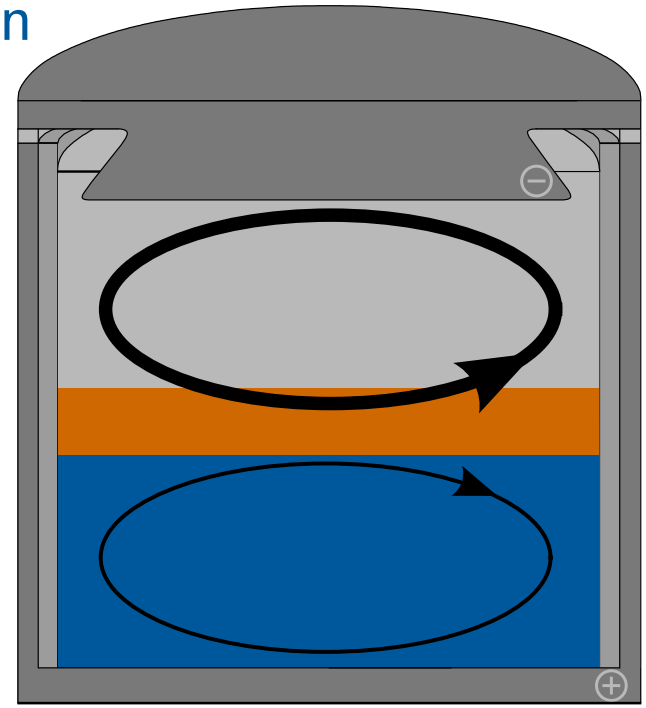


$I > I_{crit}$



Tayler instability
Introduction

Brian James (2007)



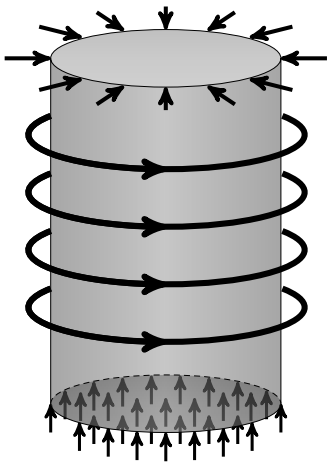
characteristic parameters:

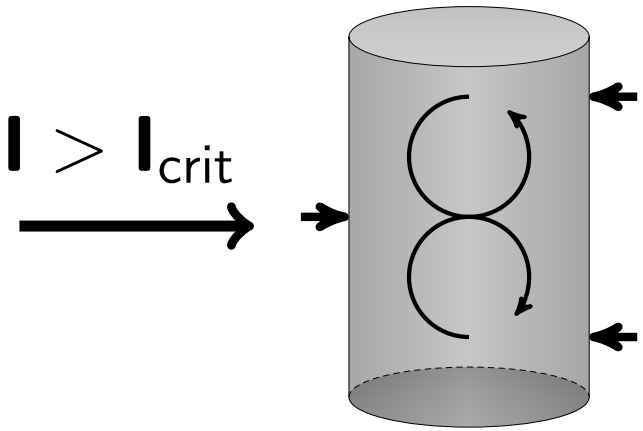
1. critical current I_{cr}
2. growth rate p
3. velocity u

Lorentz force **F**

magnetic field **B**

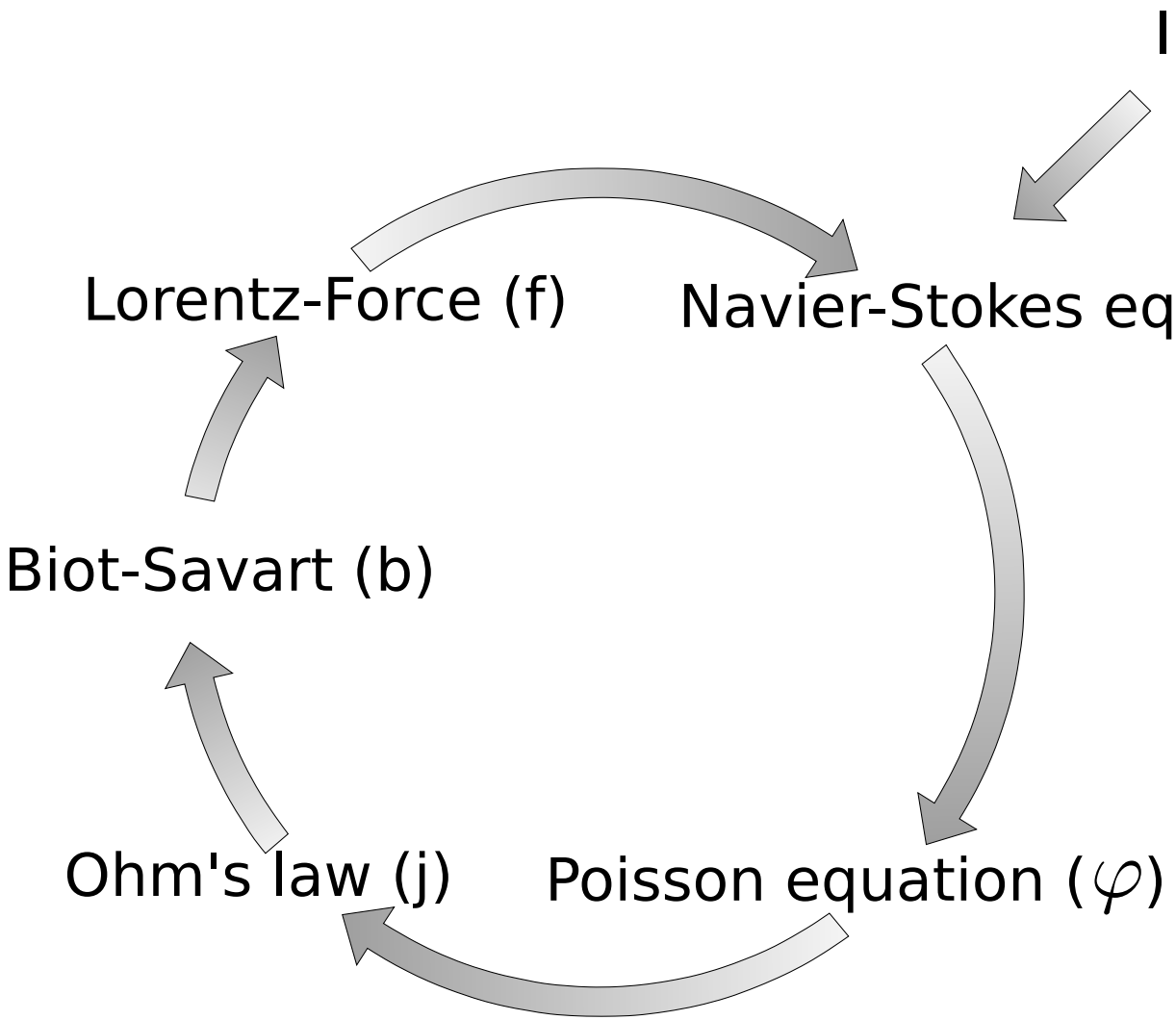
current density **J**

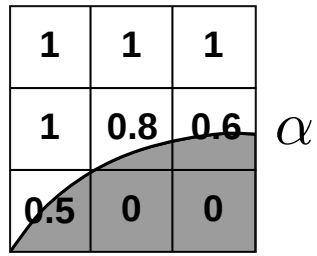




Numerics

Multiphase-simulation: example Al and cryolith



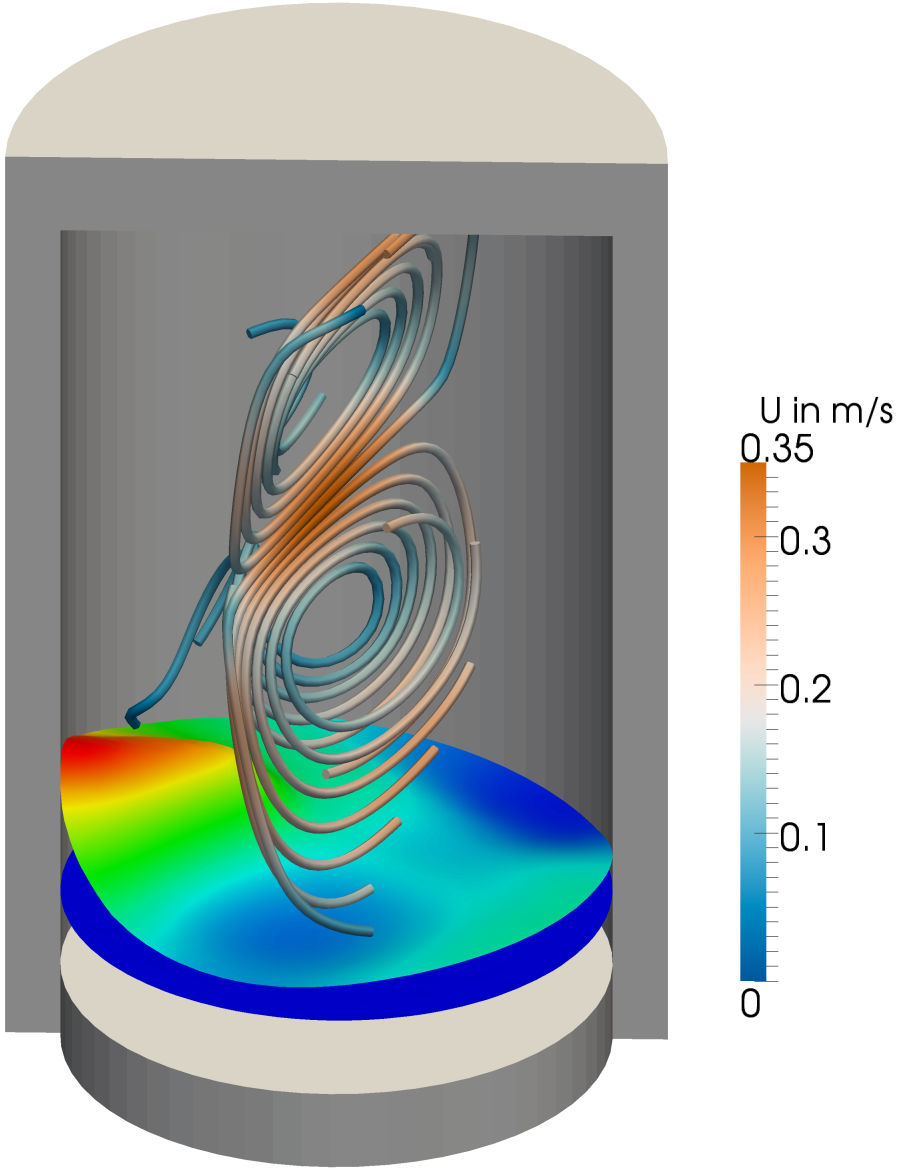


$$\sigma = \alpha\sigma_1 + (1-\alpha)\sigma_2$$

$\Rightarrow$ Biot-Savart instead of induction equation

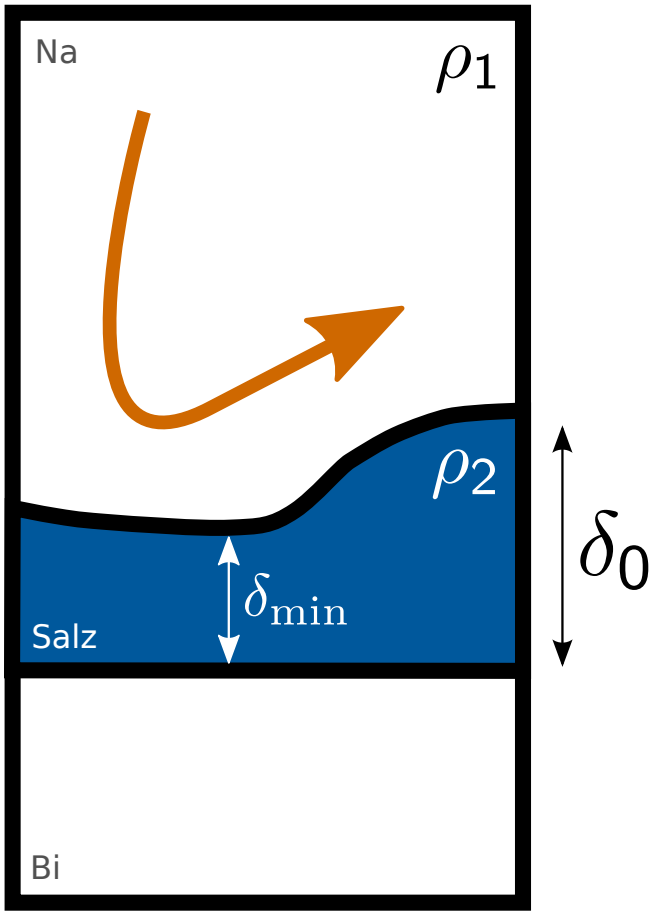
α	phase-fraction Al
$1-\alpha$	phase-fraction cryol.

Tayler instability
Multiphase simulation



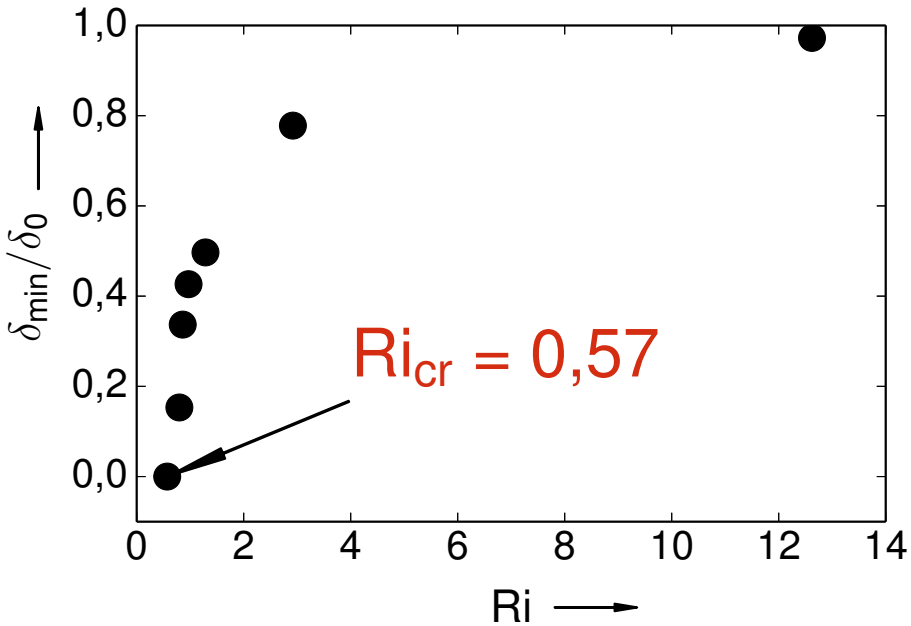
Multiphase simulation
Deformation of the electrolyte layer: scaling

Ansatz: $E_{kin} \sim E_{pot}$



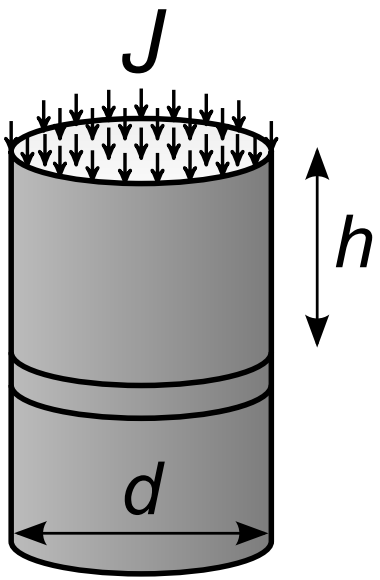
Richardson number:

$$\mathrm{Ri} = \frac{E_{pot}}{2E_{kin}} = \frac{g(\rho_2 - \rho_1)\delta_0}{\rho_1 u^2}$$



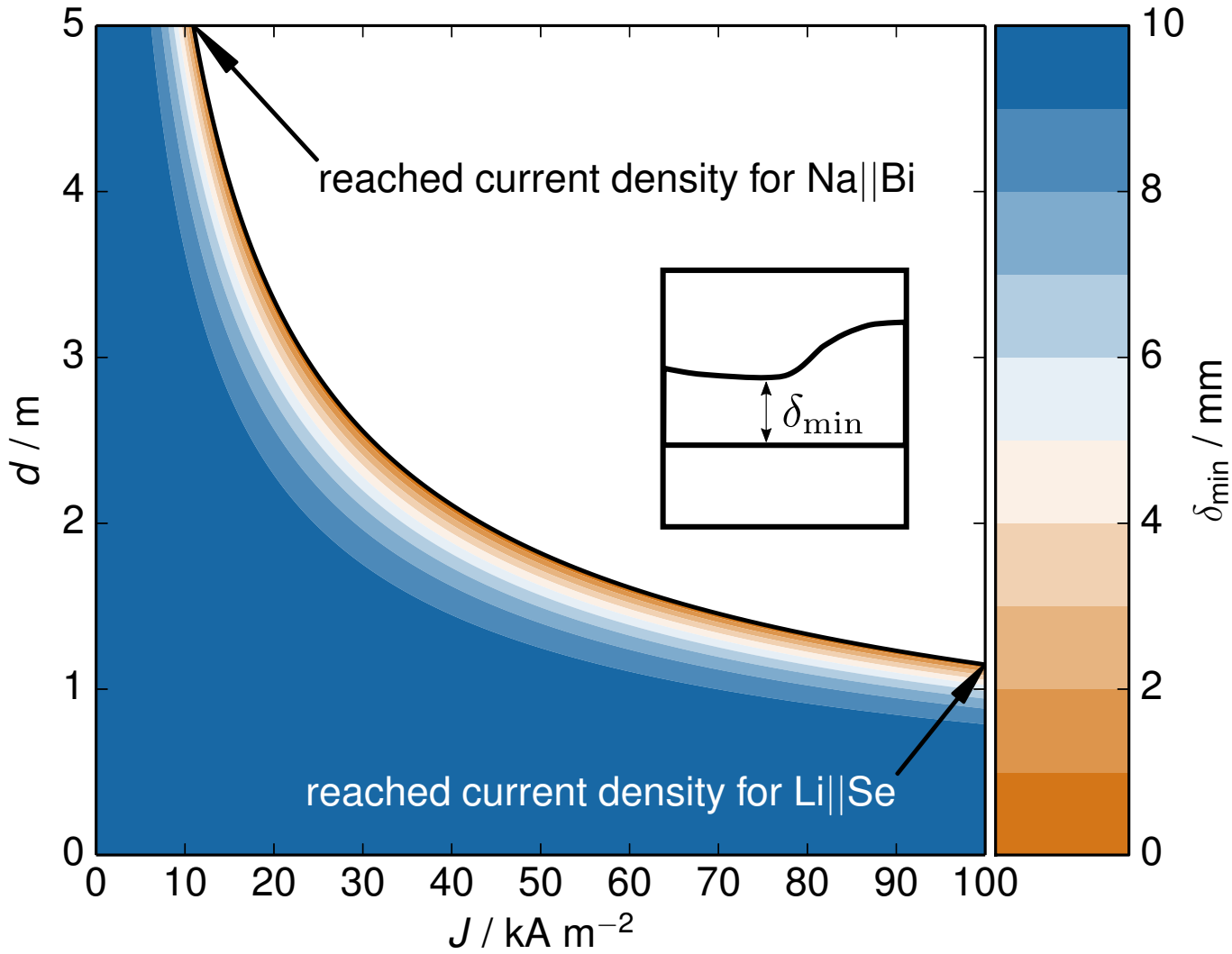
⇒Richardson number defines deformation of the interface

Multiphase simulation
How large is the deformation?



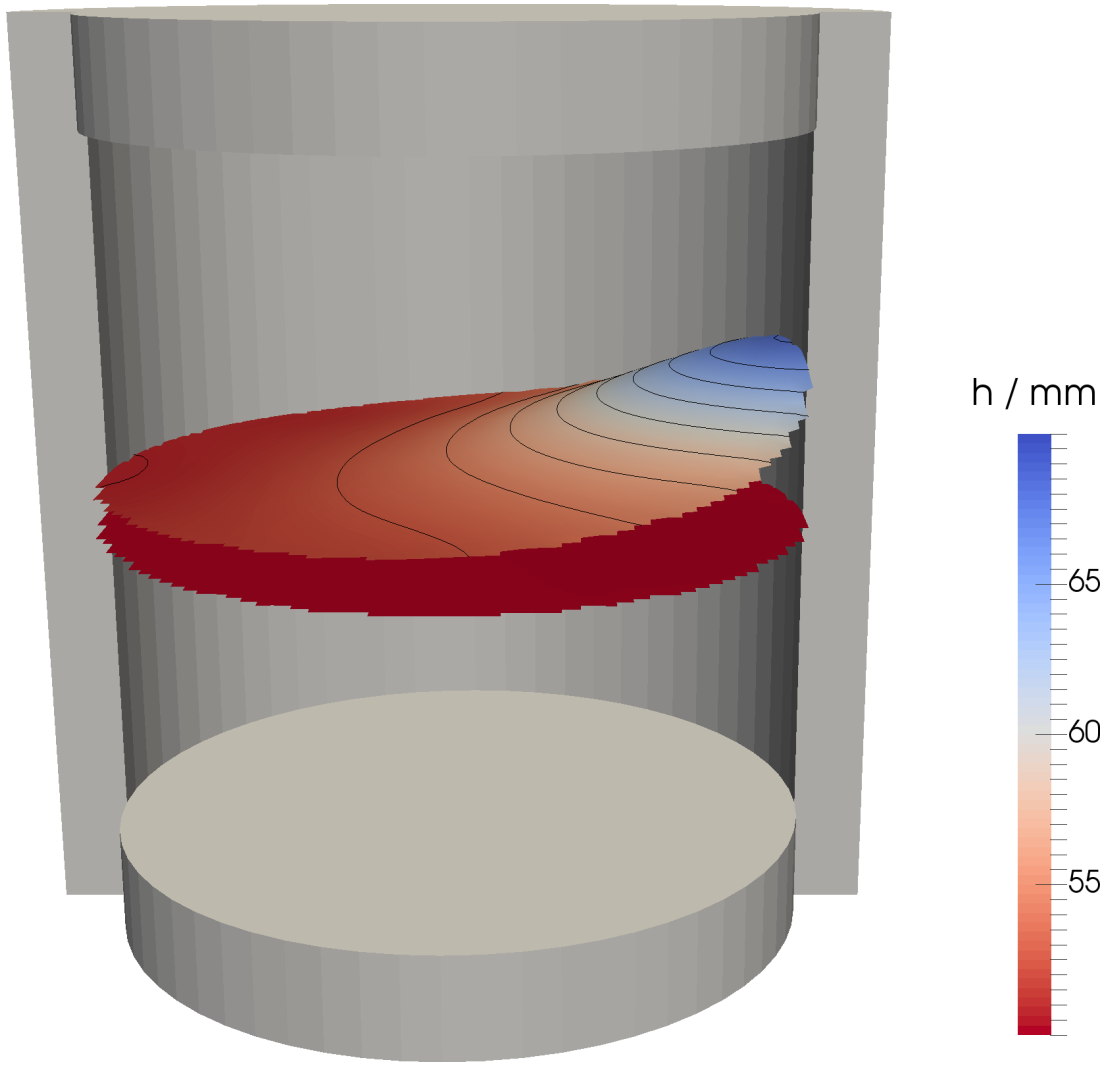
$h/d = 1{,}25$

Na|NaCl-NaF-NaI|Bi

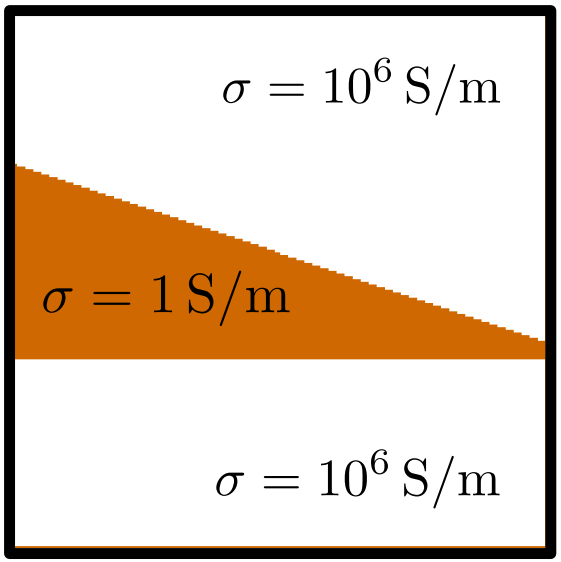


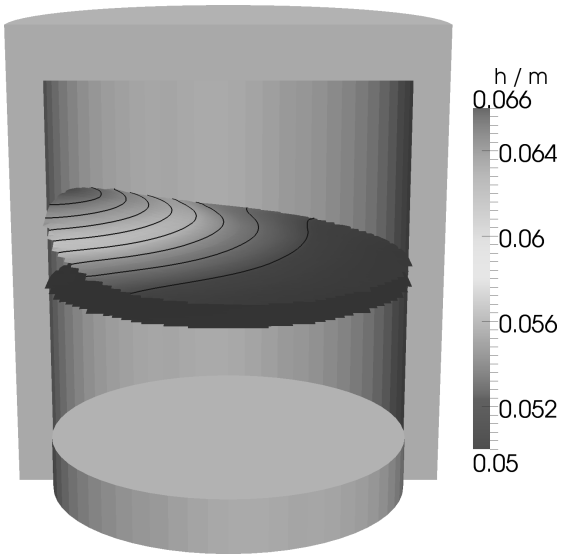
⇒ short-circuit for batteries of $d < 1\,\mathrm{m}$ unlikely

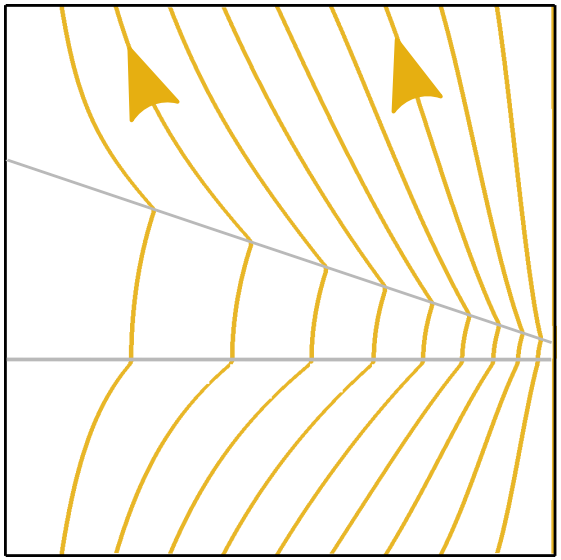
Metal pad roll instability



Metal pad roll instability







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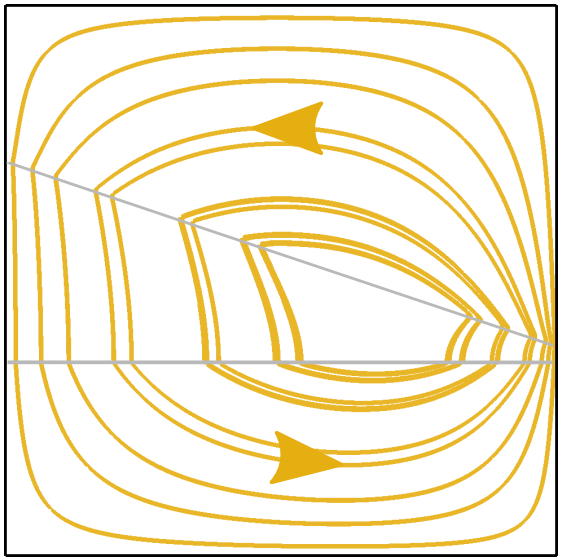
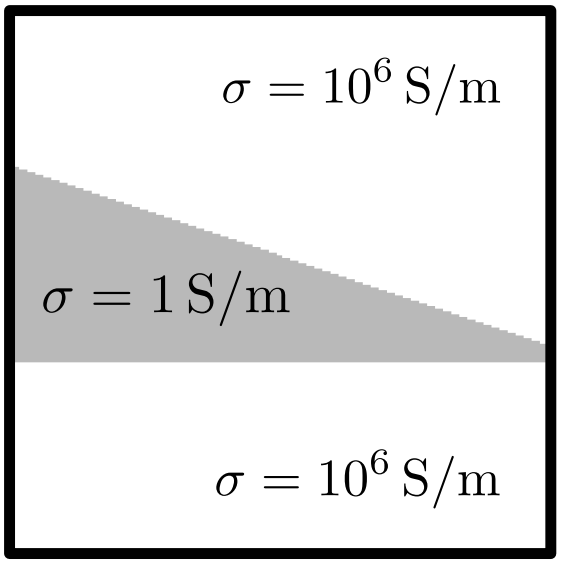
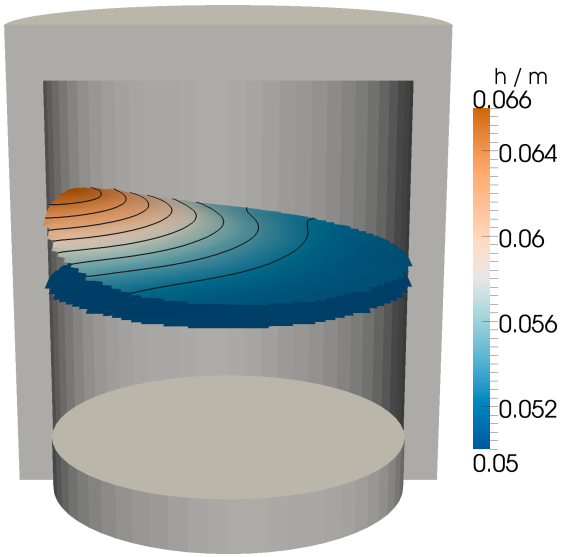
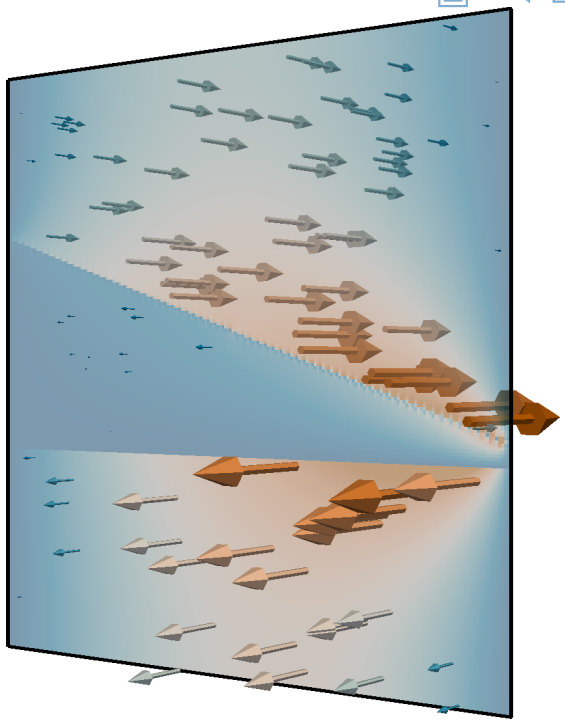
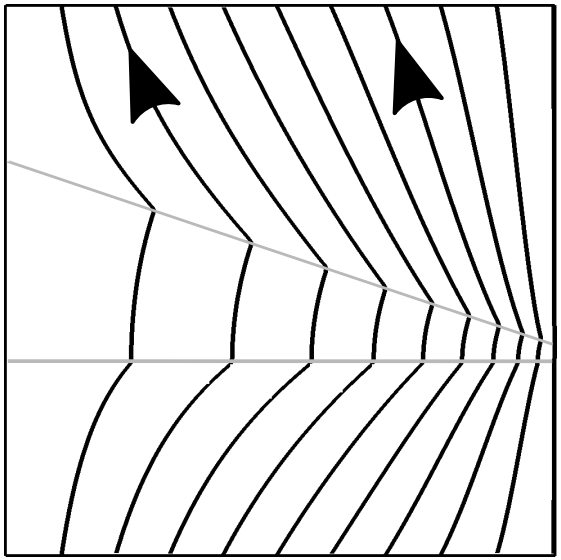


Metal pad roll instability









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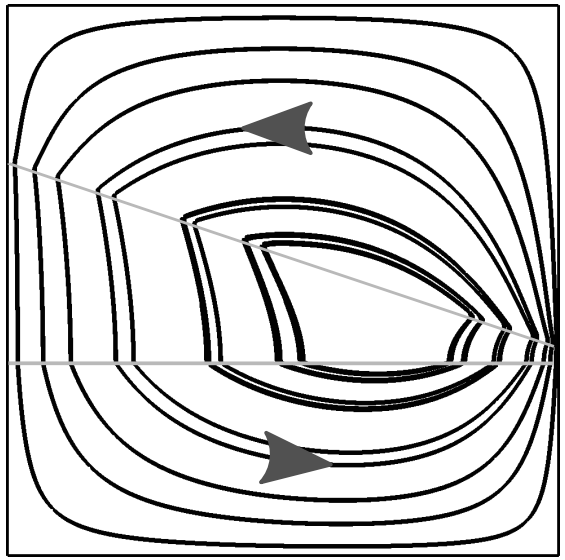

Thank you for you attention!