A computational model of the freezing of salt water

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Overview of the Talk

- Freezing Salt Water Model
- Computational Approach
- Discussion
- Summary

Motivation

- Part of a group project looking at biological phenomena in sea ice formation
- Need for a computational framework to include micro-scale phenomena at macroscopic scales

Model

Scaled Equations

- $\theta(x,t)$ is the scaled temperature
- n is the scaled local salt concentration
- ϕ is the brine fraction

$$
\begin{aligned}
(\theta+\phi)_t &= \theta_{xx} && \text{Enthalpy conservation} \\
(\phi n)_t &= d(m(\phi)n_x)_x && \text{Salt conservation} \\
\theta + bn &= 0 && \text{Cryoscopic relationship} \\
m(\phi) &= \frac{\phi-\phi_*}{1-\phi_*}
\end{aligned}
$$

Model

Scales

$$
\begin{aligned}
(\theta + \phi)_t &= \theta_{xx} \\
(\phi n)_t &= d(m(\phi) n_x)_x \\
\theta + bn &= 0
\end{aligned}
$$

Scales:

- Length: 1m
- Time: 10 days
- Temperature: 150C
- Salt: 3.5% by weight
- d: 1.6×10^{-3}
- b: 0.012

Model

Three Regimes

- $\phi < \phi_*$ Immobile brine:

$$\begin{aligned}(\theta + \phi)_t &= \theta_{xx} \\ (\phi n)_t &= 0, \;\; \theta + nb = 0\end{aligned}$$

One parabolic, one local ODE with "history".

- $\phi_* < \phi < 1$ Mushy:

$$\begin{aligned}(\theta + \phi)_t &= \theta_{xx} \\ (\phi n)_t &= d(m(\phi)n_x)_x, \;\; \theta + nb = 0\end{aligned}$$

Mixed parabolic - hyperbolic system.

- $\phi = 1$ Free brine:

$$\begin{aligned}\theta_t &= \theta_{xx} \\ n_t &= dn_{xx}\end{aligned}$$

Two parabolic.

Computations

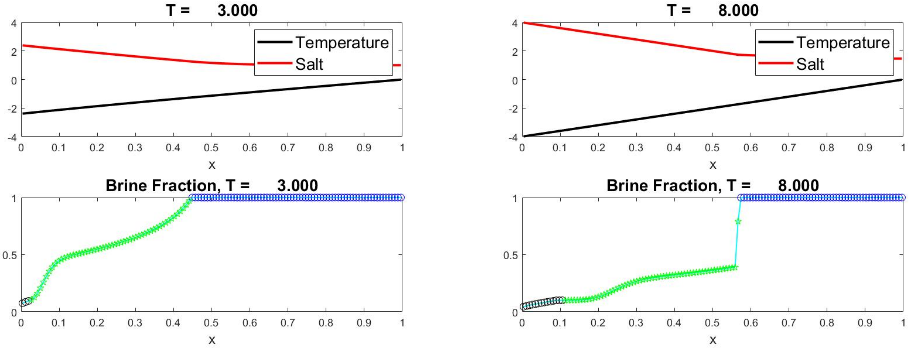
Discretization

- Conservative cell centered Finite Difference scheme
- $m_{j+1/2} = \min\left[m(s_j), m(s_{j+1})\right]$?
- Implicit (Backward Euler) time stepping
- Iterative method based on regime flag updates (two flags)
- Inner Newton iterations
- This strategy leads to a consistent solution. Theory?

Computations

Results

(Computations with relaxed parameters $d = 0.025$ and $b = 1$)



Discussion

Mushy Region

- θ obeys an equation of parabolic type
- Assuming smooth solutions, we can derive

$$(\theta + dm(\phi))_t = (dm - \phi)\theta_t + dm'\theta_x\phi_x$$

- Neglecting $O(d)$ terms in the first two terms

$$\phi_t - \frac{dm'\theta_x}{\theta}\phi_x \approx -\frac{\phi}{\theta}\theta_t$$

- We recognize a hyperbolic equation with wave speed

$$S = \frac{dm'(\phi)\theta_x}{\theta}$$

- S is small and negative in our simulation conditions.

Discussion

Mushy/Brine Interface

- The mushy zone is characterized by a mixed parabolic/hyperbolic system
- The hyperbolic component has a slow wave speed to the left
- When characteristics are exiting the interface, the interface is of implicit type and s is continuous ($s = 1$)
- When the interface is moving fast enough to the left, s is discontinuous and the interface is of explicit type (normal velocity determined by Enthalpy conservation).

Summary

More questions than answers:

- Computational method proposed to capture regime boundaries in sea ice formation as part of a larger project.
- Analysis of the model? Convergence analysis of the numerical method?
- Can the model be considered as a gradient flow with constraint

$$(\phi - 1)(\theta + nb) = 0$$

  with the phase change rate as a Lagrange multiplier?
- Does the model emerge with formal asymptotics for large phase change rate?