Computational approaches to a model problem of two phase flow in porous media with phase change and, the oxygen depletion problem revisited

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Overview of the Talk

- model problem and computed solutions
- two simpler, related problems
- revisiting the oxygen depletion problem
- computational methods for the two phase flow problem
- discussion
Model Problem

cartoon model

Heat and water transport in a porous medium:

- \( u \): temperature
- \( v \): water vapour
- \( w \): water liquid
- \( \Gamma \): condensation rate

\( S(u) \): vapour saturation (we take \( S(u) = e^u \)).

Equations:

\[
\begin{align*}
  u_t &= \Delta u + \Gamma \\
  v_t &= \nabla \cdot (D(u)\nabla v) - \Gamma \quad \text{(we take } D(u) = 2(1 + u)^2).\\
  w_t &= \Delta w + \Gamma
\end{align*}
\]

Motivation: transport in fuel cell electrodes and baking bread
Model Problem

picture: moving boundary

\begin{align*}
W &= 0 \\
W &= 0 \\
W &> 0, \\
\mathbf{u}_t &= \Delta \mathbf{u} \\
\mathbf{v}_t &= \nabla \cdot (D(\mathbf{u}) \nabla \mathbf{v}) - \Gamma \\
\mathbf{w}_t &= \Delta \mathbf{w} + \Gamma \\
\text{Saturation} \\
\mathbf{v} &= S(\mathbf{u}).
\end{align*}
Model Problem

two zone formulation

Vapour only region ($w \equiv 0$):

$$
\begin{align*}
&u_t = \Delta u \\
&v_t = \nabla \cdot (D(u)\nabla v)
\end{align*}
$$

Two phase zone region ($v = S(u)$):

$$
\begin{align*}
&S'(u)u_t + w_t = \nabla \cdot (S'(u)D(u)\nabla u) + \Delta w \\
&(1 + S'(u))u_t = \nabla \cdot ((1 + S'(u)D(u))\nabla u)
\end{align*}
$$

Interface conditions:

1. $w = 0$ (two phase)
2. $[u] = 0$
3. $v = S(u)$ (vapour)
4. $[\partial u/\partial n] = \partial w/\partial n$ (heat flux evaporates water flux)
5. $[D(u)\partial v/\partial n] = \partial w/\partial n$ (water conserved)
Model Problem

two zone formulation: discussion

- Count check: four component second order parabolic equations, five mixed Dirichlet/Neumann conditions.
- There can be a condensation delta function at the free boundary.
- There is no Stefan velocity. This is an “implicit” free boundary value problem, Crank, Free and Moving Boundary Problems, 1984.
- Earlier work, Donaldson and W, IMAJAM, 2006 and Chen and W, IMAJAM, 2008 relates to the local problem at steady state:
  - algebraic criteria for linear well posed-ness to 2D perturbations for given far field fluxes.
  - identification of artificial Stefan velocities to reach steady state with good numerical properties.
Model Problem
1D computation (using the M2 method)
Model Problem

2D computation (using the split-step method)

Movie
Two Simpler Problems

Level sets of the heat equation

Consider an interface with the variable $u$ on either side of an interface that satisfies

$$u_t = \Delta u$$

on either side of the interface. Consider “implicit” moving boundary conditions

1. $u_+ = 0$
2. $u_- = 0$
3. $[\partial u/\partial n] = 0$

- The interface is just the zero level set of solutions of the heat equation.
- The interface will be regular (for short time) if the normal derivative is nonzero at all points of the interface.
- Level sets of harmonic functions in 3D can be irregular
Two Simpler Problems

The oxygen depletion problem

- Early literature summarized in Crank
- Bergers, Ciment, Rogers, SINUM, 1975 [BCR]. Points to some theory about the problem that was never published.
- Movie
Oxygen Depletion Problem

scheme one: DAE

- Map $x \in [0, s(t)]$ to $y \in [0, 1]$, $x = ys$.
- $c_t = x_{xx} - 1$ becomes

$$s^2 c_t - y s \ddot{c}_y = c_{yy} - s^2$$

with boundary conditions $c_y(0) = c(1) = c_y(1) = 0$.
- Method of lines on a cell centred grid, $h = 1/N$, with ghost points:

$$s^2 \dot{C}_j - y s \ddot{D}_1 C_j = D_2 C_j - s^2 \text{ interior points}$$

with $C_1 - C_0 = C_N + C_{N+1} = C_{N+1} - C_N = 0$.
- Index one DAE problem, use standard MATLAB time stepping to get a high time accuracy solution, used as a benchmark for the other schemes. No theory.
Oxygen Depletion Problem

scheme two: status flag method

- Uses a fixed grid in $x$, based on Backward Euler time stepping with time step $k$.
- Each grid point at each time step has a flag set to either $A$ ($C > 0$) or $B$ ($C = 0$).
- Setting up the system for the next time step based on the flag at grid $j$:
  
  $$
  A: \quad C_j^* - C_j^n = k(D_2 C_j^* - 1) \\
  B: \quad C_j^* = 0.
  $$

- Then, the states are checked for every grid $j$:
  - If $A$ and $C_j^* < 0$ switch to $B$.
  - If $B$ and $C_j^n + k(D_2 C_j^* - 1) > 0$ switch to $A$.
- If there was a switch at any grid point, recompute $C^*$, otherwise accept $C^{n+1} = C^*$.
- First order convergence in time, $O(k)$, to benchmark solution. No theory.
- In practice, switching iterations always converge. No theory.
Oxygen Depletion Problem

scheme three: split step

- Uses a fixed grid in \( x \), based on Backward Euler time stepping with time step \( k \).

- Split Step:
  - \( C_j^* - C_j^n = kD_2 C_j^* \) at all grid points, artificial far field condition \( C_N^* = 0 \).
  - \( C_j^{n+1} = \max(C_j^* - k, 0) \).

- Theory! [BCR] for the space and time continuous (heat equation solve) version of the scheme.

- First order convergence in time, \( O(k) \), to benchmark solution.
Oxygen Depletion Problem

scheme three: split step (continued)

Apply to the steady state problem \( c(x) = (x - 1)^2/2 \), space continuous:

\[
C^* - C = kC^*_{xx}, \quad C^*(\infty) = 0
\]
\[
C(x) = \max(C^*(x) - k, 0).
\]

\( x < 1 - \sqrt{k} \):
\[
C^*(x) = (1 - x)^2/2 + k/2,
\]
\[
C(x) = (1 - x)^2/2 - k/2
\]

\( x > 1 - \sqrt{k} \):
\[
C^*(x) = ke^{-(x-1+\sqrt{k})}, \quad C(x) = 0
\]
Oxygen Depletion Problem

scheme three: split step 2D computations

Contour plotting in the 1970's [BCR]:

![Contour Plot](image-url)
Two Phase Flow Model

scheme one: M2 method

\[ u_t = \Delta u + \Gamma \]
\[ v_t = \nabla \cdot (D(u)\nabla v) - \Gamma \]
\[ w_t = \Delta w + \Gamma \]
\[ v = S(u) \quad \text{when} \quad w > 0 \]

Introduce total water \( \rho = v + w \) and “Enthalpy” \( Q = u + v \):

\[ \rho_t = \nabla \cdot (D(u)\nabla v) + \Delta w \]
\[ Q_t = \nabla \cdot (D(u)\nabla v) + \Delta u \]

Recover \( u, v \) and \( w \) from the “M2 map”:

- if \( \rho < S(Q - \rho) \), all vapour \( w = 0, v = \rho, u = Q - \rho \).
- otherwise solve \( Q = u + S(u) \) for \( u, v = S(u), w = \rho - v \).
Two Phase Flow Model

scheme one: M2 method (discussion)

- M2 map approach proposed by Wang and Beckermann, IJHMT, 1993.
- M2 map is continuous with derivative discontinuities.
- Computational convergence study Bridge and W, JCP, 2007, on a more physical model with degenerate water diffusion. No theory.
- Implemented on a fixed grid with Backward Euler time stepping and the status flag approach.
- Status flag change at each Newton iteration. Status flag iterations always converge. No theory.
- $O(k) + O(h^q) \ (1 < q < 2)$ convergence observed in $\| \cdot \|_1$ on the current model.
- Used as a benchmark for the other schemes below in 1D.
Two Phase Flow Model

scheme two: split step

Variables $u$, $v$ and $w$ kept for every $x$. Solve

\[
\begin{align*}
U^* - U^n &= k\Delta U^* \\
V^* - V^n &= k\nabla \cdot (D(U^*)\nabla V^*) \\
W^* - W^n &= k\Delta W^*
\end{align*}
\]

Then add condensation locally (each $x$) with $\gamma \approx k\Gamma$:

\[
\begin{align*}
U &= U^* + \gamma \\
V &= V^* - \gamma \\
W &= W^* + \gamma
\end{align*}
\]

where $\gamma = \max(\gamma^*, -W^*)$ and $\gamma^*$ solves

\[
S(U^* + \gamma^*) = V^* - \gamma^*
\]
Two Phase Flow Model
scheme two: split step (discussion)

- Temporal errors $O(\sqrt{k})$ observed computationally. **No theory.**
- At steady state, spatial continuous analysis of a related linear problem shows $O(\sqrt{k})$ errors. Condensation delta function approximated by width $O(\sqrt{k})$ exponentials.
- The 2D computation shown earlier is based on this formulation.
Two Phase Flow Model

scheme three: HLZ scheme

\[ u_t = \Delta u + \Gamma, \quad v_t = \nabla \cdot (D(u) \nabla v) - \Gamma, \quad w_t = \Delta w + \Gamma \]

Introduce the regularization \( H \gg 1 \):

\[
\Gamma = \begin{cases} 
0 & \text{if } w = 0 \text{ and } v < S(u) \\
H(v - S(u)) & \text{otherwise}
\end{cases}
\]

- \( \gamma = \max \left[ (\nabla^n - S(U^n)/(1 + 1/(kH)), -W^n) \right] \)
- \( W^* = W^n + \gamma, \quad W^{n+1} - W^* = k \Delta W^{n+1} \)
- \( U^{n+1} - U^n = \gamma + k \Delta W^{n+1} \)
- \( V^* = V^n - \gamma, \quad V^{n+1} - V^* = k \nabla \cdot (D(U^{n+1}) \nabla V^{n+1}) \)
Two Phase Flow Model
scheme three: HLZ scheme (discussion)

- Proposed by Huang, Lin and Zho, SIAP, 2007
- At steady state, spatial continuous analysis of a related linear problem shows $O(\sqrt{k}) + O(1/\sqrt{H})$ errors. Condensation delta function approximated by width $O(\sqrt{k})$ (vapour only) and $O(1/\sqrt{H})$ (two phase) exponentials.
- Point-wise iterations converge to $V = S(U)$ only when $kH$ is sufficiently small.
- With $H = O(1/k)$, convergence of $O(\sqrt{k})$ observed computationally.
Summary

- Presented a collection of methods for two implicit free boundary value problems with numerical evidence of convergence.
- Lots of missing theory:
  - Existence and regularity theory for the underlying problems
  - Equivalence of the formulations
  - Convergence of discretizations
  - Convergence of the discrete status iterations
- Future work:
  - Implement mapped domain technique for the condensation problem to get a high accuracy reference solution.
  - Connection to Augmented Lagrangian methods?
  - Can every implicit free boundary value problem be written in a status flag formulation, and/or as a split step method with more components?