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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MSU Applied Mathematics Seminar, May 27, 2016

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

Γ: condensation rate

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

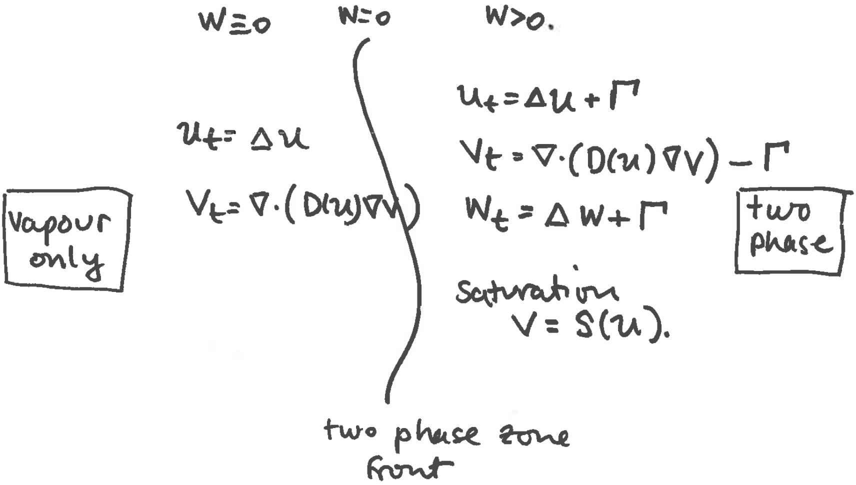
Equations:

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

Motivation: transport in fuel cell electrodes and baking bread

Model Problem

picture: moving boundary



Model Problem

two zone formulation

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

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

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

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

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)

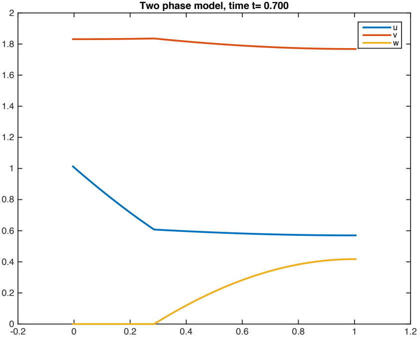
Model Problem

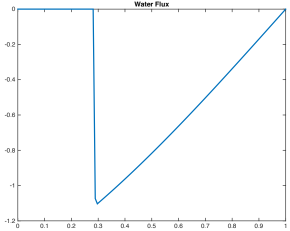
two zone formulation: discussion

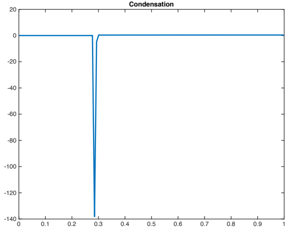
- Count check: four component second order parabolic equations, five mixed Dirichlet/Neumann conditions.
- There can be a condensation delta function at the free boundary.
- There is no Stefan velocity. This is an “implicit” free boundary value problem, Crank, Free and Moving Boundary Problems, 1984.
- 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)



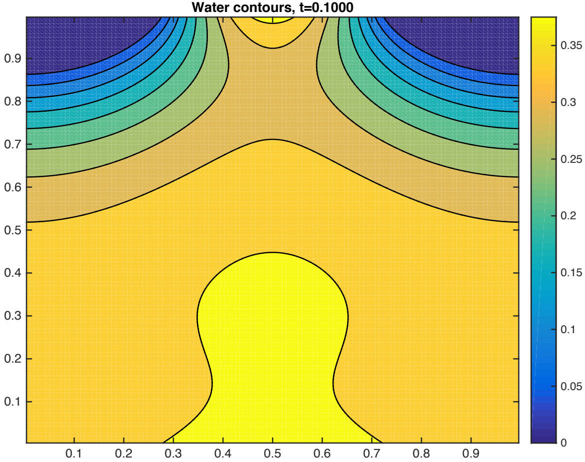




Movie

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

$$u_t = \Delta u$$

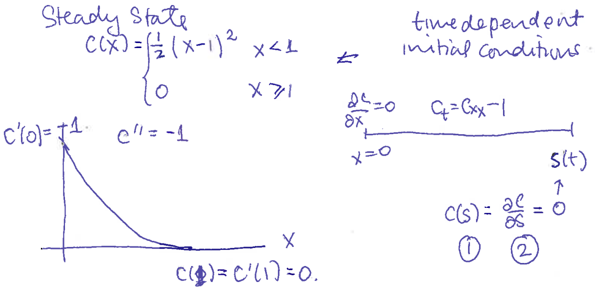
on either side of the interface. Consider "implicit" moving boundary conditions

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

$$s^2 c_t - ys\dot{s}c_y = c_{yy} - s^2$$

  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:

$$s^2 \dot{C}_j - ys\dot{s}D_1 C_j = D_2 C_j - s^2 \quad \text{interior points}$$

  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:

$$\begin{aligned} A\!: &\ C_j^* - C_j^n = k(D_2 C_j^* - 1) \\ B\!: &\ C_j^* = 0. \end{aligned}$$

- 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:

$$\begin{aligned} C^* - C &= kC^*_{xx}, \quad C^*(\infty) = 0 \\ C(x) &= \max(C^*(x) - k, 0). \end{aligned}$$

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

$x > 1 - \sqrt{k}$: $C^*(x) = ke^{-(x-1+\sqrt{k})}, C(x) = 0$

Oxygen Depletion Problem

scheme three: split step 2D computations

Contour plotting in the 1970's [BCR]:

FIG. 5.2. *Truncation ADI*, 1000 × *computed solution at* $t = .05$; $\Delta x = \Delta y = .04$, $\Delta t = .005$

Two Phase Flow Model

scheme one: M2 method

$$
\begin{aligned}
u_t &= \Delta u + \Gamma \\
v_t &= \nabla \cdot (D(u)\nabla v) - \Gamma \\
w_t &= \Delta w + \Gamma \\
v &= S(u) \ \ \text{when } w > 0
\end{aligned}
$$

Introduce total water $\rho = v + w$ and "Enthalpy" $Q = u + v$:

$$
\begin{aligned}
\rho_t &= \nabla \cdot (D(u)\nabla v) + \Delta w \\
Q_t &= \nabla \cdot (D(u)\nabla v) + \Delta u
\end{aligned}
$$

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

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

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

$$\begin{aligned} U &= U^* + \gamma \\ V &= V^* - \gamma \\ W &= W^* + \gamma \end{aligned}$$

where $\gamma = \max(\gamma^*, -W^*)$ and γ^* 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 $H \gg 1$:

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

- $\gamma = \max\left[(V^n - S(U^n)/(1 + 1/(kH)), -W^n\right]$
- $W^* = W^n + \gamma$, $W^{n+1} - W^* = k\Delta W^{n+1}$
- $U^{n+1} - U^n = \gamma + k\Delta W^{n+1}$
- $V^* = V^n - \gamma$, $V^{n+1} - V^* = k\nabla \cdot (D(U^{n+1})\nabla V^{n+1})$

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?