Equivalent formulations of the oxygen depletion problem, other implicit moving boundary value problems, and implications for numerical approximation

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Overview of the Talk

- Motivating Problem
- Oxygen Depletion Problem
  - Problem
  - Equivalent Formulations
  - Computational Approximation
  - Conjecture on 1D dynamics
- Biharmonic Problem
- Generalized Problems (only questions)

https://arxiv.org/abs/2105.03538

A mixture formulation for numerical capturing of a two-phase vapour interface in a porous medium Bridge and W, JCP (2007)

Motivating Problem

two phase flow in porous media (easy bake 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:

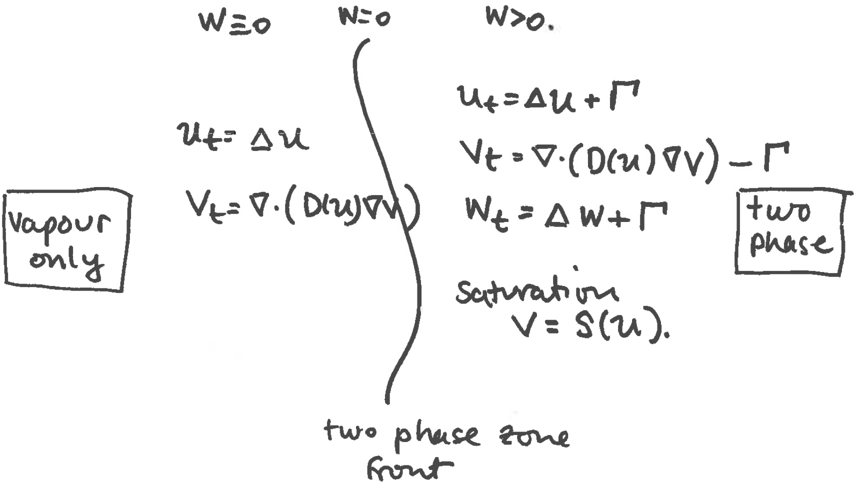
$$
\begin{aligned}
u_t &= \Delta u + \Gamma \\
v_t &= \nabla \cdot (D(u) \nabla v) - \Gamma \\
w_t &= \Delta w + \Gamma
\end{aligned}
$$

Motivation: Transport in fuel cell electrodes and baking bread

HH: "It's a 1D problem, how hard can it be?"

Motivating 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)

Motivating Problem

two zone formulation: discussion

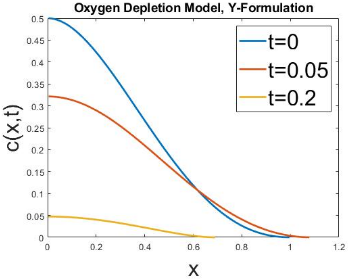
- Count check: four component second order parabolic equations, five mixed Dirichlet/Neumann conditions.
- There is no Stefan velocity. This is an "implicit" moving boundary value problem. Crank, Free and Moving Boundary Problems, 1984.

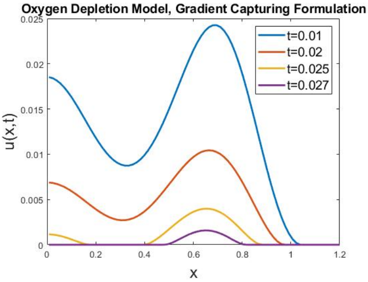
Oxygen Depletion Problem

problem in 1D

$$u_t = u_{xx} - 1$$

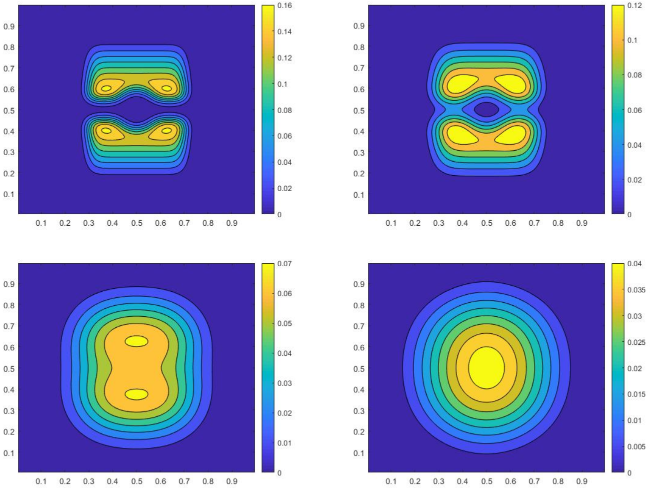
- Unknown $u(x,t)$ for $x \in [0, s(t)]$
- Free boundary $x = s(t)$ at which $u = 0$ and $u_x = 0$ (*implicit*)
- Consider the Cauchy problem or $u_x = 0$ at $x = 0$.
- The steady state problem is the *Elliptic Obstacle Problem*.





Oxygen Depletion Problem

2D results



Open question: Generic limiting end state $u \to 0$?

Oxygen Depletion Problem

fixed topology formulations

Five formulations, all equivalent (rigorous arguments by Xinyu).

I: Stefan formulation

- $v = u_t$ satisfies $v_t = v_{xx}$ with $v = 0$ at the moving boundary and an explicit normal velocity of $-v_x$.
- Equivalent to a explicit normal velocity of $-u_{xxx}$ in the original variables.

II: Mapped domain formulation

- Mapped coordinate $y = x/s(t)$, $y \in [0, 1]$
- $u_{yy} + \dot{s}syu_y - s^2 u_t - s^2 = 0$
- Numerical method using DAE time stepping
- No analysis for this formulation

The oxygen diffusion problem: Analysis and numerical solution, Mitchell and Vynnycky (2015)

Oxygen Depletion Problem

variable topology formulations

III: Variational inequality formulation

$$\int_0^t \int u_t \cdot (v - u) + \int_0^t \int \nabla u \cdot \nabla (v - u) \geq \int_0^t \int u - v$$

for all v in $L_2(0, T, H^1_+)$. Augmented Lagrangian methods.

IV: Gradient flow formulation (new)

L_2 gradient in flow in H^1_+ on $\mathcal{E}(t) = \int_\Omega \frac{1}{2}|\nabla u|^2 + u$

V: Regularized formulation

$$\partial_t u_\epsilon = \Delta u_\epsilon - f_\epsilon(u_\epsilon) \text{ with } \; f_\epsilon(u_\epsilon) = \begin{cases} 1 & u_\epsilon > \epsilon \\ \dfrac{u_\epsilon}{\epsilon} & u_\epsilon \leq \epsilon, \end{cases}$$

Berger, Ciment, and Rogers, Numerical Solution of a Diffusion Consumption Problem with a Free Boundary, SINUM (1975)

Oxygen Depletion Problem

gradient flow time stepping

- Time step k from u^n to $u \in H^1_+$ minimizes

$$E[u] = \int_\Omega \frac{1}{2}|\nabla u|^2 + \frac{1}{2k}(u - u^n)^2 + u$$

- $\mathcal{E} < \mathcal{E}^n$.
- After spatial discretization, the problem for U is a quadratic minimization problem with linear inequality constraint.
- There is a convergence proof of the fully discrete method.
- The discrete minimization is done with an index iteration strategy.
- The method has many similarities to the approach used for the two phase flow model.

Oxygen Depletion Problem

Conjecture on 1D dynamics

Assume u_0 has a finite $\mathcal{S}(0)$ where $\mathcal{S}(t)$ counts the number of free boundary points: Then

(i) $\mathcal{S}(t)$ is finite for every $t > 0$.

(ii) There exists a finite increasing sequence of times t_j, $j = 0, \ldots, M$ with $t_0 = 0$ and $\operatorname{card} \mathcal{S}(t) := n_j$ constant on every interval (t_j, t_{j+1}) and $u \equiv 0$ for $t \geq t_M$.

(iii) $\mathcal{S}(t) = \{s_1(t), s_2(t), \ldots s_{n_j}(t)\}$ for $s_l(t)$ smooth on (t_j, t_{j+1}).

(iii) $u(x,t)$ is C^1 for $t > 0$ and C^∞ except at free boundary points.

Recent related results have been shown for the Stefan problem Figali, Ros-Oton, Serra.

Biharmonic Problem

Viscoelastic beam model

- Scaled, linear, viscoelastic motion of a beam under gravity above a flat, rigid surface:

$$u_t = -u_{xxxx} - 1$$

  with $u = 0$, $u_x = 0$, and $u_{xxx} = 0$ at the free boundary $x = s(t)$ (implicit). Gwynn Elfring.

- Gradient flow on the energy

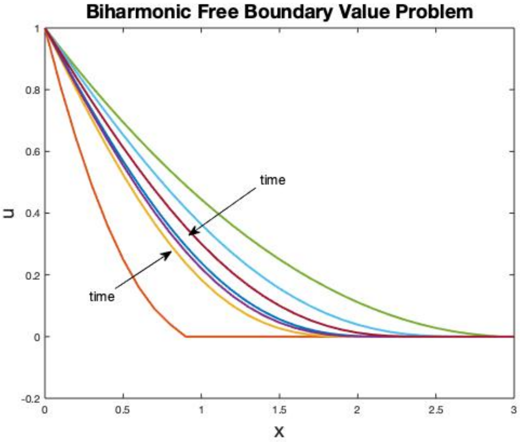
$$E(u) := \int \frac{1}{2} |\Delta u|^2 + u$$

  with $u \in H^2_+$.

- Convergent discrete capturing scheme follows the same analyis as the OD problem.

Biharmonic Problem

Computations



Physical boundary conditions $u(0) = 1$, $u_{xx} = 0$

Generalized Problems

1D second order implicit vector parabolic problems

- Consider a single free boundary at $x = s(t)$
- $\mathbf{u}^l(x,t)$ having n components for $x < s(t)$
- $\mathbf{u}^r(x,t)$ having m components for $x > s(t)$
- We take

$$\mathbf{u}^*_t = D^*\mathbf{u}^*_{xx} + \mathbf{a}^*$$

- At the boundary

$$B \begin{bmatrix} \mathbf{u}^l \\ \mathbf{u}^l_x \\ \mathbf{u}^r \\ \mathbf{u}^r_x \end{bmatrix} = \mathbf{0}$$

  B is an $(m+n+1) \times (2m+2n)$ matrix of full rank.
- The OD problem has $n = 1,\ m = 0$.
- The condensation problem has $n = 2,\ m = 2$.

Generalized Problems

Questions

- Which lead to well defined problems? (this could depend on the sign of entries of $\mathbf{a}$)
- Which have gradient flow or variational inequality structure?
- Which allow a capturing formulation with index iteration similar to the OD, condensation, and biharmonic problems?

Summary

- Motivating two phase flow problem
- Oxygen Depletion problem: five equivalent formulations, convergence of gradient flow method.
- In the arXiv paper:
  - Equivalency analysis
  - Convergence proof of the discrete gradient method
- Open problems
- Generalized implicit moving boundary value problems