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

Brian Wetton Xinyu Cheng (Fudan) Zhaohui Fu (UBC/SUSTech)

Mathematics Department, UBC
www.math.ubc.ca/~wetton

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Overview of the Talk

- Motivating Problem
- Oxygen Depletion Problem
  - Problem
  - Equivalent Formulations
  - Computational Approximation

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

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 $S(u) = e^u$).

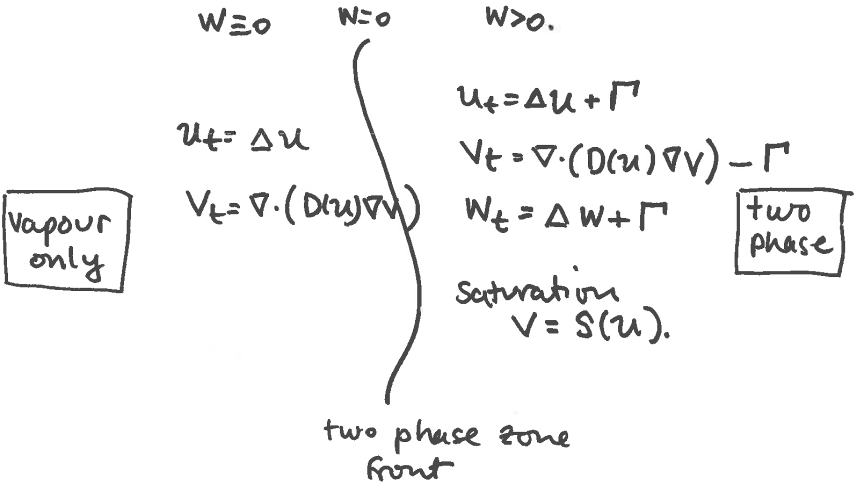
Equations:

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

Motivation: Transport in fuel cell electrodes and baking bread

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

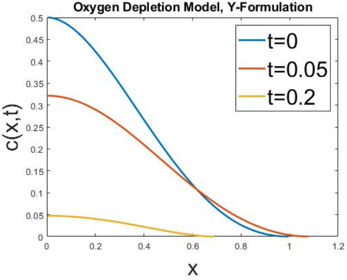
- Count check: four component second order parabolic equations, five mixed Dirichlet/Neumann conditions.
- There is no Stefan velocity. This is an "implicit" moving boundary value problem. Crank, Free and Moving Boundary Problems, 1984.

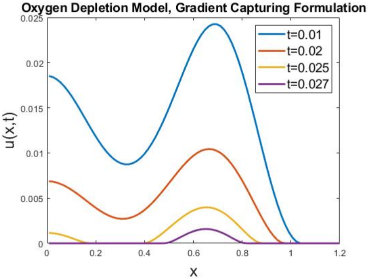
Oxygen Depletion Problem

problem in 1D

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

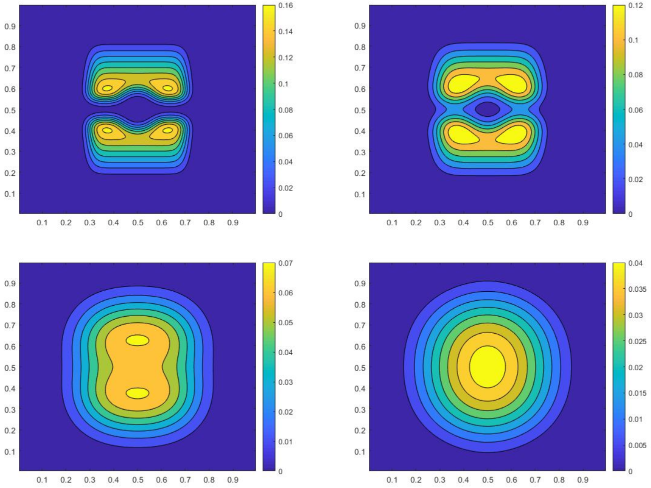
- Unknown $u(x,t)$ for $x \in [0, s(t)]$
- Free boundary $x = s(t)$ at which $u = 0$ and $u_x = 0$ (*implicit moving boundary value problem*).
- Consider the Cauchy problem or physical boundary condition $u_x = 0$ at $x = 0$.





Oxygen Depletion Problem

2D results



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

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.

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