EVAPORATION FROM POROUS MEDIA

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W.L. Gore & Associates, Inc., Elkton, MD

37th Annual MPI Workshop
Virtually hosted by The University of Vermont
June 14, 2021

Together, improving life

W. L. Gore & Associates

- Founded in 1958 by Bill and Vieve Gore in Newark, DE
- 10,000+ associates
- Privately held
- Manufacturing in U.S., Germany, Scotland, Japan, and China and sales offices in many other countries
- Repeatedly listed on “Best Companies to Work For” lists in the U.S., U.K., Germany and Italy

Gore’s 3 Divisions

Fabrics	Medical Products	Performance Solutions

GUARANTEED TO KEEP YOU DRY
GORE-TEX® PRODUCTS
GORE

GORE® WINDSTOPPER® PRODUCTS

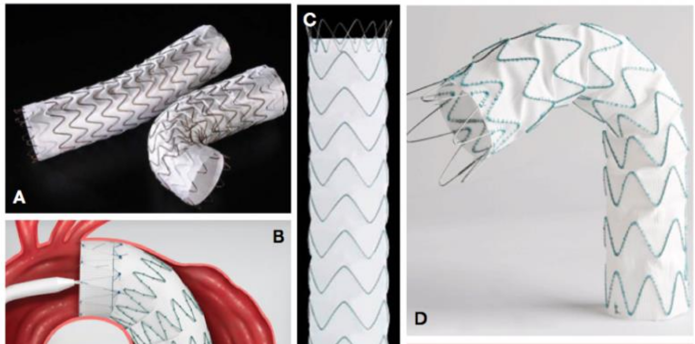
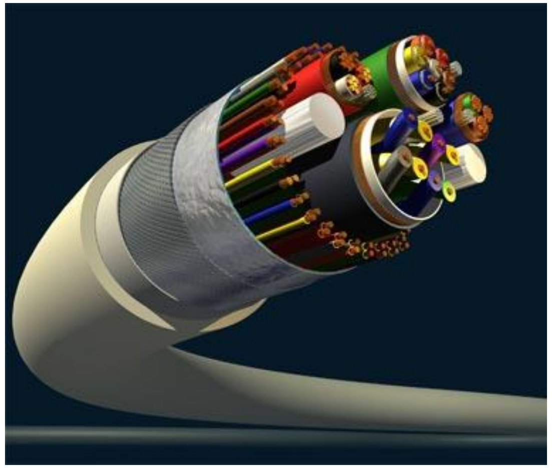


Figure 1. Approved thoracic stent grafts: C-TAG (A), TX2 ProForm (B), Valiant (C), Relay (D).



GORE

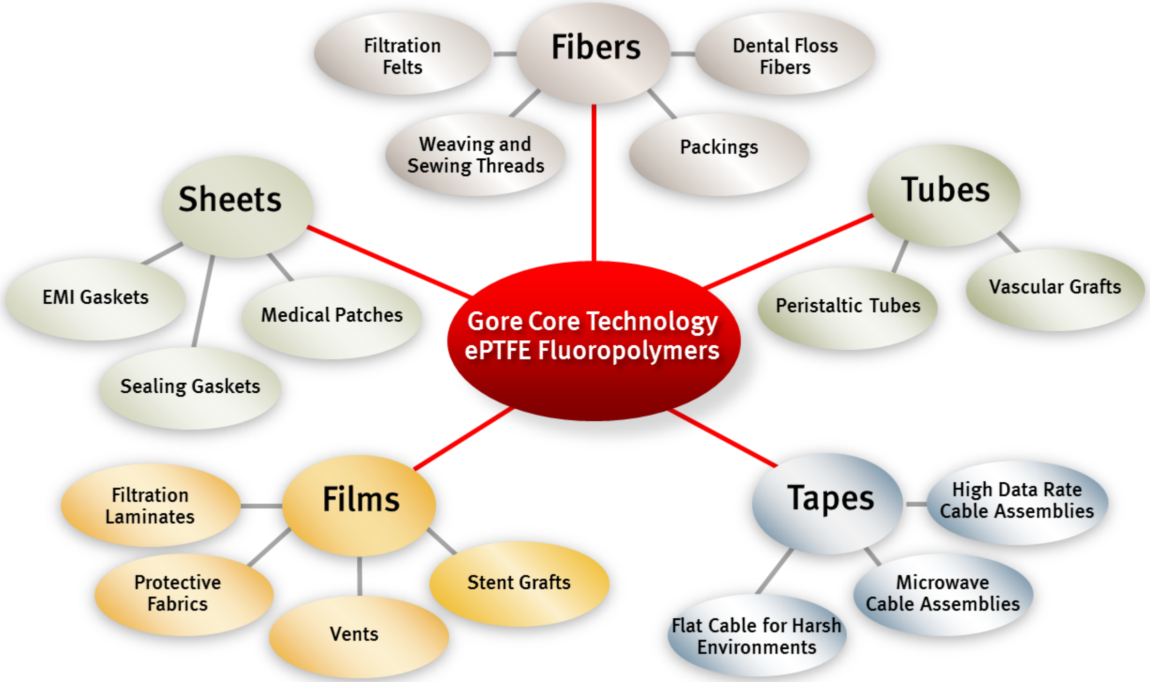
Commitment to fitness for use

Our Materials

- Biocompatible
- High thermal resistance
- Chemical resistance
- Low flammability
- Hydrophobicity
- Consistent product quality
- Optical and acoustic properties

Our Products

- Do what we say they will do — the first time and every time
- Adhere to our standards of high quality and product integrity
- Are derived from a comprehensive understanding of our customers' needs and end-use applications



Bob Gore demonstrates PTFE's ability to stretch when pulled quickly
http://www.gore.com/en_xx/technology/story.html?isAjax=true

GORE

Gore’s history with MPI

2002 — Gore’s first participation in MPI. Uwe Beuscher presents problem on multiphase flow in porous media

2009 — Uwe meets Sumanth at MPI. Network model for filtration

2011 — Sumanth starts at Gore. Beginning of dedicated modeling and simulation team

2013 — Sumanth meets Zhenyu and Vasu. Kerplunk model for filtration

2014 — Vasu starts at Gore with the modeling and simulation team

2015 — Zhenyu starts at Gore with the modeling and simulation team

2016 — InFoMM collaboration starts on a problem from 2015 study group (Kris Kiradjiev)

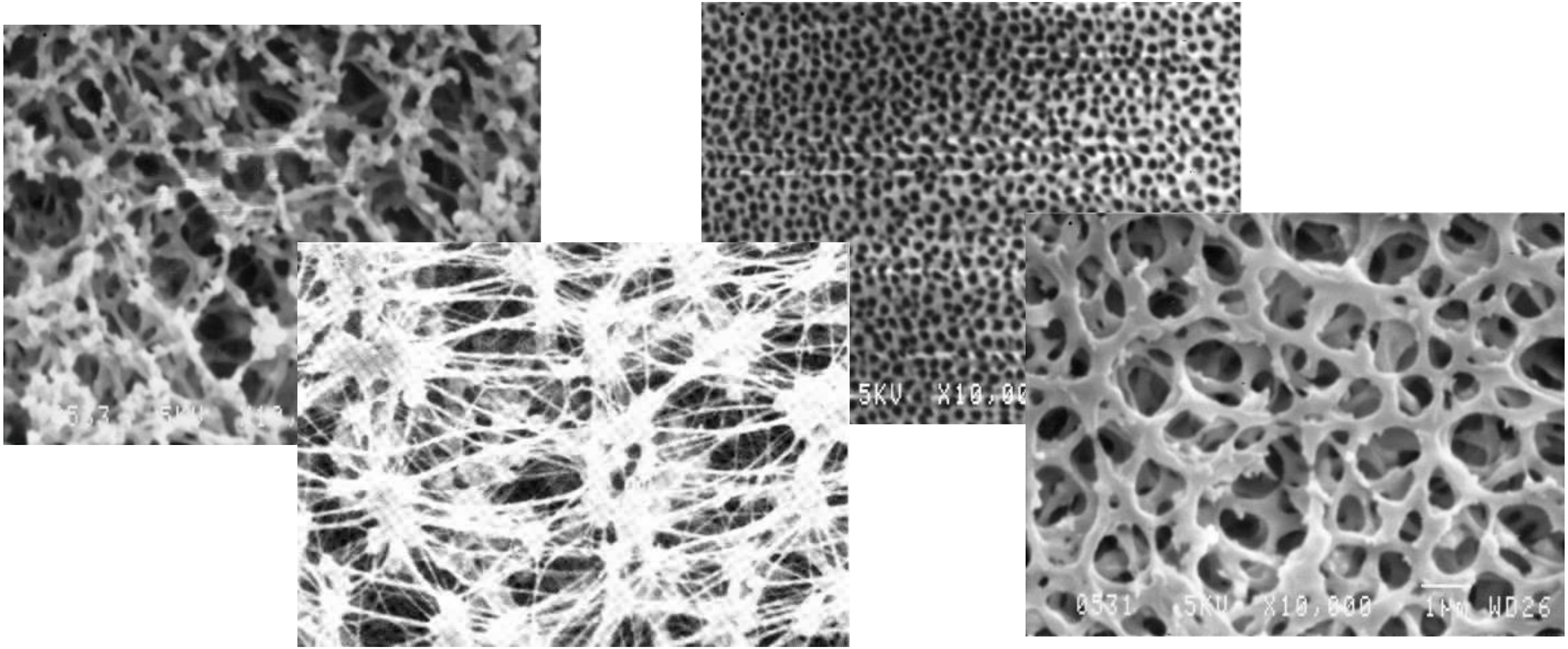
2020 — Kris finishes PhD thesis

First fully virtual MPI with global participation

2021 — Sadly, doing math by the shores of Lake Champlain will have to wait for a few more years

In more than one decade of participation, we have worked on problems in multiphase flow, heat transfer, reactions, filtration, and quantitative image analysis/microscopy.

The wide range of microstructure in porous media



Ho, C. and Zydney, A., J. Membr. Sci. 155 (1999) 261-275

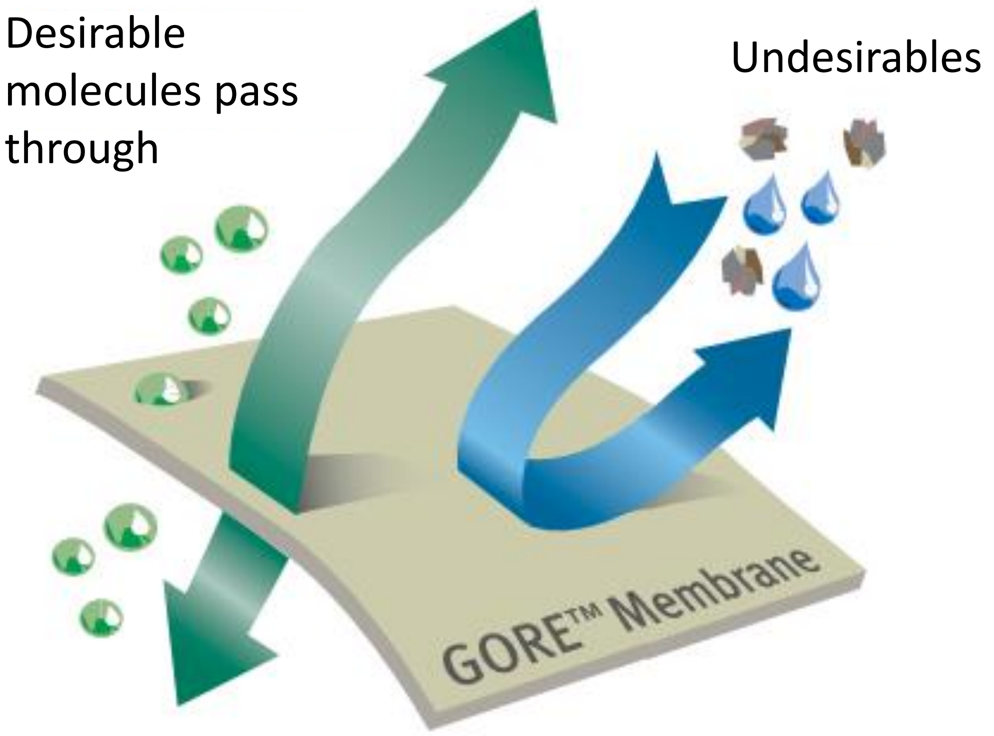
Porous materials as barriers

Filters, clothes, architectural fabrics,….

- Selective permeability is desirable quality in many applications
- Materials undergo wetting and drying cycles through their lifetime

Wetting → Impurities enter material → Drying →
- Impurity deposition
- Change in pore size
- Change in wetting properties

→ Easier wetting → Eventual material failure with undesirable breakthrough



- Breakthrough of impurities can be harmful to other system components

Drying of a porous material

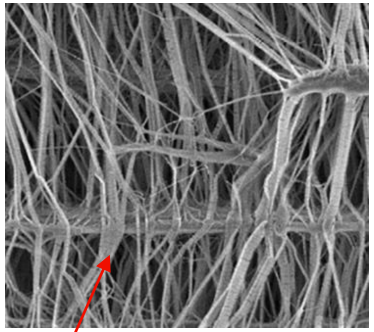
We have a porous material that is filled with a liquid solution containing solute molecules (can be multiple species) with known concentration. As the solvent evaporates solute molecules deposit on the internal pore walls within the material.

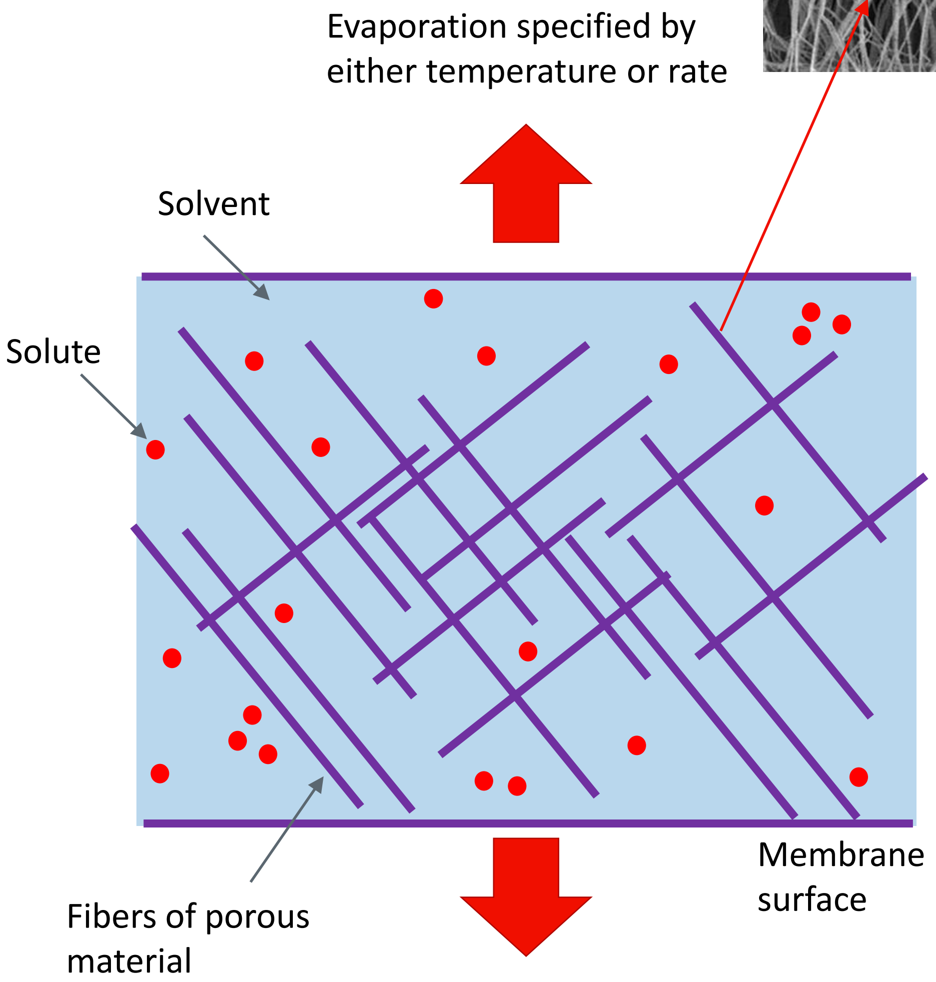
Develop a mathematical model that will predict the mass distribution of solutes inside a porous medium after the solvent has evaporated.

How does the mass distribution change upon subsequent cycles of wetting?

How do the following parameters affect the solute distribution

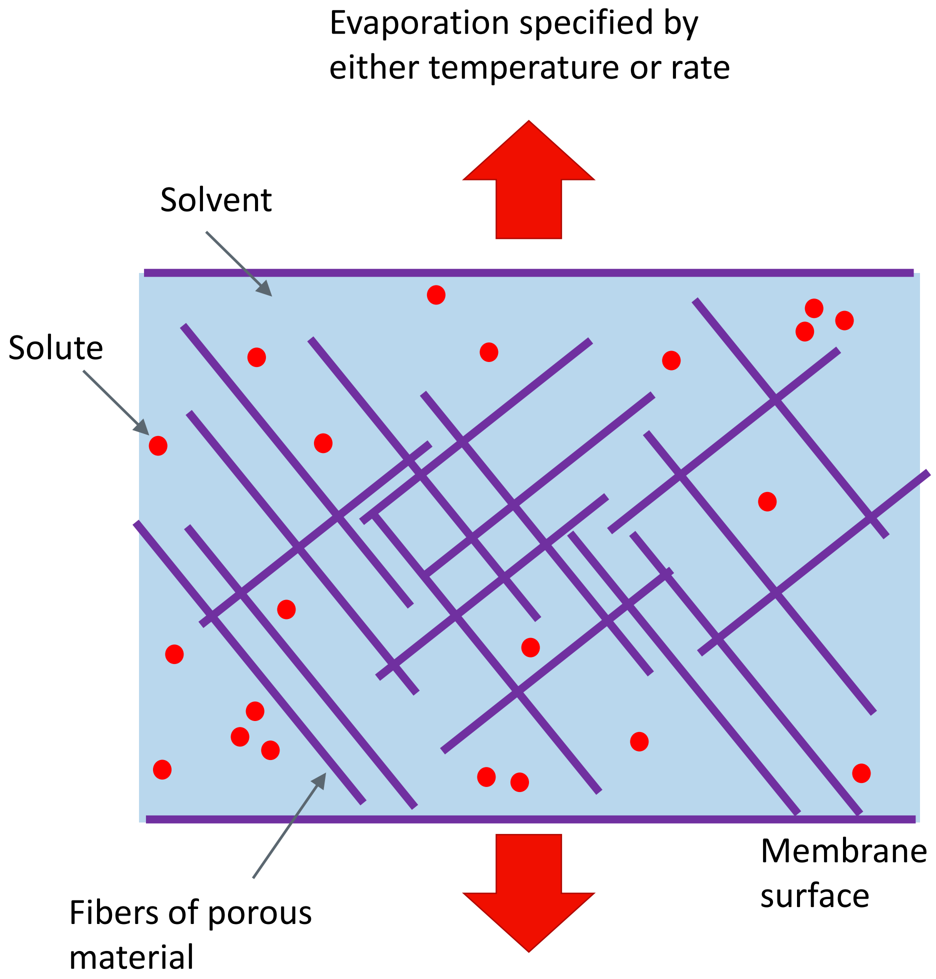
a. Porosity and pore size distribution of the porous material
b. Starting concentration of solute species
c. Evaporation rate





Boundary conditions and assumptions

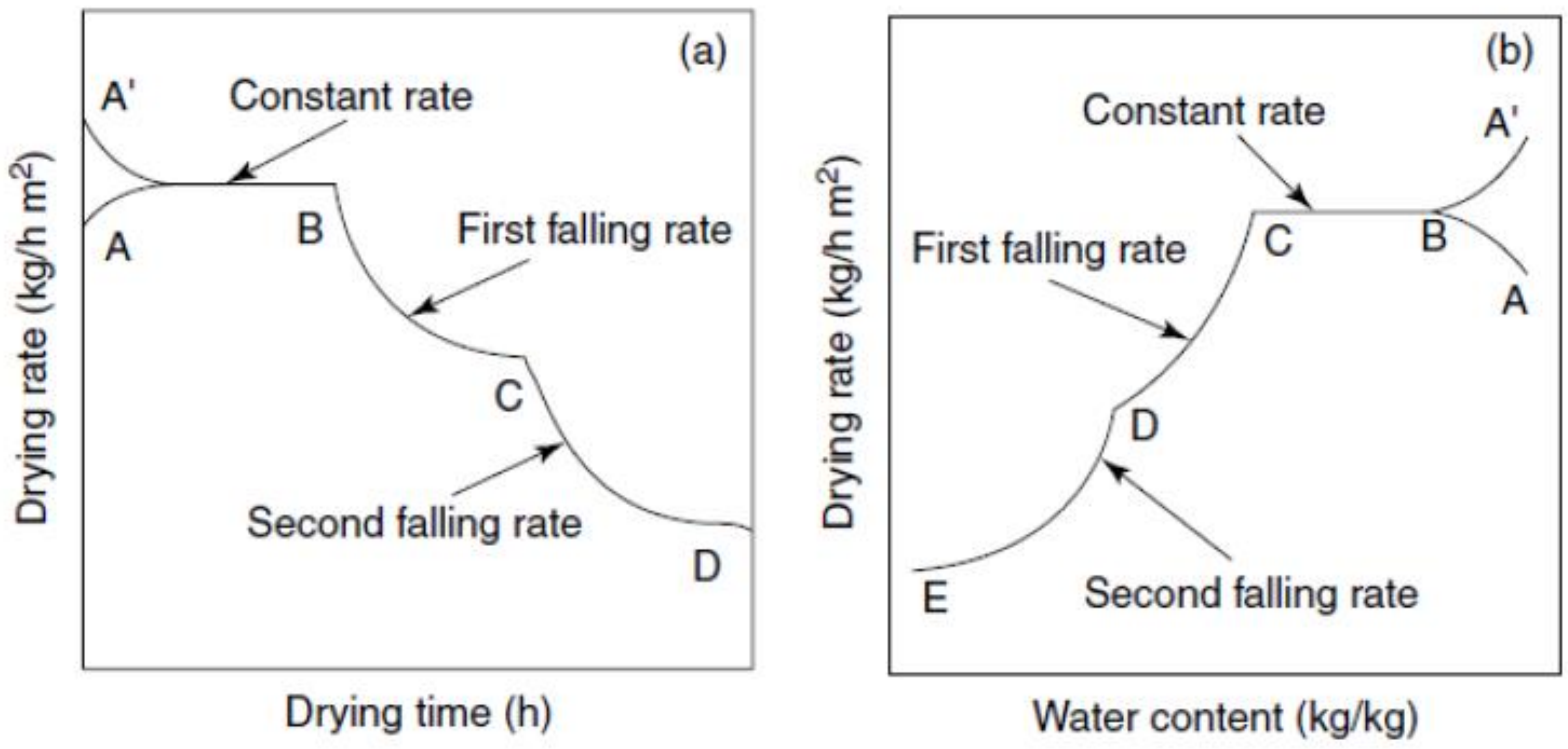
- Porous material initially completely wetted by fluid
- Species deposition can be treated by either of the following methods
  - Saturation concentration, i.e., if $C > C_{sat}$, deposition occurs until $C = C_{sat}$
  - Equilibrium boundary condition (similar to Henry's law) between deposit layer and solution
- Assume that the porous medium is rigid and does not deform under forces exerted by evaporating fluid, i.e., no poroelasticity
- Start with 1 species. If time permits consider N total species with initial concentrations $\{C_1, C_2, \ldots, C_N\}$ that are uniformly distributed through the solution phase.



Model inputs

- Porosity, Pore size distribution, Fiber size distribution, and thickness of porous material. For more complicated model we can assume anisotropy in pore distribution between x-y and z directions
- Starting concentration of solute species
- Solubility/Saturation concentration of solute species
- Solution properties – density and viscosity. Assume simple laws for change in viscosity and density with concentration
- Evaporation rate under isothermal conditions
- For a more complicated model we can specify the temperature outside the medium and account for heat transfer

A typical drying process

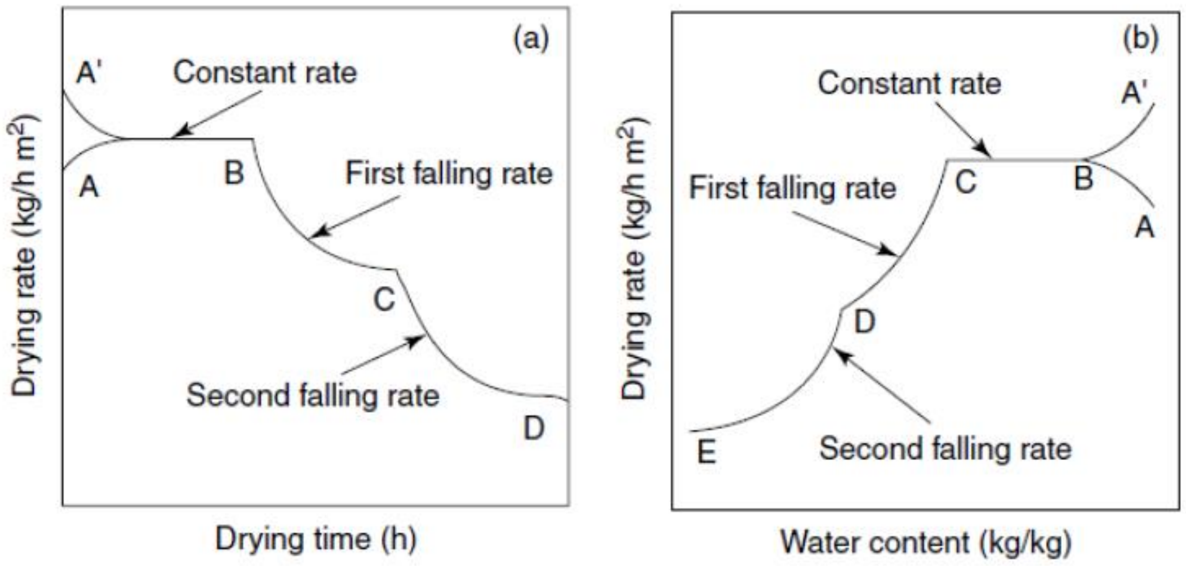


https://moisturecontrol.weebly.com/drying-curve.html

MPI 2021 – Effected of connected capillaries

Accounting for capillary flow and particle diffusion in continuous liquid phase

In certain drying regimes, timescale for capillary effects can be smaller than/comparable to evaporation. Hence not all menisci recede during the constant drying rate period.



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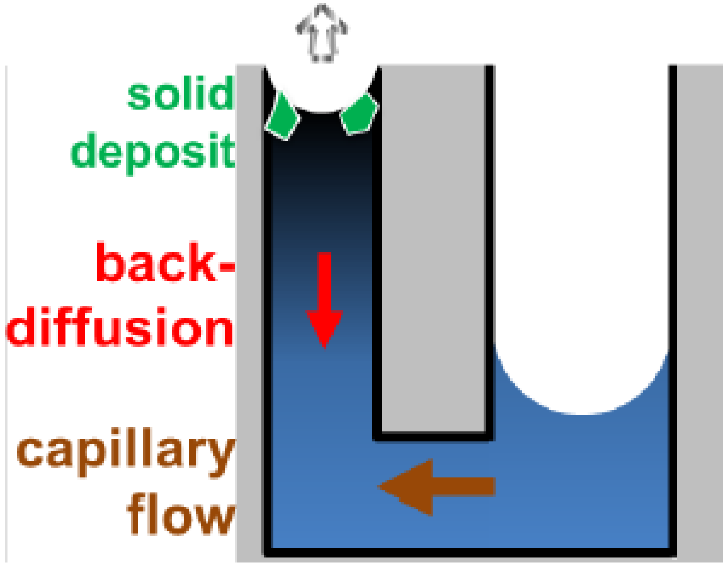
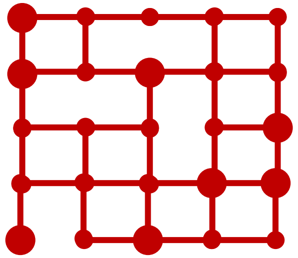
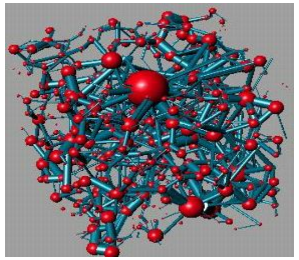
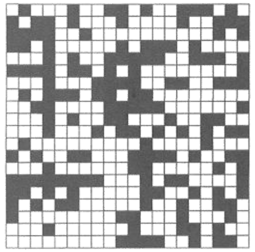
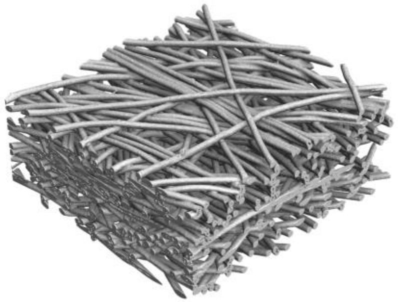


A. Kharaghani, Drying and wetting of capillary porous materials : insights from imaging and physics-based modeling, PhD Thesis

Modeling porous materials

Compromise between mathematical simplicity and accurate description.

Continuum	Depth filtration models Effective medium approximations Field-theoretic models	$Flux \propto K_{eff}\ (Intensity)$
Idealized porous structure	Network Models	  
Actual porous structure	CFD simulations, Pixel/Voxel based calculations	

MPI 2020 – Single equivalent pore drying model

- Simple equivalent cylinder geometry
- Single drying cycle
- No connected pores/liquid flow
- Various adsorption/deposition conditions
- Numerical simulation and asymptotics

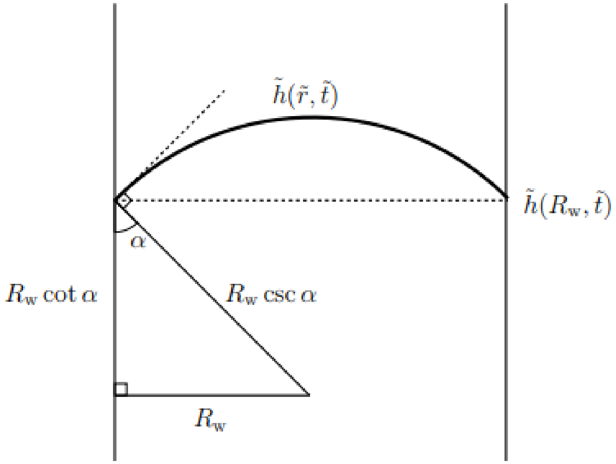


Figure 1.1: Cross-sectional schematic of top of evaporating drop.

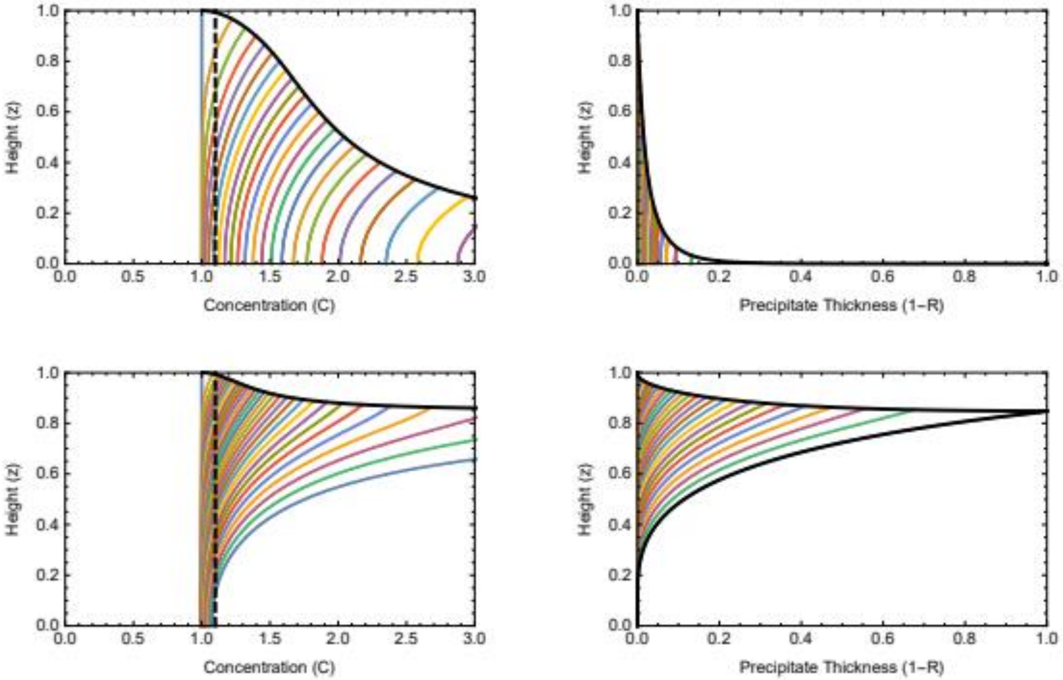


Figure 3.5: Comparison of effect of deposition coefficient λ on solution profiles, which are as in Fig. 3.3, except $D = 1$. Top: small deposition coefficient ($\lambda = 0.1$). Bottom: large deposition coefficient ($\lambda = 10$).

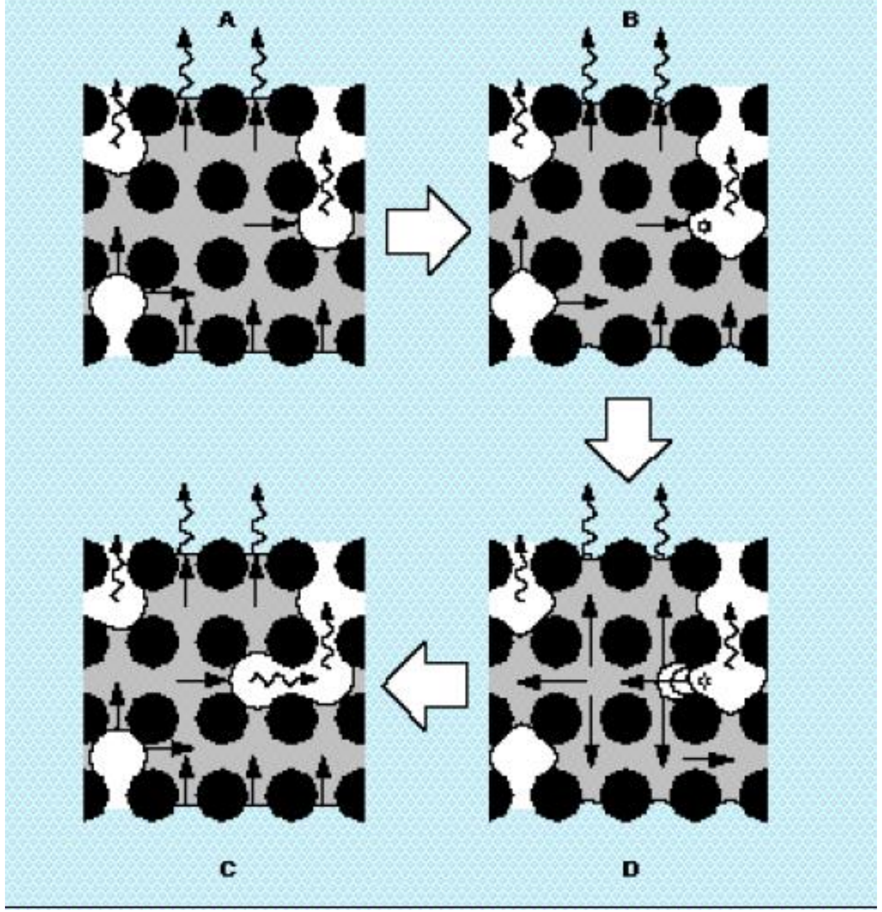
See MPI 2020 report

Other models – Network model with Haines jump

The works of L. E. Scriven and coworkers

- Scriven and coworkers used a network model approach with a simple cubic network to study the drying on inks on paper.
- Paper is treated as a porous medium that is filled with an ink solution. As ink dries, “binder” particles deposit.
- They write down equations for
  - Liquid flow between liquid filled pores and vapor diffusion in vapor filled pores
  - Binder diffusion in liquid phase
  - Binder precipitation based on saturation condition
  - Haines jump mechanism to redistribute liquid as menisci move
- Calculate binder mass distribution as a function of time

5. Illustration of drying mechanisms. A: Liquid flows › to the menisci, where liquid evaporates. B: The fastest receding meniscus reaches a pore throat *. C: Haines jump causes liquid to flow away from the jumping meniscus, and the liquid cluster redistributes the liquid by adjusting its menisci. D: Drying continues and vapor diffuses away from evaporating menisci through old and new paths.



Pan et. al., TAPPI Journal, 1995

Goals for MPI 2021

- Key question remains - *How does the mass distribution of molecules change upon cycles of wetting and drying*?
- Further examine the dependence of the mass distribution of molecules through pore and drying rate/time on pore diameter, pore length, fluid wetting properties, and evaporation conditions using MPI 2020 model.
- Extend the model to a porous structure that has a distribution of pore sizes specified by a pore size distribution.
  - Fluid moves within this pore space and between pores due to capillary force.
  - Track the meniscus and molecule deposition
  - *We are interested in different approaches, viz. continuum, network, and network homogenization, towards this problem.*
  - *Subgroups can potentially work on expanding MPI2020 and Scriven approaches and comparing.*

Thank you!

Some notes:

- Zhenyu He and Vasu Venkateshwaran will be in and out of the teams channels based on some other meetings. Uwe Beuscher will join from Wednesday.
- We will also be stopping by UD to check in with the campers as schedule permits.
  - Vasu will be in tomorrow (15 June 2021) morning for a couple of hours. Planning on coming by Wednesday and Thursday as well.
  - Zhenyu will also be stopping in tomorrow
- Please use the teams chat feature for any questions. We will be checking the chat regularly.