

Stochastic Modelling of Sieving

B. Gu¹

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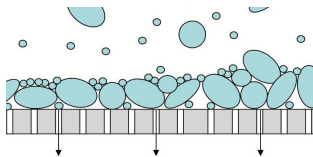
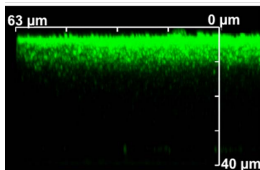
²Department of Mathematics, New York Institute of Technology

Outline

- 1 Overview
- 2 Modelling
- 3 Results
- 4 Summary

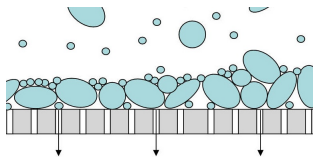
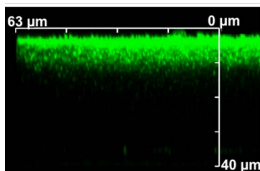
Fouling Mechanisms

- Adsorption: Deposition of **small** particles on the pore walls within membrane;
- Sieving: Deposition of **large** particles covering the top of membrane or plugging pores;
- Cake formation: Stacking of particles on top of each other, during later stages of filtration.



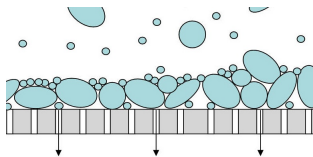
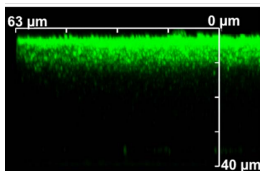
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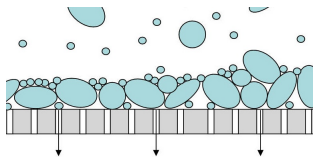
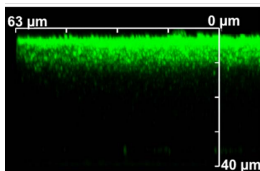
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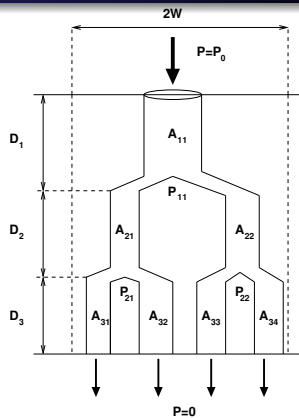


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Flow and Adsorption (Sanaei & Cummings (2017))



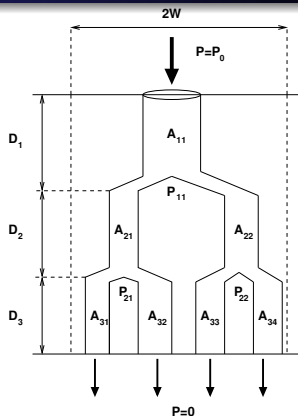
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Hagen Poiseuille

$$\pi A_{ij}^2 \bar{U}_{p,ij} = -\frac{1}{\mu R_{ij}} \frac{\Delta P}{D_i}$$

Conservation of Flux

$$\sum_{j=1}^{\nu_i} \pi A_{ij}^2 \bar{U}_{p,ij} = (2W)^2 U.$$



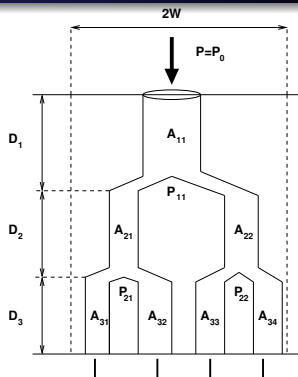
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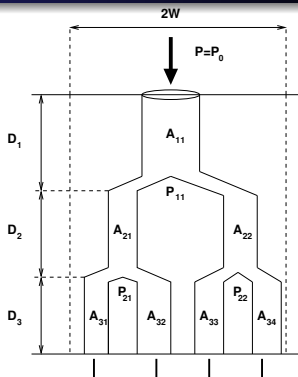
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The Basics of Sieving

Discrete Properties

- Takes one large particle to have an effect
- View the underlying geometry as a connected graph.

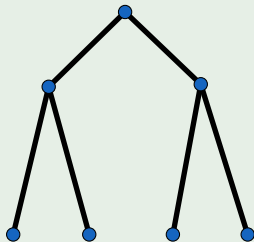
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A connected graph



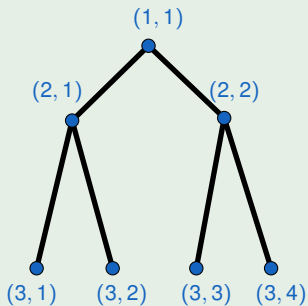
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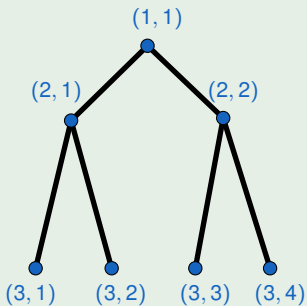
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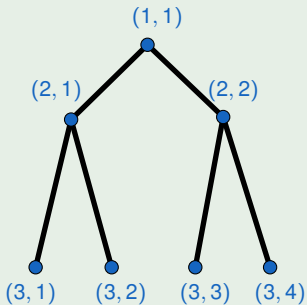
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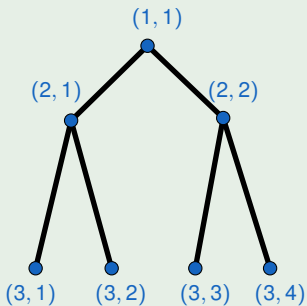
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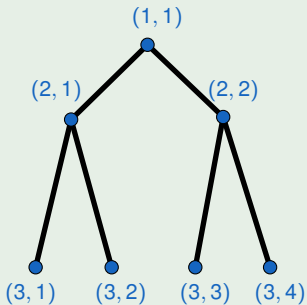
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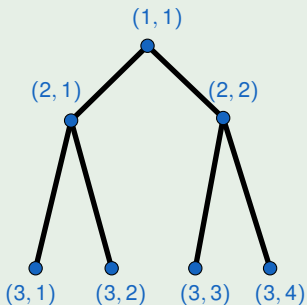
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- Determination of blocking state by size comparison between particle and pore size

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- **Additional** particles arriving at an already blocked site add **negligible resistance** to the pore.
- The size and arrival of particles are independent.

Effect of Local Sieving

State Characterization

$$\chi_{ij}(T) = \begin{cases} 1, & T \geq T_{ij} \text{ (blocked)}, \\ 0, & T < T_{ij} \text{ (open)}, \end{cases}$$

where T_{ij} is the blocking time of a pore at location (i, j) .

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Local Resistance due to Sieving

$$R_{ij, \text{blocking}} = \Xi \mathbb{E} [\chi_{ij}]$$

Ξ : Severity of sieving.

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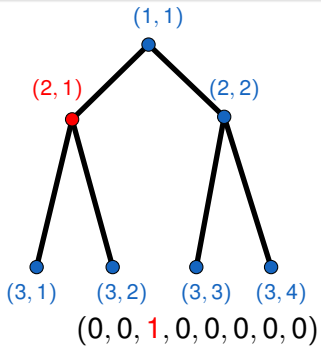
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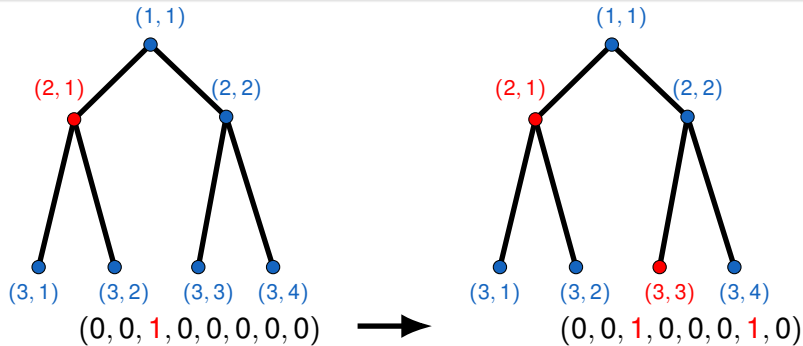
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Solution: condition on the state of the ensemble.

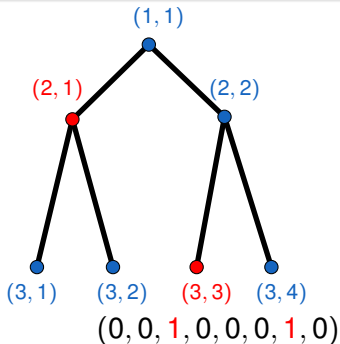
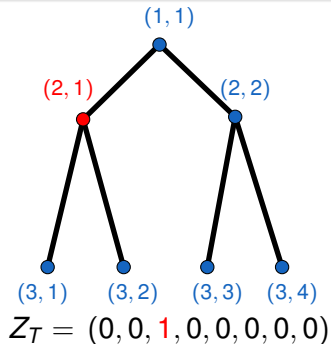
Continuous-time Markov Chain (CTMC)



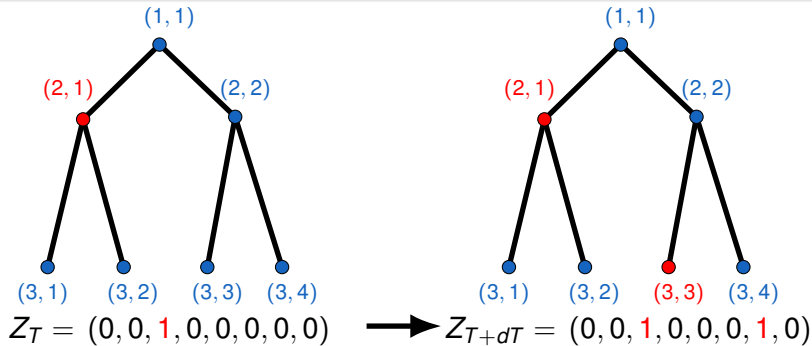
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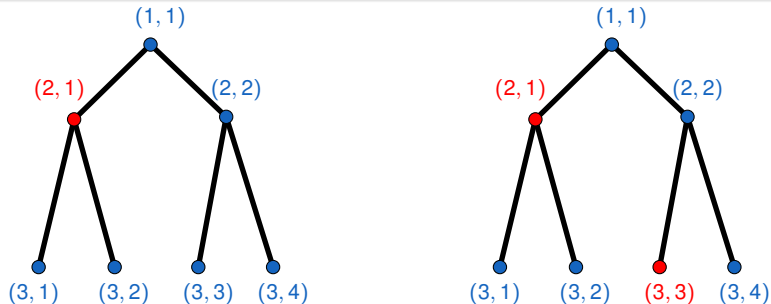
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$Z_T = (0, 0, \mathbf{1}, 0, 0, 0, 0, 0)$ \longrightarrow $Z_{T+dT} = (0, 0, \mathbf{1}, 0, 0, 0, \mathbf{1}, 0)$
 Z_T : time-inhomogeneous CTMC with transition density \mathcal{P} and rate \mathcal{Q} , satisfying the master equations,

$$\frac{d\vec{P}}{dT} = \mathcal{Q}(T) \vec{P}(T), \vec{P}(0) = (1, 0, \dots, 0).$$

\vec{P} lists the probability of the ensemble being in a possible state, contributing to a new formula for $\mathbb{E}[T_{ij}]$.

Resistance in Series

- Resistance by the two fouling modes are put in series,

$$R_{ij} = R_{ij,a} + R_{ij,b} = R_{ij_a} = \frac{8}{\pi A_{ij}^4} + \Xi \mathbb{E} [T_{ij}] .$$

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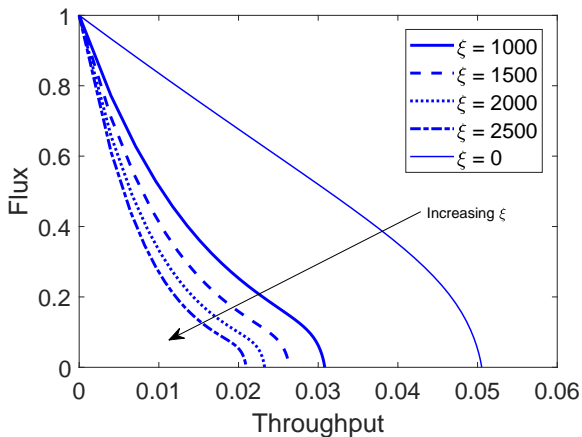
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- Fix initial resistance for fair comparison of different membranes.
- Initialize pore size (for symmetric case – pores in the same layer have equal initial radii):

$$a_i(0) = a_0 \kappa^{i-1} .$$

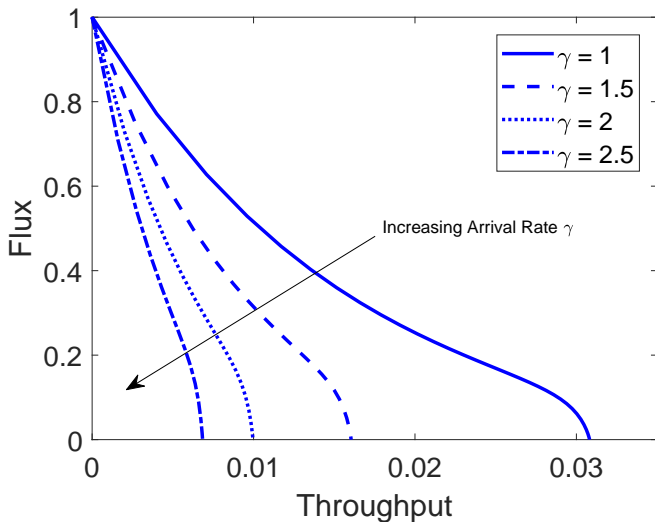
Variations in Sieving Severity ξ

Throughput:

$$v(t) = \int_0^t u(s) ds.$$



Variations in Arrival Rates γ



Model Predictions and Extensions

- Increasing blocking strength and arrival rate reduces total throughput, as expected.
- Sieving severity parameter can be further improved.
 - Radius dependent, e.g. sieving impact is small when pore radius is small.
- Apply the method to more general connected graphs.
- Investigate the dependence of membrane performance on graph parameters.

Acknowledgments

- “Flow and fouling in membrane filters: effects of membrane morphology”, Sanaei, P. & Cummings, L. J., Journal of Fluid Mechanics, 818, 744–771 (2017).
- “Membrane filtration with complex branching pore morphology”, Sanaei, P. & Cummings, L. J., Physical Review Fluids, 3(9), 094305 (2018).”

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