A multiscale model for particle filtration

Arkady Wey – arkady.wey@maths.ox.ac.uk
Mathematical Institute, University of Oxford
C.J.W. Breward, S.J. Chapman, I.M. Griffiths,
U. Beuscher, V. Venkateshwaran

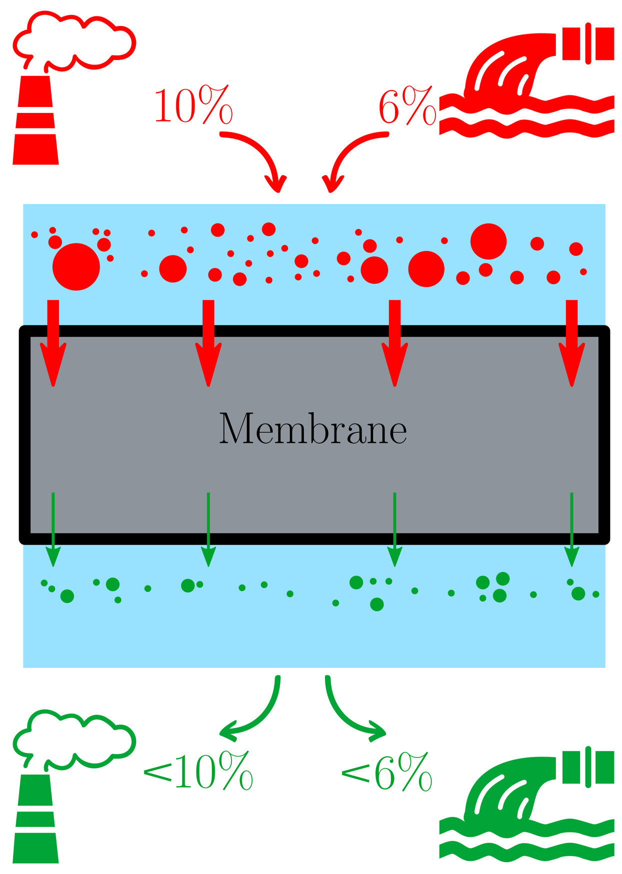
1. Filtration

Problem:

- Fluids that contain harmful particles pose a serious threat to humanity.
- 10% of deaths worldwide are attributed to polluted air.
- 6% of deaths in low-income countries are caused by contaminated water.

Solution:

- Filtration is a method for the removal of harmful particles from fluids by driving them through a semi-permeable membrane.
- Optimisation of this process using mathematical models is essential, to help to decrease the severity of air pollution and water contamination.



2. Multiscale membranes

Macroscale:

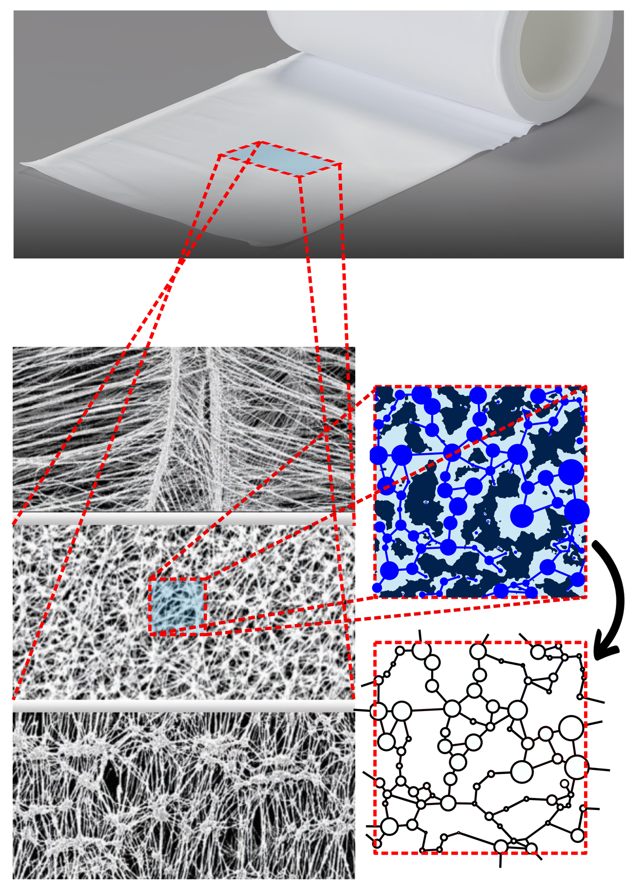
- Many filtration membranes are composed of a material called ePTFE.
- On the macroscale, ePTFE is a thin plastic sheet.

Microscale:

- On the microscale, ePTFE consists of tiny fibres that are woven together randomly.
- This creates tunnels of space between fibres, called pores, through which fluid and particles can travel.

Networks:

- Algorithms sort pore space into nodes and edges of different sizes.
- These nodes and edges form a network with highly complex structure.



3. Microscale model

Model:

- Particles deposit on the walls of pores as they flow through them. This decreases their size.
- We model pores as cylinders with radii that decrease uniformly when deposition occurs.
- Cylinders are network edges. Deposition decreases their sizes until they are removed, which changes the structure of the network.

Equations:

Fluid is conserved as it moves through the network:

$$\sum_{j=1} \boxed{G_{ij}(P_i - P_j)} = 0$$

Velocity

Particles deposit in edges as they move through the network:

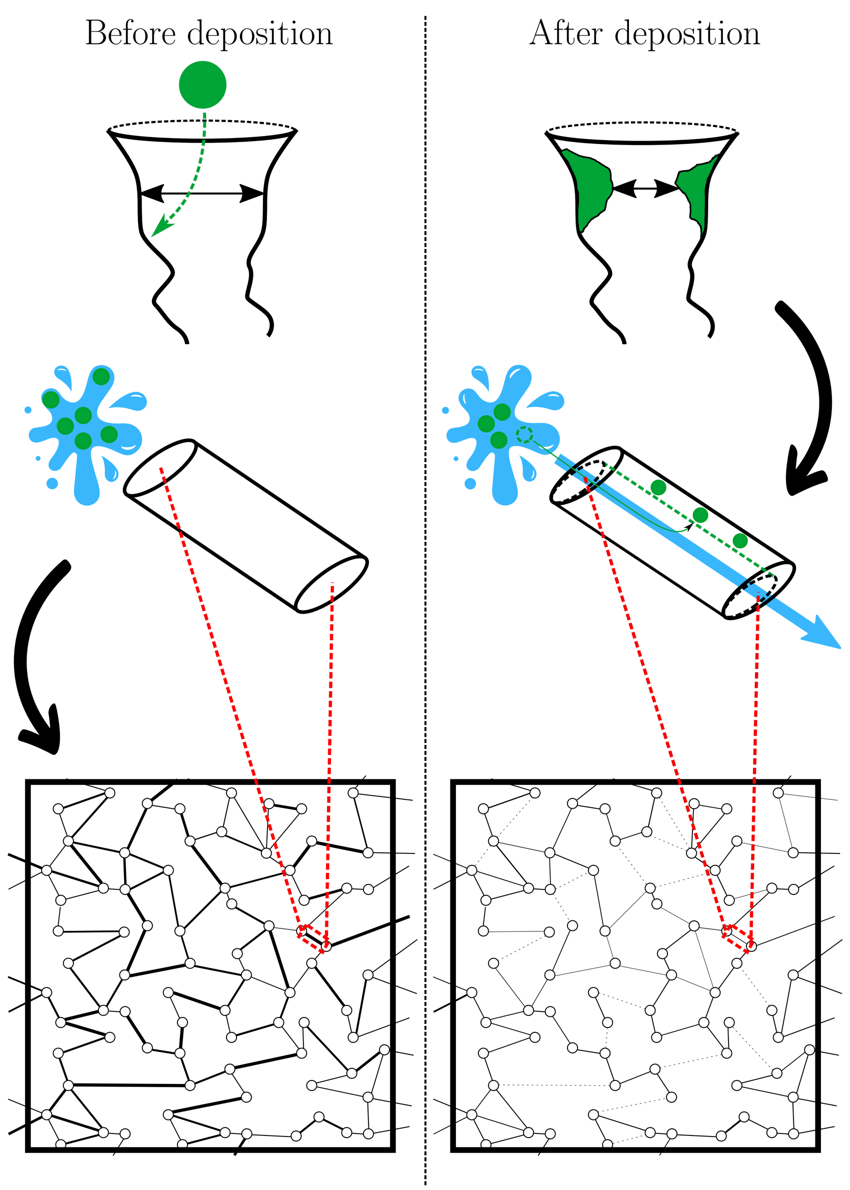
$$\frac{\partial C_i}{\partial t} = \sum_{j=1} \left((1 - \boxed{\alpha\varepsilon}) G_{ji}(P_j - P_i) C_j H_{ji} - \boxed{G_{ij}(P_i - P_j) C_i H_{ij}} \right)$$

Particle concentration — Deposition — Advection

Edges shrink as particles deposit in them:

$$\frac{\partial G_{ij}}{\partial t} = \boxed{-\alpha\beta} C_{ij} (G_{ij})^{\frac{3}{2}} \boxed{|P_i - P_j|}$$

Edge size — Deposition — Pressure drop



Problem:

- The model predicts important properties, like particle concentration and fluid velocity.
- This is accurate but too computationally expensive for filtration optimisation.

4. Multiscale model

Model:

- To decrease the computational expense, we choose a cell that is representative of the network.
- We then define a new network that consists of many repetitions of this representative cell.
- We obtain a multiscale geometry. Each macroscale continuum point contains a microscale cell.

Equations:

Fluid is conserved as it moves through the continuum:

$$\nabla \cdot \boldsymbol{u} = 0$$

Velocity

Particles deposit in edges as they move through the continuum:

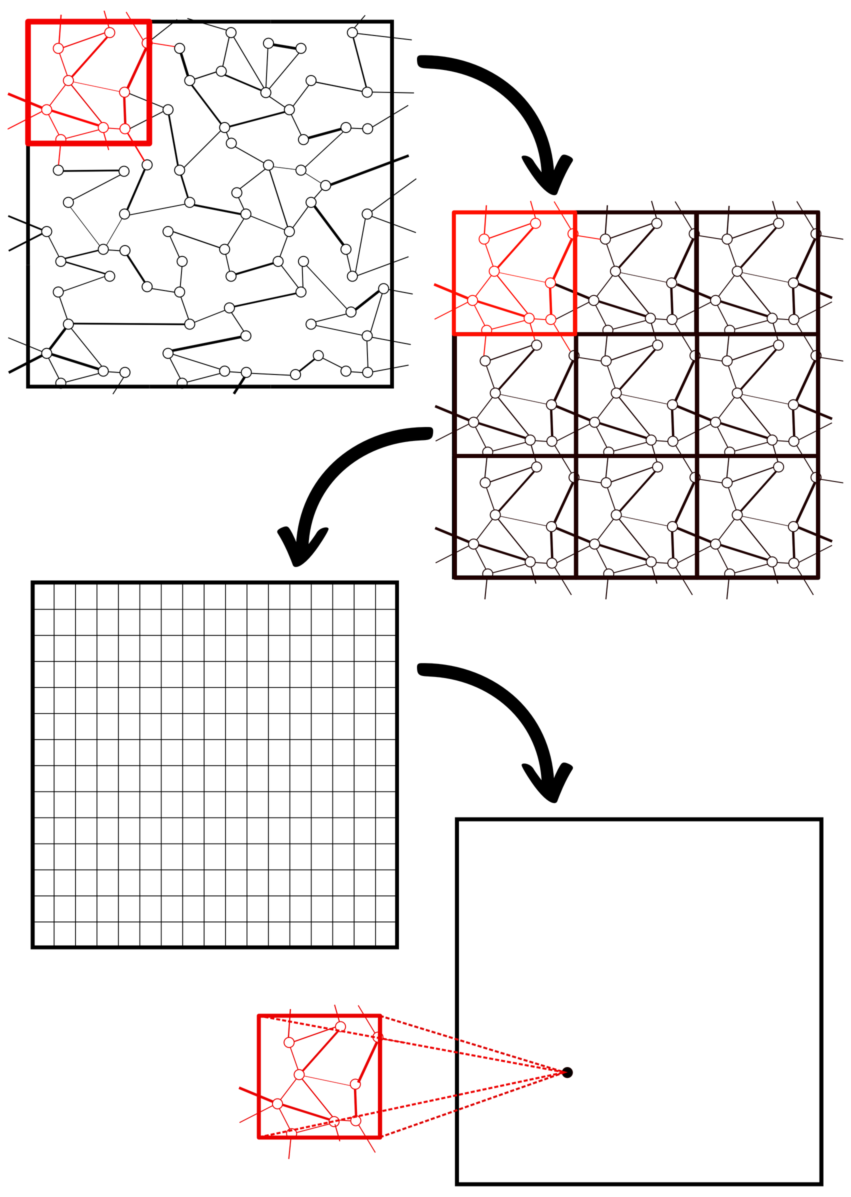
$$\frac{\partial c}{\partial t} + \boxed{\nabla \cdot \frac{\boldsymbol{u}}{\phi} c} = \boxed{-\frac{\psi}{\phi} c}$$

Particle concentration — Advection — Deposition

Edges shrink as particles deposit in them:

$$\frac{\partial G_{ij}}{\partial t} = \boxed{-\alpha\beta} c \left(G_{ij}\right)^{\frac{3}{2}} \boxed{\sum_{n=1}^{D} \left|\Delta_{ji}^{-r^n}\right| \left|\frac{\partial p}{\partial x^n}\right|}$$

Edge size — Deposition — Pressure drop



Solution:

- The multiscale model is more computationally cheap than the microscale model.
- Yet it is still accurate provided that the cell is representative of the network.

5. Representative cell

Choosing the cell:

The repeating cell must be representative of the network in two ways:

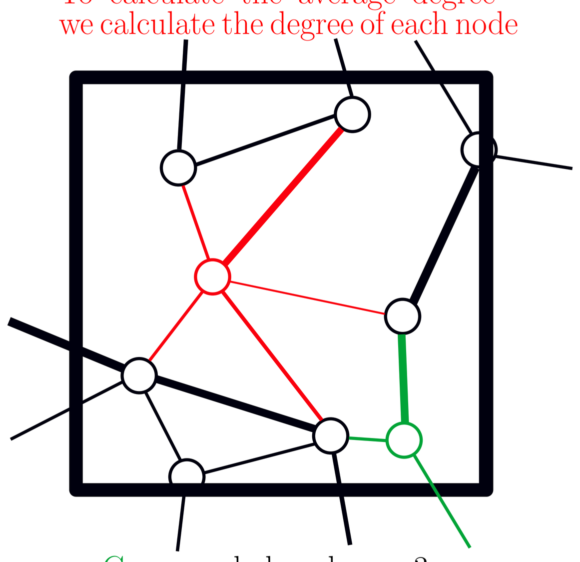
1. The average degree of the cell must be the same as that of the network.

   *"**Average degree:** The average number of edges that are connected to each node."*

2. The average conductivity and adhesivity of the cell must be the same as that of the network. This depends on the number of nodes in the cell, N.

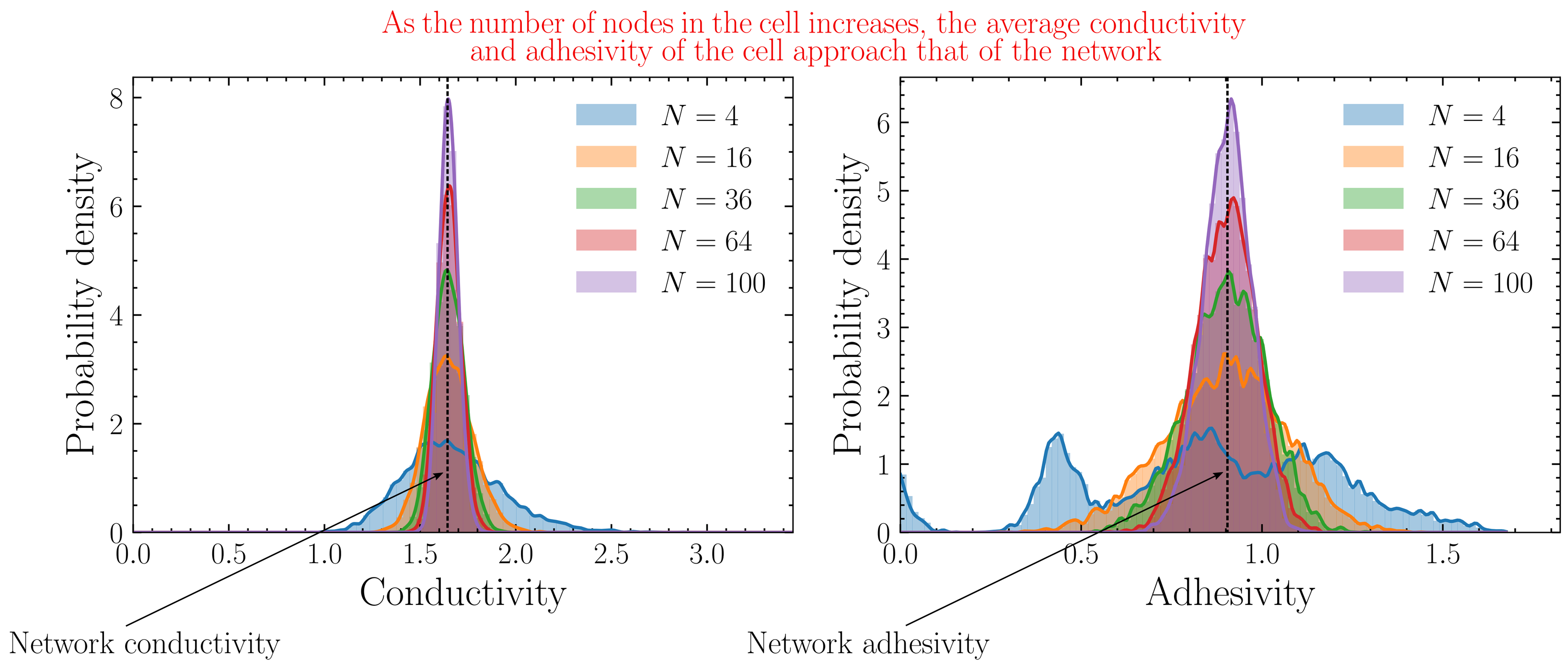
   *"**Conductivity:** Ability to conduct fluid for advection."*
   *"**Adhesivity:** Ability to attract particles for deposition."*

To calculate the average degree we calculate the degree of each node



Green node has degree 3
Red node has degree 5

As the number of nodes in the cell increases, the average conductivity and adhesivity of the cell approach that of the network

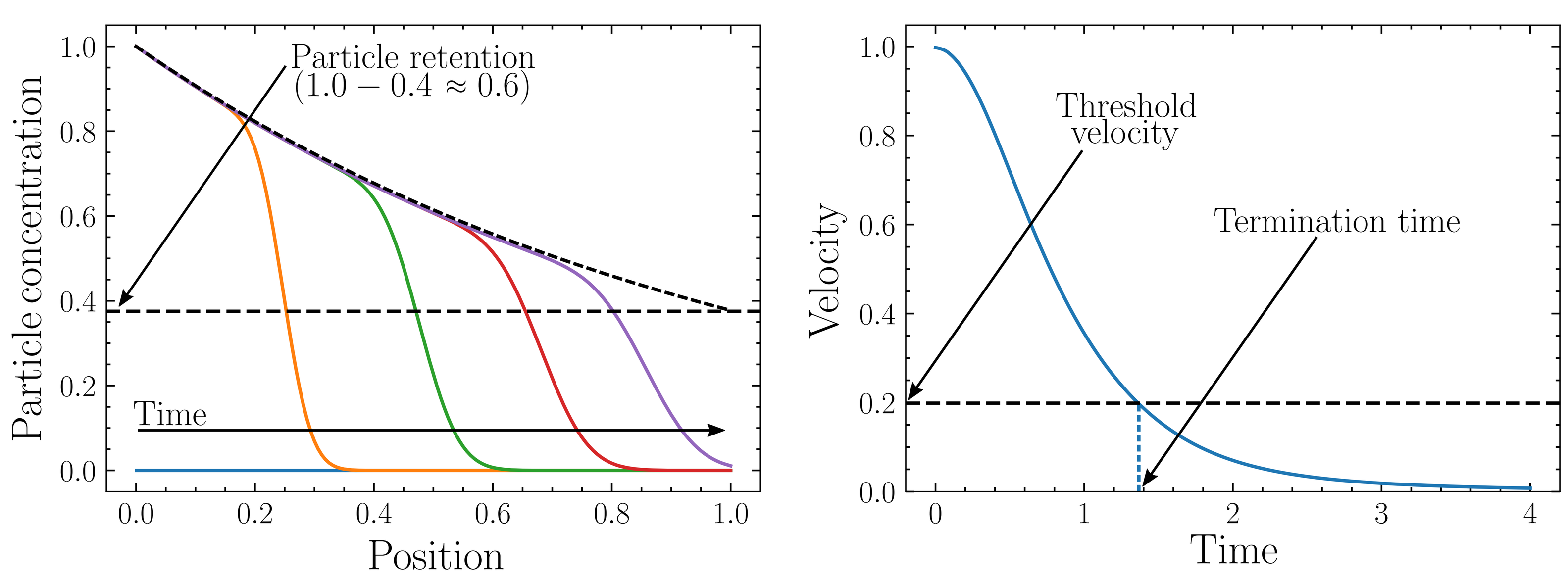


6. Solution

Solution:

- We solve the multiscale model using a representative cell with the correct average degree and enough nodes.
- The solution is used to calculate important filtration properties, such as the particle concentration and fluid velocity.
- From these, useful filtration process metrics, such as particle retention and termination time, are obtained.

*"**Particle retention:** The proportion of particles that are retained in the filter."*
*"**Termination time:** The time at which filtration is terminated. This is usually when the velocity falls below some threshold."*



7. Conclusions

Conclusions:

- We have developed a new mathematical model for the filtration process.
- This multiscale model predicts industrially important macroscale properties using microscale data, such as network structure.
- Solutions are computationally cheap, which means optimisation is possible.

Further work:

- We will fit solutions to industrial data, to tune model parameters.
- We will use this multiscale model to optimise the filtration process.