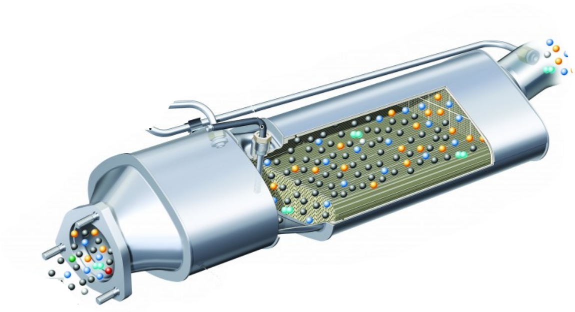
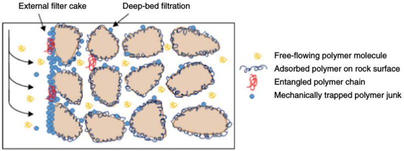
Mathematical Modeling
Project fall 2016

Diesel Particulate Filter



Background

- Loss of injectivity in polymer enhanced oil recovery



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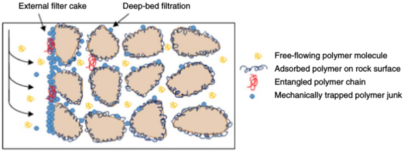

- [Master projects at SINTEF]

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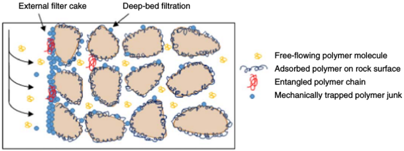
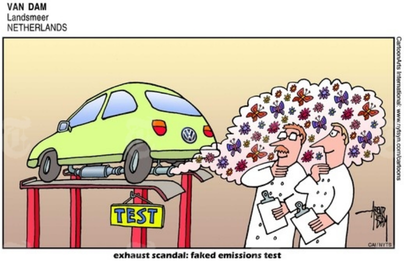


- Master projects at SINTEF
- Volkswagen emissions scandal



Filter design

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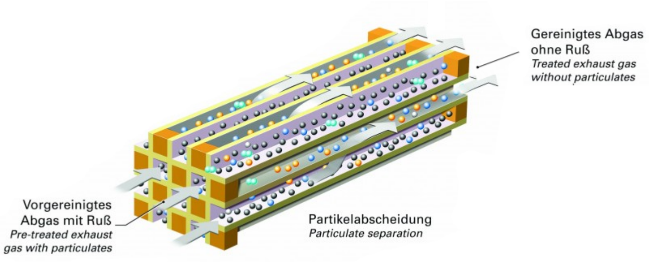
- Exhaust gas enters honeycomb structure and it forces to flow through a porous media



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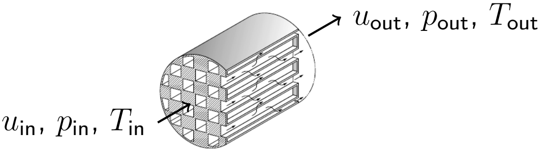
- Energy balance



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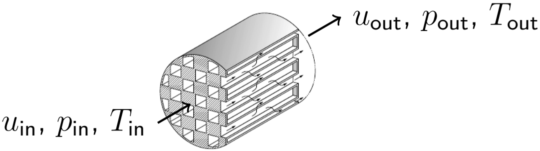

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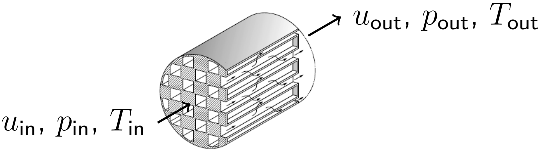

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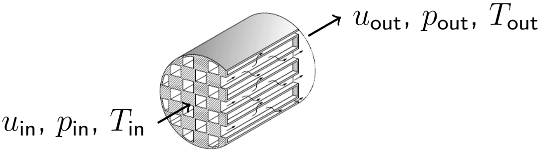

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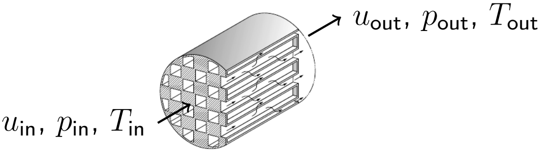

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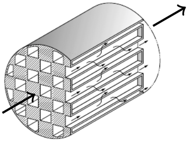

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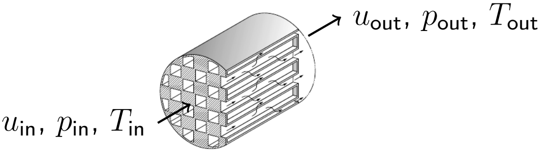

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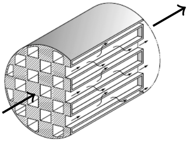

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Modeling equations

- Conservation laws
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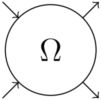

$$\left\{ \begin{matrix} \text{rate of} \\ \text{change} \end{matrix} \right\} = \left\{ \begin{matrix} \text{what} \\ \text{comes} \\ \text{in} \end{matrix} \right\} - \left\{ \begin{matrix} \text{what} \\ \text{comes} \\ \text{out} \end{matrix} \right\}$$

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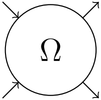

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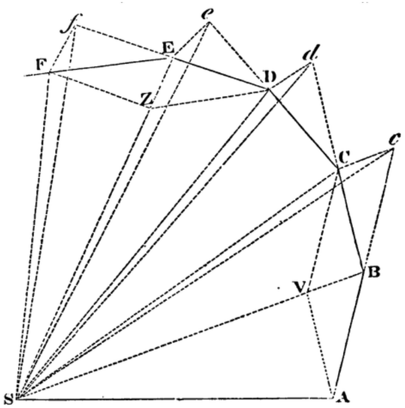
- Hence,

$$\frac{d}{dt} \int_\Omega \rho \, dx = - \int_{\partial\Omega} \rho u \cdot \boldsymbol{n} \, dx$$

implies

$$\int_\Omega \frac{\partial \rho}{\partial t} \, dx = - \int_\Omega \nabla \cdot (\rho u) \, dx$$

Conservation of momentum



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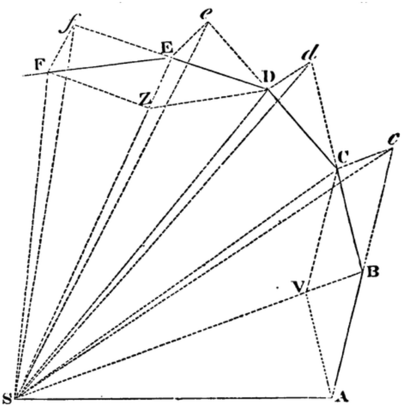

$$\text{momentum} = m\boldsymbol{v}$$

$$\frac{d}{dt}(m\boldsymbol{v}) = \boldsymbol{f}$$

Conservation of momentum

- Conservation of momentum for a fluid

$$(\rho u)_t + \nabla \cdot (\rho u \otimes u) = f.$$

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$$u \otimes u = \begin{pmatrix} u_1 u_1 & u_2 u_1 & u_3 u_1 \\ u_1 u_2 & u_2 u_2 & u_3 u_2 \\ u_1 u_3 & u_2 u_3 & u_3 u_3 \end{pmatrix},$$

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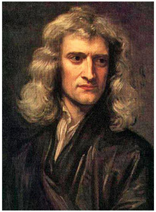
- Divergence theorem for matrices

$$\int_\Omega \nabla \cdot A(x)\, dx = \int_{\partial\Omega} A(x)\boldsymbol{n}\, dx$$

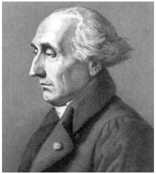
Newton and Lagrange



$$m\ddot{x} = \boldsymbol{f}$$

- Introduce kinetic and potential energy

$$E_{\mathsf{kin}} = \frac{1}{2} m \dot{x}^2 \quad \text{and} \quad E_{\mathsf{pot}}(x)$$



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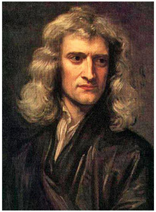

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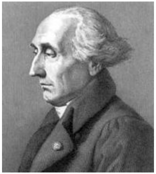

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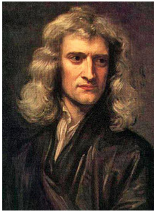

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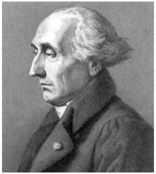

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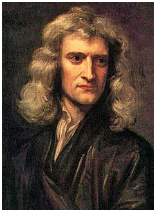

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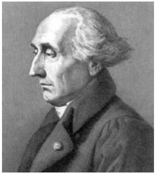

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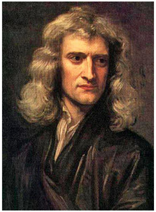

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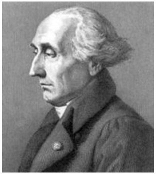

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$$\begin{aligned}\delta\mathcal{L} &= \int_0^T mx \cdot \delta\dot{x}\,dt - \int_0^T \nabla E_{\mathsf{pot}}(x) \cdot \delta x\,dt \\ &= \int_0^T (-m\ddot{x} + \nabla E_{\mathsf{pot}}(x)) \cdot \delta x\,dt\end{aligned}$$
- Hence,
$$m\ddot{x} = \nabla E_{\mathsf{kin}}$$

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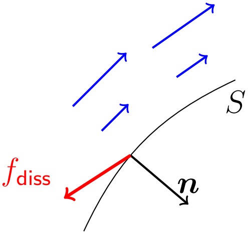

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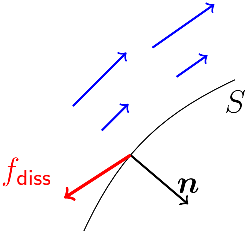
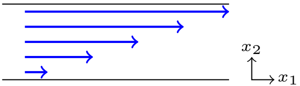


Moving plates



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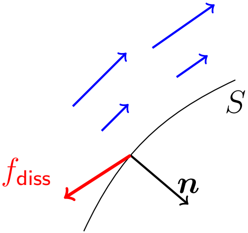

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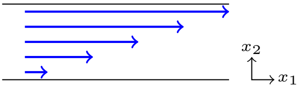

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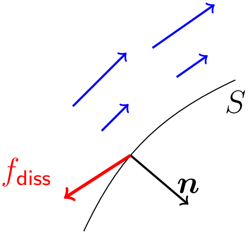

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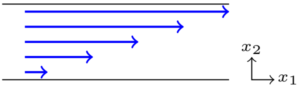

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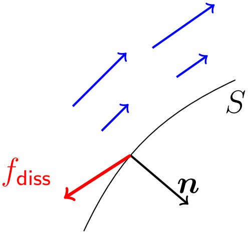

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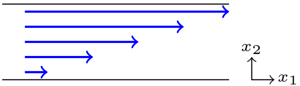

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$$f_{\text{diss}} = \mu \begin{pmatrix} 0 & v \\ v & 0 \end{pmatrix} \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -\mu v \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

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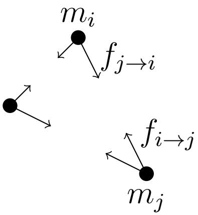
- Viscous energy
$$E_{\text{diss}} = \int_\Omega (\frac{\lambda}{2} \operatorname{tr}(\boldsymbol{\varepsilon})^2 + \mu \|\boldsymbol{\varepsilon}\|^2)\, dx$$
where $\boldsymbol{\varepsilon}$ is symmetric tensor
$$\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla u + \nabla(u)^T).$$

Conservation of momentum and angular momentum

- Newton's third law

When one body exerts a force on a second body, the second body simultaneously exerts a force equal in magnitude and opposite in direction on the first body



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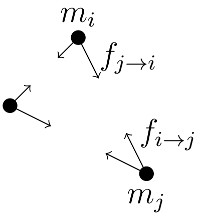

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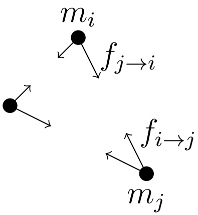

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- For a closed system, we have the conservation of momentum and of **angular momentum**

$$\frac{d}{dt} \sum_i (m_i v_i) = 0 \quad \text{and} \quad \frac{d}{dt} \sum_i m_i r_i \times v_i = 0$$

Approximation of the viscous force

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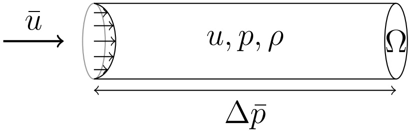

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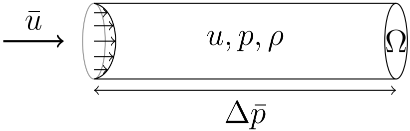

- Define average values over the cross-section,

$$\bar{u} = \frac{1}{|\Omega|}\int_\Omega u\,dx \quad \text{and} \quad \bar{p} = \frac{1}{|\Omega|}\int_\Omega p\,dx$$

Q: *Express f_{diss} as a function of $\bar{u}$. Show that $f_{diss} = -a\bar{u}$, for a constant a that depends only on the shape Ω.* You have to compute the velocity profile.

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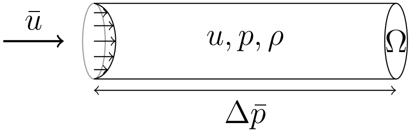

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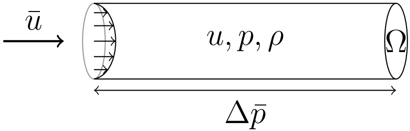

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- Similar approach to obtain Darcy approximation $\bar{u} = -K \frac{\Delta \bar{p}}{\Delta x}$.
- **Q**: *Compute the coefficient a for Ω given by a cylinder, a square or an hexagon.*

One dimensional approximation

Instead of considering

$$\rho_t + \nabla \cdot (\rho u) = 0,$$
$$(\rho u)_t + \nabla \cdot (\rho u \otimes u) = -\nabla p - au,$$

we consider the one dimensional approximation

$$\rho_t + (\rho u)_x = 0,$$
$$(\rho u)_t + (\rho u^2)_x = -\frac{\partial p}{\partial x} - au.$$

Q: *How are the one-dimensional equations obtained? What are the approximations that we are doing?*

One dimensional approximation (2)

- We consider an ideal gas law, with constant temperature. Then p is proportional to ρ,

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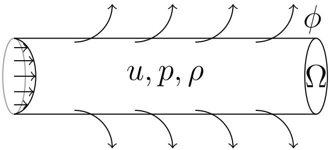
- After that, we only consider steady-state.

mass loss from the walls

- We incorporate in the model mass loss along the walls



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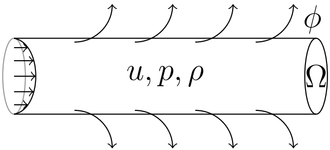

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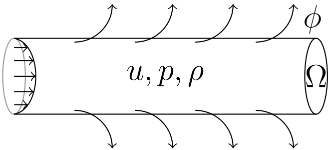

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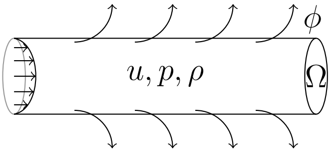

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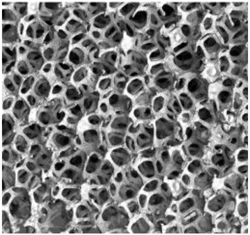
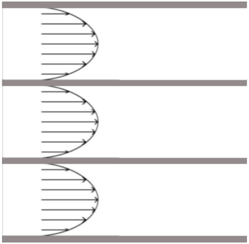
- **Q**: *How are the full 3D equations changed?*
- **Q**: *How are the 1D equations changed?*
- **Q**: *Solve numerically the 1D equations in the stationary case.*

Porous media

- Linear relation between velocity and pressure drop

$$u = -\frac{K}{\mu}\frac{\Delta p}{\Delta x}$$





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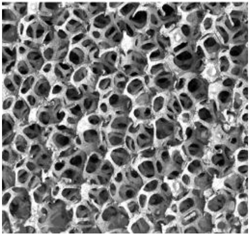
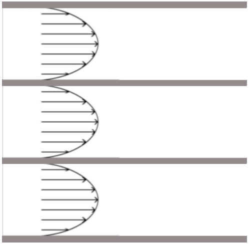
The scalar (or matrix) K is called the *permeability*.





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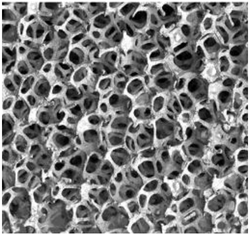

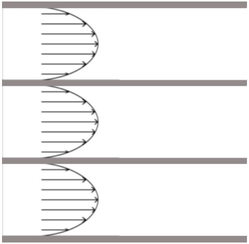

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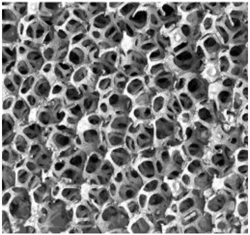

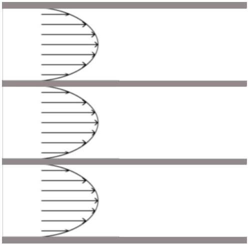

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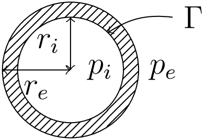
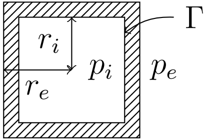


Cylindrical channel



Square channel

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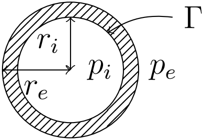

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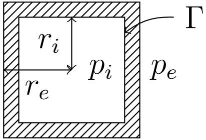


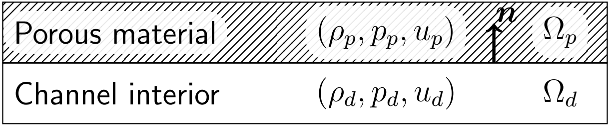
Square channel

- **Q**: *Find the relation between U and $p_e - p_i$ for the steady state. Compute κ for a cylinder and a square.*

$$U = \kappa(p_e - p_i)$$

Coupling of the channel with a porous layer

- At the interface, we should have conservation of mass and force balance. **Q**: *What are the interface condition?*



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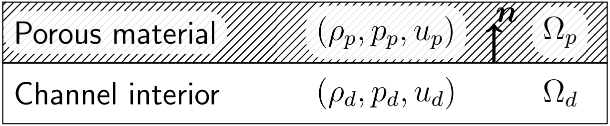
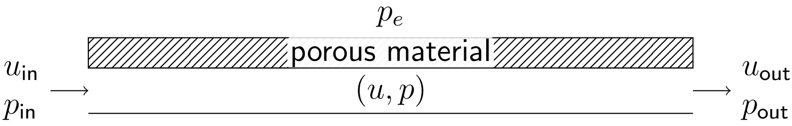


- We consider pressure continuity at the interface (consistent with previous approximation). **Q**: *Set up the one dimensional equations.*



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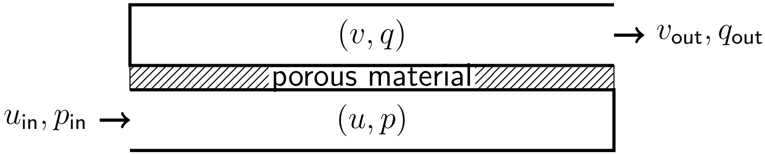

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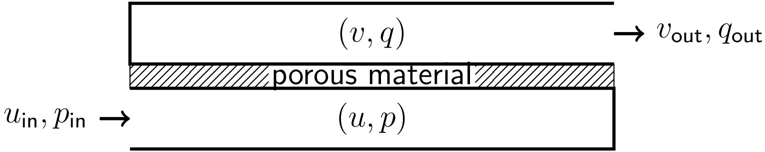

- **Q**: *Setup the equations for the one dimensional model in the stationary case.*

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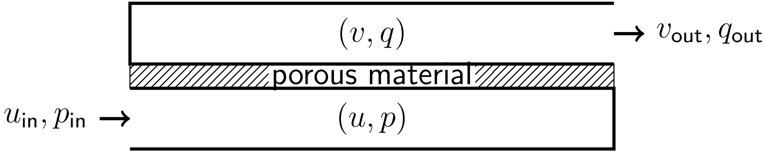

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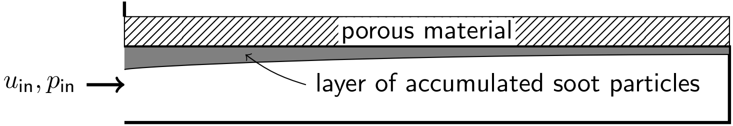
Accumulation of particles

- We denote by c the concentration of soot particles ($c = \text{mass(soot)}/\text{mass(gas)}$)



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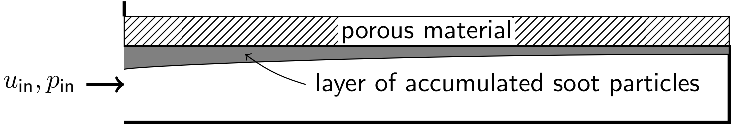

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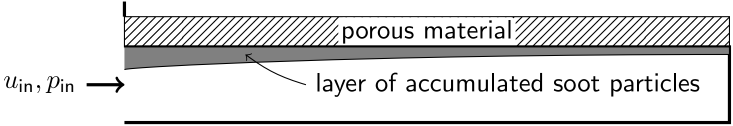

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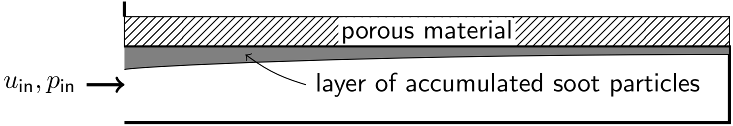

- **Q**: *What is the modeling equation that governs c, for the 3D model and the one-dimensional model.*
- **Q**: *Find a formula for the amount of accumulated particles as a function of t and x*
- **Q**: *Compute this value numerically (one-dimensional case).*

Filter clogging

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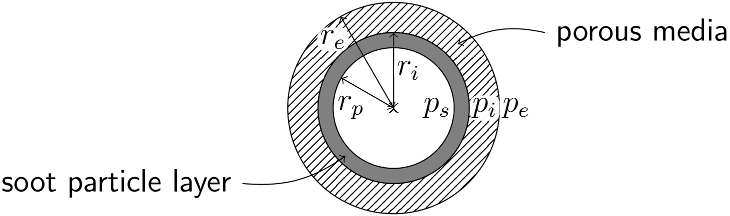

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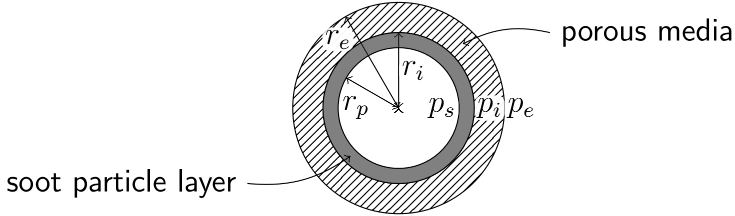

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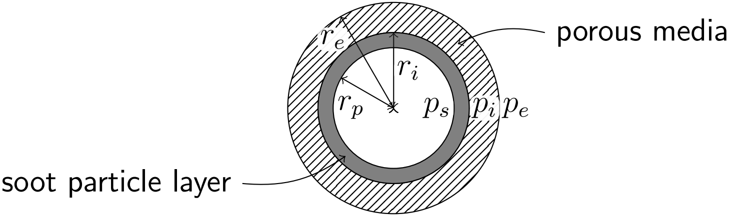


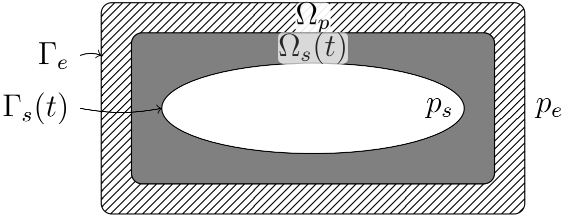
- **Q**: *Compute the new coefficient κ.*

$$U = \kappa(p_e - p_i)$$

- The coefficient κ depends on the amount of accumulated soot and the amount of accumulated soot depends on κ.
  Q: *Set up the coupled equations.*

Filter clogging - general cross-section

- For a general geometry of the cross-section, the particles do not accumulate uniformly at the interface



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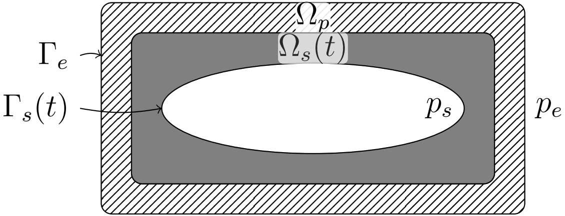

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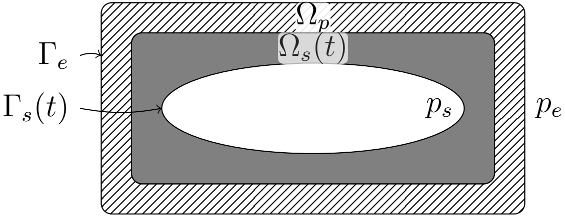

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- **Q**: *Derive the equation for $x(\tau, t)$.* Find an equation that guarantees the conservation of the mass of soot.
- **Q**: *Design and implement a scheme to solve the governing equations for this problem.*