EPSRC
Engineering and Physical Sciences Research Council

InFoMM
Industrially Focused Mathematical Modelling

Homogenisation of agents and cleansers interacting on the microscale

Ellen Luckins

Supervised by Chris Breward, Ian Griffiths, Zach Wilmott, and Ross Heatlie-Branson (DEFRA), and with Oliver Whitehead

Background

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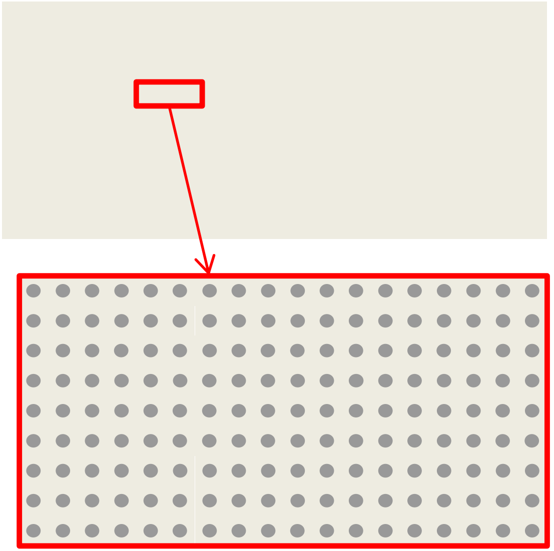
- DEFRA has responsibility for coordinating the **decontamination** of these porous materials.
- We want to optimise the decontamination methods to be as **effective** and **efficient** as possible.
- We therefore want to model the **mechanics the decontamination process**, including
  - the **diffusion of chemicals** through the porous medium,
  - the movement of the **chemical reacting fronts** through the contaminant.

Aim:

- It is **computationally expensive** to solve for the diffusion and chemical interaction of fluids through a porous medium.
- We're interested in the behaviour over the **scale of the chemical spill.**



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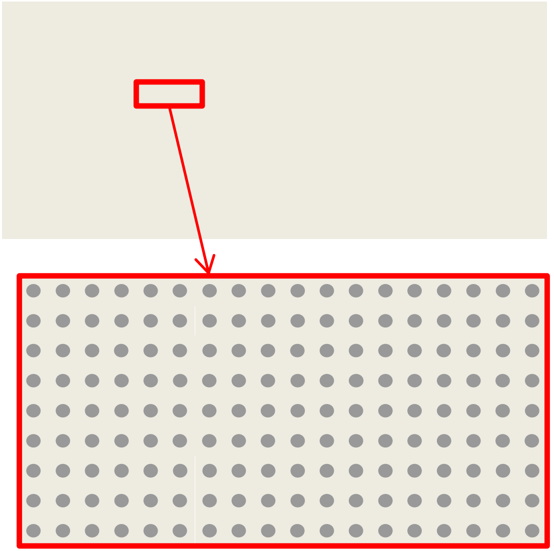
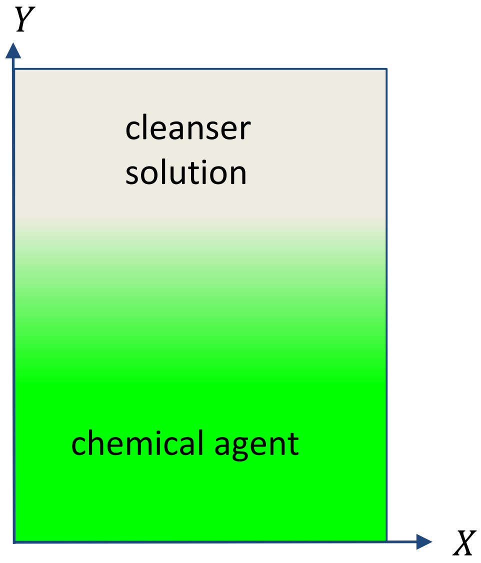


The aim of this project is:

- to model the **pore-scale interaction** of the agent and cleanser within a porous medium,
- to **average** this model in order to **develop simple and accurate models for the macroscale behaviour.**

Model description



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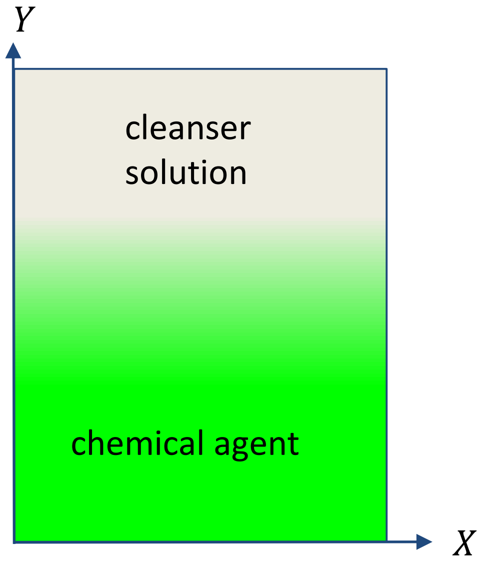

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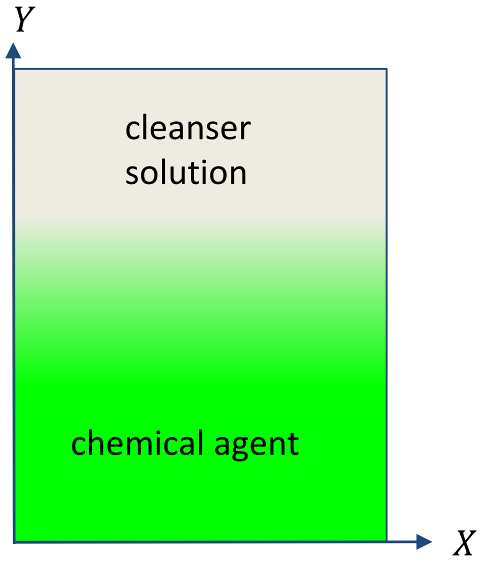

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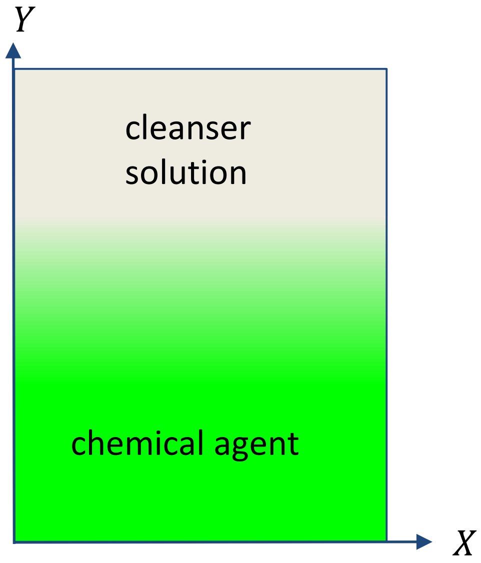

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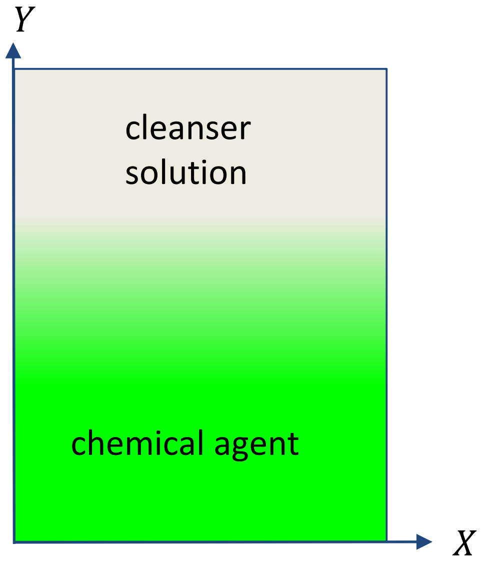

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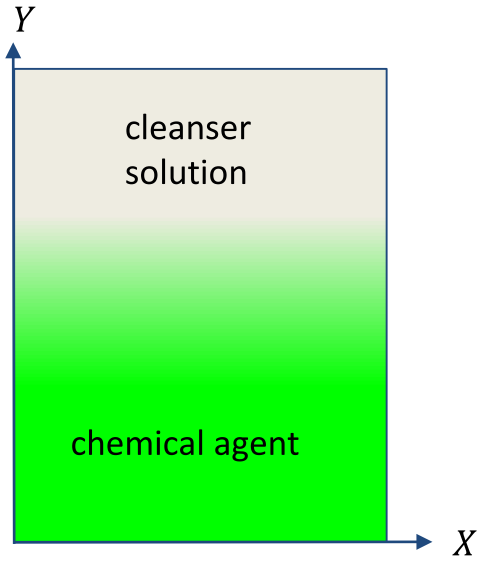

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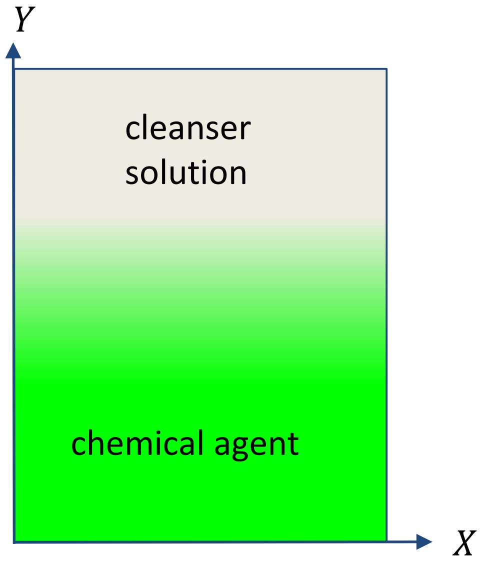

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- Cleanser **diffuses** through the solution.
- When in contact with the agent the **chemical reaction** occurs at the interface.
- The **product** of the chemical reaction is **only soluble in the cleanser** (not the agent).
- There is **no fluid flow**.

Mathematical model

Within the pores, Ω, and where the fluid is the cleanser solution:

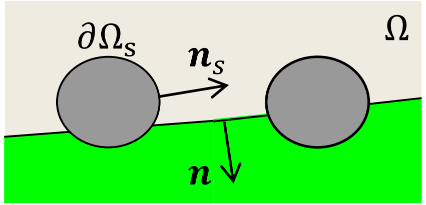
$$c_t = D\nabla^2 c,$$

on the solid boundary $\partial\Omega_s$:

$$\nabla c \cdot \boldsymbol{n}_s = 0,$$

and at the cleanser-agent interface:

$$-c\boldsymbol{v}\cdot\boldsymbol{n} + D\boldsymbol{n}\cdot\nabla c = -kc,$$
$$\boldsymbol{v}\cdot\boldsymbol{n} = -\chi kc.$$



c is the concentration of cleanser,

D is the diffusivity of cleanser,

k is the reaction rate,

χ is the molar volume of the agent,

$\boldsymbol{v}$ is the velocity of the interface

Stoichiometry:

Agent + Cleanser → Product

Mathematical model

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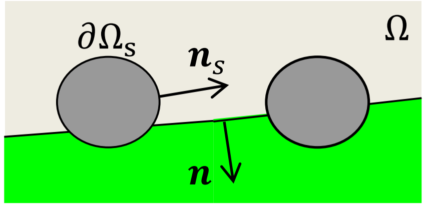

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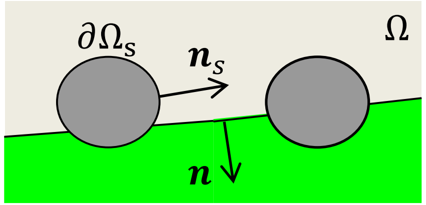

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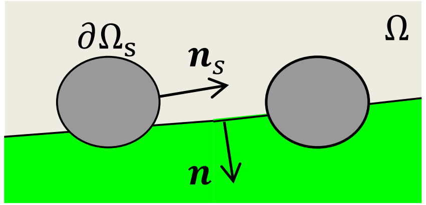
Conservation of cleanser, and of agent



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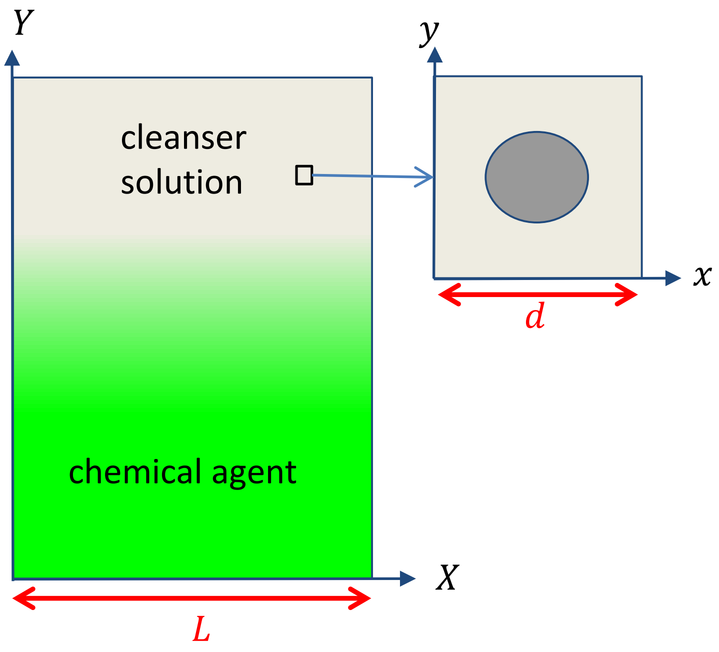

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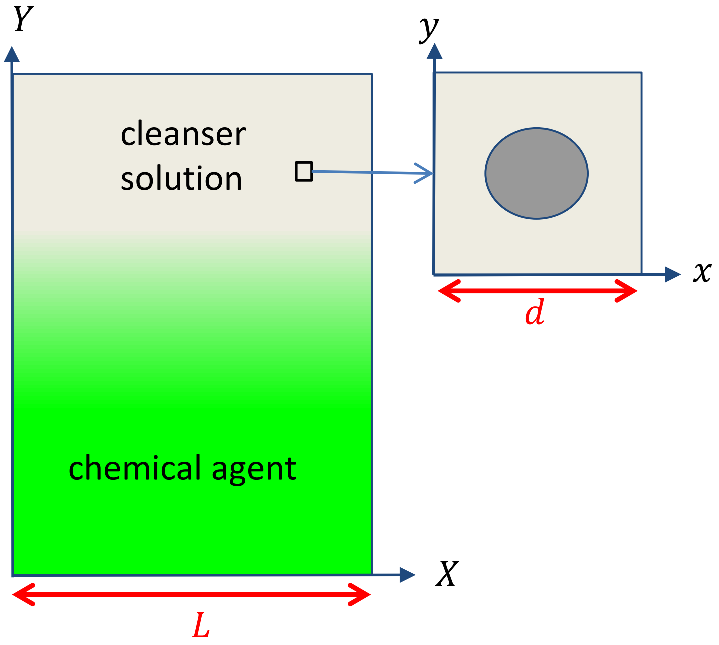

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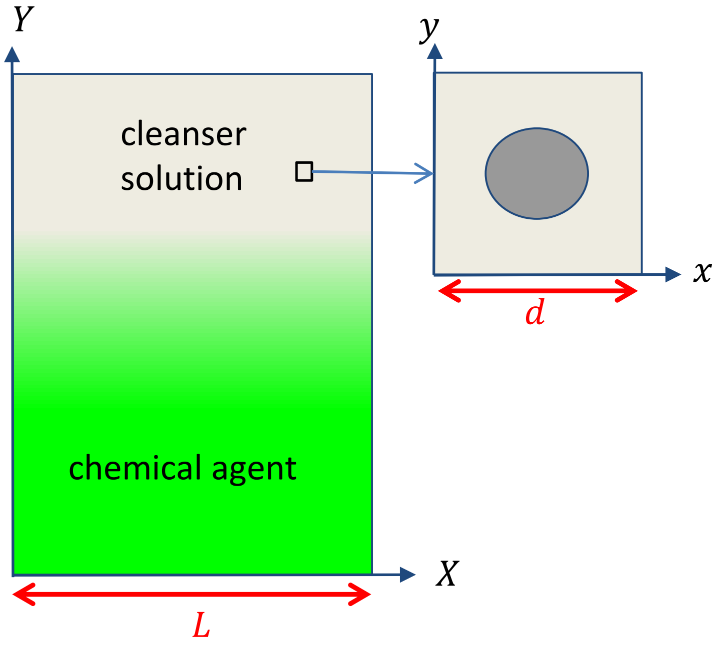

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Assume the problem depends on **both** the microscopic and macroscopic variables, **independently.**

Homogenisation approaches

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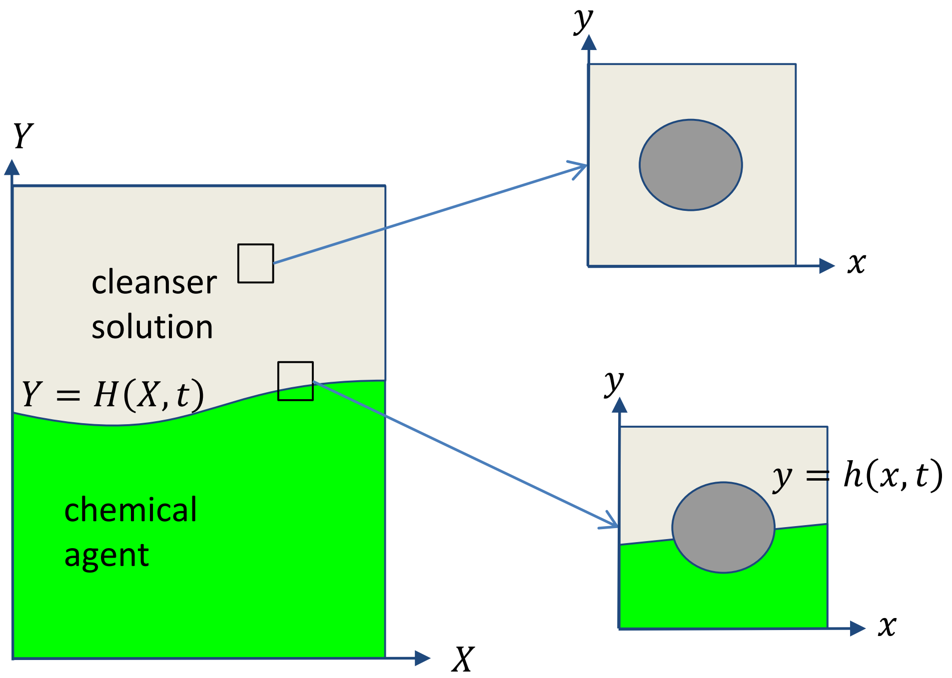
1. Sharp interface
   - The homogenisation gives a **standard macroscale diffusion equation** for the cleanser
   - The chemistry comes into the averaged boundary conditions at $Y = H(X,t)$



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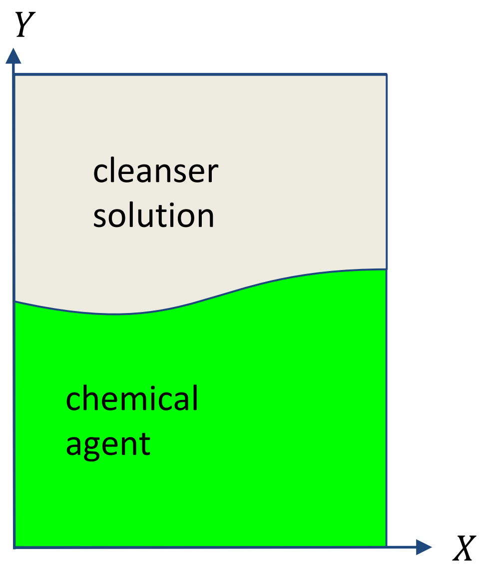

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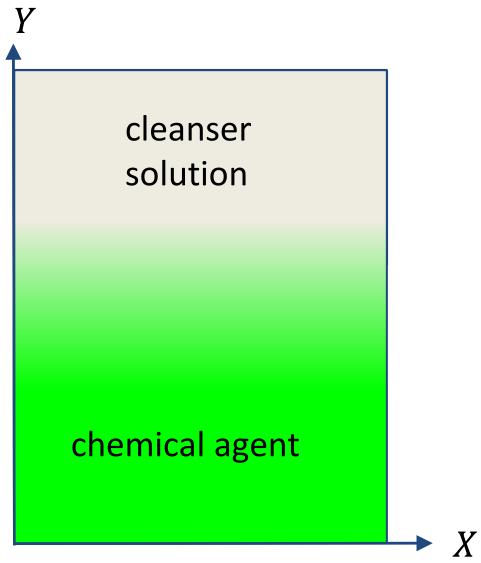

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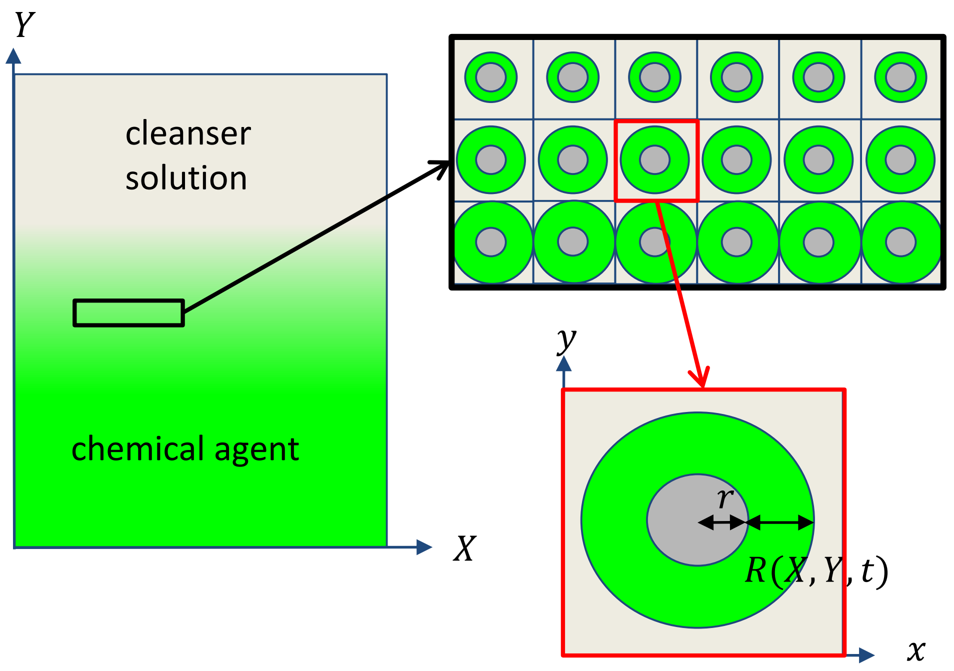

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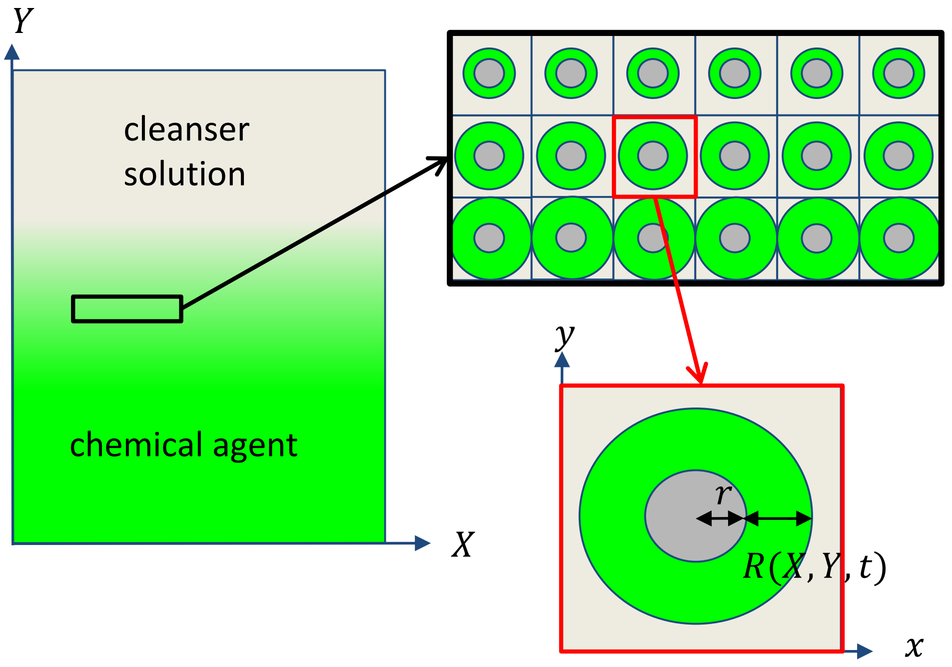

Today we'll focus on option 2

Dimensionless model

Away from the interface:

$$\epsilon^2 c_t = \nabla^2 c,$$

on the interface:

$$\text{if } R > 0 \begin{cases} -\epsilon^2 c R_t - \boldsymbol{n} \cdot \nabla c = -\epsilon^2 \beta c, \\ R_t = -\gamma c. \end{cases}$$

$$\text{if } R = 0, \quad \nabla c \cdot \boldsymbol{e}_r = 0,$$

Scalings:

$$x, y, R \sim d, \qquad c \sim c^*, \qquad t \sim \frac{d^2}{\epsilon^2 D}.$$

Dimensionless parameters

$$\beta = \frac{kd}{\epsilon^2 D}, \qquad \gamma = \chi c^* \qquad \sim O(1)$$

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We're looking at a situation with small enough reaction rate k

Multiple scales analysis

The problem is modified to account for the two lengthscales by setting

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We assume that c and R are **periodic over a microscale cell**, and

- $c = c(x, y, X, Y, t)$ depends on micro- and macroscale variables **independently**
- $R(X, Y, t)$ **varies slowly in space**, over the macroscale.

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Periodicity is crucial to the homogenisation procedure.

Look for an asymptotic expansion solution

$$c = c_0 + \epsilon c_1 + \epsilon^2 c_2 + \cdots,$$
$$R = R_0 + \epsilon R_1 + \epsilon^2 R_2 + \cdots.$$

We'll be interested in the leading order behaviour of c and R.

Leading-order problem

The $O(1)$ problem is:

away from the interface

$$0 = \nabla_x^2 c_0,$$

on the interface

$$\nabla_x c_0 \cdot \boldsymbol{e}_r = 0.$$

and c_0 is periodic over the cell.

Diffusion dominates to leading order

No flux of c into the interface

We conclude that $c_0 = c_0(X, Y, t)$ is **independent of the microscale.**

First-order problem

The $O(\epsilon)$ problem is:

away from the interface

$$0 = \nabla_x^2 c_1,$$

on the interface

$$(\nabla_X c_0 + \nabla_x c_1) \cdot \boldsymbol{e}_r = 0.$$

and c_1 is periodic over the cell.

The effect of the solid structure on the overall problem comes in here

This allows us to write $c_1 = \boldsymbol{w} \cdot \nabla_X c_0$, with w_i satisfying a cell problem:

$$\begin{cases} \nabla_x^2 w_i = 0, & \text{away from the interface,} \\ \boldsymbol{e}_r \cdot (\nabla_x w_i + \boldsymbol{e}_i) = 0, & \text{on the interface,} \\ w_i \text{ periodic} & \text{over the cell.} \end{cases}$$

We can express c_1 in terms of c_0, given the solution of a cell problem (a common occurrence in homogenisation problems)

Second-order problem

The $O(\epsilon^2)$ problem is:

away from the interface

$$c_{0t} = \nabla_X^2 c_0 + (\nabla_x \cdot \nabla_X + \nabla_X \cdot \nabla_x) c_1 + \nabla_x^2 c_2,$$

on the interface

$$\text{if } R_0 > 0\,, \begin{cases} -c_0 R_{0t} + \nabla_X R_0 \cdot (\nabla_X c_0 + \nabla_x c_1) \\ \qquad -\boldsymbol{e}_r \cdot (\nabla_x c_2 + \nabla_X c_1) = -\beta c_0, \\ R_{0t} = -\gamma c_0, \end{cases}$$

$$\text{if } R_0 = 0\,, \ (\nabla_X c_1 + \nabla_x c_2) \cdot \boldsymbol{e}_r = 0,$$

and c_2 is periodic over the cell.

The time derivative of c_{0t} and the chemistry at the interface appear at this order.

Macroscale equations for c_0 and R_0 are derived by:

1. **integrating** the diffusion equation over the cell
2. applying the **Divergence Theorem**
3. substituting in the **boundary conditions**
4. simplification using **Reynolds Transport Theorem**

The macroscale equations

The resulting equations are:

when $R_0 > 0$:

$$c_{0t} = \nabla_X \cdot (D^* \nabla_X c_0) - \frac{2\pi(r + R_0)}{1 - \pi(r + R_0)^2}(\beta + \gamma c_0)c_0,$$

$$R_{0t} = -\gamma c_0,$$

when $R_0 = 0$:

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The standard homogenised diffusion equation in porous media

D^* depends on R_0 via the solution of the cell problem.

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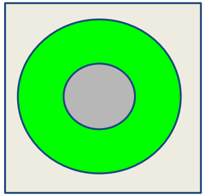

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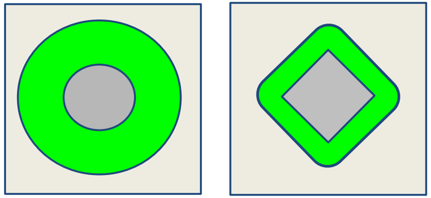

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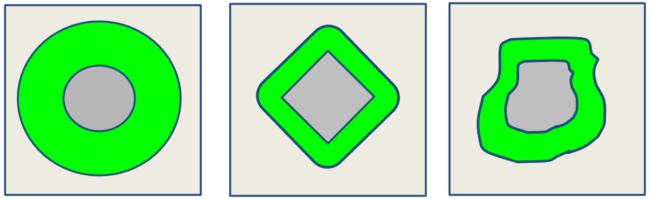


The macroscale equations

The resulting equations are:

when $R_0 > 0$:

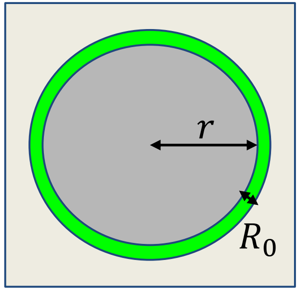
$$c_{0t} = \nabla_X \cdot (D^* \nabla_X c_0) - \frac{2\pi(r + R_0)}{1 - \pi(r + R_0)^2}(\beta + \gamma c_0)c_0,$$
$$R_{0t} = -\gamma c_0,$$

when $R_0 = 0$:

$$c_{0t} = \nabla_X \cdot (D_0^* \nabla_X c_0),$$

where $D^* = D^*(R_0)$ is an adapted diffusivity, and $D_0^* = D^*(0)$.

If $r \gg R_0$ then the blue terms are **approximately constant**, and we may be able to make analytical progress with this model.



Conclusion

Two homogenisation approaches:

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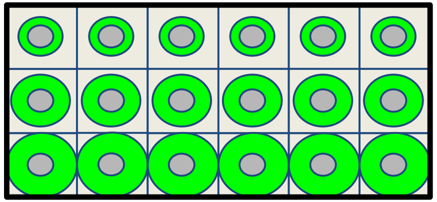
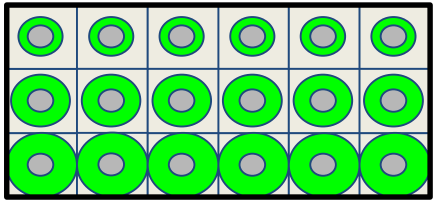
- With the **agent stuck to solid**
  - Showed the homogenisation procedure
  - Discussed the resulting macroscale equations

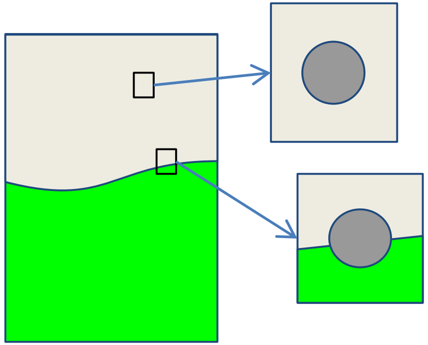


Conclusion

Two homogenisation approaches:

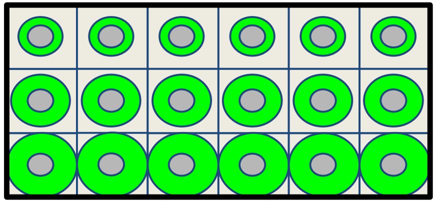
- With the **agent stuck to solid**
  - Showed the homogenisation procedure
  - Discussed the resulting macroscale equations
- For the **sharp interface** the homogenisation is more complicated:
  - Careful change of variables to the interface, like a **travelling wave**
  - Periodicity is no longer applicable everywhere

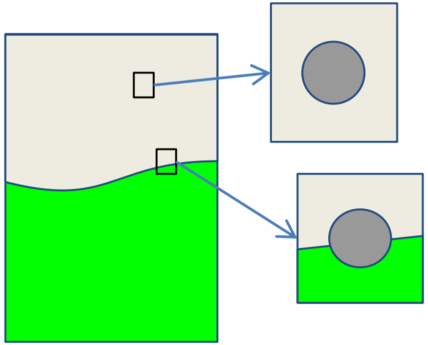




Conclusion

InFoMM
Industrially Focused Mathematical Modelling





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Next steps:

- **Solutions** of the derived model
- Homogenisation of the **sharp interface** problem
- **Comparison** of methods