EPSRC
Engineering and Physical Sciences Research Council

InFoMM
Industrially Focused Mathematical Modelling

Homogenisation Problems in Reactive Decontamination

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

Background

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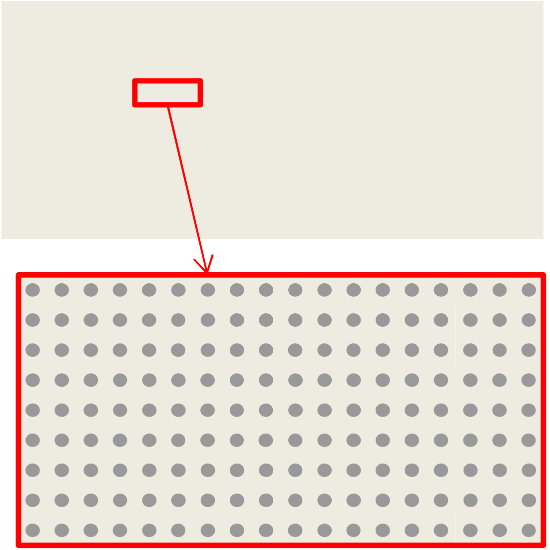
- DEFRA has responsibility for coordinating the clean-up of hazardous chemicals, for instance after a chemical attack.
- We are interested in decontaminating a **porous building material** (eg: concrete) into which a **hazardous agent** has seeped.
- An immiscible **cleanser** is applied on top, and allowed to react into the agent.
- We want to model the mechanics the decontamination process:
  - **diffusion of chemicals,**
  - movement of the **chemical reacting fronts.**

Aim:

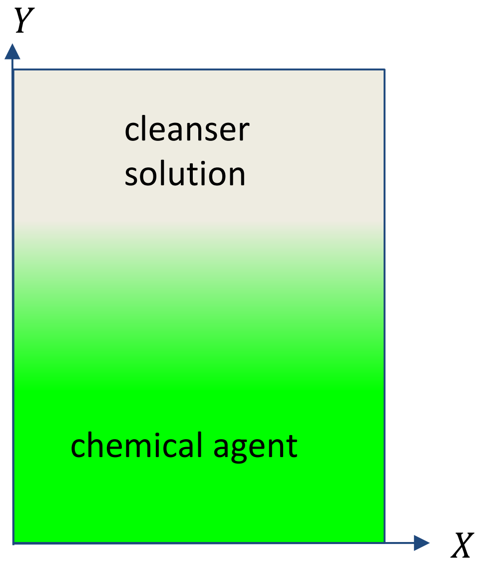
- It is **computationally expensive** to solve for the diffusion and chemical interaction of fluids through a porous medium
- We're interested in the behaviour over the **scale of the chemical spill.**



Our aim:

- 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



- A 2D **porous medium** is saturated with a **neat chemical agent** (the contaminant).
- A **dilute cleanser** is applied on top.
- The fluids are **immiscible.**
- Cleanser **diffuses** through the solution.
- Where the cleanser is in contact with the agent the **chemical reaction** occurs.
- The **product** of the chemical reaction is **not soluble in the agent**.
- There is **no fluid flow**.

Mathematical model

Within the pores, in the cleanser solution:

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

Diffusion equation

on the solid boundary:

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

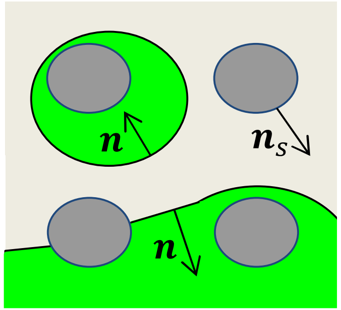
No flux of cleanser into the solid

and at the cleanser-agent boundary:

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

$$\boldsymbol{v} \cdot \boldsymbol{n} = -\chi k c.$$

Conservation of cleanser, and of agent



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 homogenisation

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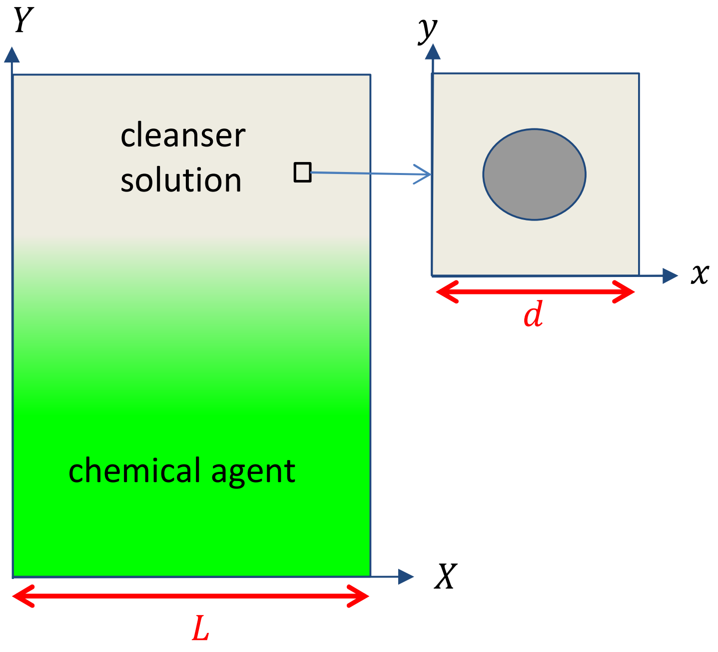

Mathematical homogenisation relies on a problem having **multiple lengthscales.**

- For our problem, we have the pore scale, d, and the spill scale L.

Define $\epsilon = \frac{d}{L} \ll 1$, and the macroscopic and microscopic variables, related by:

$$x = \frac{X}{\epsilon}, \qquad y = \frac{Y}{\epsilon}.$$

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

Homogenisation approaches

There are two natural ways to set up the homogenisation problem:

Homogenisation approaches

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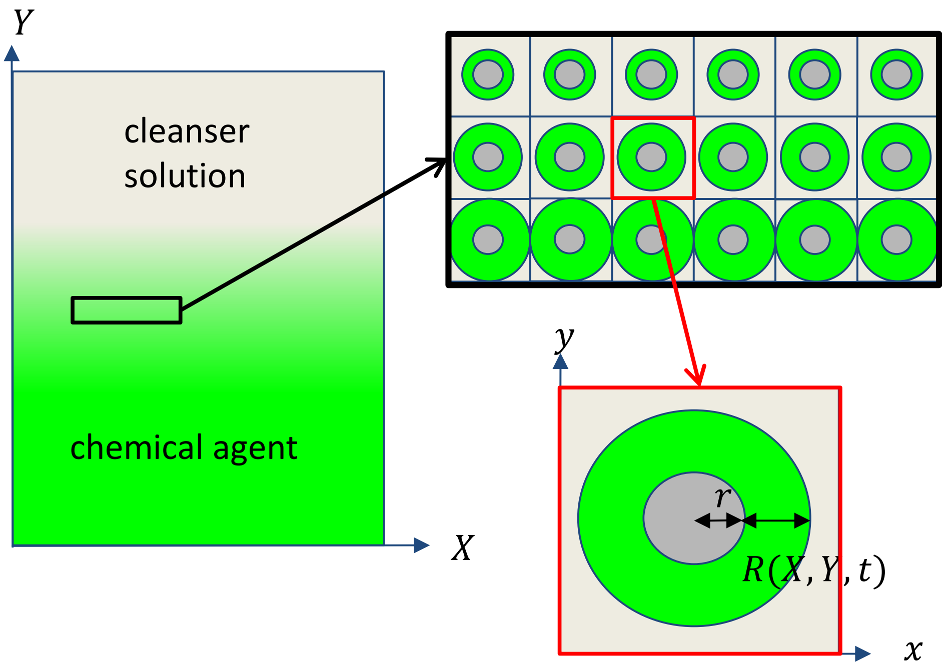
There are two natural ways to set up the homogenisation problem:

1. Agent stuck to solid
   - In a 2D region we have both agent and cleanser
   - Agent is stuck to solid structure, and is eaten away by the cleanser
   - The chemistry will come into the problem as **sink term in the cleanser diffusion equation**



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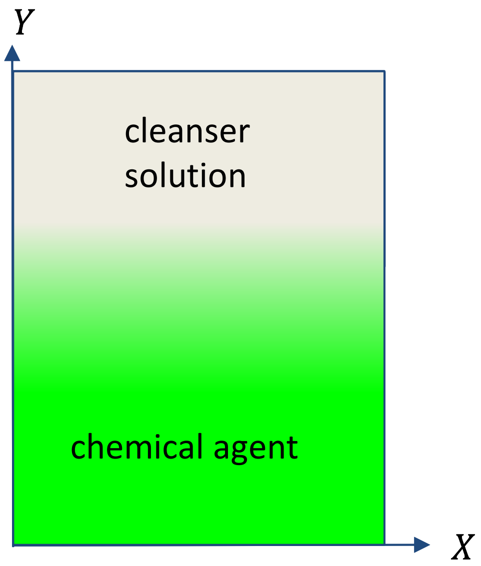

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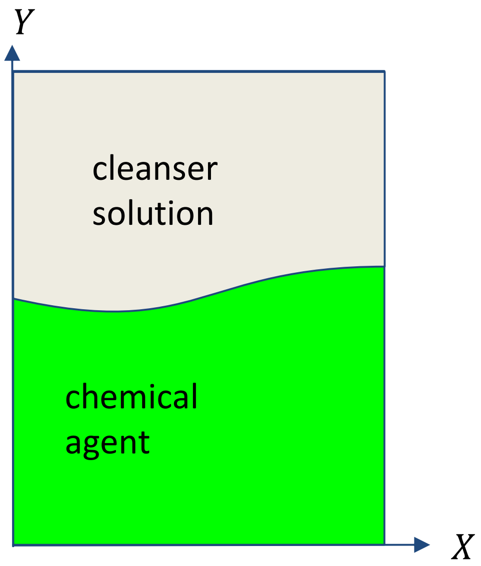
2. Sharp interface



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   - The homogenisation gives a **standard macroscale diffusion equation** for the cleanser
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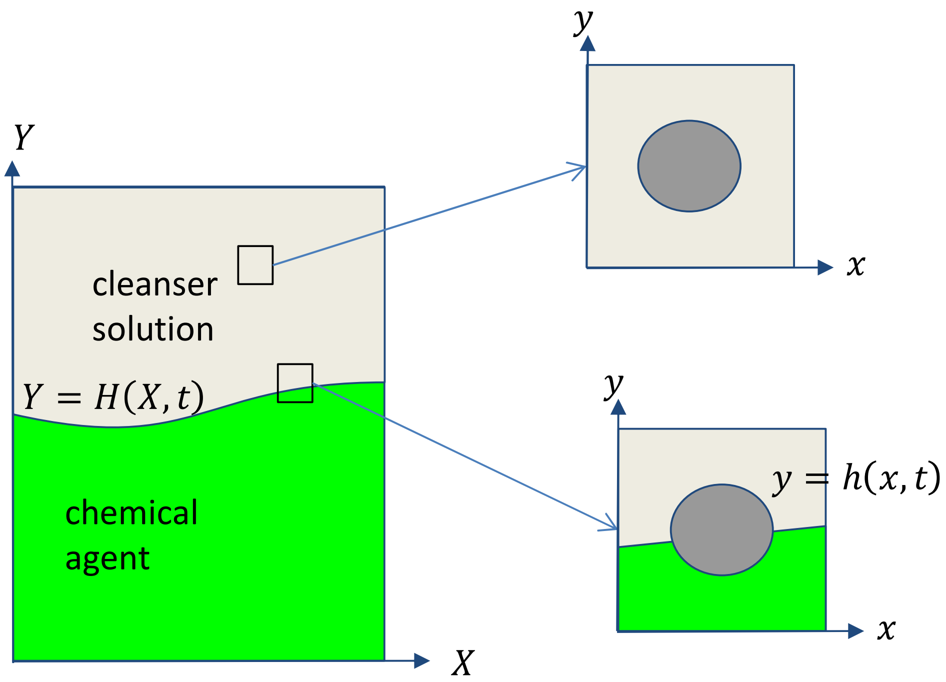

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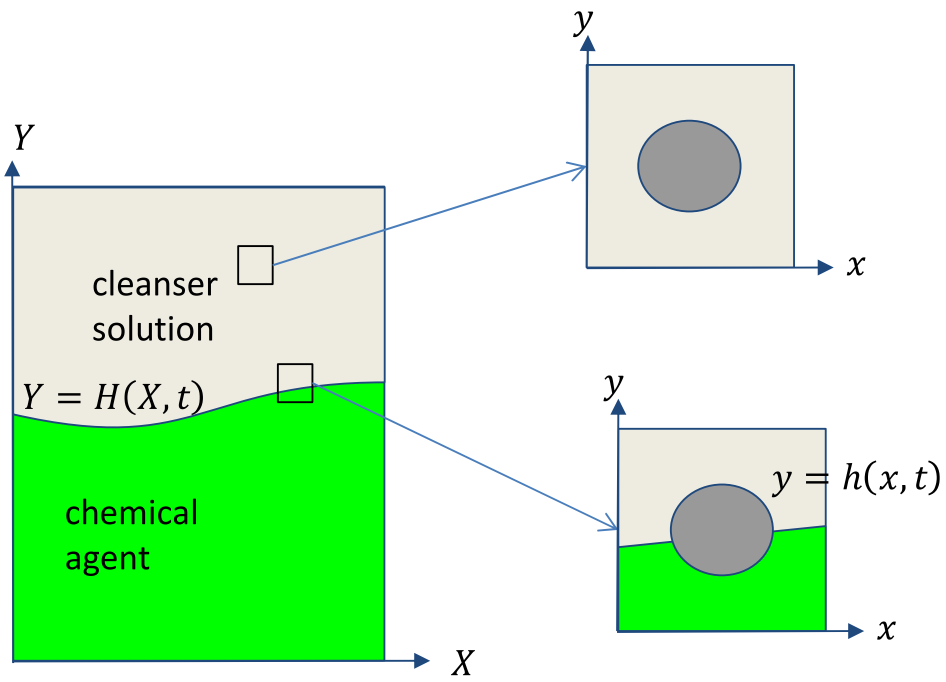

TODAY:

- Skim through the homogenisation for case 1,
- Highlight the differences in case 2, and discuss the resulting equations

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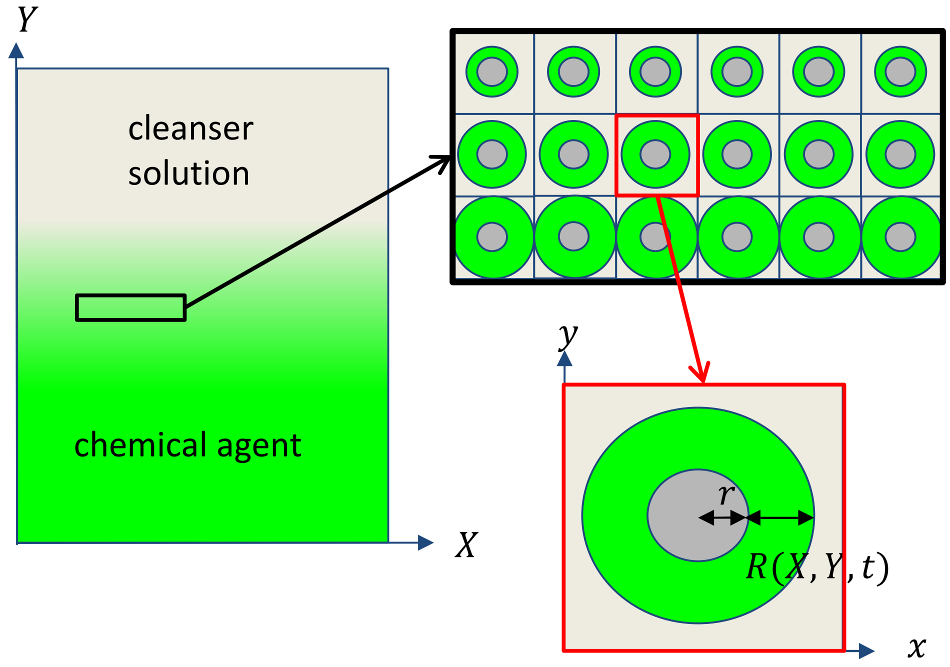

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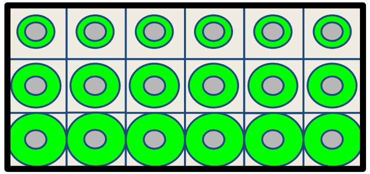

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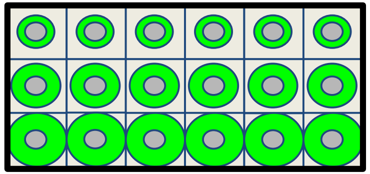

Original Model:

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

on the solid boundary $\partial\Omega_s$:

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

on the interface:

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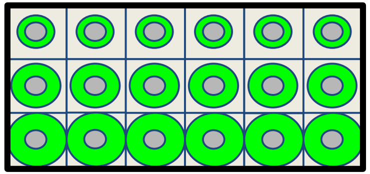

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Scalings:

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

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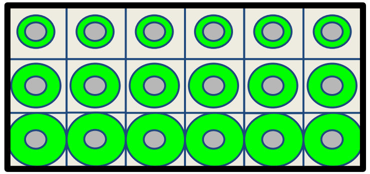

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Choose the diffusive timescale for the macroscale (this is also the timescale over which the interface moves)

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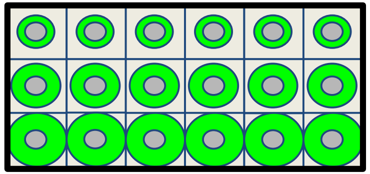

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Dimensionless Model:

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

on the interface:

if $R > 0$ $\quad -\epsilon^2 c R_t - \boldsymbol{n}\cdot\nabla c = -\epsilon^2 \beta c,$

$$R_t = -\beta\gamma c,$$

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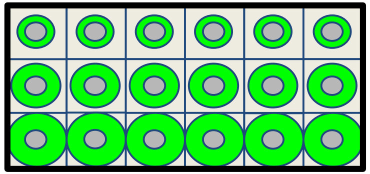

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$$\beta = \frac{kd}{\epsilon^2 D}, \qquad \gamma = \chi c^* \qquad \sim O(1)$$

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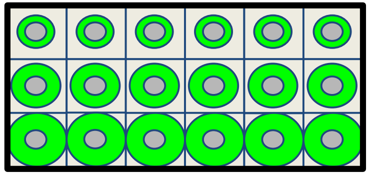

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These are assumed to be $O(1)$ so that we obtain a distinguished limit

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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.

Periodicity is crucial to the homogenisation procedure.

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Periodicity is crucial to the homogenisation procedure.

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

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.

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

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No flux of c into the interface

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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.

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

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

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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

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

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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**

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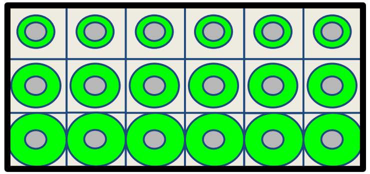

The resulting equations are:

when $R_0 > 0$:

$$c_{0t} = \frac{1}{V}\nabla_X \cdot (V D^* \nabla_X c_0) - \lambda(1 + \gamma c_0)\beta c_0,$$

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

when $R_0 = 0$:

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

where $D^* = D^*(R_0)$ is an adapted diffusivity, $D_0^* = D^*(0)$, and $V(R_0)$ is the area of cleanser.

For the circular solid structure $\lambda = \frac{2\pi(r+R_0)}{1-\pi(r+R_0)^2}$.

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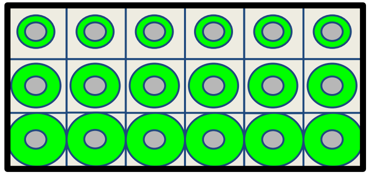

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The standard homogenised diffusion equation in porous media

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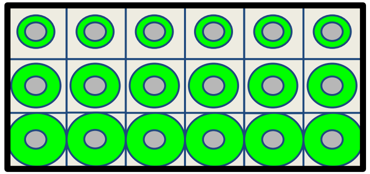

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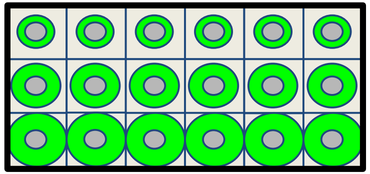

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The chemistry appears as **body** terms

The standard homogenised diffusion equation in porous media

D^* depends on R_0 via a canonical problem on the pore-scale

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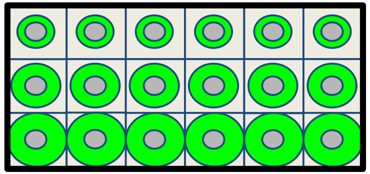

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when $R_0 = 0$:

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

where $D^* = D^*(R_0)$ is an adapted diffusivity, $D_0^* = D^*(0)$, and $V(R_0)$ is the area of cleanser.

For the circular solid structure $\lambda = \frac{2\pi(r+R_0)}{1-\pi(r+R_0)^2}$.

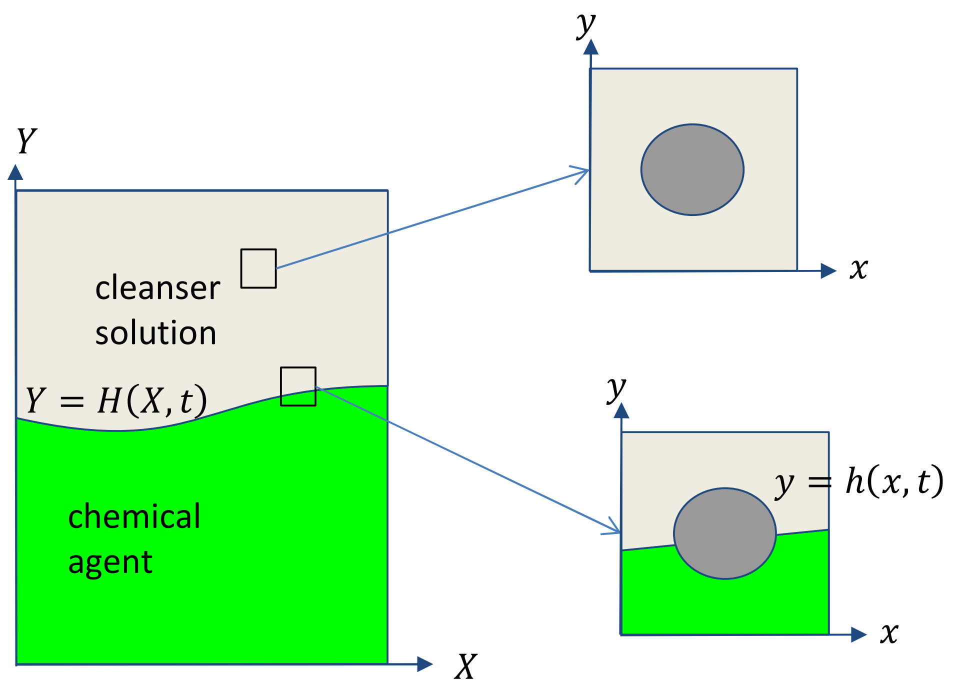
The chemistry appears as **body** terms

The standard homogenised diffusion equation in porous media

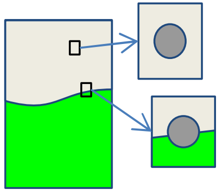
D^* depends on R_0 via a canonical problem on the pore-scale

λ is the ratio of the length of the cleanser-agent boundary to the area occupied by cleanser

Sharp interface



Sharp interface



Original Model:

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

on the solid boundary $\partial\Omega_s$:

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

on the interface:

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

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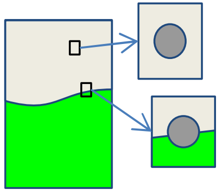
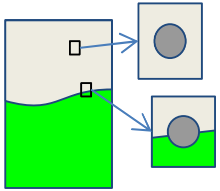


Scalings:

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

Sharp interface



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The timescale is chosen to match the interface motion

Sharp interface

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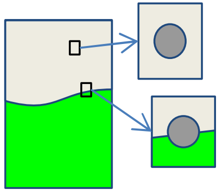


Dimensionless Model:

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

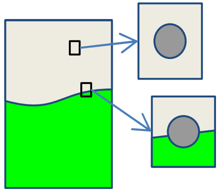
on the solid boundary:

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

on the interface:

$$-\epsilon c \frac{h_t}{\sqrt{1 + h_x^2}} + \boldsymbol{n} \cdot \nabla c = -\epsilon \beta^* c,$$
$$\frac{h_t}{\sqrt{1 + h_x^2}} = -\beta^* \gamma c,$$

Sharp interface



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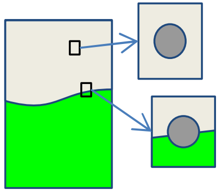
Dimensionless parameters

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

Sharp interface

InFoMM Industrially Focused Mathematical Modelling



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Scalings:

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

$\beta^* = \epsilon\beta$ here, but we now need this to be O(1), since we are interested in the macroscale interface motion

Dimensionless Model:

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

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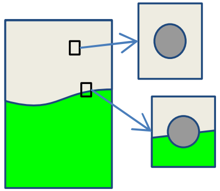
Sharp interface



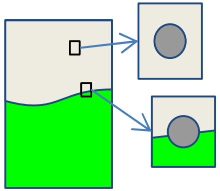
As before we have multiple spatial scales:

$$x = \frac{X}{\epsilon}, \qquad y = \frac{Y}{\epsilon}.$$

but now we also need multiple **timescales**:

$$t = \frac{T}{\epsilon}.$$

Sharp interface



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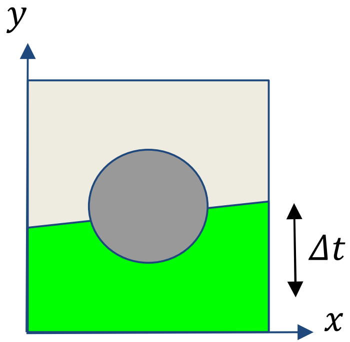
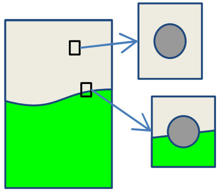
t is the **short** timescale, chosen to match the speed of the interface on the **microscale**



Sharp interface



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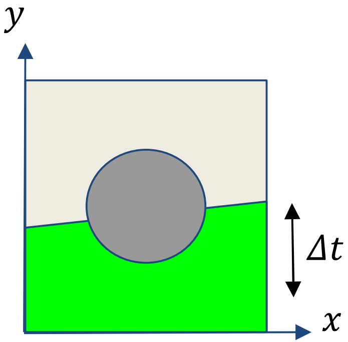
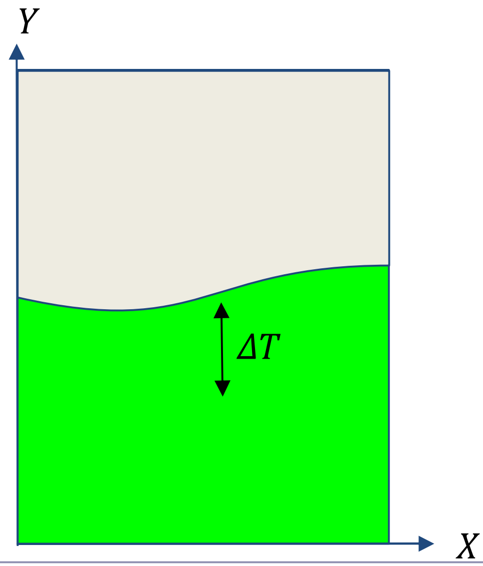


T is the **long** timescale: this matches the speed of the interface on the **macroscale**



Sharp interface

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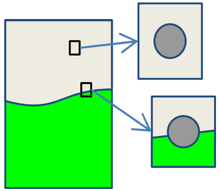
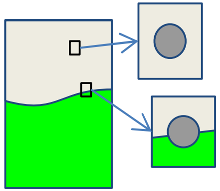


The chemistry happens at an **interface** rather than over the entire (macroscale) region

This means we need a **boundary layer** analysis as well as the homogenisation.

Sharp interface



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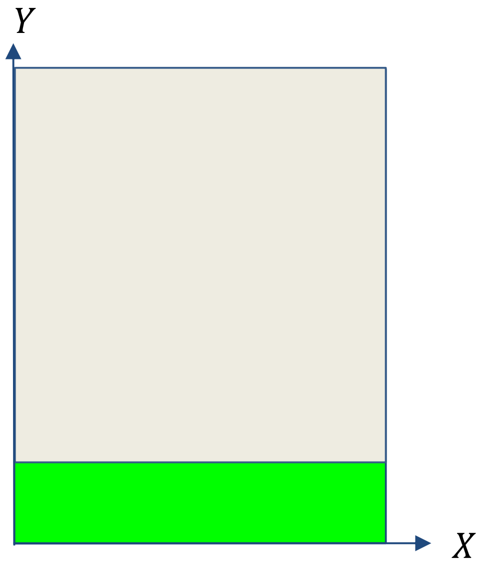
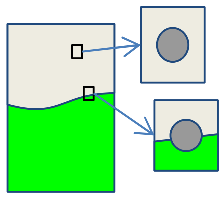


To make things easier, we look at a **flat** macroscale interface

Sharp interface



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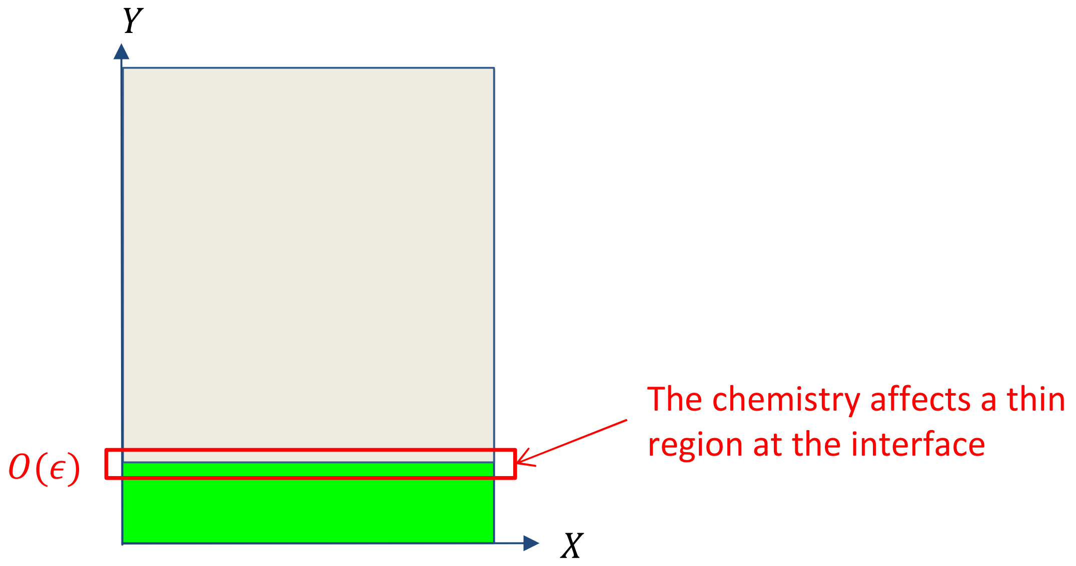

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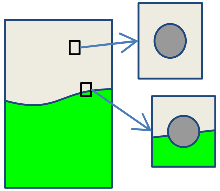

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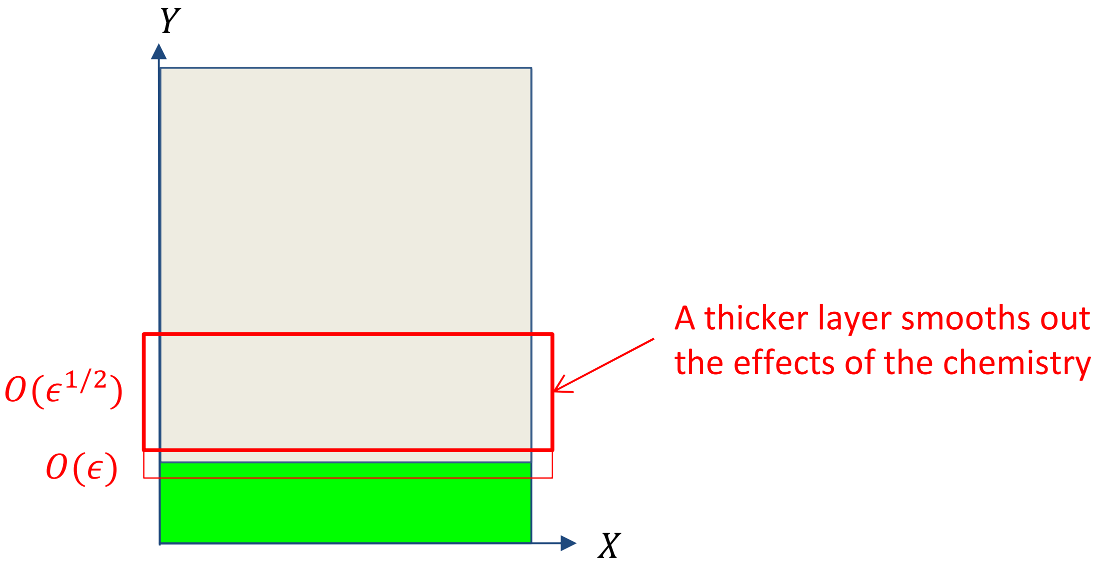

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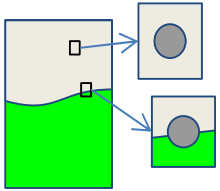

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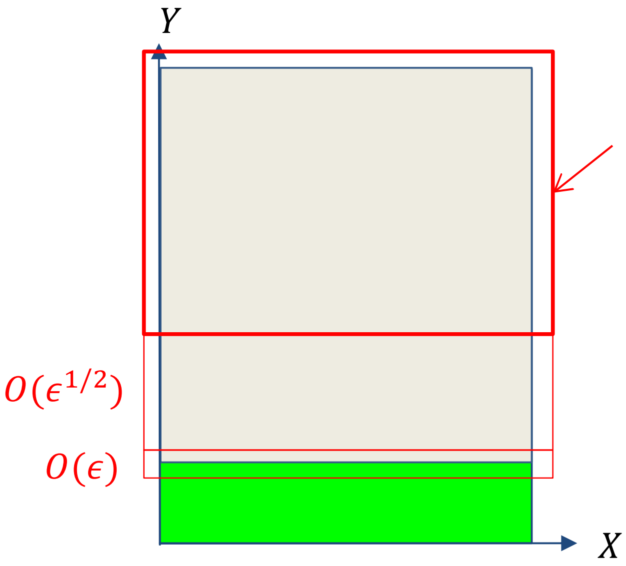
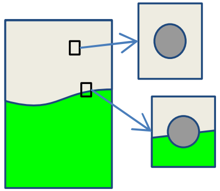


Away from the interface the effects of the chemistry can be matched to the macroscale behaviour of the cleanser

Sharp interface



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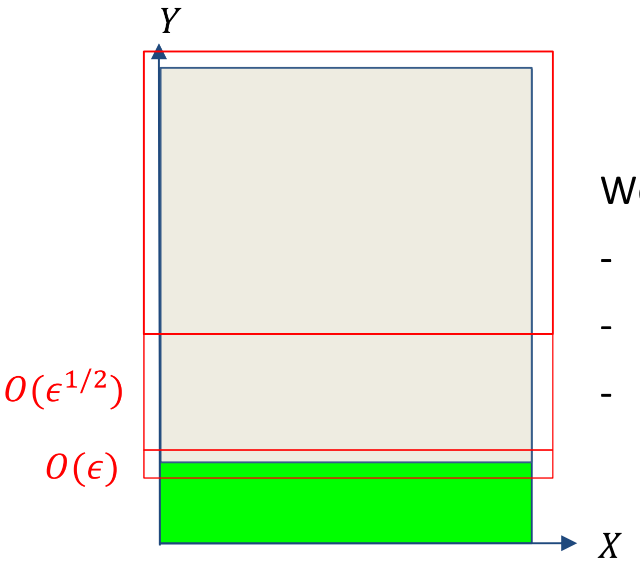
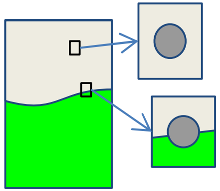
This means we need a **boundary layer** analysis as well as the homogenisation:



We homogenise:

- in **all 3** of these regions,
- in **time** and in **space**,
- **matching** the analysis carefully between the regions

Sharp interface



The resulting macroscale equations are:

in $Y > H(T)$

$$C_T = D_0^* C_{YY},$$

on $Y = H(T)$

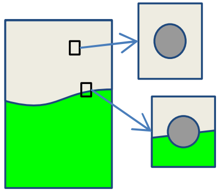
$$H_T = -\beta^* \gamma C,$$
$$C H_T + \mu C_Y = \beta^* C,$$

where D_0^* is the altered diffusivity, and μ is a new flux-factor.

The new factors D_0^* and μ take into account the **microscale**:

- D_0^* takes into account the **solid structure** (as before)
- μ is an average of the **length of the microscale interface** over time

Sharp interface



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Same form of the diffusion equation

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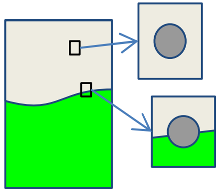

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Same form of the diffusion equation

Same form of the boundary conditions

The new factors D_0^* and μ take into account the **microscale**:

- D_0^* takes into account the **solid structure** (as before)
- μ is an average of the **length of the microscale interface** over time

Comparison of dimensional models:

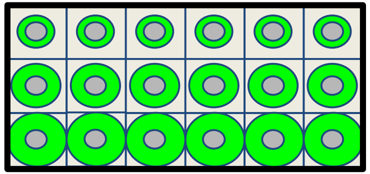
Agent stuck to solid:

when $R = 0$:

$$C_T = D_0^* C_{YY},$$

when $R > 0$:

$$C_T = \frac{1}{V}(VD^* C_Y)_Y - \lambda(1 + \chi C)kC,$$
$$R_T = -\chi kC.$$



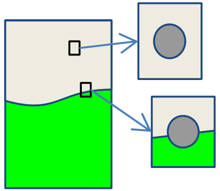
Sharp interface:

in $Y > H(T)$

$$C_T = D_0^* C_{YY},$$

on $Y = H(T)$

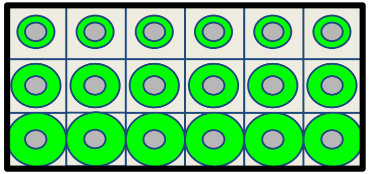
$$H_T = -\chi kC,$$
$$CH_T + \mu C_Y = kC.$$



Implications

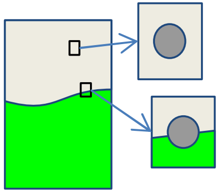
Agent stuck to solid:

- This model is **different** to previous reactive decontamination models
- Analysis of this model could give new insight in the decontamination of **unsaturated agent spills**
- In certain limits, **this could behave like a sharp interface model**



Sharp interface:

- This model has the **same structure** to that used previously
- Previous work could be extended to cover different values of D_0^* and μ.
  - The porous structure is taken into account systematically
  - Allows for situations where the porous structure varies spatially



Conclusion

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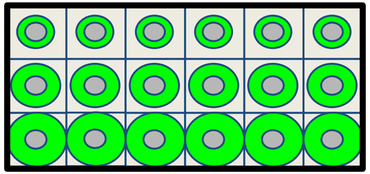
Two homogenisation approaches:

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

  This is a new model for **unsaturated decontamination**



- For the **sharp interface**
  - Discussed the differences and complications
  - Presented the resulting macroscale equations

  Extends sharp-interface decontamination to include the effects of the porous structure