Modelling The Decontamination Of A Porous Material

Lyllian Chanerley
University of Warwick

Introduction

- **Chemical spills** can often be disastrous, regularly being both environmentally damaging and expensive to clean and clear. Developing an understanding of different clean up protocols and their efficacy, is vital to quick and efficient **decontamination**.
- The decontamination process of cleaning a chemical spill on a **porous material** like concrete often involves pouring a neutralising cleanser over where the hazardous agent has been spilt.

Fig. 1: Person pouring cleanser over a chemical spill [1].

- We developed a **mathematical model** to investigate this decontamination process and to assess which physical properties in a cleanser we need for the most effective decontamination

Model

Our model is heavily based on the one used in [2]. We assume both the cleanser, $\bar{c}$ [mol m^{-3}], and agent, $\bar{a}$ [mol m^{-3}], **diffuse** through the porous medium with diffusion constants $\bar{D}_c$ [m^2 s^{-1}] and $\bar{D}_a$ [m^2 s^{-1}] respectively. We impose a no flux condition at the top and bottom boundary. At the interface, we assume the agent and cleanser react irreversibly and **assume all product formed dissolves into the oily phase**. From these assumptions we derive the following model:

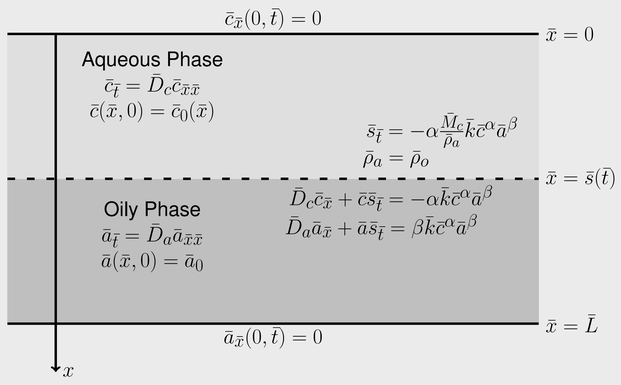

Fig. 2: Governing equations over diagram of a porous material with a layer of agent and cleanser

Where $\bar{k}$ [mol$^{1-(\alpha+\beta)}$ m$^{3(\alpha+\beta)-2}$ s^{-1}] is the effective rate constant, $\bar{\rho}_a$ [kg m^{-3}] and $\bar{\rho}_o$ [kg m^{-3}] are the densities of the aqueous and oily phase respectively. $\bar{M}_c$ is the molar mass of the cleanser. $\bar{L}$ [m] is the depth of the porous medium and $\bar{s}$ [m] is the position of the interface between the two phases.

Nondimensionalisation

After deriving the model, we then make a choice of **dimensionless** variables:

$$\xi = \frac{\bar{x}}{\bar{s}(\bar{t})}, \qquad \eta = \frac{\bar{L} - \bar{x}}{\bar{L} - \bar{s}(\bar{t})}, \qquad t = \frac{\bar{L}^2}{\bar{D}_c},$$
$$\bar{c}(\bar{x},\bar{t}) = \bar{a}_0 c(\xi,\eta), \qquad \bar{a}(\bar{x},\bar{t}) = \bar{a}_0 a(\xi,\eta), \qquad \bar{s}(\bar{t}) = \bar{L} s(t).$$

choosing them in such a way that we rescale the problem in order to **remove the moving boundary**, allowing for easier numerical simulation. We then substitute these dimensionless variables into our model's equations to get:

$$\begin{aligned}
s^2 c_t &= c_{\xi\xi} + \xi c_\xi s s_t && \text{for } \xi \in (0,1),\\
a_t (1-s)^2 &= D_a a_{\eta\eta} - \eta a_\eta s_t (1-s) && \text{for } \eta \in (0,1),\\
c_\xi + s s_t c &= -\alpha Q s c^\alpha a^\beta && \text{for } \xi = 1,\\
D_a a_\eta - (1-s) s_t a &= -\beta Q (1-s) c^\alpha a^\beta && \text{for } \eta = 1,\\
s_t &= -\alpha Q M c^\alpha a^\beta && \text{for } t \in (0,\infty),\\
c_\xi(0,t) &= 0 && a_\eta(0,t) = 0,\\
s(0) &= d \qquad c(\xi,0) = \frac{\bar{c}_0(\xi \bar{s}_0)}{\bar{a}_0} && a(\eta,0) = 1 \quad .
\end{aligned}$$

With the nondimensional constants being:

$$d = \frac{\bar{s}_0}{\bar{L}}, \qquad D_a = \frac{\bar{D}_a}{\bar{D}_c}, \qquad Q = \frac{\bar{a}_0^{\alpha+\beta-1} \bar{k} \bar{L}_0}{\bar{D}_c}, \qquad M = \frac{\bar{M}_c \bar{a}_0}{\bar{\rho}_a}.$$

We are now ready to do some numerical simulation and analysis.

Time Until Decontamination

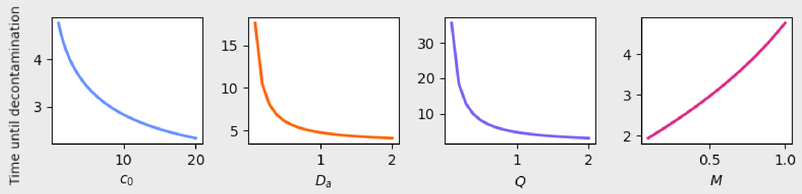

Fig. 3: Time taken for reaction to complete for different parameter values of c_0, D_a, Q and M

The figure above shows how changing different constants affects the speed at which the reaction was complete. If the maximum concentration of agent was ever less than 0.01, the reaction was considered complete. We can see the most impact constants are D_a and Q, meaning **high agent diffusivity** and **high effective rate constant** are most important to have a quick reaction

Late-Time Analysis

Assuming that the system has come to rest and that all time dependant terms are zero, we can investigate the **final concentrations** of cleanser and agent. We find that the concentration of either the cleanser or agent goes to **zero** and we can calculate the concentration of the non zero chemical using the initial conditions:

$$\text{if } \beta d c_0 - \alpha(1-d) a_0 >= 0: \qquad c = \frac{1}{2}(\beta d c_0 - \alpha(1-d) a_0),$$
$$\text{if } \beta d c_0 - \alpha(1-d) a_0 <= 0: \qquad a = \frac{1}{2}(\beta(1-d) a_0 - \alpha d c_0).$$

Reaction Progression

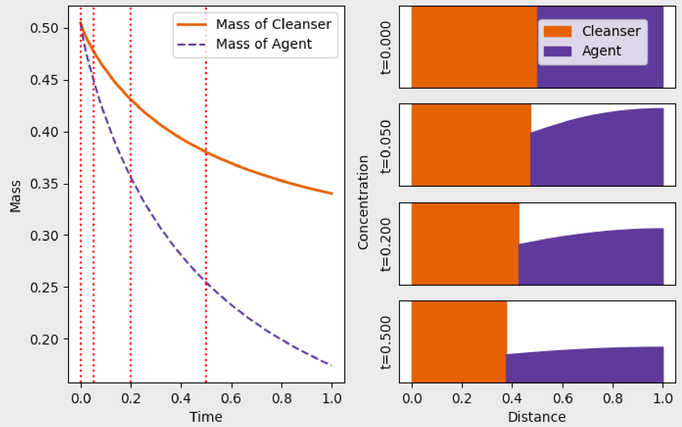

Fig. 4: Mass of chemicals over time with concentration distributions sampled at $t = 0.000, 0.050, 0.200, 0.500$

The shown results are from a simulation where all constants are 1 except for $\beta = 2$ and $d = 0.5$. We can see in the left graph the mass of the agent **decreases** at twice the rate of the cleanser decreasing, which is what we expect. On the right, we can see how the agent concentration decreases over time, but the cleanser **concentration remains constant** as the interface moves towards the left.

Conclusion

This project has allowed me to gain valuable insight into this area, with a few key conclusions:

- Tracking how this neutralisation reaction progresses is incredibly difficult due to it happening inside a porous material, although some methods have been developed [4].
- This means identifying an effective decontamination protocol is very challenging [3].
- Using our model, we were able to investigate reaction times and determine that low diffusivity of cleanser and high effective rate constant contribute to a lower reaction time.

Acknowlegments and References

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[1] Creative Safty Supply. *chemical-spill*. [Online; accessed September 23, 2024] [eddited slightly to make power look like a liquid]. 2019. URL: https://www.creativesafetysupply.com/content/images/articles/chemical-spill.jpg?setCurrencyId=1.

[2] Mohit P Dalwadi et al. "Mathematical modeling of chemical agent removal by reaction with an immiscible cleanser". In: *SIAM Journal on Applied Mathematics* 77.6 (2017), pp. 1937–1961.

[3] Ellen Raber and Raymond McGuire. "Oxidative decontamination of chemical and biological warfare agents using L-Gel". In: *Journal of hazardous materials* 93.3 (2002), pp. 339–352.

[4] Amanda R Wilmsmeyer et al. "Multifunctional ultra-high vacuum apparatus for studies of the interactions of chemical warfare agents on complex surfaces". In: *Review of Scientific Instruments* 85.1 (2014).