# Modelling The Decontamination Of A Porous Material

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## 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 and agent **diffuse** through the porous medium. We impose a no flux condition at the top and bottom boundary, meaning no concentration of agent or cleanser can leave through the boundaries. At the interface, we assume the agent and cleanser react irreversibly and **assume all product formed dissolves into the oily phase**.

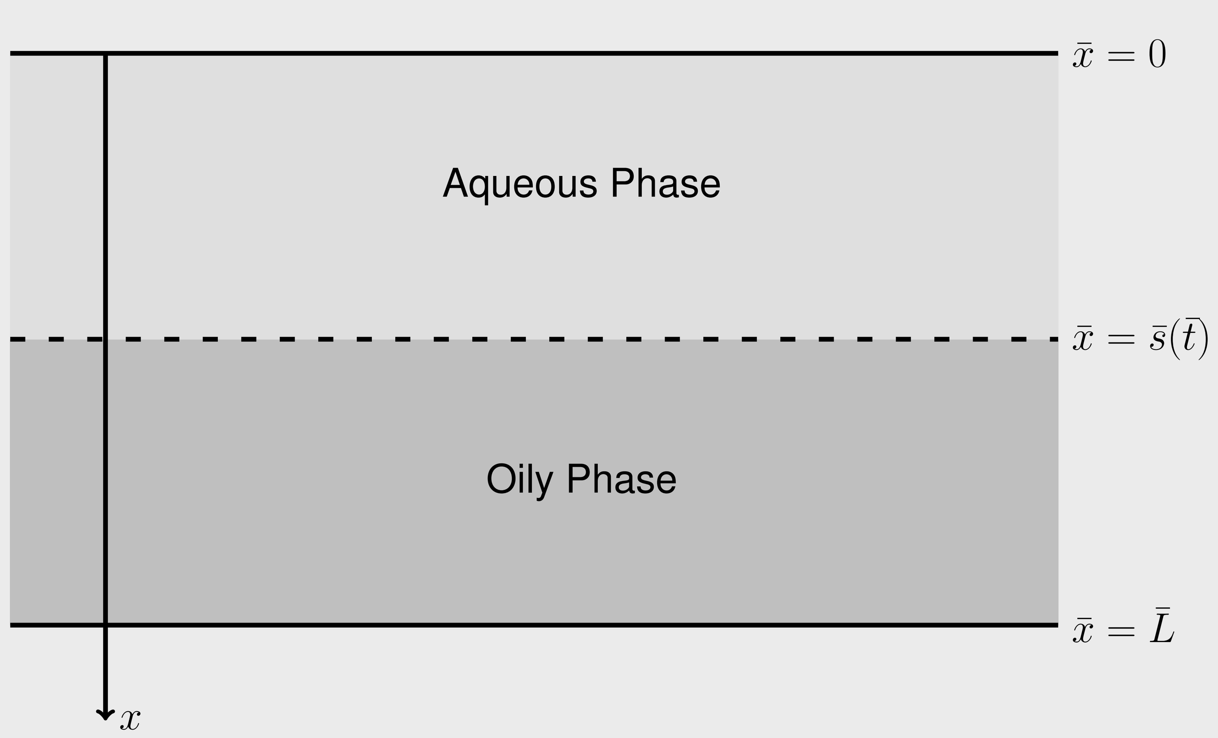


Fig. 2: Governing equations over diagram of a porous material with a layer of agent and cleanser

After deriving the model we end up with 4 dimensionless constants: $c_0$, which is the initial concentration of cleanser; $D_a$, which is the ratio between how fast the cleanser diffuses compared to the agent; $Q$, which is the ratio between reaction rate and length of medium; and $M$ which is the ratio between the mass of cleanser times concentration of agent and density of oily phase.

## Reaction Progression For Constant Initial Cleanser

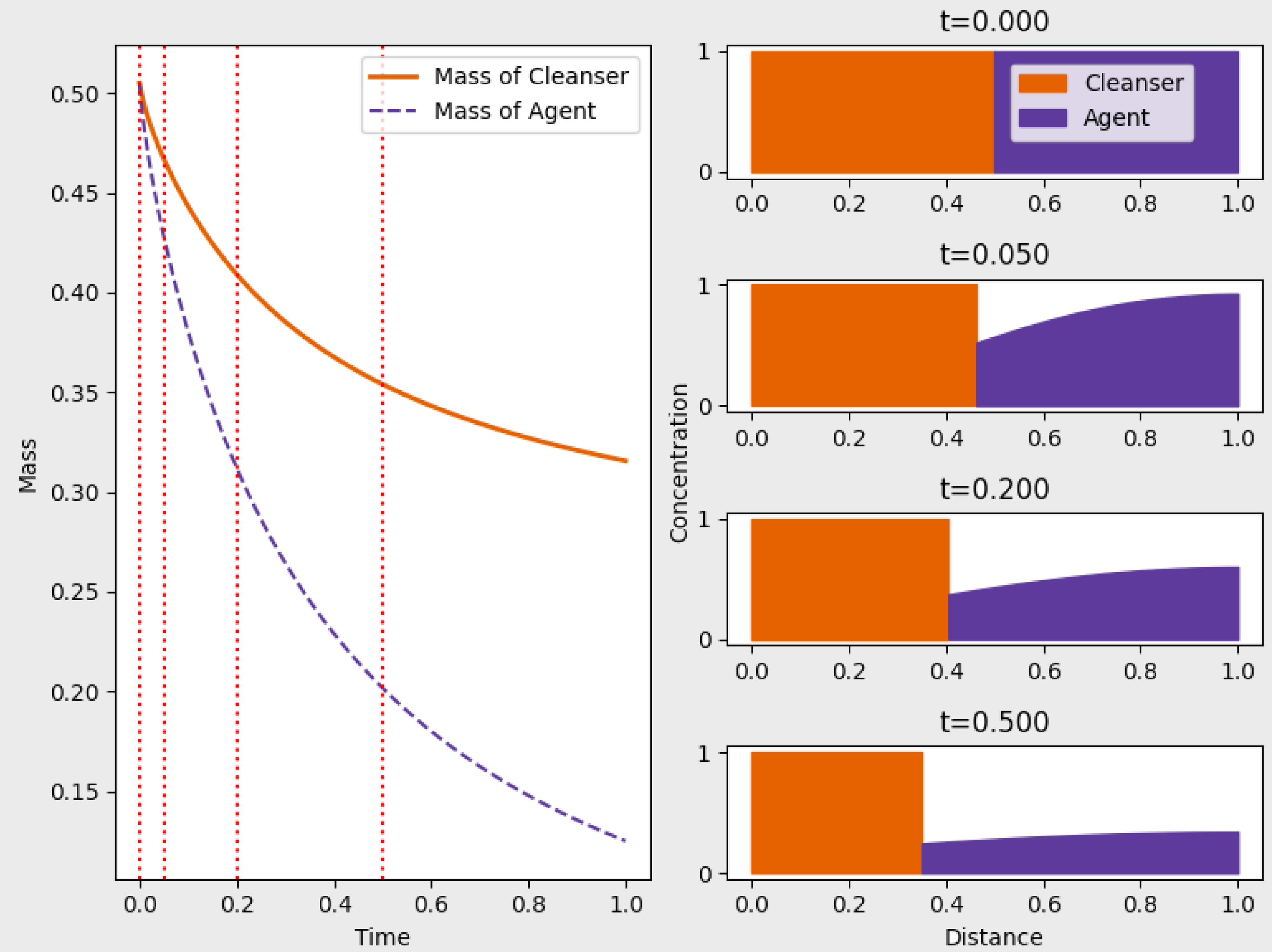


Fig. 3: Mass of chemicals over time with concentration distributions sampled at $t = 0.000, 0.050, 0.200, 0.500$

The shown results are from a simulation where the agent reacts twice as fast as the cleanser. 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.

## Time Until Decontamination

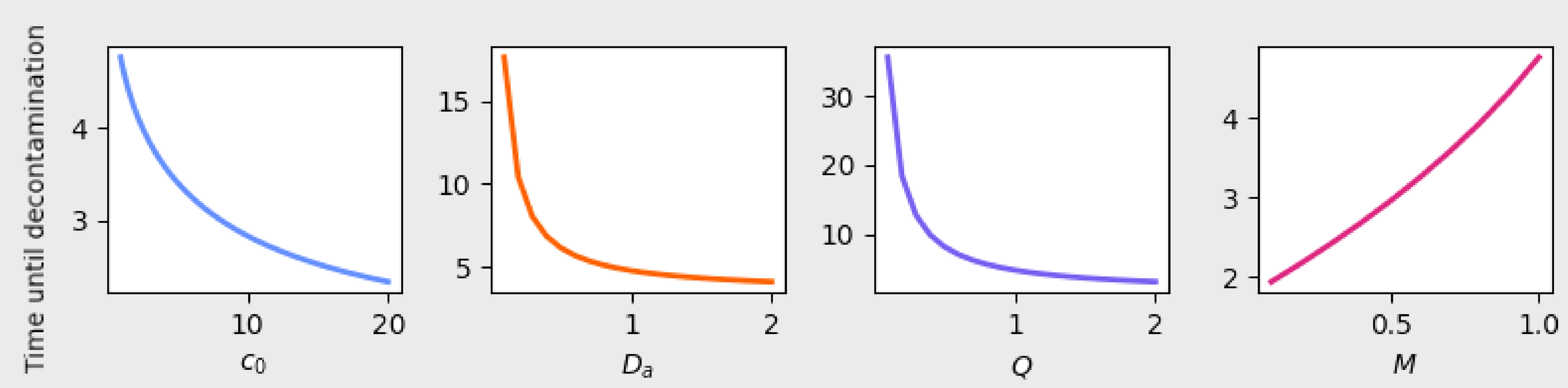


Fig. 4: Time taken for reaction to completed for different parameter values of $c_0, D_a, Q$ and $M$

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 reaction rate** are most important to have a quick reaction.

## QR code for animations and source code

## Reaction Progression For Linear Initial Cleanser

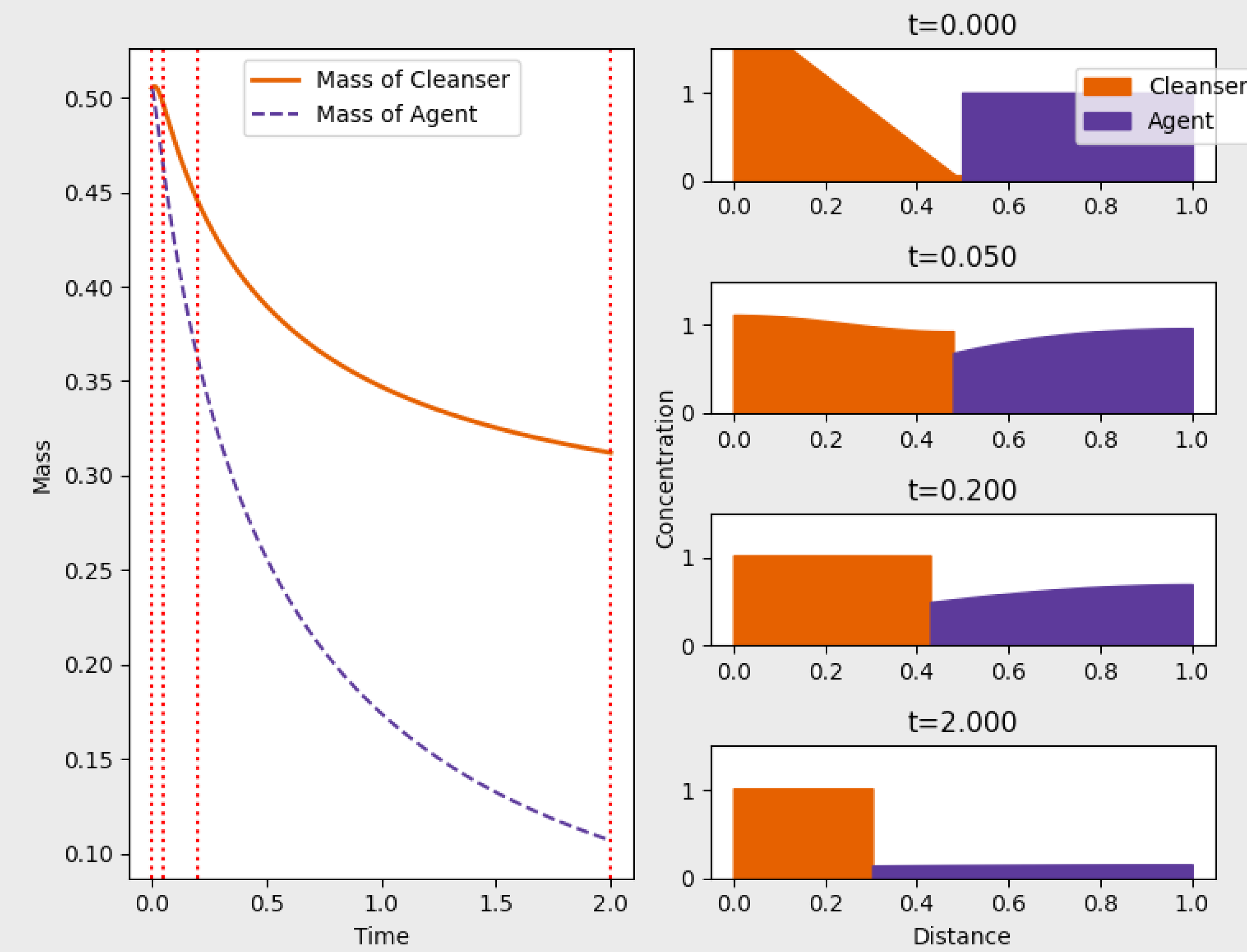


Fig. 6: Mass of chemicals over time with concentration distributions sampled at $t = 0.000, 0.050, 0.200, 2.000$

This Figure is similar to Fig 3 except for the fact the initial concentration of cleanser decreases linearly. The graphs on the right very clearly show how the **cleanser concentration smooths** to become constant in a short amount of time.

## 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 reaction rate constant contribute to a lower reaction time.

## Acknowlegments and References

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[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).