Mathematical modelling for environmental challenges

Dates: 21st-22nd March 2024

Locations:
- Talks: Room B3.02, Zeeman Building, University of Warwick
- Coffee, lunch, drinks: Common room, Zeeman Building, University of Warwick

Schedule

Day 1: Thursday 21st March

9.30	Set up
10.00-10.15	Welcome by the organisers

Session 1: Natural flows

10.15-11.00	**Thomasina Ball** (Unravelling wrinkle formation in natural flows)
11.00-11.45	Coffee
11.45-12.30	**Katarzyna Kowal** (Slippery flows in nature)
12.30-14.00	Lunch

Session 2: Decontaminating the environment

14.00-14.45	**Doireann O'Kiely** (Decontaminating the Environment: Modelling Infiltration)
14.45-15.30	**Ellen Luckins (**Reactive decontamination of porous media)
15.30-16.00	Coffee
16.00-16.45	**Francesco Conto** (Surface-washing of porous surfaces)
17.00-18.30	Drinks in the Common Room
19.00	Dinner

Day 2: Friday 22nd March

Session 3: Energy

10.00-10.45	**Ferran Brosa Planella** (Modelling thermal energy storage: challenges and opportunities)
10.45-11.15	Coffee
11.15-12.00	**Adam Butler** (Modelling Flow Dynamics and Geological Heterogeneities in Subsurface CO2 Sequestration)
12.00-12.45	**Smita Sahu** (A continuum model for lithium plating and dendrite formation in lithium-ion batteries: formulation and validation)
12.45-13.00	Wrap up and close

Abstracts

Session 1: Natural flows

Thomasina Ball: Unravelling wrinkle formation in natural flows

Wrinkles or creases in the surface of a material are indicative of compression. For example, on Earth, mountain ranges formed due to the plate tectonics exhibit regular spaced folds on the surface; and buckles on the surface of ice sheets are observed due to compression from sea ice. Both examples have a layered structure with contrasting rheological behaviours where compression leads to an instability causing the stiff surface to buckle.

To model this system, often an elastic beam is considered. However, in many cases where the stiff layer is significantly broken-up, or forced to deform well beyond its yield point, other models may be more relevant, such as a substantially more viscous fluid, or a plastic material. In this talk, we consider a viscoplastic beam which is compressed while lubricated below by a thin layer of viscous fluid. We investigate the wavelengths observed, the impact of introducing a yield stress, and discuss future developments of the model to consider non-uniform layers.

Katarzyna Kowal: Slippery flows in nature

Slip, as seen in various natural and industrial applications, strongly depends upon the length scales involved. Examples range from the small scales of lotus leaves and fabricated hydrophobic surfaces to the large scales of ice sheets, such as Greenland and Antarctica, which generally slide at their base. Owing to difficulties associated with scaling glacial processes to the laboratory, it remains a challenge to design analogue fluid-mechanical experiments of ice sheets that slide at their base. The main challenge is the design of a substrate that is slippery enough for appreciable sliding to be seen in the laboratory. This talk goes through the design of such a substrate and the development of a theoretical and experimental framework for generating slip underneath viscous fluids on the large scale while minimising the effects of unwanted fluid-mechanical instabilities. We build into this framework the freedom to adjust slip, as desired, and capture it by a macroscopic sliding law. We test our sliding law experimentally and relate it to the sliding of ice sheets.

Session 2: Decontaminating the environment

Doireann O'Kiely: Decontaminating the Environment: Modelling Infiltration

Mathematical modelling can support decontamination processes in a variety of ways. In this talk, we focus on the *contamination* step: understanding how much of a chemical spill has seeped into the Earth or a building material, and how far it has travelled, are essential for making good decisions about how to clean it up.

We consider an infiltration problem in which a chemical is poured on an initially unsaturated porous medium, and seeps into it via capillary action. Capillarity-driven flow through partially-saturated porous media is often modelled using Richards' equation, which is a simplification of the Buckingham-Darcy equation in the limit where the infiltrating phase is much more viscous than the receding phase. In this talk, I will explore the limitations of Richards equation, and discuss some scenarios in which predictions for small-but-finite viscosity ratios are very different to the Richards simplification.

Ellen Luckins: Reactive decontamination of porous media

Following a chemical weapons attack, it is crucial for public safety that any hazardous chemical agent remaining in the environment is properly removed, which is especially difficult if it has seeped into porous building materials. For one type of remediation protocol, a cleanser solution is applied to the surface and allowed to react in, neutralising the hazardous agent in a chemical reaction. The cleanser and agent fluids are typically immiscible, so the reaction takes place at the fluid-fluid interfaces within the pores of the material. We present models for this decontamination process for two different initial distributions of the agent through the porespace and compare their relative decontamination times. We also build understanding of the factors limiting both the speed and efficiency of the decontamination procedure, and the trade-off between these desired properties.

Francesco Conto: Surface-washing of porous surfaces

The cleaning of porous surfaces is a challenging problem in everyday life and industrial practice since it can lead to redistribution of the absorbed contaminant within the porous material instead of a complete removal of the unwanted agent. The role of decontamination is particularly crucial when contaminants (such as chemical weapons agents and pathogens) pose serious risks to human health.

In this work, I present surface-washing experiments modelling the decontamination of porous substrates. A surface-washing apparatus is equipped with camera-based and in-line UV-Vis diagnostics. A dyed fluid is placed onto the porous substrate to simulate the region of contamination. The surface-washing is simulated by a thin gravity-driven film of water flowing over an inclined porous-glass surface. The resulting interaction between the cleansing film flow and the contaminating dye is then tracked using direct image analysis based on dye-attenuation techniques, enabling to study the space-time evolution of the contaminant field over the porous medium. The camera visualization is complemented with a UV-Vis spectrometer monitoring in real-time the contaminant concentration in the effluent during the washing.

Our experiments, together with a simple two-dimensional analytical model and numerical simulations performed in COMSOL, provide insights on the role of initial conditions and the relevant transport mechanisms of the contaminant. Moreover, they demonstrate a decontamination-induced redistribution of the contaminant in the porous medium. Importantly, they are useful to assess and optimize the efficiency of the decontamination process and the impact of cleaning strategies on industrial performance.

<u>Session 3: Energy</u>

Ferran Brosa Planella: Modelling thermal energy storage: challenges and opportunities

In 2022 heat accounted for almost half of total final energy consumption and 38% of energy-related CO_2 emissions worldwide. Decarbonising its production will be fundamental if we are to achieve the current net zero emissions goals. Thermal energy storage technologies will be key to decouple supply and demand, but they are still not ready for broad commercial deployment.

Modelling can play a crucial role in speeding the development of these technologies, but there are still many open challenges. State-of-the-art models are overly complicated and computationally expensive. Therefore there are many challenges and opportunities to develop a new generation of fast and accurate models that can be used to design, control and optimise thermal energy storage solutions. In this talk we will present a multi-scale modelling approach for encapsulated thermal energy storage devices that provides accurate simulations at a low computational cost.

Adam Butler: Modelling Flow Dynamics and Geological Heterogeneities in Subsurface CO2 Sequestration

Subsurface CO_2 sequestration represents a crucial step in reaching Net Zero targets as a method for securely storing emissions from processes that cannot be fully decarbonised. This involves injecting CO_2 into porous geological formations rather than releasing it into the atmosphere. Over time, the CO_2 will become permanently trapped through a series of processes including dissolution in groundwater and chemical reactions with the surrounding minerals. However, the behaviour of the CO_2 while mobile is strongly influenced by geological heterogeneities, such as variations in porosity and permeability, for which only limited measurements are available. These uncertainties present major challenges in the design of injection locations and strategies for a given storage site.

In this talk, I will discuss a vertically integrated modelling approach for simulating CO_2 flow through these porous geological formations. This simplifies the governing equations while retaining the key physical mechanisms involved, such as residual trapping, dissolution, and deformation. These vertically integrated models allow us to simulate the flow in a fraction of the time of the standard industry approach, and so evaluate more extensively the impact of different reservoir heterogeneities and injection strategies.

Smita Sahu: A continuum model for lithium plating and dendrite formation in lithium-ion batteries: formulation and validation

This work presents a novel physics-based model for lithium plating and dendrite formation in lithium-ion batteries. The formation of Li metal is an undesirable side-effect of fast charging and a primary contributor to cell degradation and failure. The model distinguishes between three types of plated Li metal, namely: (a) Li metal plated within the pores of the solid electrolyte interphase (assumed to be electronically connected to the anode and therefore recoverable); (b) dendrites protruding outside the SEI that remain electronically connected (and are therefore dangerous, potentially leading to a short circuit), and (c) electronically disconnected/ "dead'' Li metal outside the SEI contributing to capacity fade. The model is validated against \bl{two independent experiments. First, measurements of: (i) the cell voltage and current during a constant-current-constant-voltage charge and subsequent discharge, and (ii) the Li metal intensities (derived from operando NMR) which directly quantifies the time-resolved quantity of Li metal in the cell during use. Second, against voltage measurements during galvanostatic discharge at a range of C-rates and temperatures. Favourable agreement is demonstrated throughout; particularly in terms of the proportions of reversible and irreversible plating. We also demonstrate that the model reproduces the well-documented trends of being more prevalent at increased C-rate and/or decreased temperature.