Liquid interactions with porous media and the environmental fate of toxic materials

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Summary

- Introduction
- Previous / related work
- Problem definition
- Specific questions
- Wider topics of interest

Defence Science and Technology Laboratory (Dstl)

- Part of the UK Ministry of Defence (MoD)
- Responsible for science and technology in UK defence
- Conduct R&D on defence and security related subjects
- Three key sites
  - Porton Down
  - Fort Halstead
  - Portsdown West
- 3700 staff > 70% active scientists, engineers and analysts
- Over £100M work placed with industry / academia
- Integral part of the UK Government and MoD

Why does Dstl exist?

- Dstl's purpose is to maximise the impact of S&T on UK Defence and Security.

- Dstl sits within Government to provide essential, impartial, high quality and timely advice on science and technology issues.

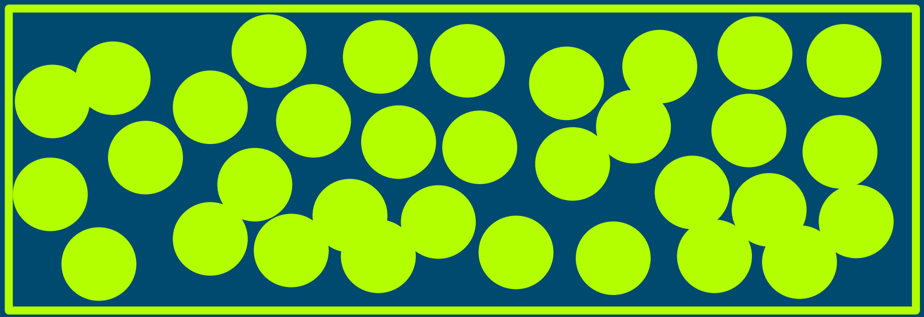
- Our expertise enables our colleagues across government and the UK Armed Forces to determine potential issues and threats.

- Dstl is primarily focused on defence S&T and continues to be strongly aligned with MoD's overall mission.
  - But we also work with Other Government Departments to exploit our expertise and knowledge, with the aim of enhancing the safety and security of UK citizens and interests.

Protection against toxic materials

- Protection of UK forces and civilians from accidental or deliberate release of:
  - Chemical warfare agents (CWAs) e.g. sarin, VX
  - Toxic industrial chemicals (TICs) e.g. chlorine
- Hazards can be airborne (gases/vapours) or surface based (liquids)
  - Liquid agents have a range of properties, e.g. volatility, reactivity, viscosity etc.
- Improve hazard assessment, mitigation and clean up
  - Understand the way materials interact with the environment

Porous materials



- Porous materials consist of:
  - *solid matrix* – the solid mass of the material structure
  - *pores* or *voids* – the open volume within the matrix
- Interconnected pore volumes allow fluids to travel through the matrix
  - Flow is typically laminar
  - Pores can act as capillaries
  - Range of length scales
- Materials of interest are usually porous to some extent, e.g. soil, sand, concrete

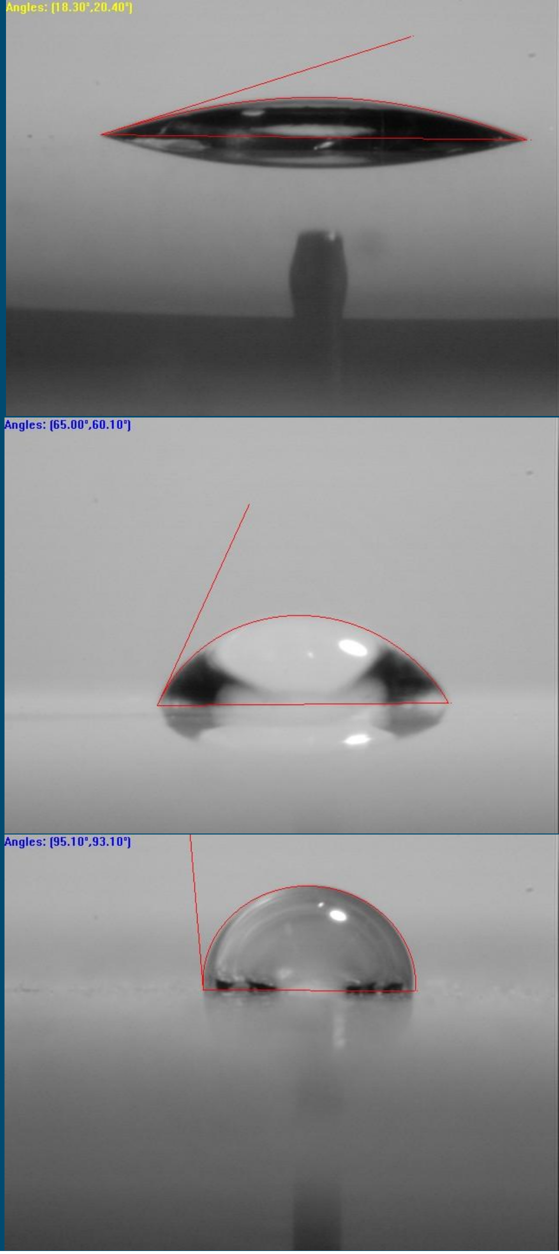
Dstl programme

- Joint modelling and experimental programme
  - Develop models for fluid interaction with porous surfaces
  - Specific data for liquid-porous material pairs
  - Validate using experimental data

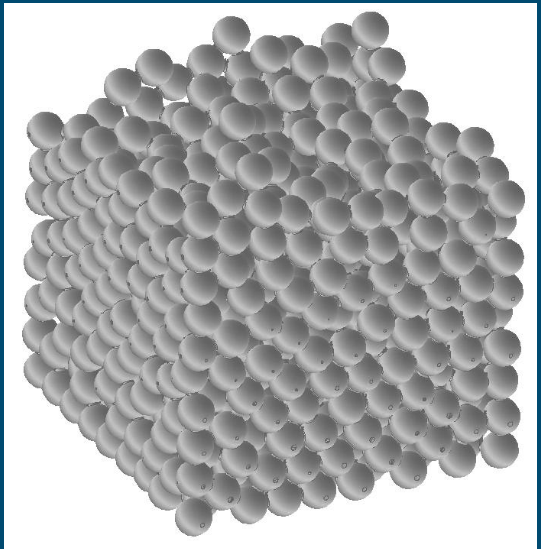
- Improve understanding to:
  - Evaluate persistence
  - Assess risk to human health
  - Improve mitigation and cleanup techniques
  - Understand the effect of fundamental physical and chemical properties of liquids and surfaces
  - Allow prediction of fate without specific experiments
  - Identify lower toxicity simulants

Experimental techniques

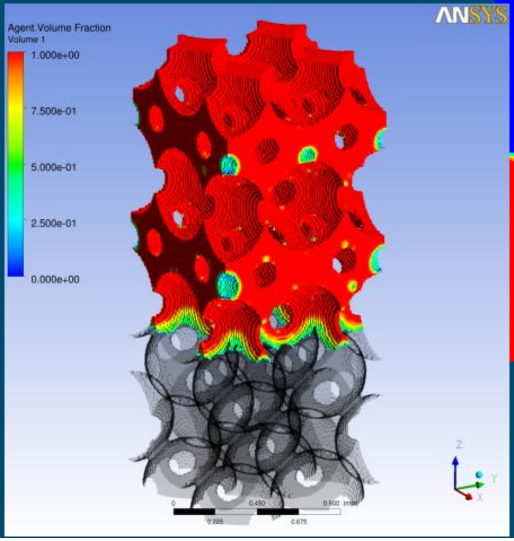
- Visualisation of liquid in matrix
  - e.g. using non-invasive imaging techniques
- Although
  - Required for each material-liquid pairing
  - Potentially large numbers of experiments
  - Potentially long experiments
  - Small scale
  - Parameters can be difficult to measure
  - Expensive
- Validation of numerical models
- Determination of liquid and matrix properties

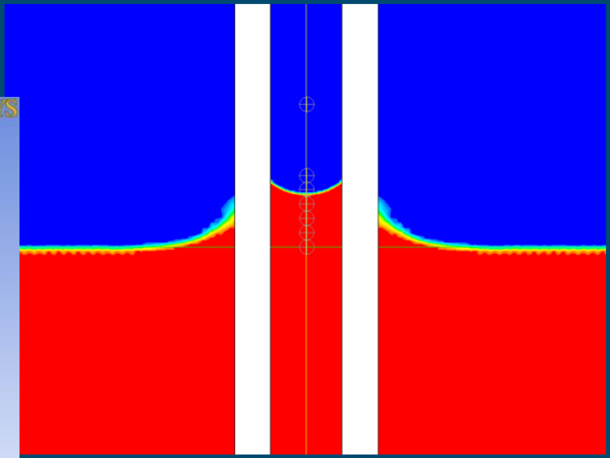


High resolution modelling



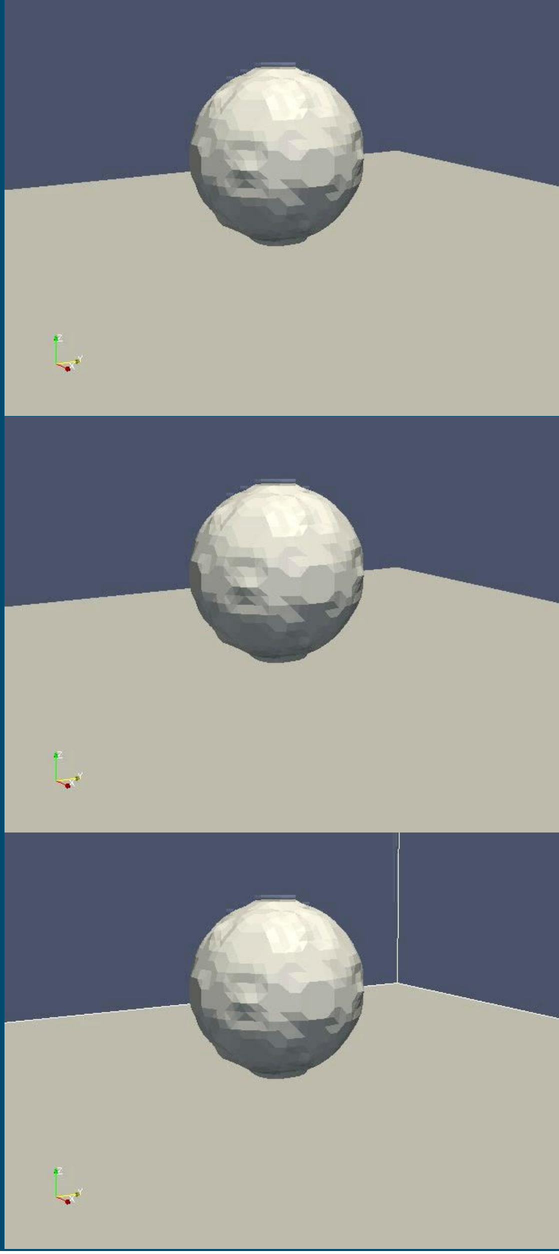
- Explicit models
  - e.g. computational fluid dynamics (CFD)
  - Model liquid and porous material explicitly
  - Interface tracking (e.g. VOF, level set)
    - Contact angle
    - Surface tension
    - Pore size





High resolution modelling

- Explicit models
  - e.g. computational fluid dynamics (CFD)
  - Model liquid and porous material explicitly
  - Interface tracking (e.g. VOF, level set)
    - Contact angle
    - Surface tension
    - Pore size
  - Droplets on surfaces
  - Computationally expensive / time consuming



Averaged approach

- Both experiments and high resolution modelling can yield good results but can be expensive and time consuming
- Need an approach which is quicker and cheaper
  - Model based on fundamental parameters
  - Should be spatially and temporally resolved to capture evolution
  - Only needs to model the important processes on relevant timescales
  - Should take fundamental parameters of the matrix and chemical as input

Fundamental parameters

- droplet size
- liquid density
- droplet impact velocity
- droplet impact angle
- gravity
- surface orientation
- surface tension
- contact angle
- substrate porosity
- viscosity
- pore size
- reactivity
- volatility
- vapour density
- vapour-surface interactions
- diffusion coefficient
- temperature

Fundamental parameters

Droplet impaction

- droplet size
- liquid density
- droplet impact velocity
- droplet impact angle
- gravity
- surface orientation
- surface tension
- contact angle
- substrate porosity
- viscosity
- pore size
- reactivity
- volatility
- vapour density
- vapour-surface interactions
- diffusion coefficient
- temperature

Fundamental parameters
Transport within matrix

- droplet size
- liquid density
- droplet impact velocity
- droplet impact angle
- gravity
- surface orientation
- surface tension
- contact angle
- substrate porosity
- viscosity
- pore size
- reactivity
- volatility
- vapour density
- vapour-surface interactions
- diffusion coefficient
- temperature

Fundamental parameters

Vapour considerations

- droplet size
- liquid density
- droplet impact velocity
- droplet impact angle
- gravity
- surface orientation
- surface tension
- contact angle
- substrate porosity
- viscosity
- pore size
- reactivity
- volatility
- vapour density
- vapour-surface interactions
- diffusion coefficient
- temperature

Specific questions

1. How does the persistence of the chemical in the surface vary as a function of the liquid and surface properties and the impact parameters?
2. Can the surface interaction process be divided into discrete stages?
3. If so what timescales are expected for each stage?
4. Can we apply the model to heterogeneous surfaces? i.e. those with a distribution of pore structures and/or multiple materials.

Wider topics of interest

1. How might temperature variation be used to optimise the removal of a liquid through evaporation for decontamination within a maximum temperature limit?
2. Can the model be extended to consider a porous material with another liquid present (e.g. water)?
3. Can we estimate how much material might be available for surface contact?