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

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1.1 Introduction

Toxic liquid chemicals released into the environment may pose an immediate risk to human health through contact or related vapour hazards. However, they can also interact with surfaces and remain in situ, potentially presenting a subsequent hazard. Understanding the fate of these materials in different environments is important in order to understand how long they may persist and the likely impact they may have. Understanding the hazard may allow it to be avoided or mitigated.

Experimental studies can provide information on persistence and behaviour for individual liquid-substrate pairings. However, there is a need to understand how the fundamental physical and chemical properties of substrates and chemicals determine their behaviour so that predictions can be made when extrapolating to other materials. This information is also important in selecting simulants with lower toxicity that can be used more easily in experimental tests.

1.2 Liquid surface model

We are looking to establish a model describing the time-dependent behaviour of the interactions that can account for a range of system properties. These include but are not necessarily limited to:

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

- vapour-surface interactions,
- diffusion coefficient,
- temperature.

These are not necessarily ranked in order of priority.

The model might include a number of stages to represent different phenomena, such as:

- initial impact where the droplet impacts a surface at some angle to its trajectory,
- droplet movement on the surface following impaction,
- absorption into the material,
- migration as a liquid through the material,
- evaporation from the surface and evaporation within the porous material,
- vapour interactions with the material,
- airborne transfer away from the surface.

We are interested in understanding the relevant timescales for the different processes and what properties govern them. Typical droplet sizes of interest are in the region of 0.1 mL, but we are interested in the effect of this parameter over a wider range.

Whilst liquid interaction can in principle be simulated using an explicit representation of a porous geometry, we are interested in a modelling approach that does not require such detail but can still account for the range of scales of porous structure. For example, the approach of Reis *et al.* [1] to droplets impinging normally on porous surfaces appears to be a useful one. Required model outputs include the mass of chemical within the different phases at any given time, spatial profile of the liquid, vapour and any reaction products within the surface and the emission from the surface as vapour.

We would be interested in the effect of variation in temperature over time. For example, due to diurnal heating and cooling or due to deliberate manipulation of temperature for decontamination. This might require an additional model of heat transfer for the surface and possibly its surroundings.

An understanding of the possible transfer of material due to surface contact is a secondary requirement but would also be of interest.

We have a developing experimental programme designed to collect data for idealised and real surfaces. However, this data will not be available in time for the workshop.

1.3 Specific questions

We would be interested in developing one or more models to represent the processes described above. In addition we would like to answer the following 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.

1.4 Wider topics of interest

There are a range of wider questions of interest that we would be happy to receive comments and input on.

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?

References

[1] REIS JR., N. C., GRIFFITHS, R. F., SANTOS, J. M., *Parametric study of liquid droplets impinging on porous surfaces*, Applied Mathematical Modelling, 2008, **32**(3), 341 – 361.