Novel ionic liquid dyes for fluid dynamics and decontamination studies

Merlin A. Etzold, DAMTP, Cambridge[1]
Stephen N. Marriott, Dstl, Porton Down

In this SRV, we conducted experiments to explore the suitability of a novel ionic liquid dye as a simulant in decontamination experiments of complex surfaces. The purpose was to model the removal of a viscous drop from a small gap, representing a feature typical for many man-made structures. Common surface washing techniques induce a flow within gaps aligned with the dominant flow direction, which aids the dissolution and removal of the contaminant (Figure 1). A *viscous contaminant* is a contaminant sufficiently viscous and adhesive to prevent its immediate removal by the shear forces imposed by the decontaminant film. We are not aware of any other non-hazardous dye with these properties which could act as model contaminant.

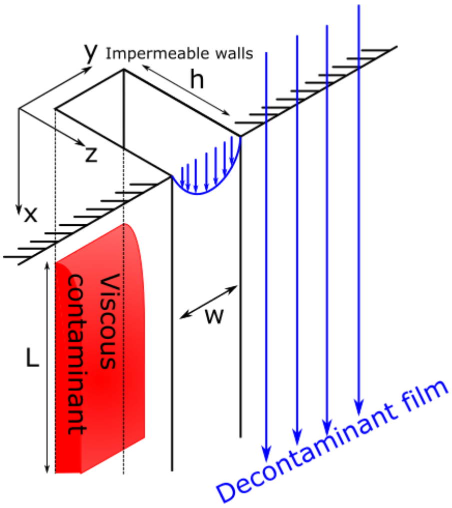

Figure 1: Sketch of the problem investigated in this SRV.

We simplified the situation described in Figure 1 by using a rectangular duct with dimensions $w = 1.3\text{mm} \times h = 40\text{mm}$. The flow was pressure-driven from an elevated reservoir and directed against gravity. This configuration was chosen so that air bubbles can easily leave the channel when the flow is switched on.

In all cases, we observed dissolution of the droplets, in some cases fragmentation, presumably due to the shear imposed by the liquid. If the droplet was not mobilised due to the shear, we found two different regimes. Depending on the flow rate and the height of the droplet (exact analysis will be supplied later), we found two different regimes.

In the first regime (Figure 2), the droplet shrinks progressively, approximately around its centre. It appears that this regime is dominated by mere dissolution at the droplet interface. Note that the shape of the droplet remains constant after a rapid initial adjustment.

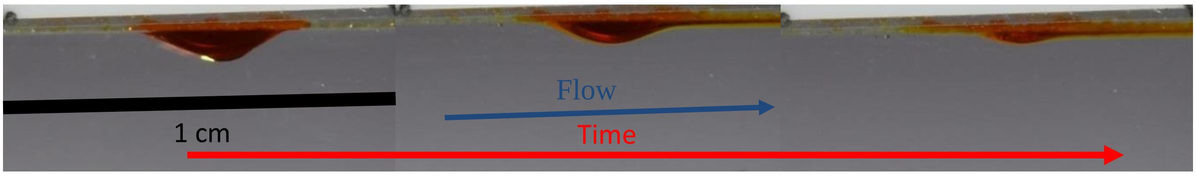

Figure 2: Typical behaviour of a flat droplet. After an initial shape adjustment, the shape remains constant and the droplet dissolves.

In the second regime, we observe the formation of a corner flow as shown in Figure 3. The initially smooth droplet is deformed and a relatively sharp corner is formed. At the down-stream edge of the droplet, a corner flow is formed. At present, it is unclear whether the corner flow enhances the mass transfer. Figure 2 indicates that the dye concentration in the corner flow is initially high, as indicated

---

[1] Contact: mae38@cam.ac.uk

by the dark red colour). As time progresses, the concentration of dye in the corner flow decreases, as indicated by the fluorescein colour. After most of the droplet has vanished, the remaining flat droplet is eroded as in the first regime. We note that some droplets seem to be eroded in the corner flow region only, whilst in other cases with corner flow the droplet is predominantly eroded at the trailing edge.

We believe that the first regime can be modelled using boundary layer theory to compute the dissolution rate at the interface, whilst for the second regime the corner will have to be taken into account.

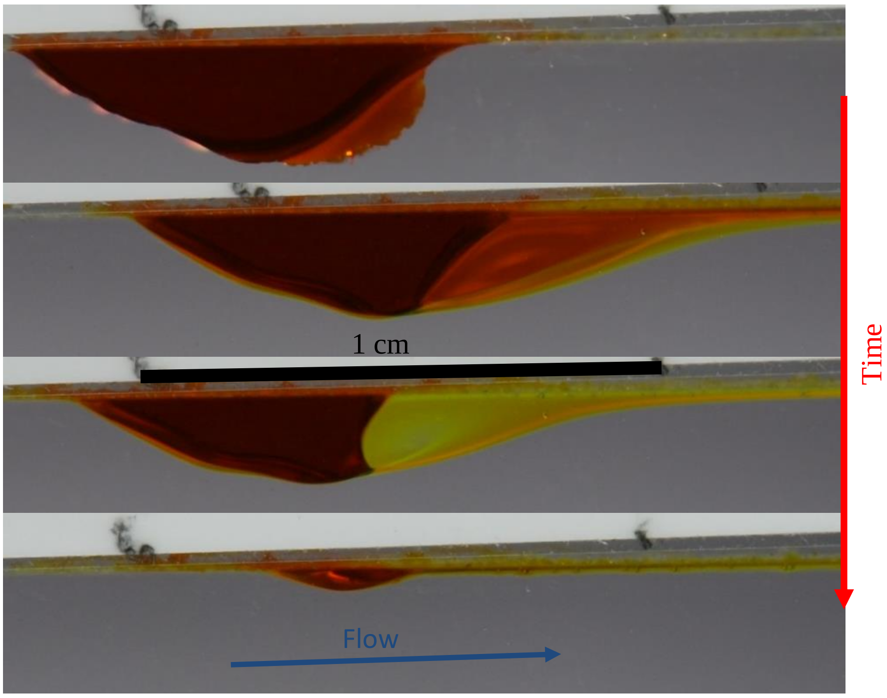

Figure 2: Typical formation of a corner-flow during droplet decontamination. The initially smooth droplet (top) is deformed towards a sharp edge (second from top) which forms a corner flow. The red colour indicates a high dye concentration in the corner

We will update this report as further analysis has been made. We will also present these results at the next SIG meeting in Cambridge.

We conclude that the dye is indeed highly suitable as a model decontaminant. It has proven to adhere strongly to the glass surface and be of good viscosity (note: the cation of the ionic liquid dye can be modified to control viscosity and solubility). The colour change of the dye during dissolution ensures easy distinction between dissolved dye and the remaining droplet. Since the dye turns essentially into fluorescein when dissolved, low concentrations can be detected. Thus, alternative strategies to track the decontamination progress by measuring the concentration of dye in the decontaminant as a function of time using UV-Vis spectroscopy can be used. Since fluorescein can be detected at very low concentrations, the dye has also potential to explore secondary contamination (spreading of the decontaminant as result of decontamination efforts). While the dye is currently not commercially available, MAE learned how to make the dye from SNM, so that it will be available in DAMTP for further experiments.