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SHORT ABSTRACT

Abstract title: MODISAFE – Modelling of Dry Gas Deposition

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Abstract text *(maximum 350 words.)*

Predicting the dispersion of toxic industrial chemicals (TICs) following a loss of containment is an important element of safety studies across a number of industries. Modelling is widely used to investigate various aspects of the release and dispersion process. The release characteristics are highly variable, from different storage types (tanks, pipelines, rail cars, tanker trucks), to different locations (military bases, industrial facilities, fertiliser plants, or in transit).

One variable influencing dispersion behaviour is the characteristics of the ground or substrate. There can be a transfer of material from the cloud via the process of dry deposition, thus removing mass from the cloud and potentially reducing the hazard extent. Dry deposition is generally parameterised by a deposition velocity, which accounts for a flux of gas to the ground. The deposition velocity is highly dependent on the interaction between the substrate and the chemical. It is near-zero for inert chemicals but increases with more reactive chemicals and also depends on the substrate type (concrete, soil, grass, etc.).

There is uncertainty around the extent to which dry deposition influences cloud behaviour. Estimates for the amount of material removed via deposition have been presented in the literature, often using simplified modelling approaches which do not take saturation into account. If a surface becomes saturated, it is no longer able to absorb contaminant. Any method without a saturation mechanism could lead to an over-prediction in deposition, and therefore an under-prediction in the cloud's extent.

In dispersion models, setting the correct deposition velocity and 'saturation control' is important. Recent experiments undertaken at the University of Arkansas provide experimental data for ammonia and chlorine dispersion over various substrates and

vegetation. The current study incorporates these experimental findings, and presents a saturation-deposition sub-model for application within a CFD model. This model is compared to a range of benchmark cases and can be applied to more complex, bespoke geometries of specific interest. This work forms part of the deposition work package within the MODISAFE project.