

**23rd International Conference on
Harmonisation within Atmospheric Dispersion Modelling
for Regulatory Purposes
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EXTENDED ABSTRACT

MODISAFE – Project Overview

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Introduction

MODISAFE (Modelling of Sources and Agent Fate) is an international collaborative project undertaking research on three technical topics related to atmospheric dispersion of hazardous substances: evaporation from porous and non-porous substrates, deposition and resuspension, and buoyant dispersion in urban areas.

MODISAFE is a collaboration between the Swedish Defence Research Agency (FOI), the Norwegian Defence Research Establishment (FFI), the French Direction générale de l'armement (DGA), the GB Health and Safety Executive (HSE), the French Institut national de l'environnement industriel et des risques (INERIS) and the University of Surrey, UK.

The overall aim of the project is to improve our understanding of source characteristics, loss processes and the fate of agents after release. In each research area, new experimental data have been produced, which will be made publicly available.

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Evaporation from porous and non-porous substrates

The amount of agent that evaporates from a surface is dependent on the absorption properties of that surface. An experimental programme investigating the evaporation of pools and droplets from 1 m² substrates (two concrete surfaces with different porosities and a glass surface) has been carried out at medium scale in the INERIS fire tunnel in Verneuil-en-Halatte, France. Substances with a wide range of vapour pressures were studied: acetone, *n*-heptane, *n*-octane and TEP (triethyl phosphate).

The experimental data have been simulated using integral and CFD models. Figure 1 shows the experimentally measured vaporisation rate as a function of time for a pool of *n*-heptane on a glass substrate. The wind speed was 1 m/s at a height of 1 m. Also shown are simulations from the integral models GASP (Webber, 1990), SLOPS (Batt and Tickle, 2020) and PEARL (Björnham, 2011), and CFD predictions using the RANS (Reynolds-averaged Navier-Stokes) turbulence model coupled to the Brutsaert (1975) model for pool evaporation. SLOPS is an implementation of the GASP model with an extension to include treatment for porous surfaces using the Green-Ampt model for infiltration. For evaporation from an impermeable glass substrate, the SLOPS and GASP outputs are almost identical.

All the model predictions are in good agreement with the experimental data for the initial phase of the evaporation up to 4 hours. At this time, the pool starts to recede, leading to a decrease in the vaporisation rate. This behaviour is captured by the PEARL model, but pool shrinkage is not incorporated in the GASP or SLOPS models. The CFD simulation did not model this stage, but rather stopped after 2 hours during the steady-state plateau.

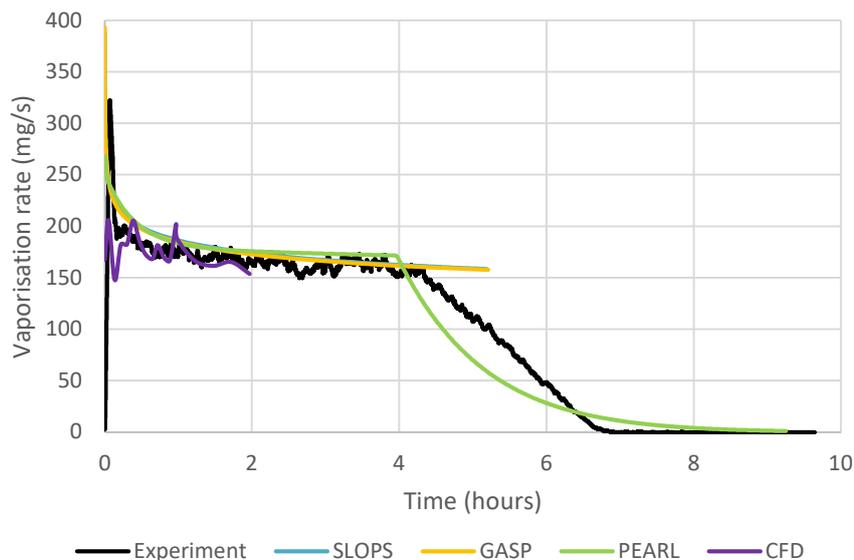


Figure 1 Experimental measurements and model predictions for evaporation of *n*-heptane from a glass substrate for a wind speed of 1 m/s at a height of 1 m.

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Deposition and resuspension

The research on deposition and resuspension aims to better understand the fate of biological aerosols or radioactive particles dispersed in an urban environment. A preliminary study of the deposition of particles on horizontal and vertical building surfaces has been carried out at HSE's dust tunnel in Buxton, UK. A schematic of the dust tunnel is shown in Figure 2. This study focused on methodology development and investigation of sampling methods.

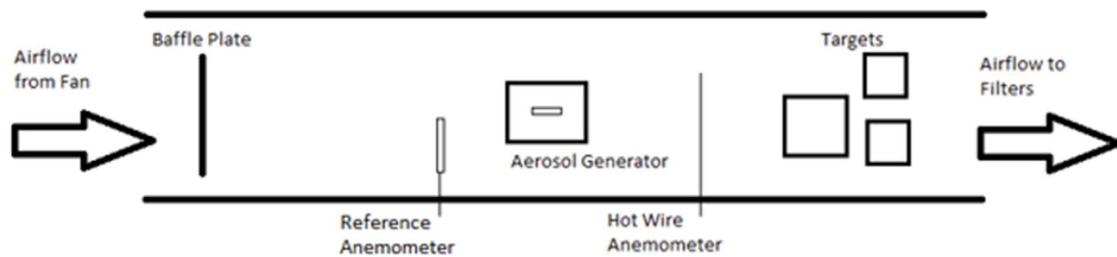


Figure 2 Schematic of HSE's dust tunnel, indicating key internal features. Top view (not to scale).

In parallel with this, modelling methodologies have been developed to simulate the deposition of particles on a small array of blocks, accounting for factors such as the roughness and orientation of the surfaces. Lagrangian and Eulerian approaches have been used to simulate the deposition of particles on vertical and horizontal walls.

Figure 3 shows simulations of a theoretical test case in which particles of diameter $10\ \mu\text{m}$ are injected vertically upwards from the floor at a mass rate of $100\ \text{mg}/\text{min}$. The bulk flow speed through the domain is $1\ \text{m}/\text{s}$ and the blocks are assumed to have a surface roughness of $1\ \text{mm}$. The left-hand panel shows the predictions from a hybrid RANS/Lagrangian model implemented in OpenFOAM, with a deposition velocity based on the Giardina and Buffa (2018) model. The right-hand panel shows the results obtained using a dispersion transport model based on the Diffusion Inertia Model (DIM) of Zaichik et al. (2010), with particle deposition modelled using the approach of Nerisson (2009).

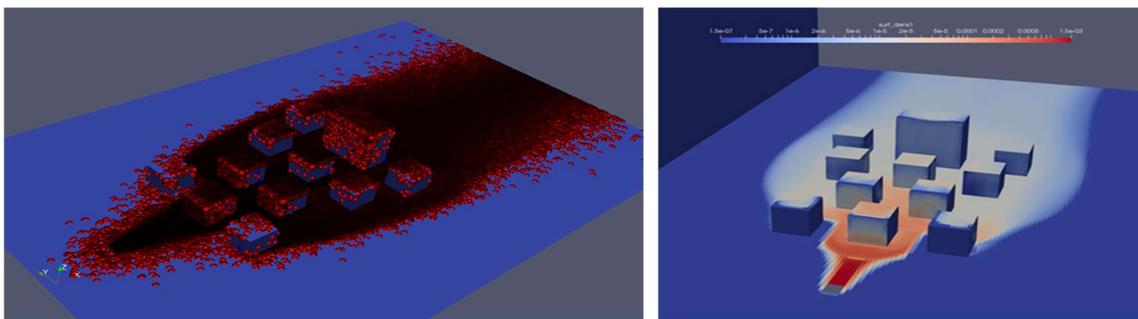


Figure 3 Simulations of particle deposition on an array of blocks using a hybrid RANS/Lagrangian model (left-hand panel) and a Diffusion Inertia Model (right-hand panel).

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Buoyant dispersion in urban areas

The final research area aims to improve understanding of the transport of positively and negatively buoyant gases through an urban environment. This has been studied in the EnFlo wind tunnel at the University of Surrey, UK, using a scale model of a 2 km² area of central Oslo, shown in Figure 4. This study builds on the MODITIC project (Modelling the dispersion of toxic industrial chemicals in urban environments, Endregard et al., 2016).



Figure 4 Scale model of central Oslo in the EnFlo wind tunnel.

CFD simulations of the experimental scenarios have been carried out using RANS equations and large eddy simulation (LES). Figure 5 shows the predicted gas concentrations from a RANS k- ϵ and a LES simulation for neutral gas dispersion from a source at the intersection between street canyons. For such a complex geometry, there is generally good agreement between the experimental data and the CFD predictions over the full range of scenarios modelled. LES performs better than RANS, particularly for predictions of concentration and turbulent kinetic energy.

Conclusions

For all three topics, the experimental outputs have been used to enhance understanding of the underlying physical processes that are occurring and to improve modelling capability. They provide a platform for model intercomparison exercises and model validation.

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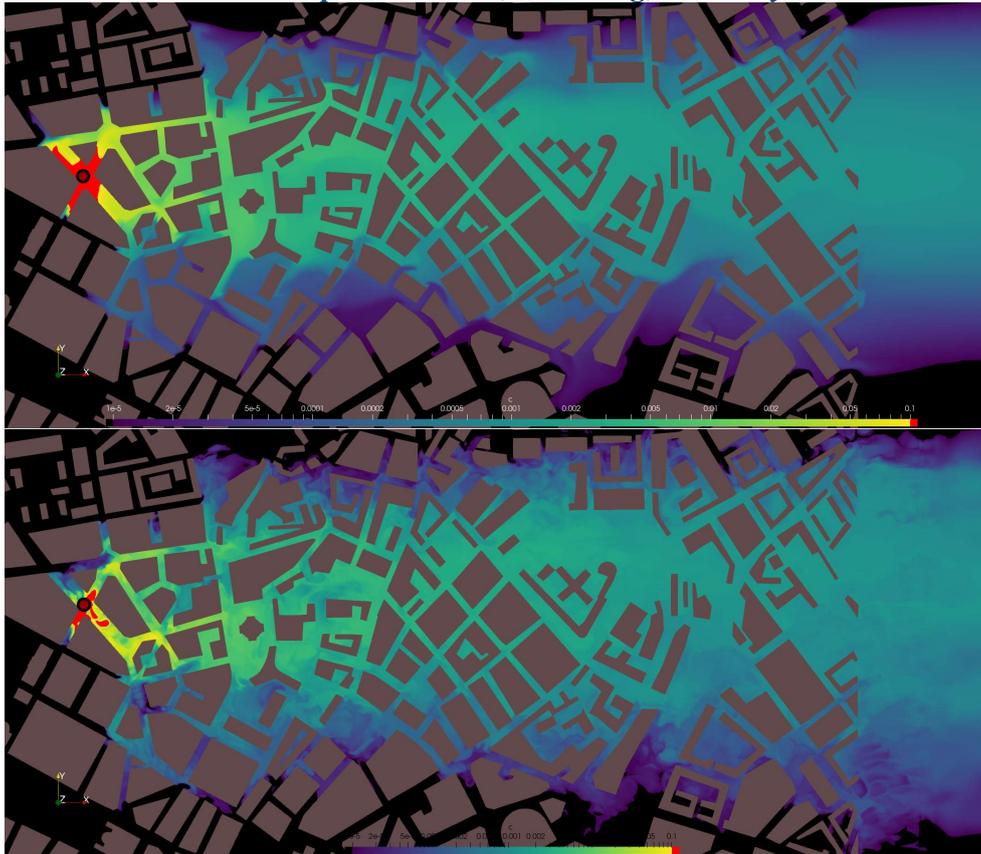


Figure 5 CFD simulations of neutral gas dispersion from a source at the intersection between street canyons (shown as a circle on the figure). The RANS (k - ϵ) and instantaneous LES predictions are shown in the top and bottom panels, respectively.

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