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EXTENDED ABSTRACT

MODISAFE - Modelling of evaporation from porous and non-porous substrates

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Introduction

Time dependent simulations of pool evaporation are an important source term when performing dispersion modelling. In this presentation, the capability of models to predict the characteristics of pool evaporation is assessed. Specifically, simulations of the MODISAFE pool and droplet experiments (Leroy et al., 2025) were performed by a consortium of four partner organisations using a range of tools (empirical, analytical, integral and CFD models). The basis of comparison is the evaporation rate and pool temperature as these values are key parameters for ensuring that the subsequent dispersion modelling is valid.

Models incorporate and describe the contributing physical processes in various ways. For pool evaporation, the liquid temperature, which depends on many different modes of heat transfer, is an important underlying factor affecting the evaporation rate and was therefore studied explicitly. For droplet evaporation, the geometric shape of the droplets on non-porous substrates is an important factor for accurately predicting evaporation rates. When porous substrates are considered, additional and more complex physical processes must be considered. For pools, this includes mass transport within the substrate as the pool dries out. For droplets, this includes the change in effective surface area as the droplets are absorbed into the substrate.

The bases of the applied models are presented to provide an understanding of the differences in assumptions and methodology. By comparing model outputs to experimental data, insights are gained into the capabilities of different evaporation models under varying conditions and the effects of differences in model formulations.

Models

The model comparison exercise compared model predictions for currently used models, as well as models developed during the MODISAFE project. The modelling tools used in this study are now detailed.

HSE models

Gas Accumulation over Spreading Pools (GASP) and Spreading Liquid Over Porous Surfaces (SLOPS) are both integral models that can predict the spread and vaporisation of hazardous liquids that form pools due to a loss of containment event. GASP was developed by Webber (1990) and is currently maintained by ESR Technology. GASP assumes an axisymmetric pool and can model pool spreading and vaporisation on both land and water. Other modelling assumptions in GASP are that the stability of turbulent air flow above the pool is neutral and the thickness of the ground is semi-infinite. SLOPS (Batt, 2020) is based on the fundamental land spreading and vaporisation model of GASP, with an extension to include treatment for porous surfaces using the Green-Ampt model for infiltration.

DGA model

Code Saturne v6.0 (EDF) CFD proposes several turbulence models. The RANS turbulence model k-ε linear production model was chosen, coupled to the Brutsaert model (Brutsaert, 1975) for pool evaporation on impervious surfaces, which expresses the Dalton number (mass transfer coefficient) in terms of local Re and Sc numbers. For the pool infiltration into a porous medium, a Washburn type law was used and for subsequent evaporation from the porous surface, a home-made model was developed, based on the “step porous” approach. Regarding droplet evaporation, the Brutsaert expression is still used over the droplet’s surfaces. Evaporation of droplets from a porous medium is handled from an initial instantaneous infiltration shape, and the subsequent receding front is obtained from a bimodal or step like porous formulation, depending on its sorption characteristics. The evaporation is driven by vapor diffusion inside the porous medium and transfer into the interfacial boundary layer (Daïan, 2014).

FFI model

Vik and Reif (2011) developed an evaporation model which is sensitive to boundary layer turbulence. The model is developed from first principles and the friction velocity is naturally included. Temperature effects are currently only taken into account implicitly through model parameters. Because of this, the model is expected to be more suited for relatively low volatile substances than for high volatility substances, since the thermal effects are relatively more important for substances with low boiling point. The model does not take substrate parameters into account. The model can be used analytically, but can also be included in a CFD analysis, where the friction velocity from the simulation is used as input to the evaporation calculation.

FOI model

The Swedish Defence Research Agency, FOI, has previously developed a model for pool evaporation called Pool Evaporation with Atmosphere and gRound Linkages (PEARL) (Björnham et al., 2011). The model can handle either pure substances or mixtures leaking from a container, and the subsequent open pool evaporation using the mass transfer formulations presented by Sutton (1934) and Pasquill (1943). Since pool temperature is a key component, particular emphasis is placed on representing the heat budget. The heat budget components included in PEARL are solar radiation, convective heat transfer from the air, longwave radiation, latent heat loss due to evaporation, and heat transfer through the ground. PEARL was further developed during the MODISAFE project to include effects of porous substrates. The method for evaporation of sub-surface liquid considers two stages: Stage I, where evaporation mainly occurs at the surface and liquid is supplied by channels connecting to the wet front, and Stage II, where evaporation slows as these channels are disrupted and vapour diffusion becomes the limiting process. In total, PEARL includes three different phases of the evaporation process for a pool on porous substrate, all connected into a seamless simulation providing a continuous estimate of the evaporation rate.

Experiments

An experimental campaign investigating evaporation was conducted as part of the MODISAFE project (Leroy et al., 2025). This involved a series of pool and droplet evaporation experiments in a medium-scale wind tunnel (‘fire gallery’) at an INERIS facility in France. A key motivation for this effort was to investigate evaporation from porous substrates, as this is a common scenario in uncontrolled outdoor releases of hazardous materials. The experimental programme was designed to examine the impact of local conditions given an imposed wind. The conditions included variations in substrate porosity (using glass, permeable concrete and coated concrete), the type of substance and the state of the liquid (droplets/pools). A total of 30 experimental tests (24 of which featured unique setups) were carried out, resulting in a comprehensive data set.

Table 1 Experimental test case conditions prioritised

Test #	Type	Substance	Substrate	U (m s^{-1}) at 1 m	T_a (°C)	T_s (°C)
1	Pool	Heptane	Glass	1	5.3	6.2
7	Pool	Acetone	Concrete	2	12	10.6
8	Pool	Heptane	Concrete	1	7.1	15.7
11	Pool	Heptane	Coated Concrete	2	8	7.8
22	Pool	Acetone	Concrete	1	4.6	3.6
15a	Droplet	Heptane	Glass	1	13.6	13.6
16	Droplet	Octane	Concrete	1	12.2	12.2
19a	Droplet	Heptane	Concrete	1	6.9	6.9

Of the 30 experimental tests performed, a subset consisting of 8 tests was prioritised using the models described previously. The tests were selected to span the key experimental parameters: pool/droplet, substance, substrate type and environmental conditions. The conditions of the tests are given in Table 1.

Model Comparison

Preliminary model predictions have been produced and compared to the experimental data for the different tests. Due to the time needed for the CFD simulations, only the model predictions for test 1 are included here.

Test 1 – n-heptane pool on glass

The model evaporation rate and temperature predictions compared to the experimental measurements for test 1 are shown in Figure 1. For the n-heptane pool experiments, the evaporation measurements show three distinct regimes:

1. An initial "short" thermal equilibrating regime (0 h – 0.1 h)
2. A steady evaporation regime (0.1 h – 4.3 h)
3. Pool shrinkage regime (4.3 h – 6.4 h)

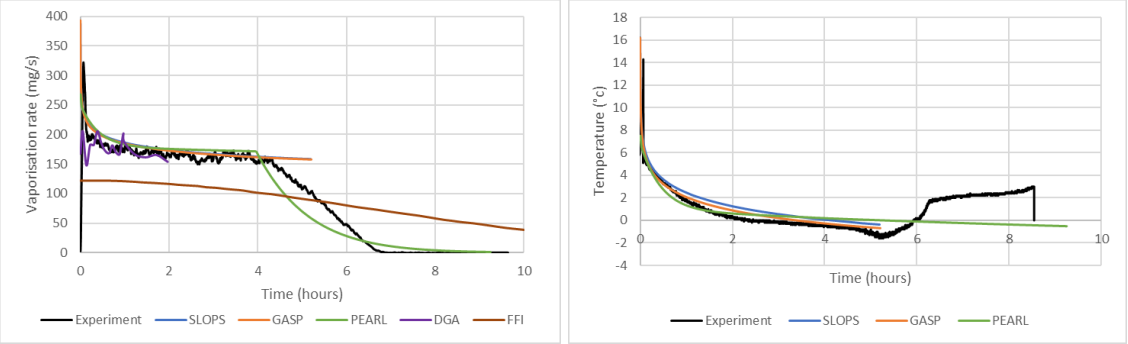

Figure 1 Experimental measurements and model predictions for Test 1, left - evaporation rate, right - pool temperature.

During the initial phase, the measurements indicate that the initial liquid temperature value used within some model assumptions may be too low. A temperature greater than the ambient, as assumed in GASP, SLOPS and PEARL, gives better agreement for the pool temperature in the very early stages.

The steady evaporation rate regime in test 1 is predicted well by each of the model approaches, with GASP and SLOPS giving near identical predictions. The GASP and PEARL models have different treatment of the heat transfer to the pool but give good agreement with the experimentally measured value for test 1. FFI's model uses a prescribed initial temperature that does vary throughout the simulation. DGA's CFD model simulated the first 2 hours of test 1, achieving good agreement while capturing the transient air flow over the pool surface, whereas the other models initially prescribe an assumed boundary layer profile.

Pool recession starts at approximately 4.3 hours, resulting in a decrease in vaporisation rate. This is not captured by GASP or FFI's model and the CFD model was not run to the point where this occurred. The assumption that the pool will recede axisymmetrically leads to an exponentially decaying vaporisation rate, as seen in the PEARL model predictions, however, a linear decay is observed experimentally. This indicates other receding phenomena at play, such as possible sloping of the substrate during the experiments.

Conclusions

A model comparison study has been performed comparing predictions to an experimental dataset for both pool and droplet vaporisation on porous and non-porous substrates. The preliminary modelling predictions have demonstrated the importance of such a study, highlighting the impact of particular model assumptions across the different modelling approaches and how these assumptions influence the predictions when considering a medium scale experimental setup. A further detailed interrogation of the numerical and experimental results for droplets and porous substrates is to follow. This will dive deeper into the influence of model parameters and provide insight into which model components need consideration when modelling.

References

Batt, R. and Tickle, G. (2020). Development of a model for Spills of Liquids On Porous Surfaces (SLOPS). https://www.icheme.org/media/16859/hazards-30-paper-05-batt.pdf.

Björnham, O., Burman, J., Hammarström, L.-G. and Thaning, L. (2011) Source model for a mixture of liquids. Swedish Defence Research Agency.

Brutsaert, W. (1975). A theory for local evaporation (or heat transfer) from rough and smooth surfaces at ground level. Water Resources Research vol. 11, No4.

Daïan, J. F. (2014) Equilibre et transfert en milieu poreux. hal-00452876.

Leroy, G., Gray L., Cruse, H., Burkhart, S., Björnham, O., Vik, T. (2025). MODISAFE – Experimental studies of evaporation from porous and non-porous substrates. HARMO23, Hamburg, 2025.

Pasquill, F. (1943) Evaporation from a plane, free-liquid surface into a turbulent air stream. Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences 182; 75-95.

Sutton, O. G. (1934) Wind structure and evaporation in a turbulent atmosphere. Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character 146; 701-722.

Vik, T and Reif B A (2011). Modeling the evaporation from a thin liquid surface beneath a turbulent boundary layer. Int J. Therm. Sci. 50, 2311-2317.

Webber, D. M. (1990). A Model for Pool Spreading and Vaporisation and its Implementation in the Computer Code G*A*S*P. (SRD Report: SRD R507).