# Investigating The Influence of Vapour Pressure Correlations in Urea-Water Spray Simulations

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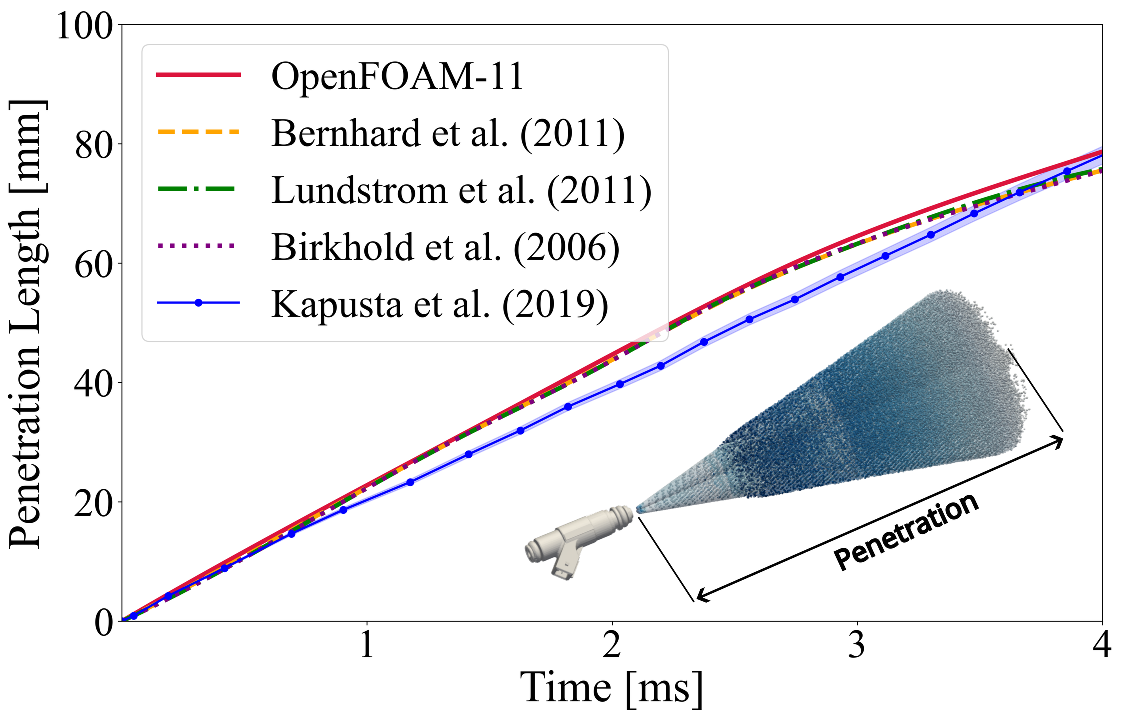
## Introduction

**Motivation:**

- Urea–water solution (UWS) is widely recognized as a promising agent for reducing NOx emissions in current and future fuel systems.
- Urea deposits challenge exhaust after-treatment systems; this work examines UWS spray evaporation to help address this issue.
- This study investigates the feasibility of using 0D multi-component evaporation models to predict global spray characteristics. Saturation vapour pressure correlations reported in the literature are benchmarked against the in-built vapour pressure correlation available in OpenFOAM-11.
- Exploring the sensitivities of multi-component evaporation models within Lagrangian–Eulerian spray simulations.

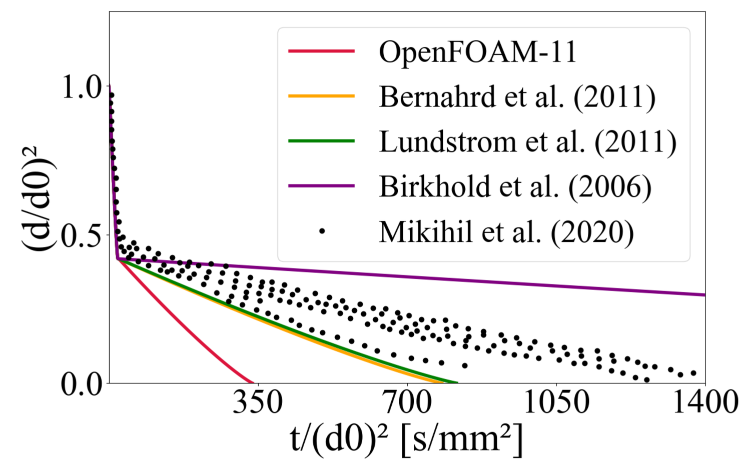
## Simulation setup and Validation

- Experimental setup and data from Kapusta et al. [1] are used to define the computational domain and validate the spray. UWS (32.5 wt% Urea) at 298 K is injected into air (77.7% $N_2$ & 22.3% $O_2$) at 573 K.
- A Lagrangian-Eulerian framework is used to model the two-phase flow.
- Simulation initialized with experimentally obtained droplet distribution, and injection profiles [1].
- Secondary breakup models and droplet coalescence are ignored.
- Turbulence is resolved through an Implicit LES method.

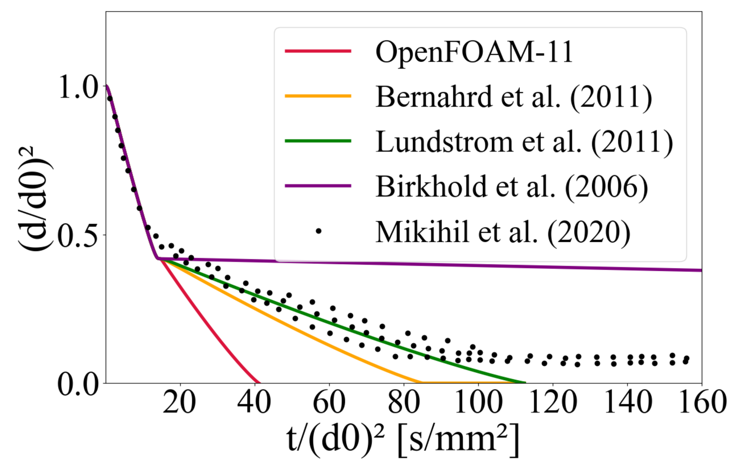



## Multi-component droplet evaporation (0D Results)

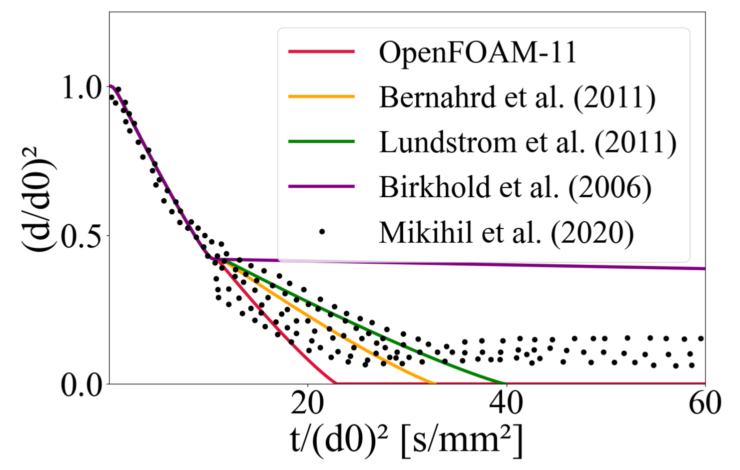
- Evaporation of a multi-component droplet under convection evaluated through a 0D MATLAB code implemented by Mikhil et al. [2].
- Saturation Vapour pressure correlations proposed by Lundström et al. [3], Bernhard et al. [4], and Birkhold [5] compared with the in-built OpenFOAM-11 correlation for the operating range of simulation (423 K - 573 K).



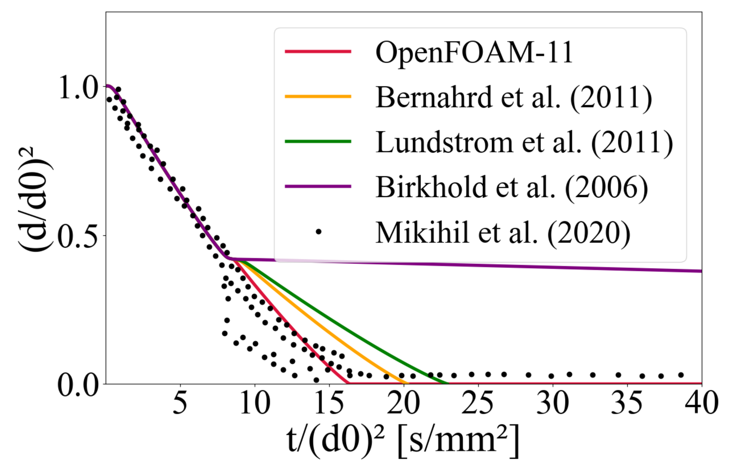

(a) $T_\infty$ = 423 K, $P_\infty$ = 1 bar, v = 1.9 m/s, $d_0$ = 1 mm




(b) $T_\infty$ = 473 K, $P_\infty$ = 1 bar, v = 2.4 m/s, $d_0$ = 1 mm



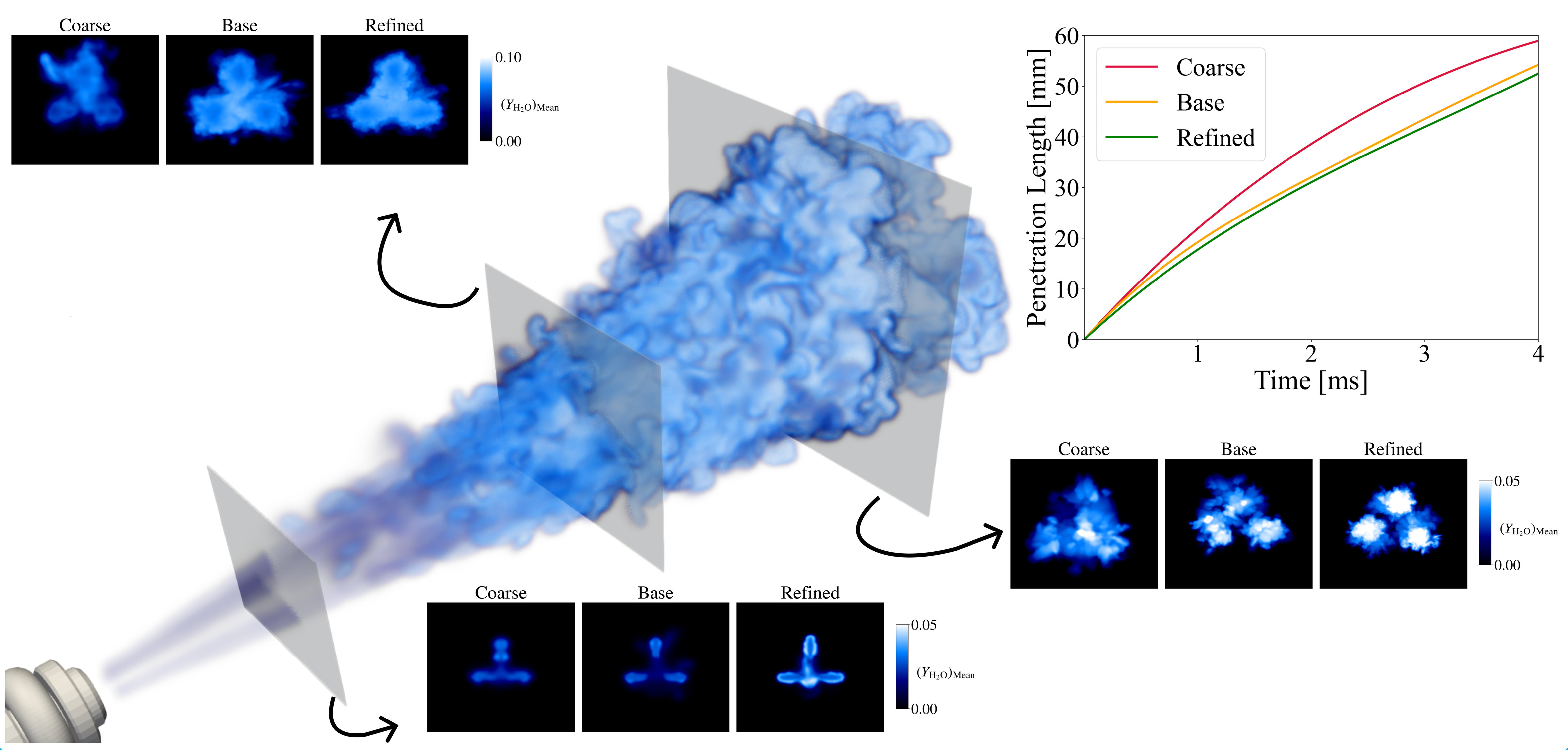

(c) $T_\infty$ = 523 K, $P_\infty$ = 1 bar, v = 2.8 m/s, $d_0$ = 1 mm




(d) $T_\infty$ = 573 K, $P_\infty$ = 1 bar, v = 3.1 m/s, $d_0$ = 1 mm

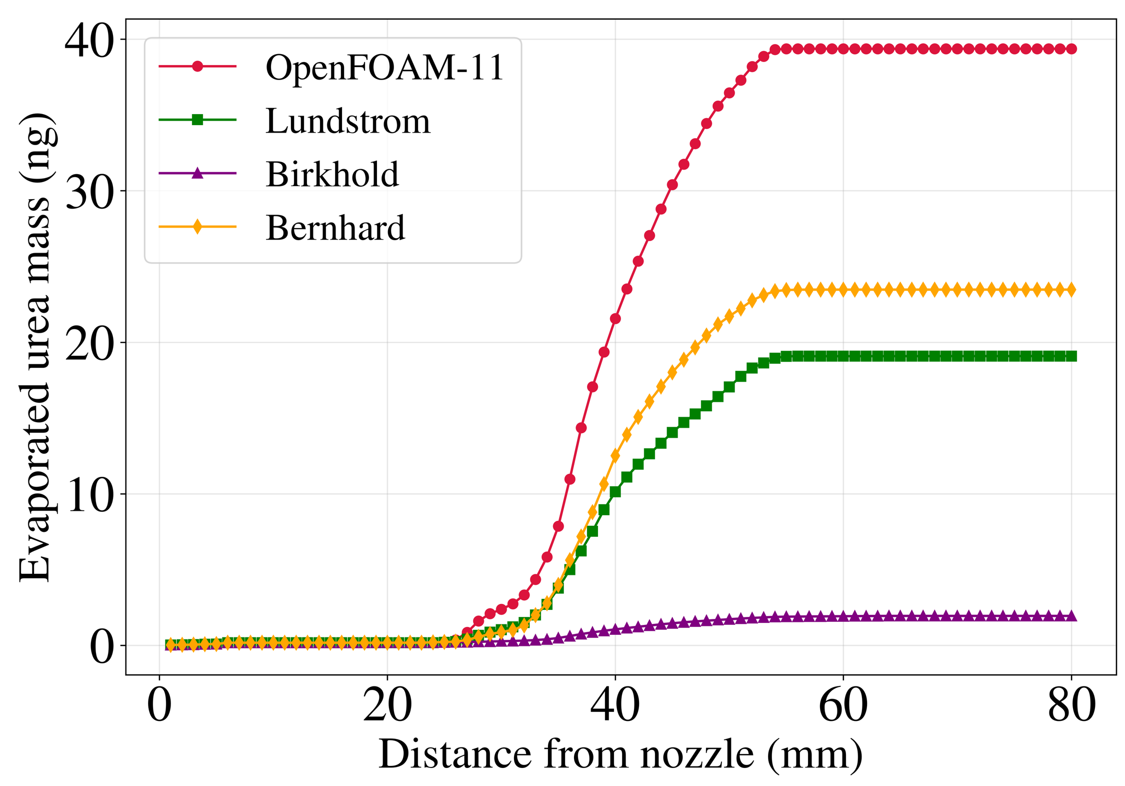
## Verification

- 3 meshes of cell sizes 250 µm (Coarse), 125 µm (Base), 62.5 µm (Refined) used to verify grid independence of results.




## Droplet evaporation (3D Results)

- Global evaporation behavior was assessed by tracking the cumulative evaporated urea mass from the nozzle onward — results shown for 4 ms of injection.
- Droplet evaporation behavior predicted by the CFD model is consistent with the 0D observations.




## Conclusions & Future Work

The study indicates that simplified 0D models are successful in predicting global evaporation characteristics. Furthermore, such tools show promise in comparing the evaporation of single droplets and droplet clusters.

Current status of research is steered towards understanding the effect of droplet sizes in the modeling of Urea-water sprays.

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Flexible Clean Propulsion Technologies

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