Ammonia Sprays and Flash Boiling

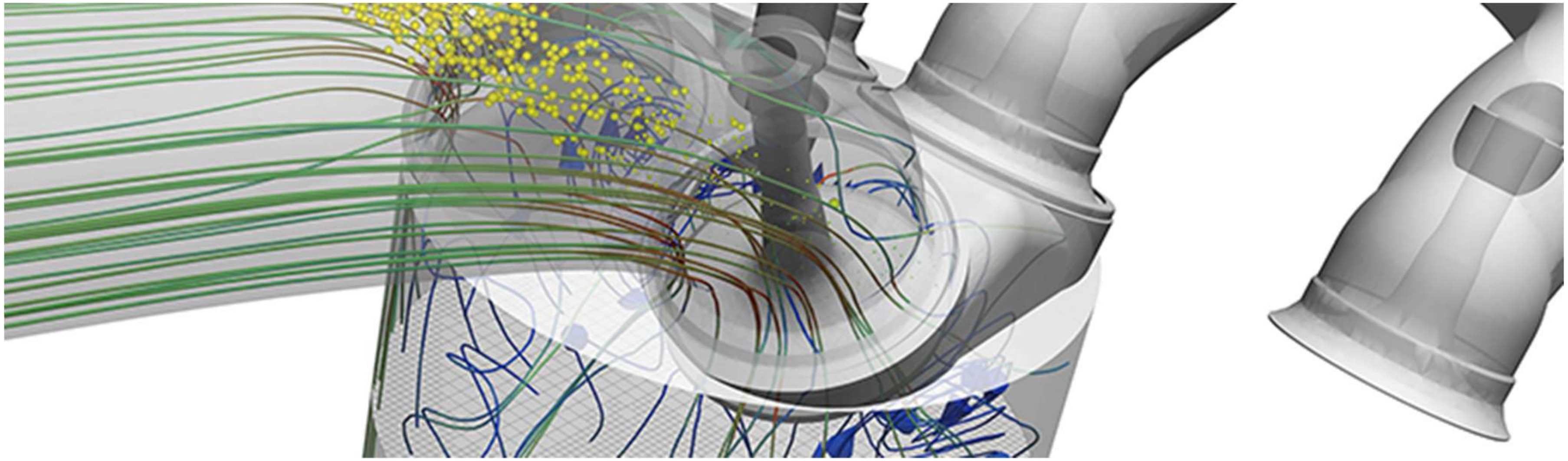
Felix Leach

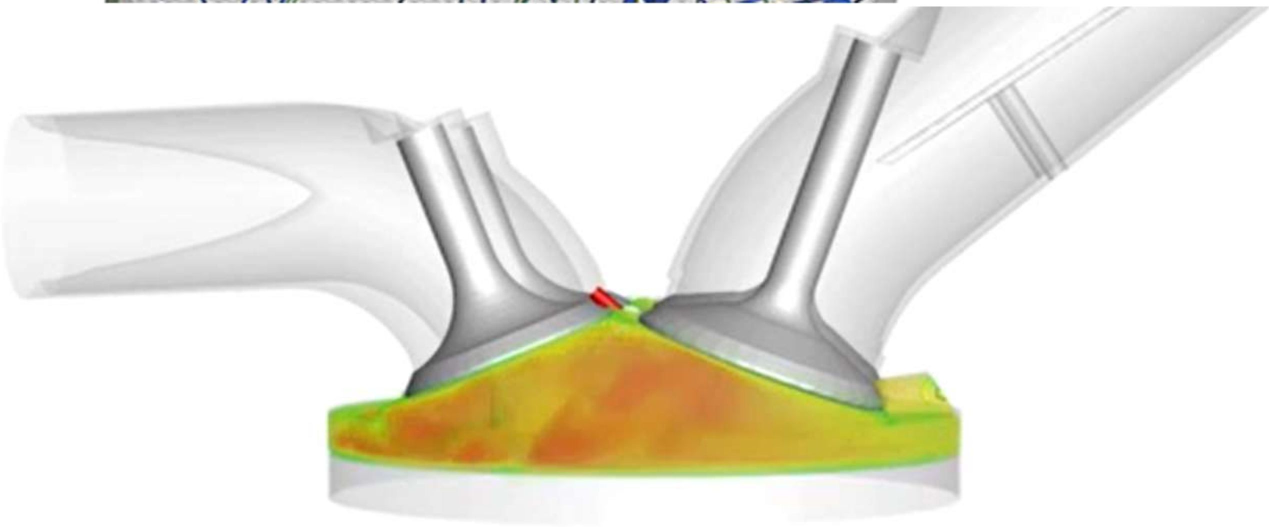
$MariNH_3$ Conference 2026

17 June 2026

DEPARTMENT OF ENGINEERING SCIENCE
UNIVERSITY OF OXFORD

How do we design new engines today?





What do we need to enable this design?

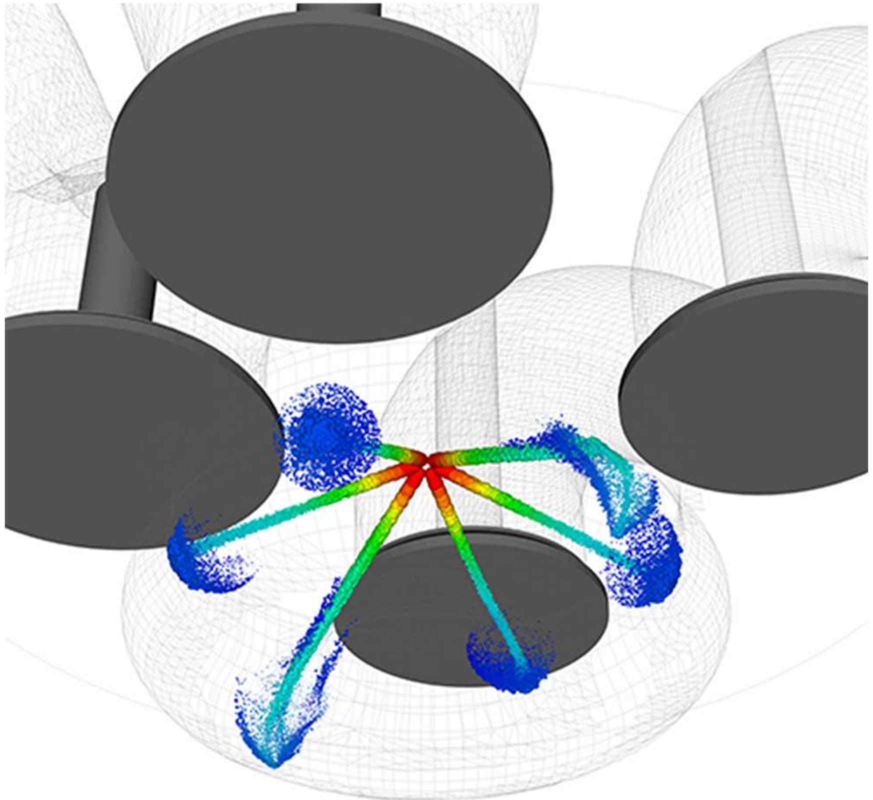
- Obtain fundamental data at as realistic as possible conditions
  - Mixing
  - Temperature
  - Combustion

- Model these fundamental experiments
  - Do existing models work?

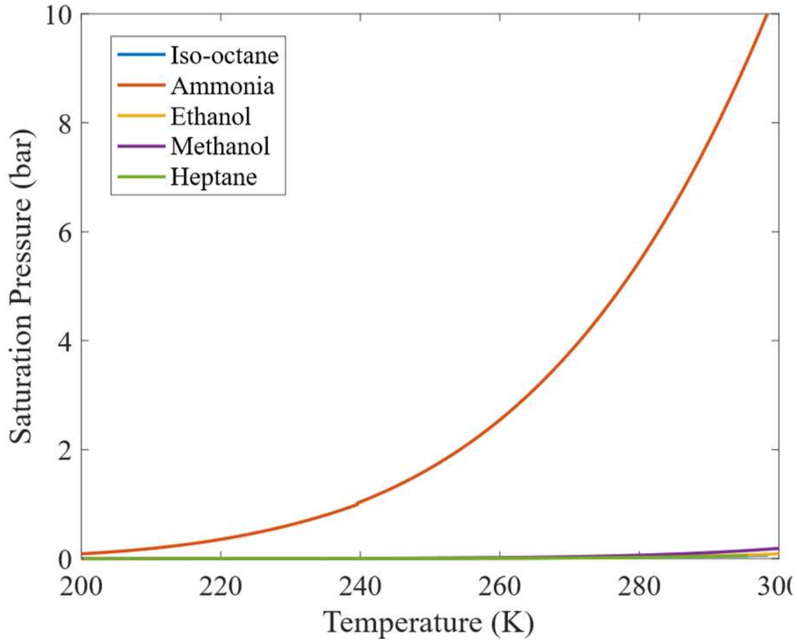
- Design in the virtual world

Why direct liquid ammonia injection?

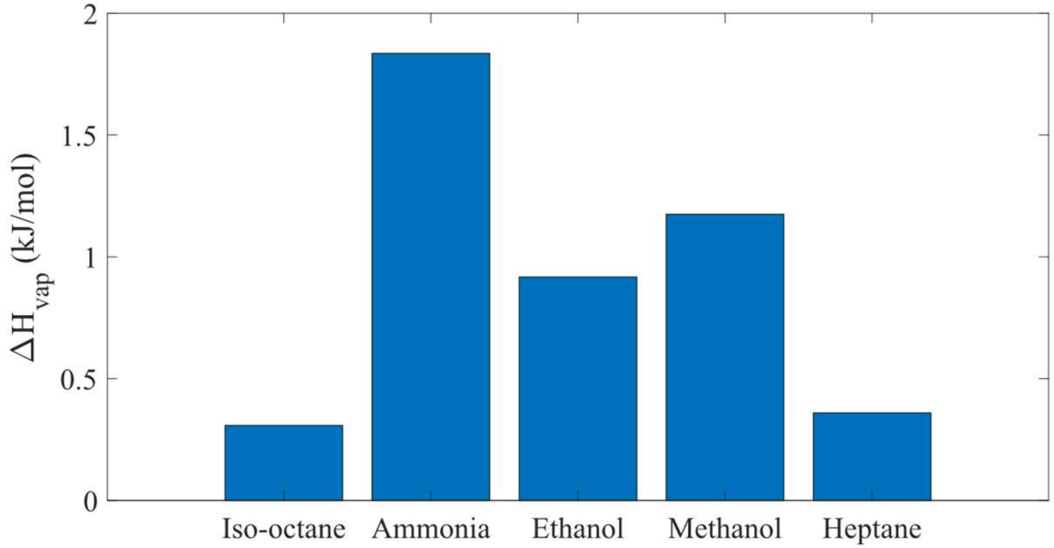
- Benefits:
    - Provide sufficient fuel quantity within limited injection window
    - Increase volumetric efficiency and power density
- Challenges:
    - Different mixing and evaporation processes compared to hydrocarbon fuels
    - New spray models are required
    - Lack of experimental data for CFD model validation



Ammonia



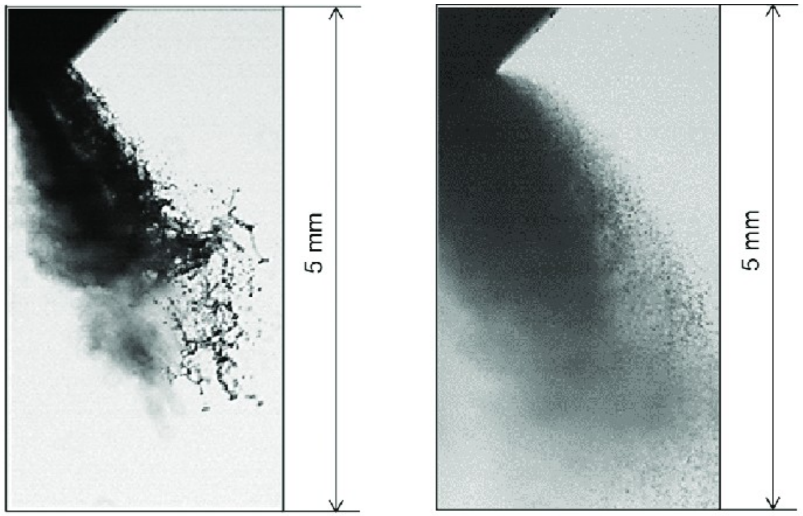
Saturation Pressure (bar)
Temperature (K)
Iso-octane
Ammonia
Ethanol
Methanol
Heptane
0
2
4
6
8
10
200
220
240
260
280
300



ΔH_{vap} (kJ/mol)
0
0.5
1
1.5
2
Iso-octane
Ammonia
Ethanol
Methanol
Heptane

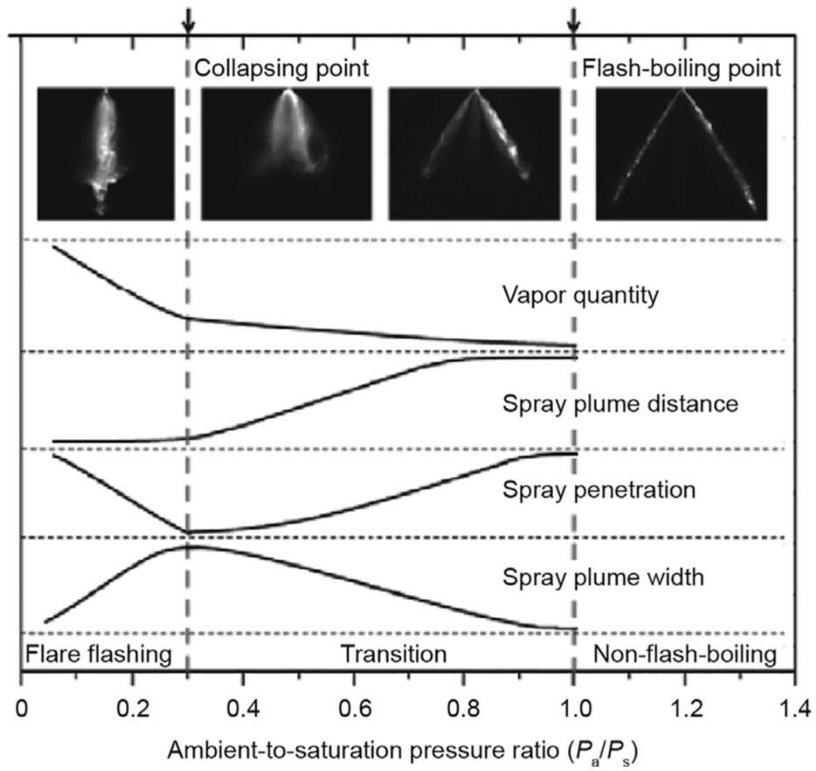
Flash Boiling Sprays

Is this a good thing?



n-heptane spray
P_{inj} =3 MPa, T_{fuel} = 25 °C,
P_a = 100 kPa, t_{ASOI} = 40 μs
(a)

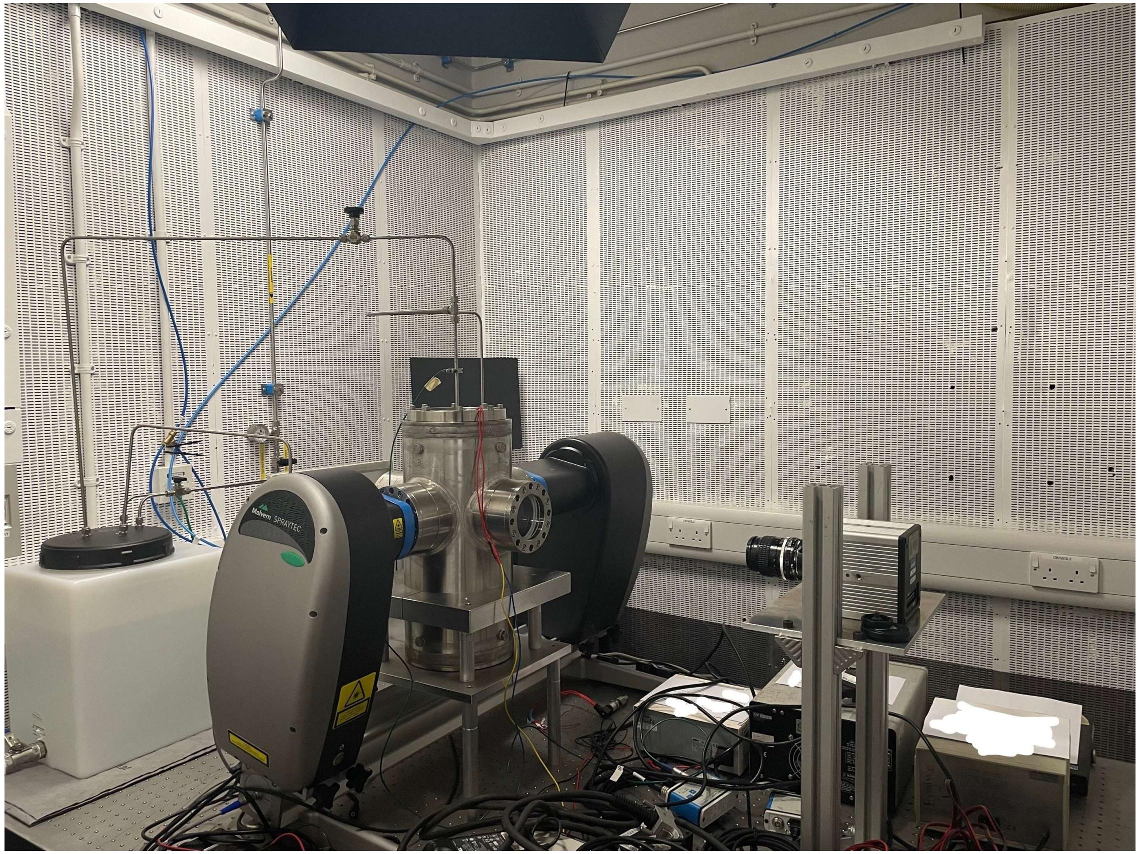
n-heptane spray
P_{inj} =3 MPa, T_{fuel} = 90 °C,
P_a = 100 kPa, t_{ASOI} = 40 μs
(b)



Arai, Masataka. (2019). The Possibility of Active Attitude Control for Fuel Spray. Engineering. 5. 10.1016/j.eng.2019.04.010.

Ammospray project

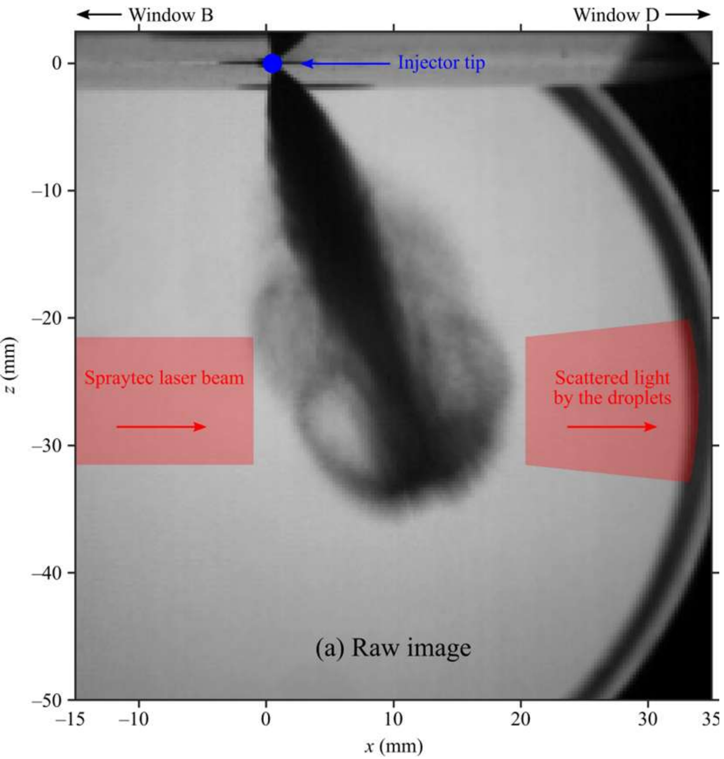
- EPSRC funded project (2022-25)
- New ammonia spray lab in Oxford
- Experimental spray measurements of ammonia with 3x different injectors:
  - Single hole
  - Bosch HDEV 5.1
  - ECN Spray M
- Modelling of ammonia sprays
  - Evaporation
  - Nozzle boundary conditions
  - Thermal Breakup



Experimental work

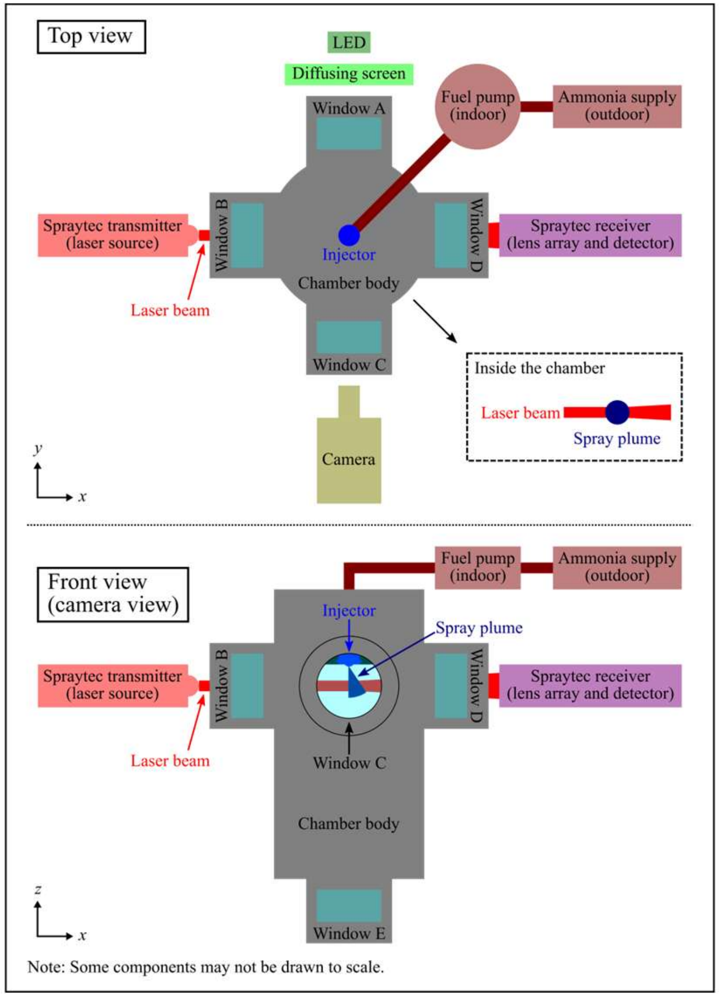
Ammonia spray measurement

- High speed backlit images (10 kfps) for spray morphology
- Droplet size distribution (SMD) in spray plumes measured by Malvern SprayTec at the same sampling rate
- Mass flow rate measurement using pressure method



Shen & Leach: SAE 2024-01-2618

Parameter	Value
Chamber dimensions	160 mm id, 282 mm height, 7.2 L
Window dimensions	80 mm
Ambient gas	N_2
Chamber pressure	1-15 bar
Chamber temperature	20°C
Injectors used	Bosch HDEV single hole, hollow cone Bosch HDEV 5.1 “GDI” (6-hole) ECN Spray M (8-hole)
Ammonia pressure	50-280 bar
Ammonia temperature	Ambient-110°C
Injection duration	0.1-7 ms
Camera	Photron FASTCAM-1024PCI, up to 125,000 fps, we use 10,000 fps (0.25 mm/pixel)
Spray particle sizing	Malvern Spraytec (10 kHz, 10 mm beam)

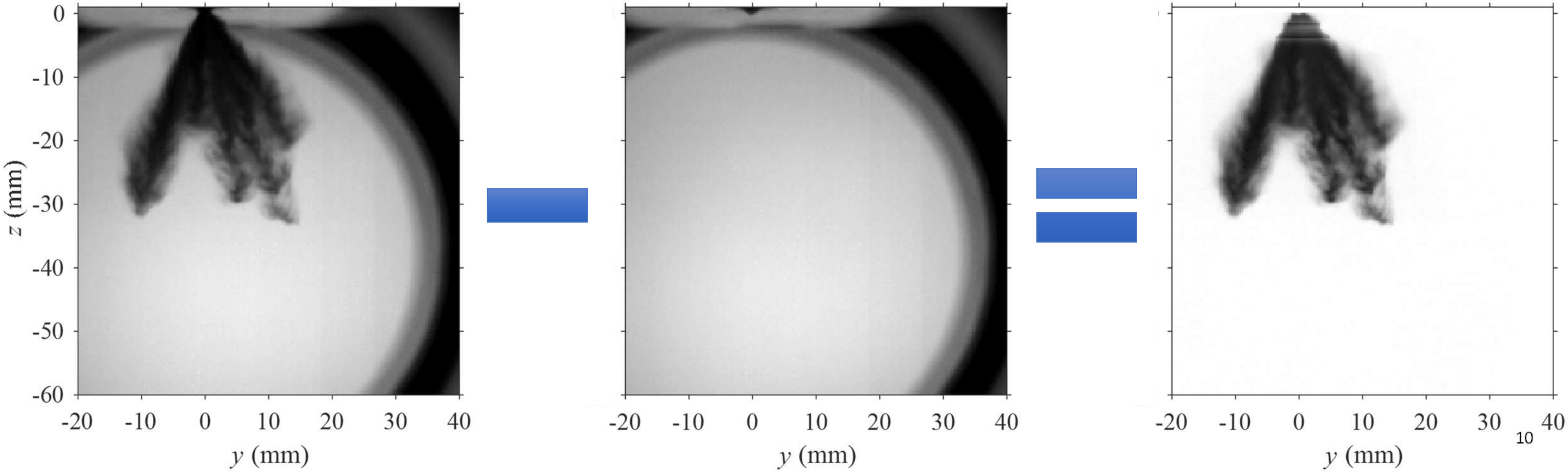


A schematic of the chamber and the experimental setup in two view orientations

Image processing

- Frame rate = 10 kFPS (0.1 ms between neighbouring images) → 10 blank images recorded before each injection
- Camera triggered 1 ms before start of injection
- Exposure time = 0.01 ms → “freezes” spray motion for sharper images

- Background subtraction using blank images → Effectively removes chamber features and isolates the plume



Calculating cone angle

- Point O: injector tip
- Point P: point in the plume furthest away from Point O

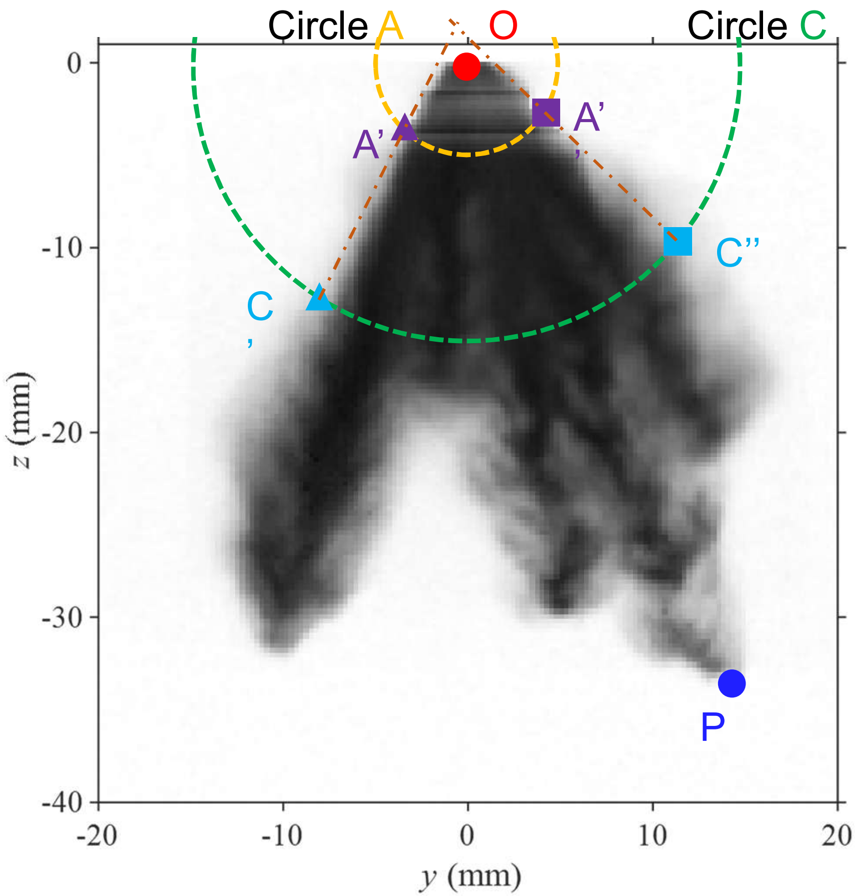
- Circle A : 5 mm away from Point O
- Point A': left intersection of Circle A
- Point A'': right intersection of Circle A

- Circle C: 15 mm away from Point O
- Point C': left intersection of Circle C
- Point C'': right intersection of Circle C

- The brown lines connects A'C' and A''C''

➡ *Plume cone angle* = Angle between the brown lines

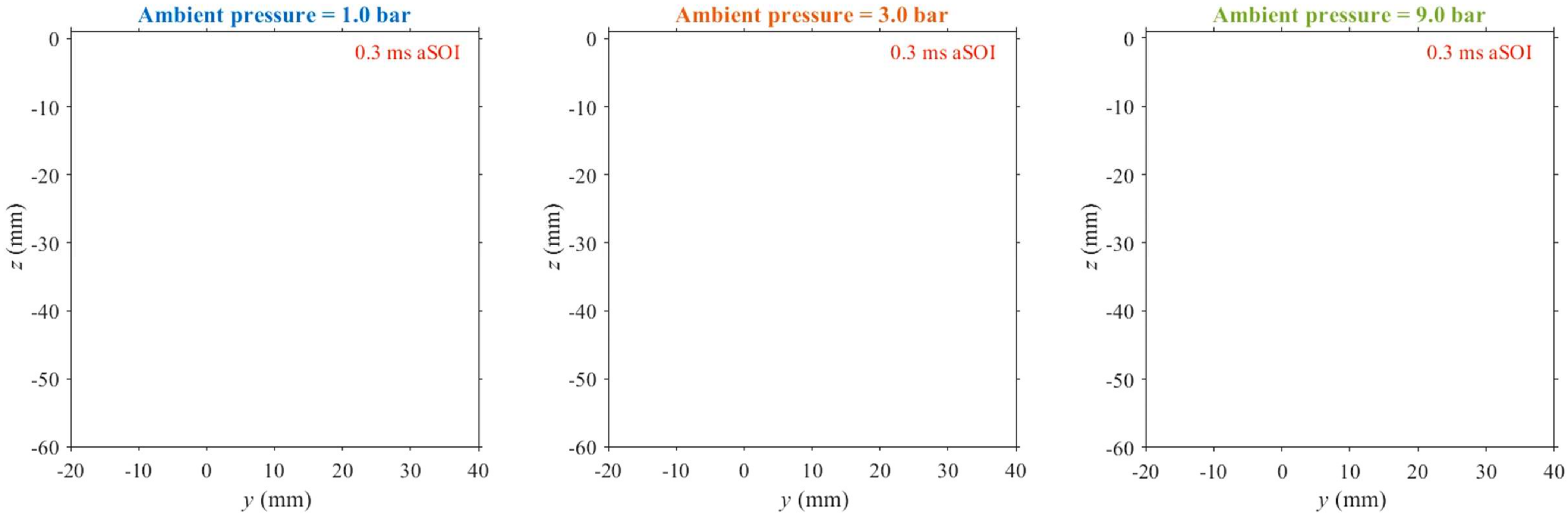
➡ *Tip penetration length* = Distance OP



* Algorithm based on the SAE J2715 standard

Initial observations

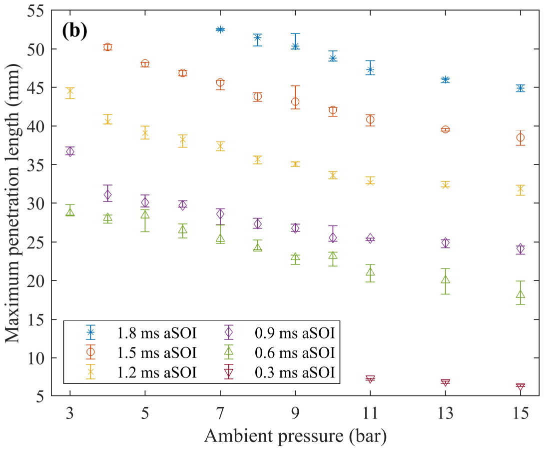
- Flash boiling case (low ambient pressure) → Spray collapse, single plume observed only
- Transition region (medium ambient pressure) → Mixed behaviour
- Non-flash boiling case (high ambient pressure) → Clear separation between plumes

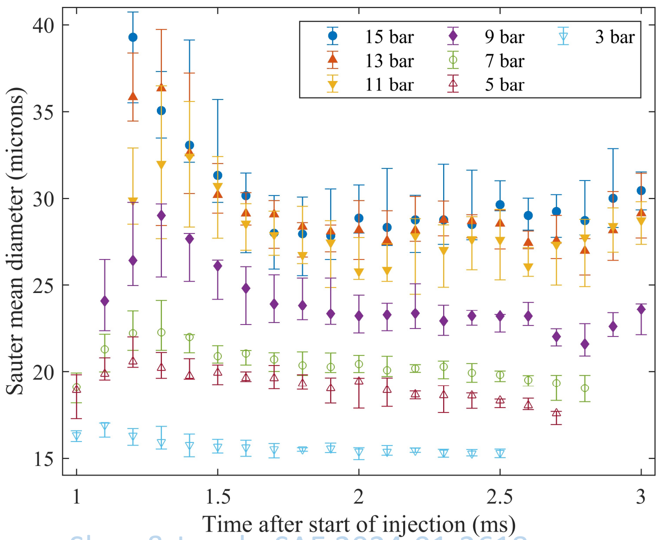


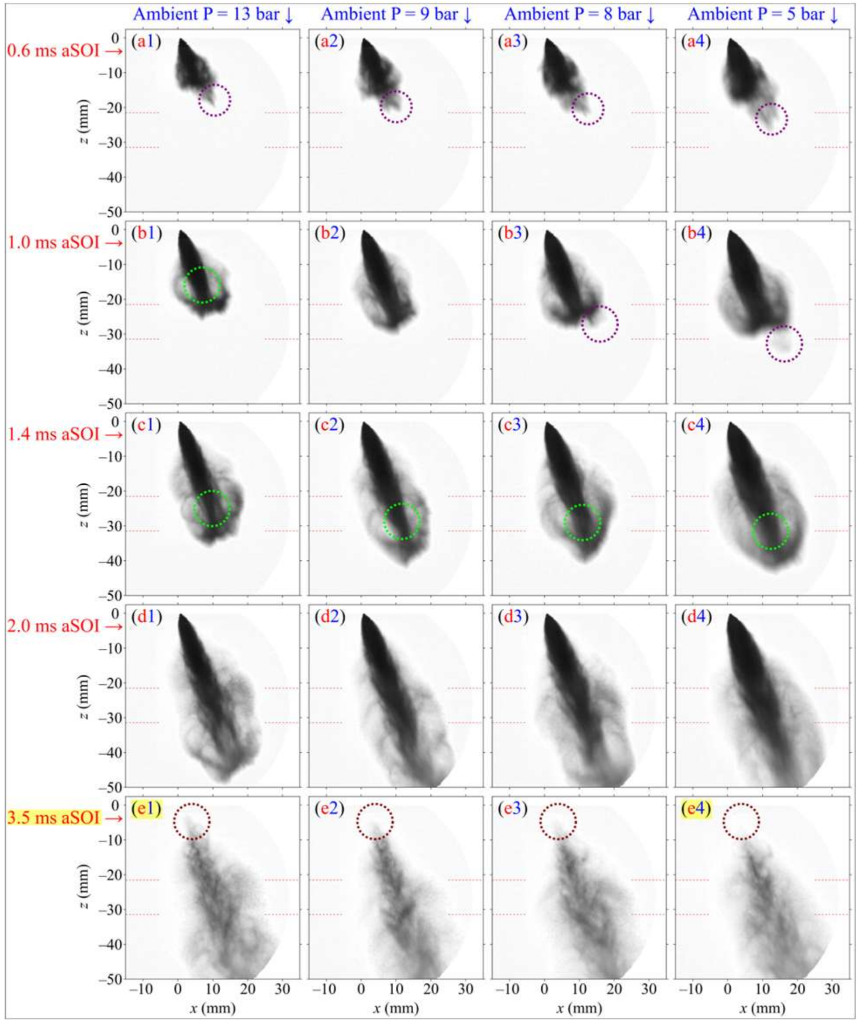
* Injection pressure = 150 bar, injection duration = 2 ms

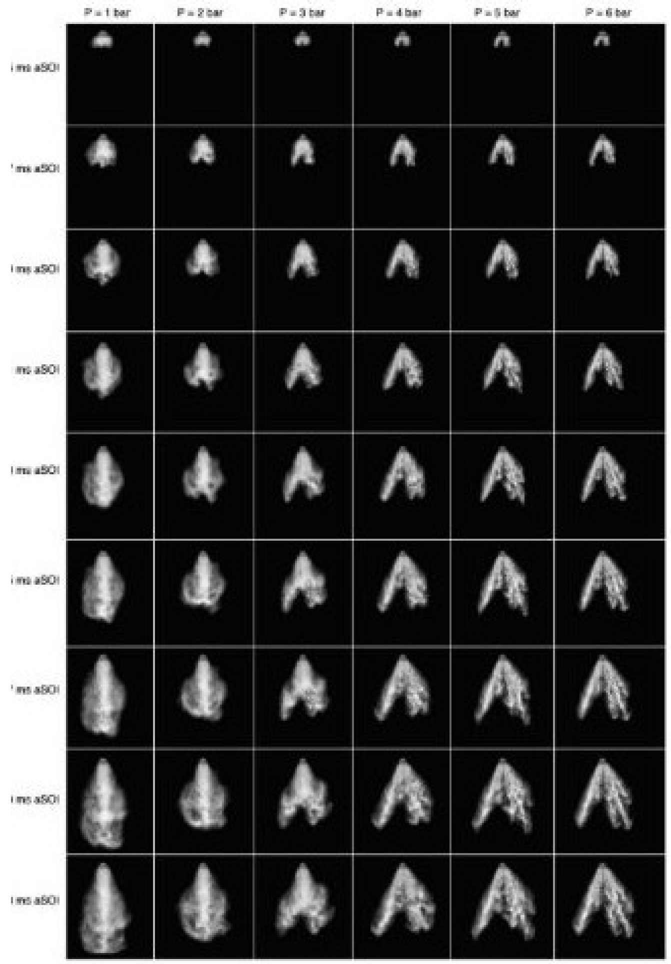
Ammonia spray measurement

Bundred and Leach, 3rd symposium on ammonia energy, 2024





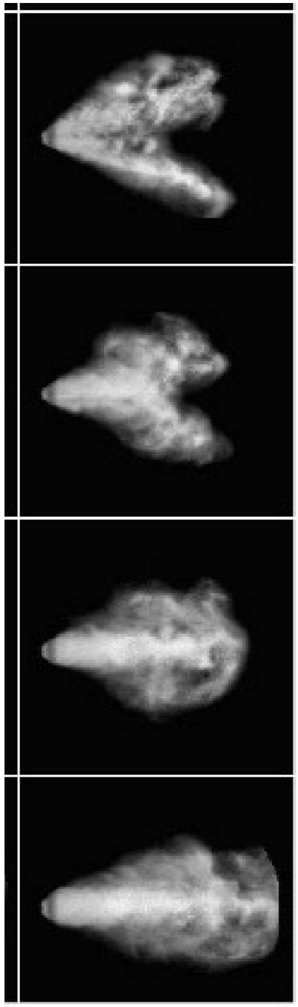




Shen & Leach: SAE 2024-01-2618

Regions of spray behaviour

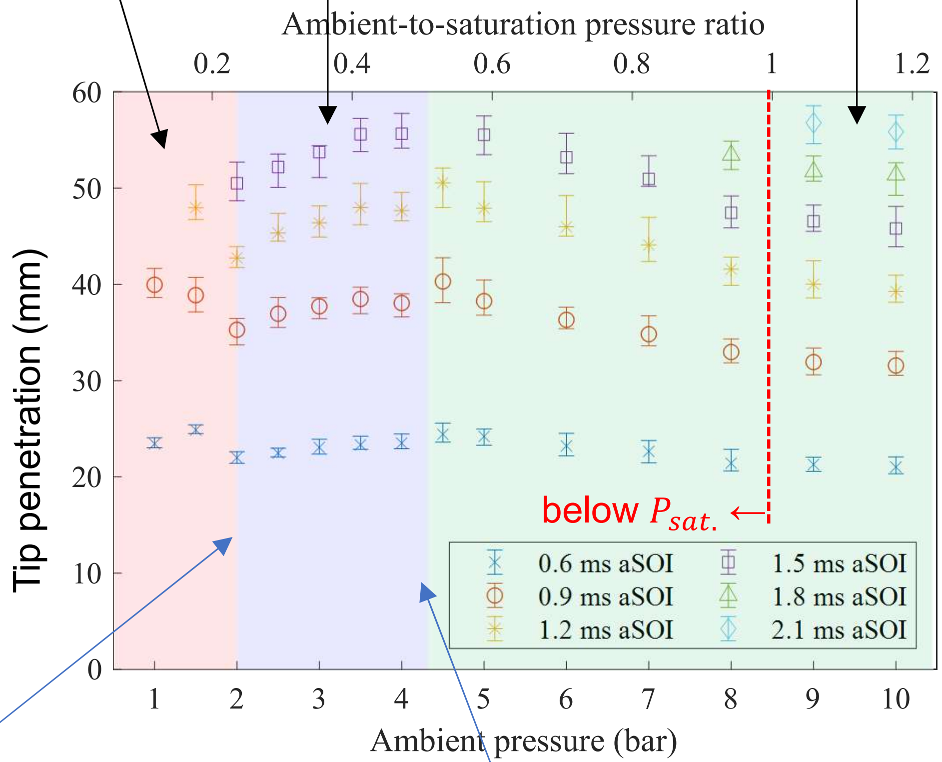
Shen and Leach, 3rd symposium on ammonia energy, 2024



flare flash boiling region

evaporation dominant

ambient resistance dominant



Does not move with P_{inj}

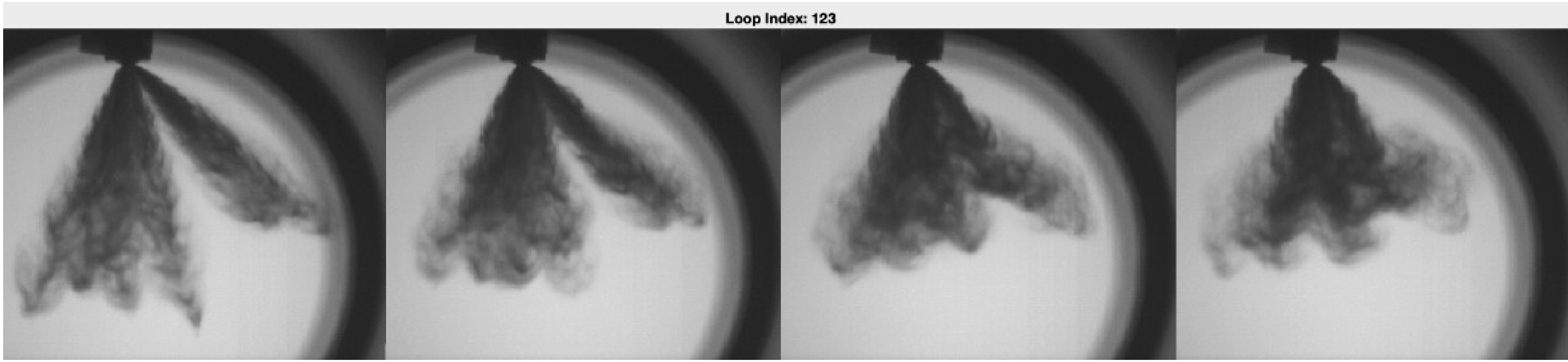
Moves with P_{inj}

Effect of ammonia temperature

Shen, Alimi, and Leach, 3rd symposium on ammonia energy, 2024

Ambient pressure : 5 bar

30°C 50°C 70°C 90°C

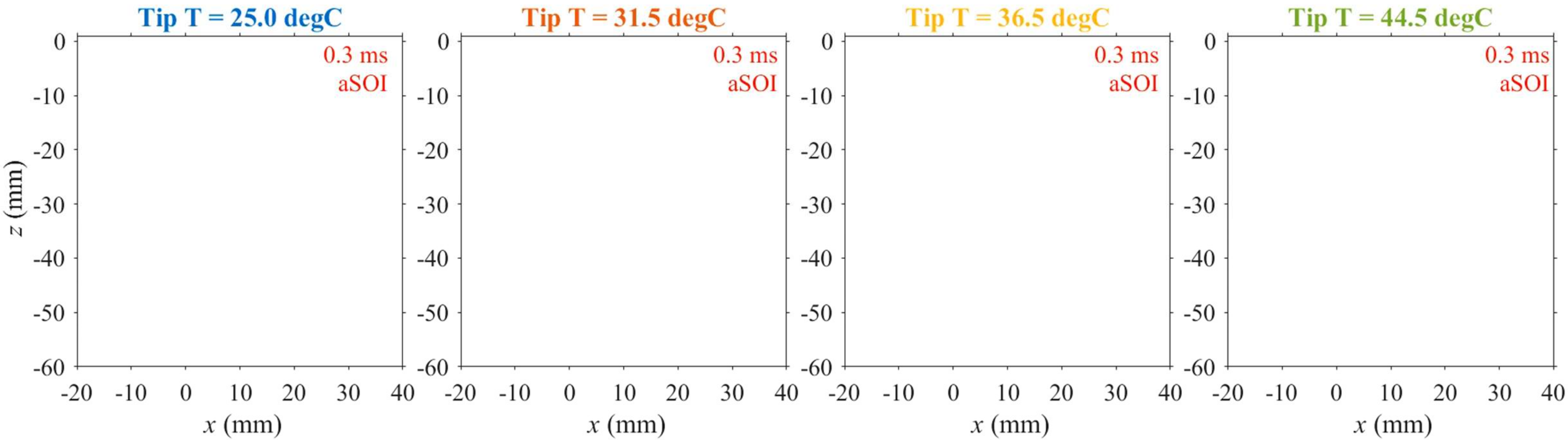


Importance of r_p

- Pressure ratio selected at evaporation dominant (transition) region
- Shortened penetration length at higher ambient P
- Similar spray shape observed at different tip T
- Minor difference due to ambient resistance variation and imperfection in r_p (test point selection)

Keeping ambient-to-saturation ratio r_p as a constant is a fairer comparison for spray behaviour at different fuel T.

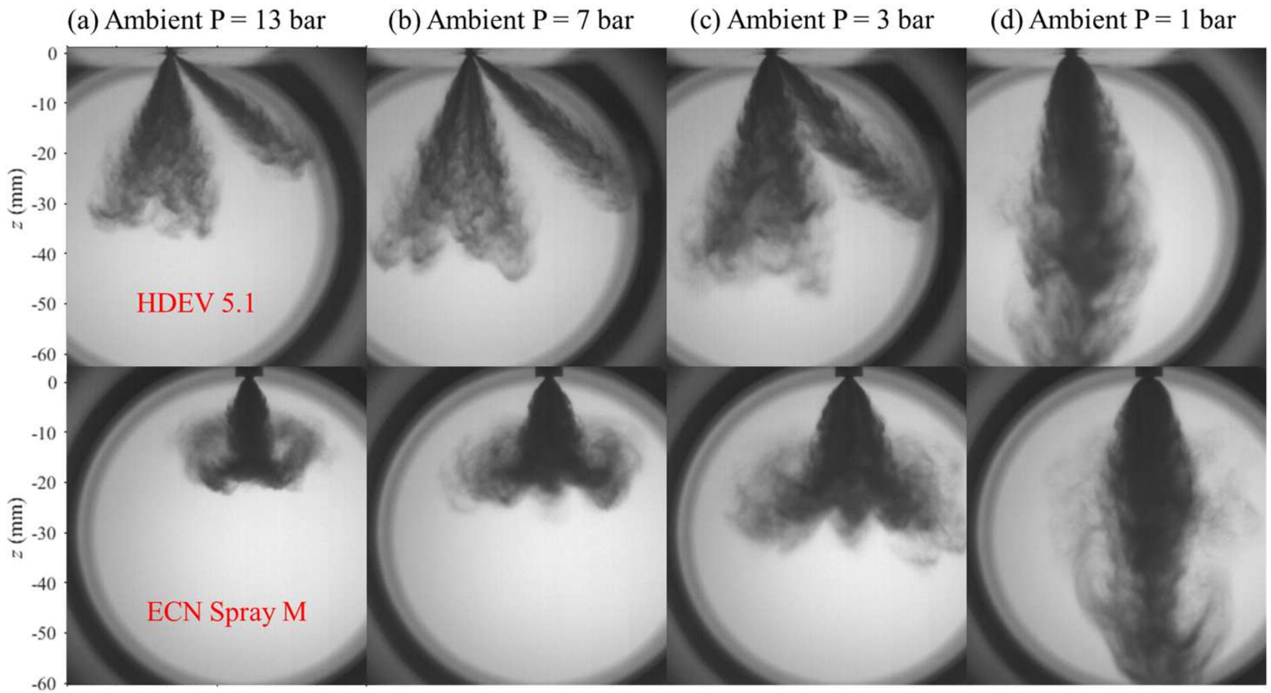
Ambient P = 3 bar, r_p = 0.31 | Ambient P = 4 bar, r_p = 0.33 | Ambient P = 5 bar, r_p = 0.35 | Ambient P = 6 bar, r_p = 0.34



* Injection pressure = 150 bar, injection duration = 2 ms

Qualitative injector comparison – 150 bar, 1.7 ms asoi

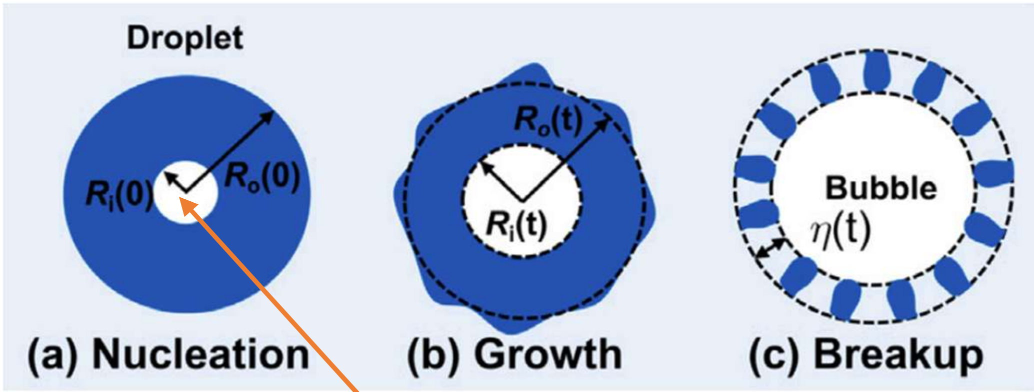
- Spray M – more holes (less plume separation), axisymmetric
- HDEV – clear plume separation, asymmetric
- Flare flash boiling (1 bar) leads to rapid increase in penetration length
- Spray M – increase in cone angle in transition region not really seen with HDEV
- Spray M lower overall penetration length (more holes) and higher tip recirculation
- ➔ Counterbore leading to more in-nozzle cavitation of the Spray M



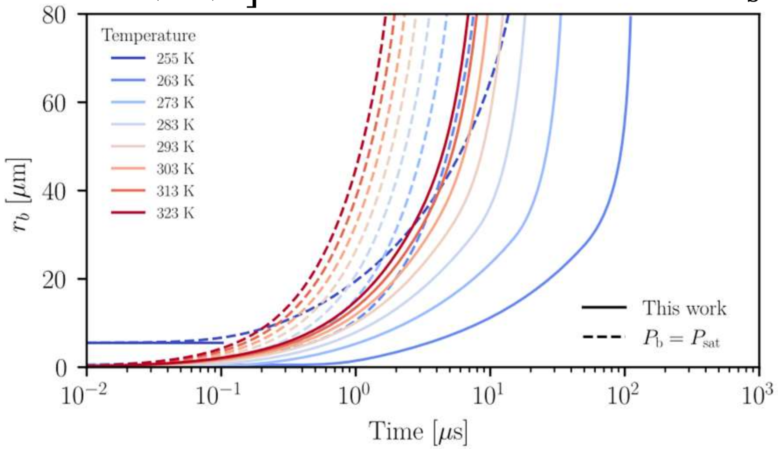
Modelling work

Why don’t Existing Thermal Breakup Models work well with ammonia?

- Lagrangian thermal breakup models typically involve the three stages shown right
- Across all models, bubble growth is governed by the Rayleigh-Plesset equation (RPE)
- This is closed by the internal bubble pressure P_b, which is typically assumed to be $P_\mathrm{sat}(T_\ell)$
- Closing the RPE in this way leads to predictions of aggressive breakup for $R_\mathrm{P} > 1$
- This breakup happens instantaneously ($\tau_\mathrm{growth} \leq 10\ \mu\mathrm{s}$) in all studied conditions, so sensitivity to R_P is still limited



$$\rho_\ell \left[r_\mathrm{b} \frac{d^2 r_\mathrm{b}}{dt^2} + \frac{3}{2}\left(\frac{dr_\mathrm{b}}{dt}\right)^2 \right] = \boldsymbol{P_b} - P_\ell - \frac{2\sigma}{r_\mathrm{b}} - \frac{4\mu}{r_\mathrm{b}}\frac{dr_\mathrm{b}}{dt} - 4\frac{\kappa}{r_\mathrm{b}^2}\frac{dr_\mathrm{b}}{dt}$$

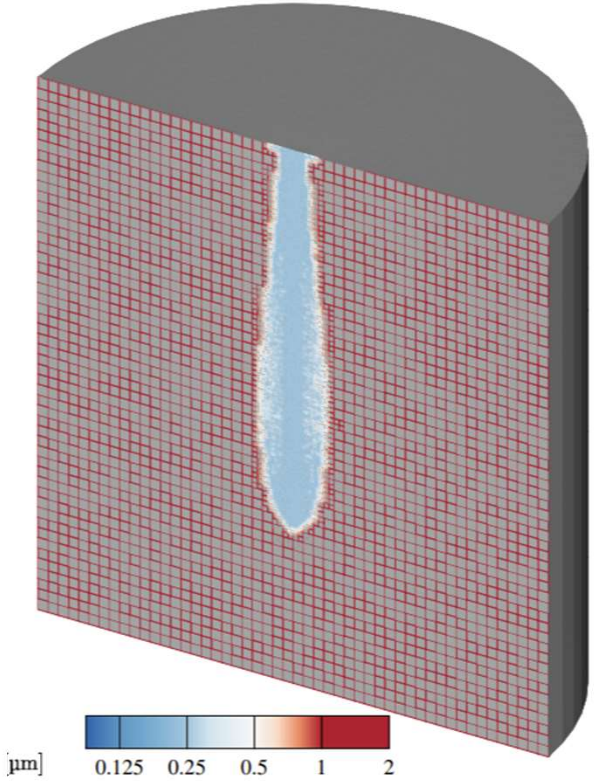


Zhang, Y., Chu, C., Liu, Z., & Jia, M. (2025). Improved dynamics, atomization, and vaporization models for liquid ammonia spray simulations under diverse ambient conditions. *International Journal of Multiphase Flow*, *188*, 105225.

Simulation Setup

Model	Parameter
Droplet Introduction	Rate of Injection
Injection	Blob
Equation of State	Redlich-Kwong EoS
Turbulence	RANS k-ε STD
Droplet Breakup	KH-RT
Droplet Collision Outcomes	No Time Counter
Droplet Drag	Dynamic

Submodel	Parameter [unit]	Value
Mesh	Base Grid, Min Grid Scale [μm]	2000, 7.8125
time-step	Min, Max, Mean [μs]	10^{-4}, 10^{0}, 10^{-1}
Lagrangian Initial Conditions	Droplet Diameter [μm]	165
Lagrangian Initial Conditions	Cone Angle [deg]	5
Kelvin-Helmholtz	Size Constant (B_0)	0.61
Kelvin-Helmholtz	Time Constant (B_1)	12.5
Rayleigh-Taylor	Breakup Length	6.25
Rayleigh-Taylor	Size Constant (C_{RT})	0.15
Rayleigh-Taylor	Time Constant (C_1)	0.1

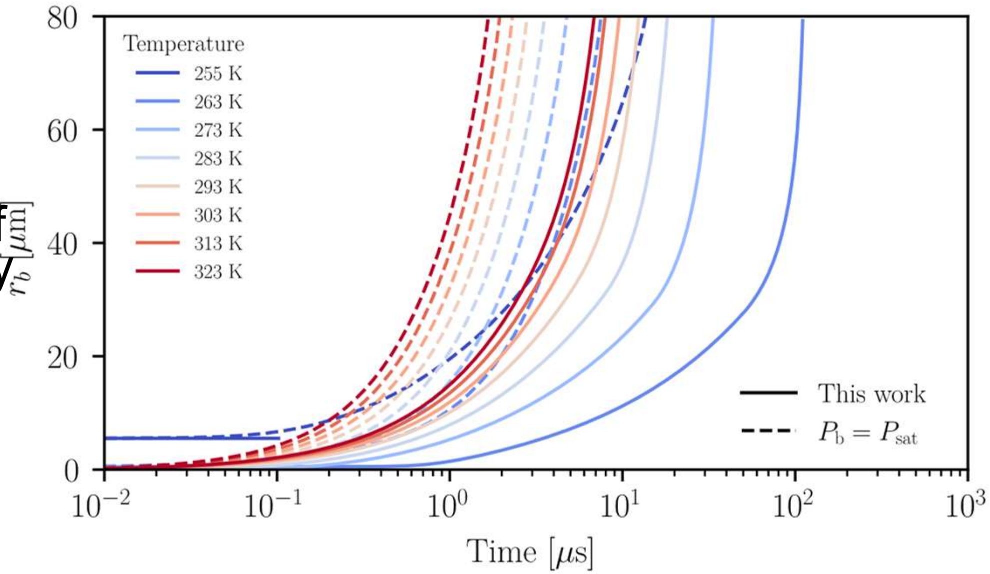


What's "New" in this model?

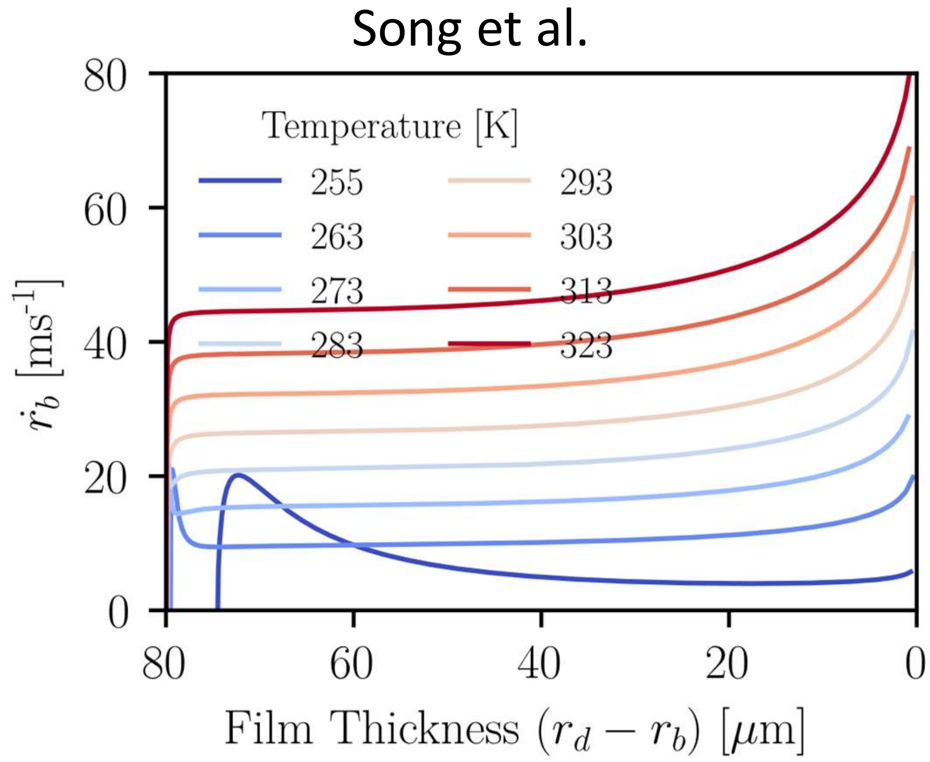
- Instead of closing the RPE with $P_{\mathrm{sat}}(T_\ell)$, the bubble pressure P_{b} is treated as a variable
- Bubble growth is assumed limited by the rate of heat transfer at the interface
- The bubble's mass and volume are used to calculate the pressure dynamically, based on an ideal gas assumption
- This links the bubble growth rate to the thermal history of the droplet (which cools rapidly due to external evaporation)
- This is necessary for ammonia because of its high saturation pressure and enthalpy of vaporisation, which otherwise lead to overly aggressive predictions of growth
- With this new closure, the RPE predicts bubble growth stalls for $R_{\mathrm{P}} < 1.3$ and happens on a timescale

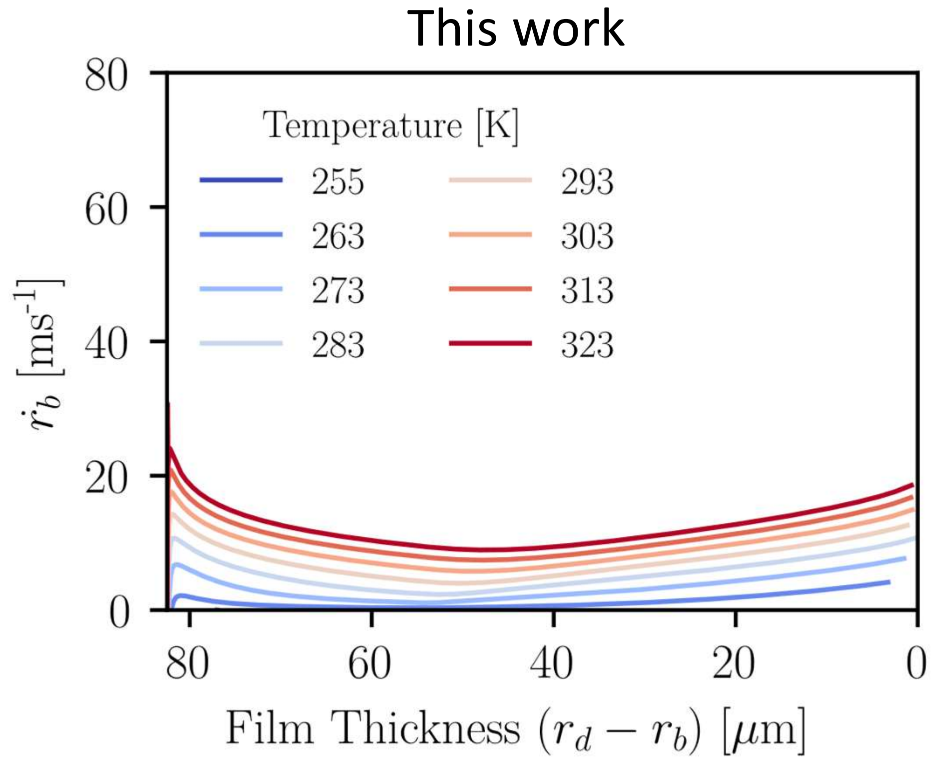
$$\rho_\ell \left[R_{\mathrm{b}} \frac{d^2 R_{\mathrm{b}}}{dt^2} + \frac{3}{2}\left(\frac{dR_{\mathrm{b}}}{dt}\right)^2 \right] = \boldsymbol{P_b} - P_\ell - \frac{2\sigma}{R_{\mathrm{b}}} - \frac{4\mu}{R_{\mathrm{b}}}\frac{dR_{\mathrm{b}}}{dt} - 4\frac{\kappa}{R_{\mathrm{b}}^2}\frac{dR_{\mathrm{b}}}{dt}$$

$$\frac{dm_{\mathrm{b}}}{dt} = \frac{4\pi\ {}_{\mathrm{b}}^{2} h_{\mathrm{b}}(T_d - T_b)}{L_{\mathrm{v}}} \quad P_{\mathrm{b}} = \frac{m_{\mathrm{b}} R T_{\mathrm{b}}}{V_{\mathrm{b}}} \quad T_b = \frac{B}{A - \log_{10}(P_{\mathrm{b}})} - C$$



Single Droplet Tests

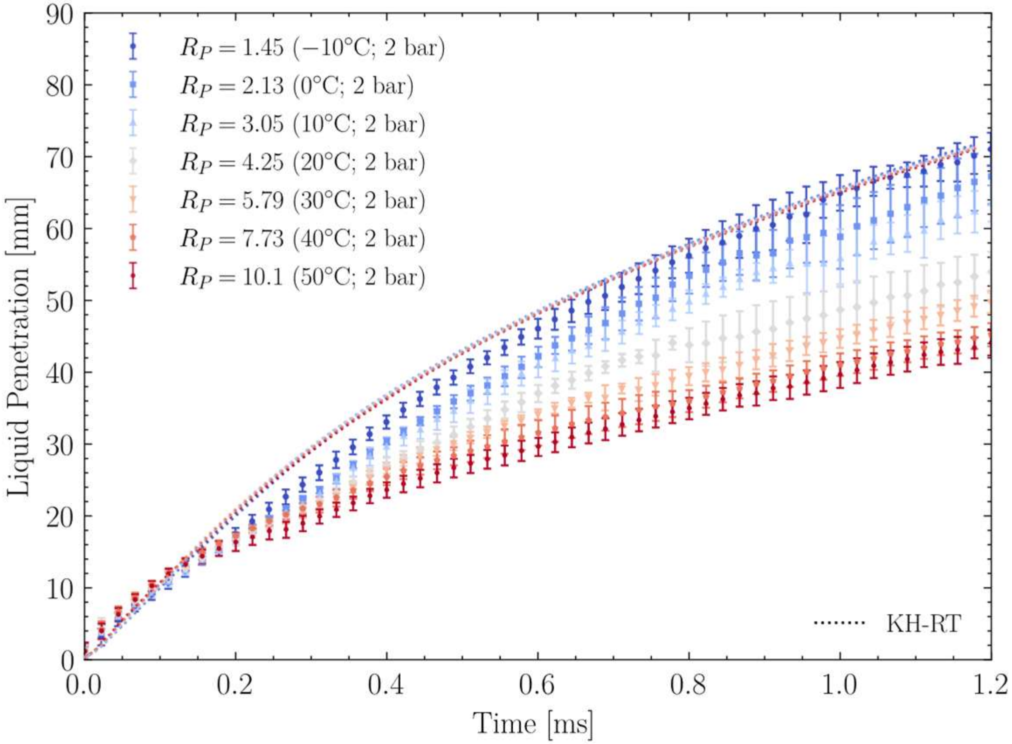




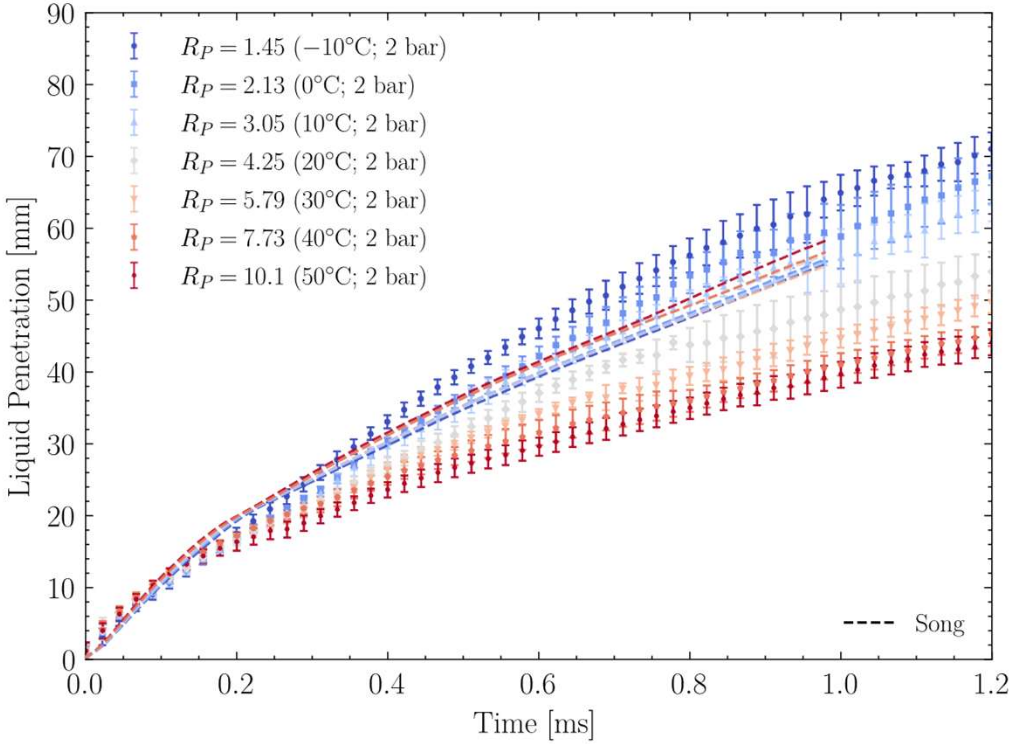
Song, X., Hu, Y., Zhao, F. and Yu, W., 2025. Modelling of liquid ammonia spray based on flash boiling break-up driven by thermal growth of multiple bubbles. Energy, 325, p.136129

Penetration Trends

KH-RT



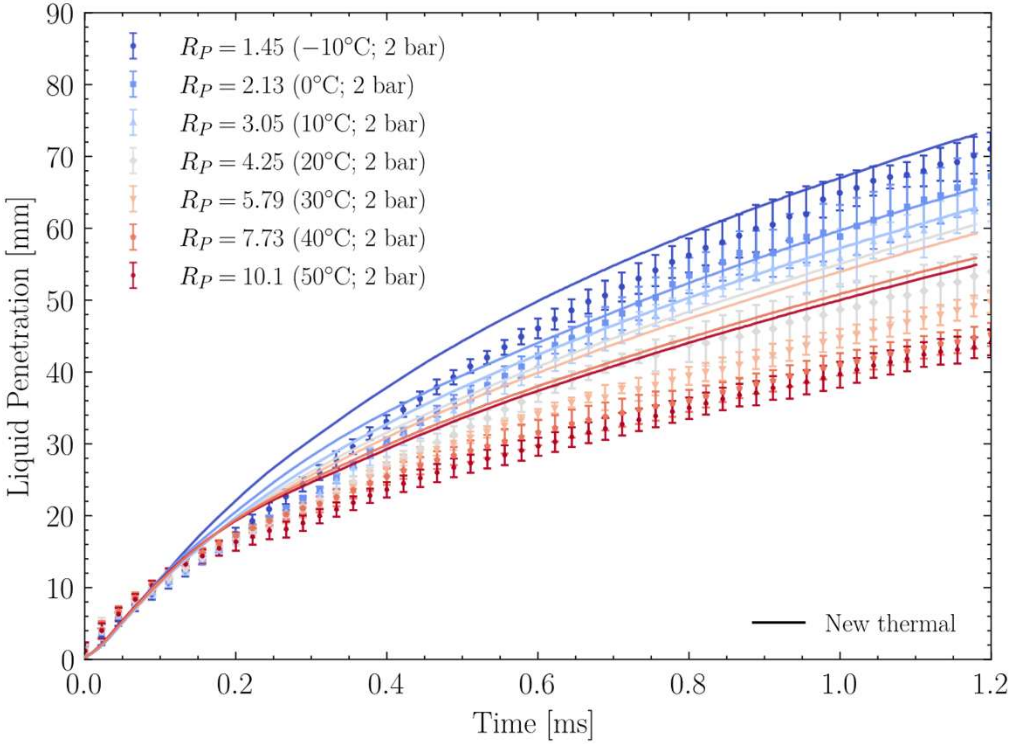
Song *et al.*



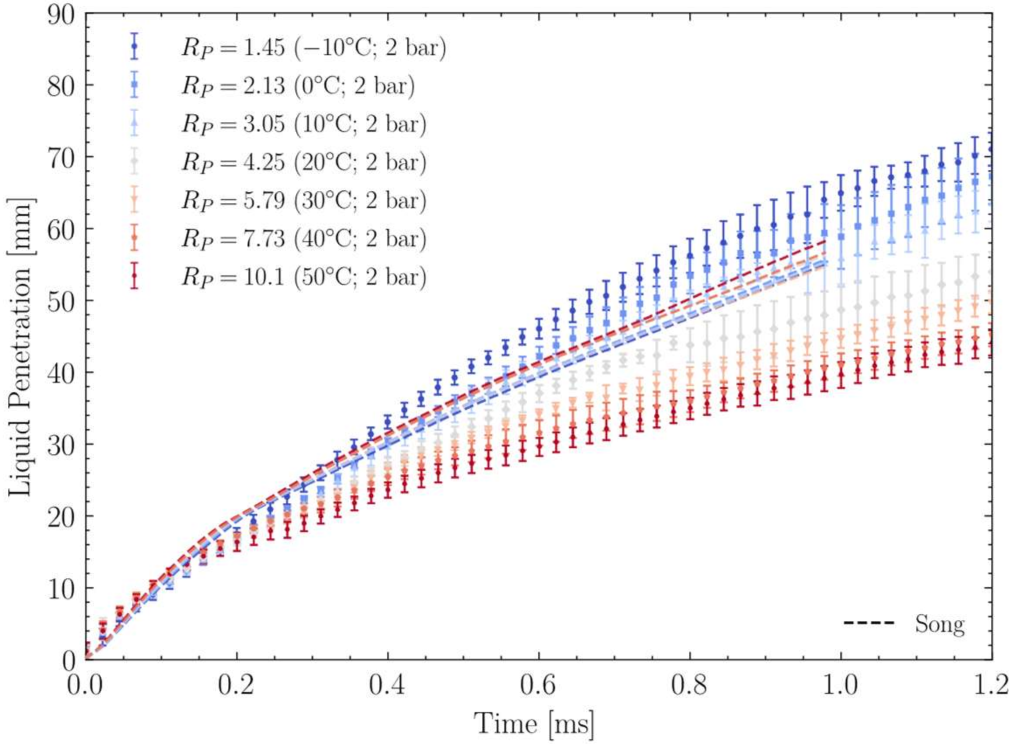
Song, X., Hu, Y., Zhao, F. and Yu, W., 2025. Modelling of liquid ammonia spray based on flash boiling break-up driven by thermal growth of multiple bubbles. Energy, 325, p.136129

Penetration Trends

New Model



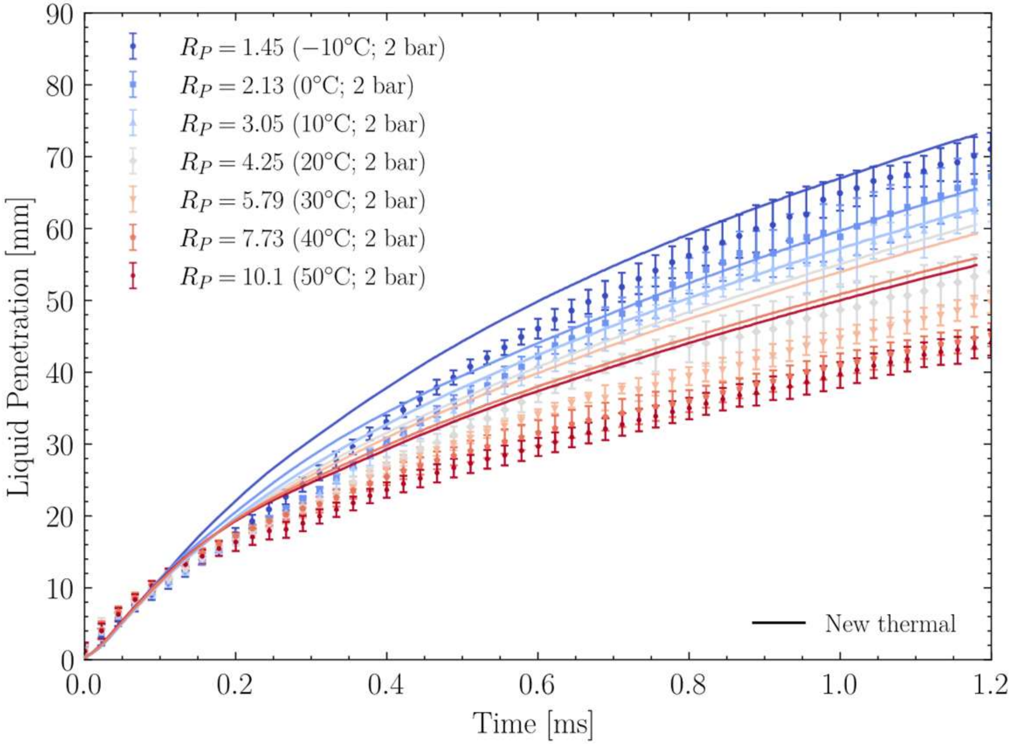
Song *et al.*



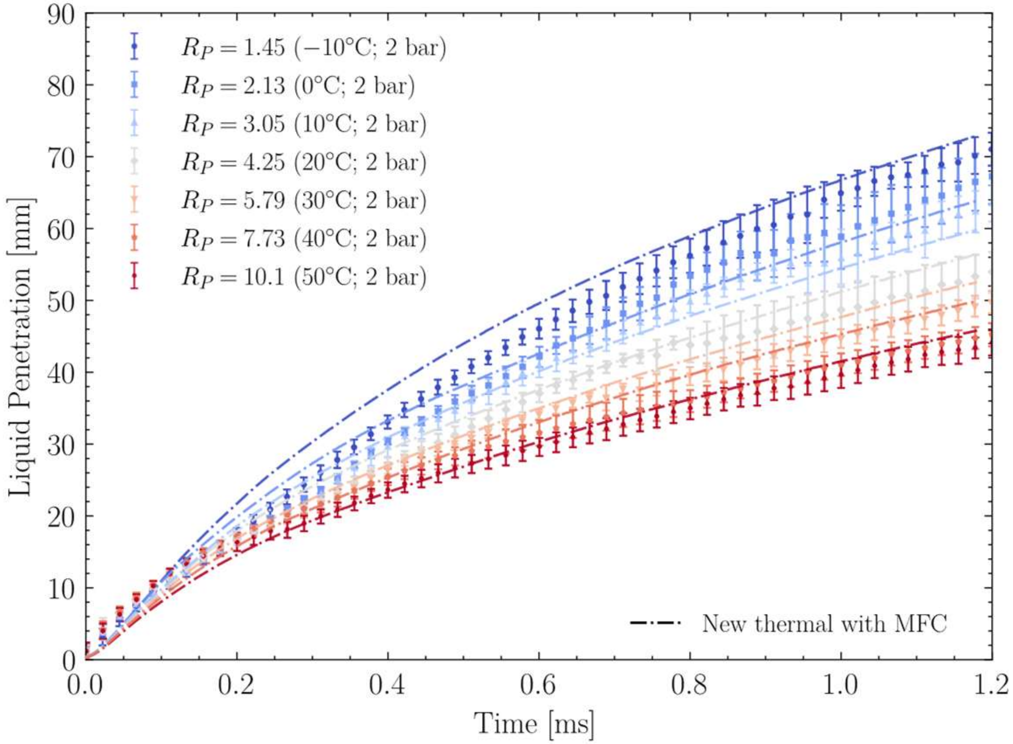
Song, X., Hu, Y., Zhao, F. and Yu, W., 2025. Modelling of liquid ammonia spray based on flash boiling break-up driven by thermal growth of multiple bubbles. Energy, 325, p.136129

Penetration Trends

New model



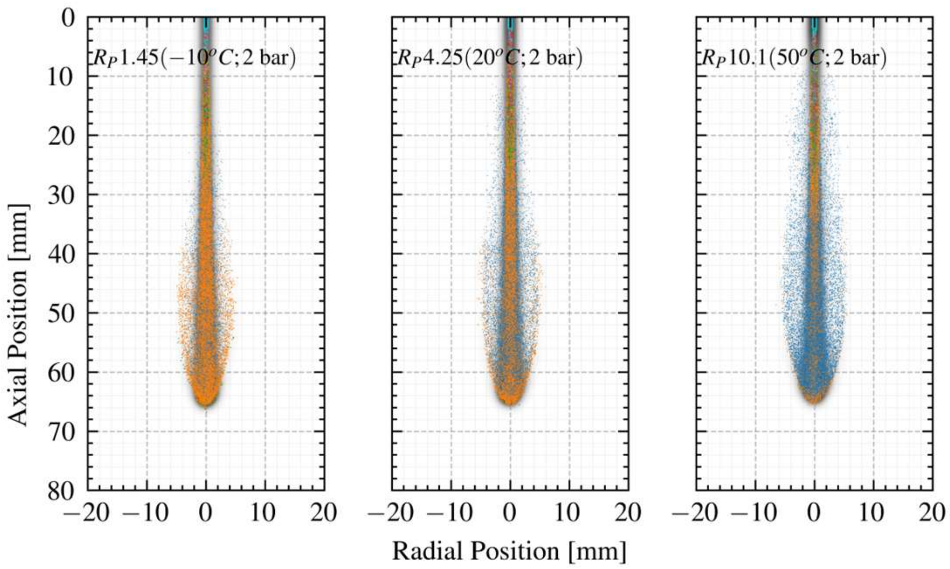
New model with injected mass correlation



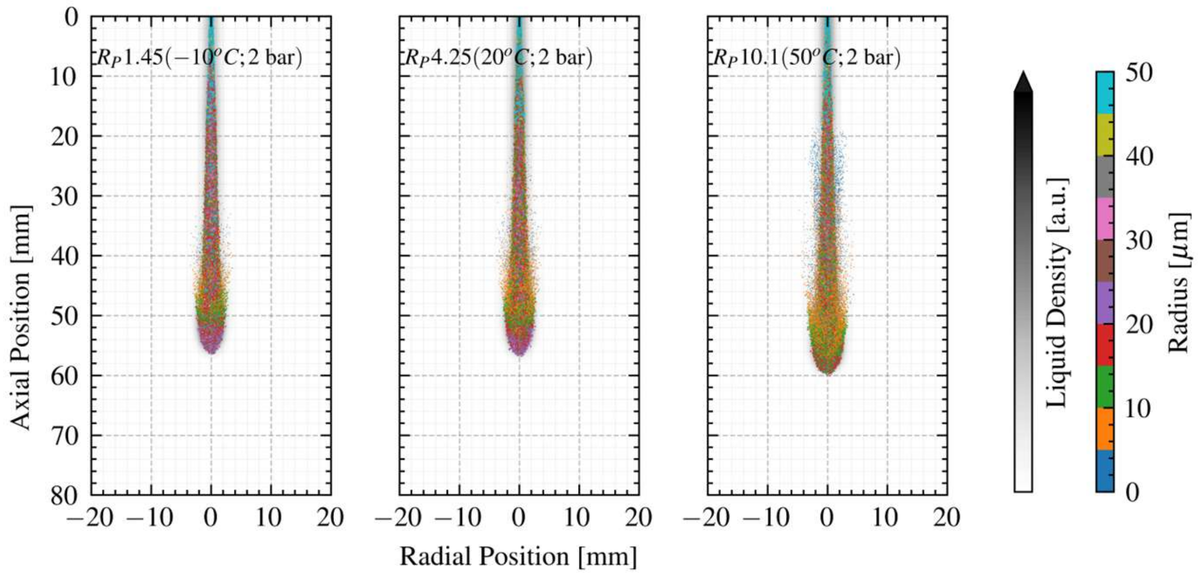
Shen L, Bajwa A, Malladi M, Davy M, Leach F. Mass flow rate measurements of liquid ammonia injections. Int J Hydrogen Energy 2026. (*under review*)

Spray Morphology at 1 ms ASOI

KH-RT



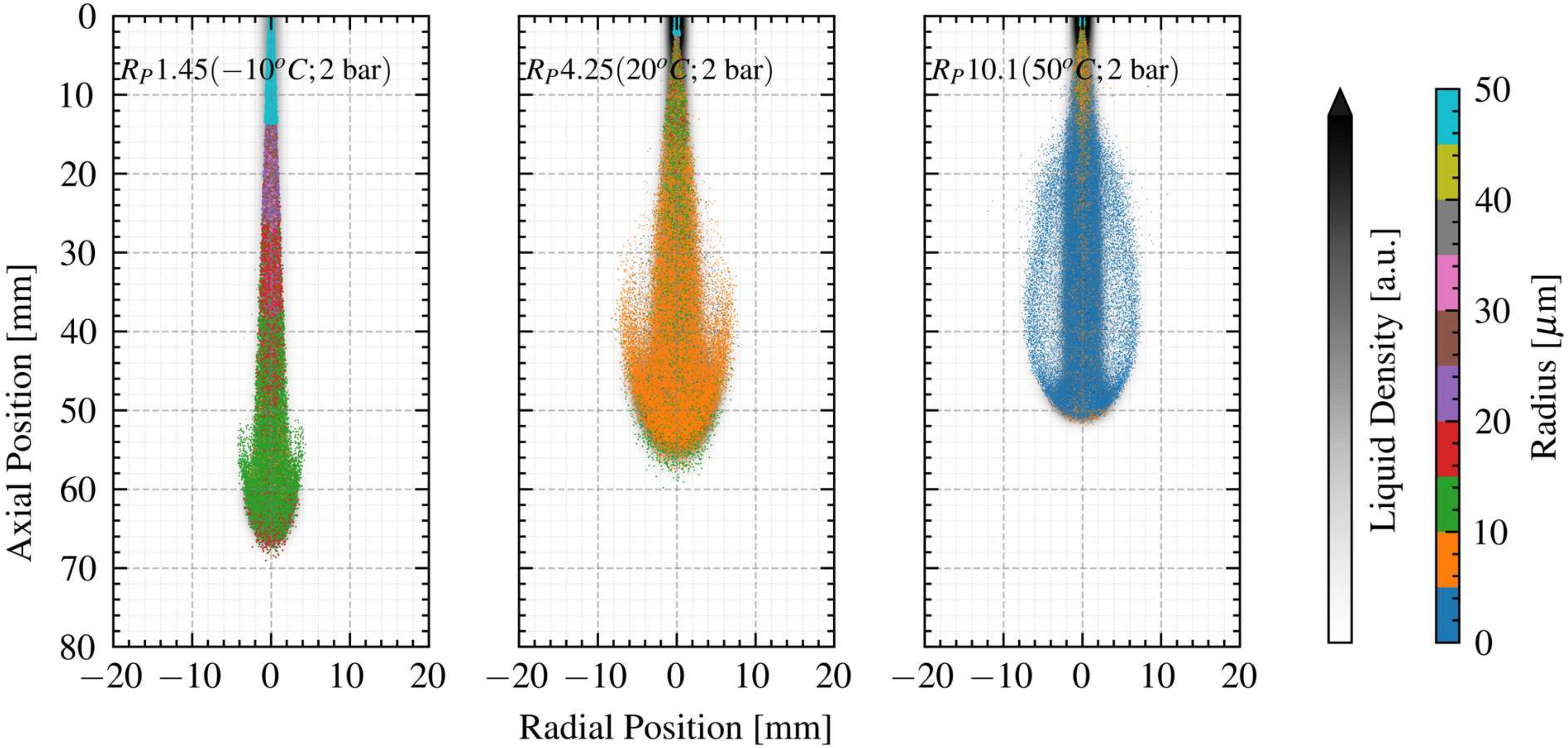
Song *et al.*



Song, X., Hu, Y., Zhao, F. and Yu, W., 2025. Modelling of liquid ammonia spray based on flash boiling break-up driven by thermal growth of multiple bubbles. Energy, 325, p.136129.

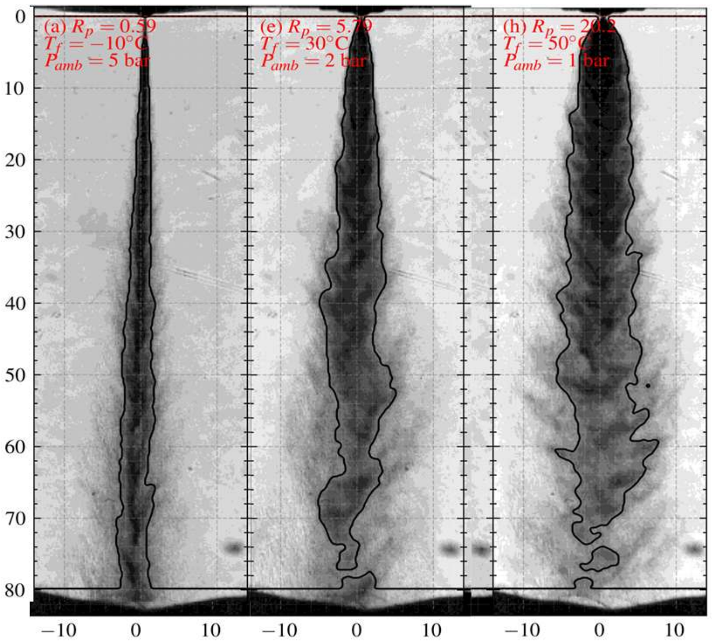
Spray Morphology

New Model at 1 ms ASOI

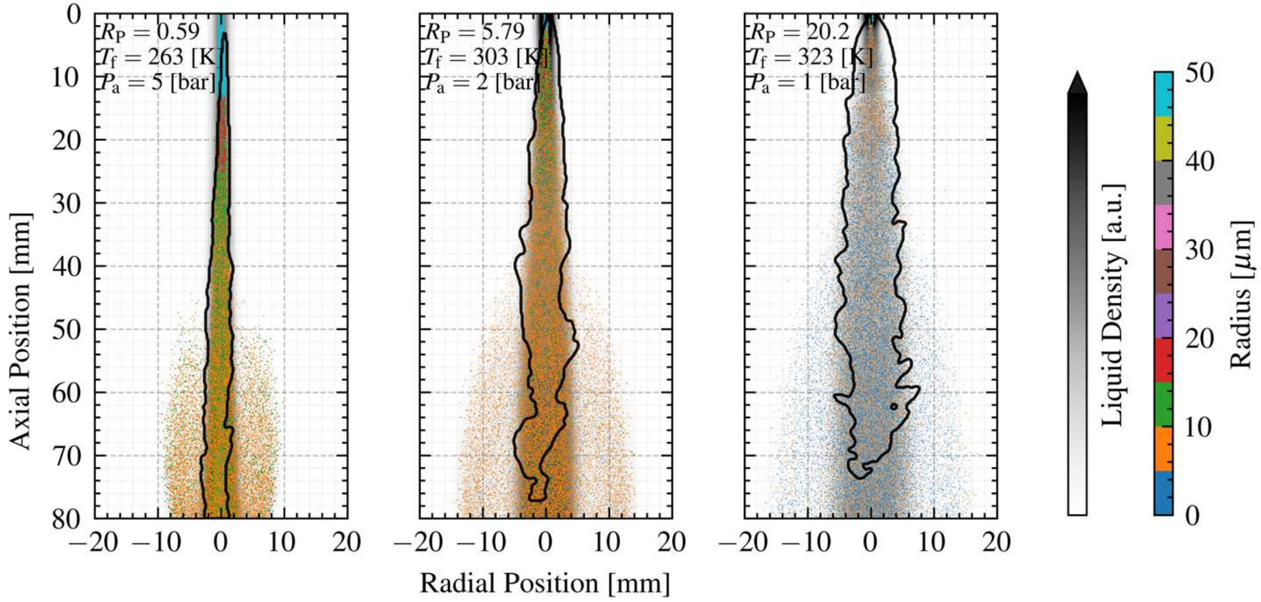


Spray Morphology

Spray images



New Model at 3.5 ms ASOI

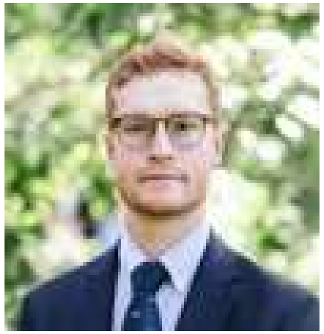


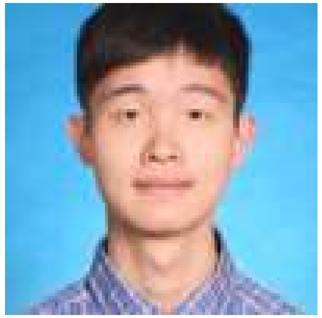
Desclaux A, Pelé R, Hespel C, Mounaïm-Rousselle C, Desclaux A, Pelé R, et al. Liquid Ammonia injection on single hole injector: effect of initial conditions on flash boiling process. 2023.

Acknowledgements

CONVERGENT SCIENCE

UKRI Engineering and Physical Sciences Research Council





References

1. Shen L, Leach FCP, “The effect of ambient and injection pressure on droplet size of ammonia sprays in a constant volume chamber”, *Fuels,* Vol 7(1), 18, 2026. doi:10.3390/fuels7010018
2. Shen L, Leach FCP, “An experimental study on the macroscopic behaviours of ammonia sprays in a constant volume chamber”. *International Journal of Hydrogen Energy,* Vol 126 pp. 386-395, 2025. doi:10.1016/j.ijhydene.2025.03.347
3. Shen L, Leach FCP, “Effect of ambient pressure on ammonia sprays using a single hole injector”, *SAE International Journal of Advances and Current Practices in Mobility* Vol 7(2):583-598, 2025. doi:10.4271/2024-01-2618
4. Shen L, Alimi K, and Leach FCP. “The effect of injection temperature on ammonia sprays” 3rd Symposium on Ammonia Energy, Shanghai, China, 23rd-26th September 2024.
5. Shen L, Bajwa A, Malladi M, Davy M, Leach F. “Mass flow rate measurements of liquid ammonia injections”, Int J Hydrogen Energy 2026.
6. Bundred D and Leach FCP. “A New Thermal Breakup Model for Ammonia Sprays” CONVERGE CFD Forum: Solutions for Low-Carbon Transportation, Torino, Italy, 11th June 2026.
7. Bundred D, Leach FCP. “Influence of Boundary Conditions on Downstream Behaviour of Eulerian Lagrangian Simulations of Ammonia Sprays”. *33rd European Meeting on Liquid Atomization and Spray Systems*, Lund, Sweden, September 2025.
8. Bundred D and Leach FCP. “Comparison of Evaporation Model Performance for Simulation of Ammonia Sprays”, 3rd Symposium on Ammonia Energy, Shanghai, China, 23rd-26th September 2024.
9. Shen L, Leach FCP. “An introduction to ammonia spray lab safety and setup” 2nd symposium on Ammonia Energy, Université d’Orléans, Orléans, France, 11th-13th July 2023.

Thank you for your attention

Felix Leach
felix.leach@eng.ox.ac.uk

DEPARTMENT OF ENGINEERING SCIENCE

UNIVERSITY OF OXFORD