

# Universität Stuttgart

Institut für Technische Verbrennung  
A. Kronenburg, D. D. Loureiro, J. W. Gärtner

Institut für Technische Verbrennung, Universität Stuttgart

HLRS Workshop  
Stuttgart,  
7-8 October 2021

Simulation und  
Modellierung von  
Zweiphasen-  
strömungen

Characteristics of  
flash-boiling

## Motivation

Flash atomization occurs when liquids are injected into environments at pressures below saturation conditions. Under these conditions, spontaneous boiling will occur, the bubbles will grow and the liquid jet will almost instantly disintegrate. This process is of relevance in e.g. upper stage rocket engines and orbital maneuvering systems where liquid reactants such as liquid hydrogen and oxygen are injected into the reaction chamber that is at vacuum conditions. The break-up characteristics and resulting droplet size distribution will determine evaporation, ignitable mixture preparation, ignition and combustion.

## Simulation Overview

The spray breakup is quantified using quasi-DNS where the interface and all flow scales are resolved. The key characteristics of the solution strategy are

- ITR code FS3D [1] with MPI parallelization
- Interface capturing with Volume-of-Fluids (VoF) and PLIC reconstruction

VoF transport: 
$$\frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{u}_T f) = \frac{-\dot{m}'''}{\rho_l}$$

Momentum: 
$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \nabla \cdot \mu [\nabla \mathbf{u} + \nabla (\mathbf{u})^T] - \nabla p + \mathbf{f}_\sigma$$

Pressure/Continuity: 
$$\nabla \cdot \left[ \frac{1}{\rho} \nabla p \right] = \frac{\nabla \cdot \mathbf{u}}{\Delta t}$$

Evaporation rate: 
$$\dot{m}''' = \alpha_T \dot{m}'' = \alpha_T \rho_v \dot{R}$$

The surface tension force is based on the continuum Surface Stress model (CSS) [2]. The evaporation rate due to phase change,  $\dot{m}'''$ , is based on the Rayleigh-Plesset equation, and the interface density,  $\alpha_T$ , is obtained from the reconstructed surface area.

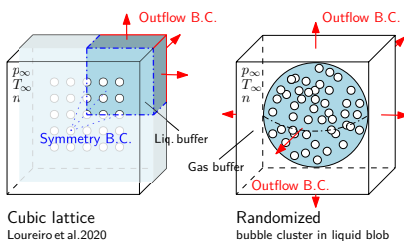
## Case Setup

The DNS domain represents a small section of the liquid within the flashing spray. This section could be part of the liquid core or a primary droplet that is still superheated. Within this droplet nucleation continues to occur.

Two setups are possible:

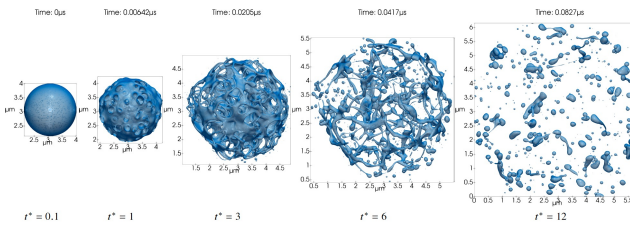
(1) Standard setup with a regular lattice arrangement of the bubbles after nucleation and

(2) randomized nucleation. Bubbles are initialized randomly with an average spacing similar to the regular lattice arrangement



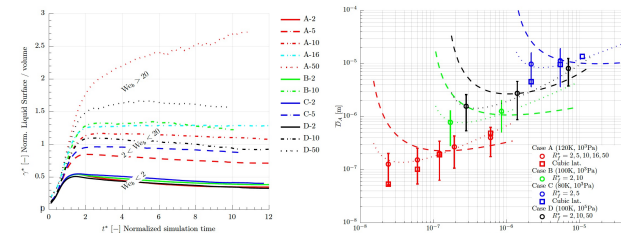
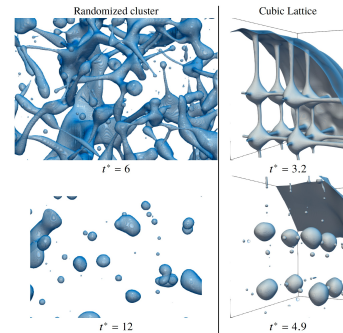
## Breakup Sequence

Time evolution of secondary droplet breakup for a reference case of cryogenic oxygen with  $p^\infty = 10^3 \text{ Pa}$ ,  $T^\infty = 120 \text{ K}$ ,  $N_{bub} = 512$ ,  $n = 1.47 \cdot 10^{20} \frac{\#}{m^3}$ .



## Results

- Qualitative and quantitative difference between the two different setups. The randomized setup leads to a droplet size distribution close to Gaussian once breakup is complete. The lattice arrangement produces a largely mono-sized distribution with additional small satellite droplets only.

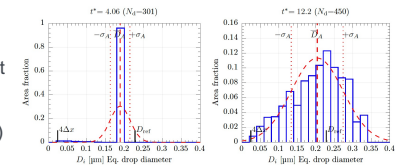


Left: Time evolution of the normalized liquid surface area. The maximum surface area generation is quickly reached. During further spray formation, contraction and breakup balance each other  
Right: Comparison of mean droplet size as function of bubble number density with a simple estimate (lines) based on force equilibrium at time of breakup.

## Results

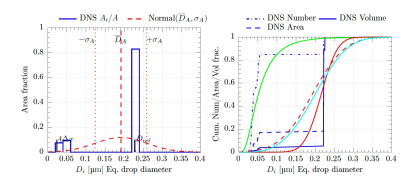
Randomized arrangement:

- Droplet size distributions at different time (blue)
- Gaussian distributions and mean diameters (red lines)



Lattice arrangement:

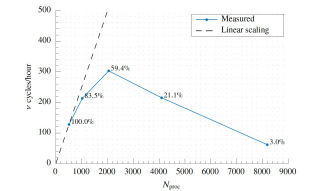
- Droplet size distribution at end of simulation
- Cumulative distributions (DNS – blue; Gaussian – red; log-normal – green; Rosin-Rammler – cyan)



## Computational Performance

Strong scaling results for 1024<sup>3</sup> grid:

Nproc	Cells/proc	Cycles/hour	$\eta$
512	2097152	128	100%
1024	1048576	213	83%
2048	524288	303	59%
4096	262144	215	21%
8192	131072	62	3%



## Conclusions

- Qualitative and quantitative differences for secondary spray breakup between lattice and randomized bubble arrangements → standard models inaccurate
- Simple estimates for resulting droplet size under certain conditions possible

## Acknowledgements

We acknowledge the financial support by DFG (grant number TRR75 - 84292822).

## References

- [1] K. Eisenschmidt, M. Ertl, H. Gomma, C. Kleer-Roth, C. Meister, P. Rauschenberger, M. Reitzle, K. Schlotke, and B. Weigand, "Direct numerical simulations for multiphase flows: An overview of the multiphase code FS3D," Journal of Applied Mathematics and Computation, vol. 272, pp. 508-517, 2016.
- [2] B. Lafaurie, C. Nardone, R. Scardovelli, S. Zaleski, and G. Zanetti, "Modelling merging and fragmentation in multiphase flows with surfar," Journal of Computational Physics, vol. 113, no. 1, pp. 134-147, 1994.