An OpenFOAM®-based tool for computational modeling of aerosol nucleation and transport

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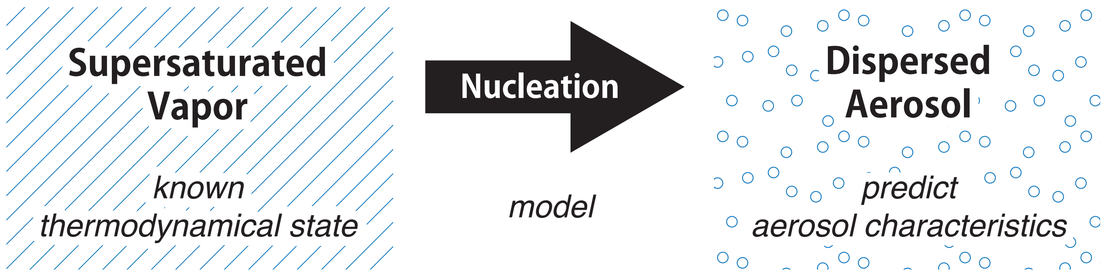
Introduction

Nucleation is the key process in the production of **dispersed aerosol** from **supersaturated vapor**.



Various parameters, such as temperature, surface tension, saturation pressure and aerosol mass density, determine the **chemical composition**, **droplet number concentration** and **droplet size distribution** of the aerosol.

To predict the aerosol characteristics, **Classical Nucleation Theory** (CNT) may be used. We present a **numerical tool** which couples CNT to **compressible flow**, describing the aerosol in an **Eulerian framework**.

OpenFOAM®-based simulation tool

Key features of the numerical simulation tool are:

- All benefits of the OpenFOAM® framework, such as **meshing tools**, **turbulence** and **thermophysical models**, **easy post-processing** and **parallel computing**
- **Specify temperature-dependent** descriptions of **thermophysical model parameters** (eg surface tension, saturation vapor pressure) as polynomial, exponential, or as a custom relation
- Easily **extendable** with **alternative nucleation models**, by adding a run-time selectable class
- Suitable for both **quick qualitative analysis** and **in-depth aerosol research**

Nucleation model

A **two-moment Eulerian representation** of the aerosol is adopted, solving for aerosol in vapor (Y) and aerosol (Z) state, and droplet number concentration N. The transport equations read [2]:

$$\partial_t(\rho Y) + \partial_j(u_j \rho Y) = \partial_j\left(D\rho\partial_j(Y)\right) - S_{v\to l} \quad (1a)$$

$$\partial_t(\rho Z) + \partial_j(u_j \rho Z) = S_{v\to l} \quad (1b)$$

$$\partial_t N + \partial_j(u_j N) = J_{nuc} - J_c \quad (1c)$$

with mixture mass density ρ, velocity field u_j, binary (vapor-carrier) diffusivity coefficient D, nucleation and coalescence rate J_{nuc} and J_c, and vapor-to-liquid source term $S_{v\to l}$.

The source term $S_{v\to l}$ accounts for the **interaction** of **nucleation** (as given by CNT [1]) and **condensation-evaporation** theory [3].

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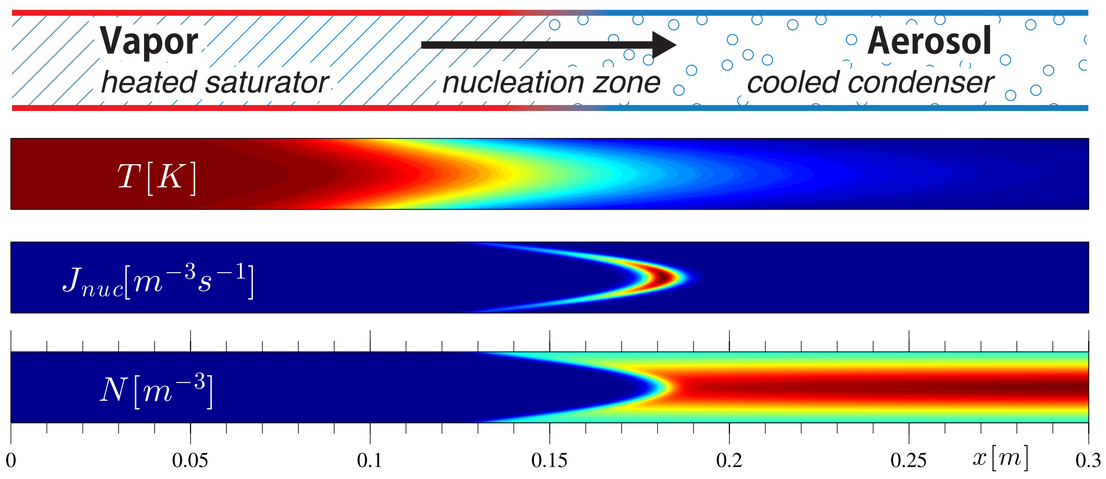
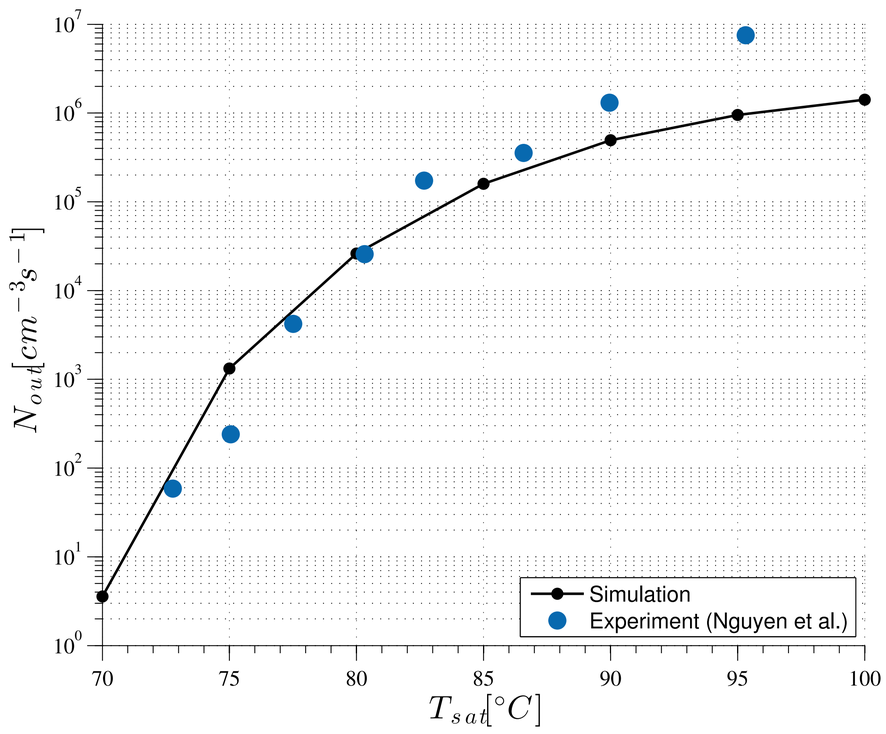
Reference case & results

We **compare** with **experimental results** of a **Laminar Flow Diffusion Chamber** (LFDC), as used in [4]. The LFDC setup consists of a **cooled pipe** through which a **saturated vapor** flows, reaching a **critically supersaturated** state, leading to nucleation.



The droplet number concentration depends on the temperature of the saturator, T_{sat}. We find a reasonable agreement between experiment and simulation:



Outlook

The development of the OpenFOAM®-based simulation tool is a stepping stone towards a **more comprehensive model**.

- A **multi-species model** to determine the **aerosol chemical composition**
- A **sectional model** to more accurate describe the **aerosol droplet size distribution**

References

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[4] H.V. Nguyen, K. Okuyama, T. Mimura, Y. Kousaka, R.C. Flagan, and J.H. Seinfeld. Homogeneous and heterogeneous nucleation in a laminar flow aerosol generator. *Journal of Colloid And Interface Science*, 119(2):491–504, 1987.

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