Multi-scale modeling of aerosol formation in pipe flow

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Motivation

- Establish **computational multiphysics model** for prediction of aerosol composition and size
- Integrate and couple aerosol formation model into **Computational Fluid Dynamics (CFD)** flow evolution simulations
- Development of **smoking products** with the potential to **reduce the risks of smoking-related diseases**
- Disease risk is related to **aerosol composition** and **deposition behavior** in the respiratory tract, related to **droplet size**

Multi-scale aerosol model strategy development

- **In-silico computational platform for development of new products**
- **Inclusion of physical phenomena specific to our applications**
- **Requirements for the aerosol model implementation:**
  - Cope with dense aerosols
  - Small number of variables
  - Good computational efficiency
- **Temporal aerosol multi-scale model:**
  - Time scale of nucleation-growth coupling is much faster than time scale of simulated flow
  - Sub-time-step model required for aerosol formation (nucleation and initial growth)
  - Larger time steps in simulations for the same accuracy of predictions

Computational Fluid Dynamics approach

Numerical simulations of Navier-Stokes equations for a multi-phase flow

Eulerian aerosol model coupled with a flow solver:

- Mass fractions for composition (gas phase Y_i and droplet phase Z_i)
- Number density N

$$\frac{d(\rho Y_i)}{dt} = -S_{nuc,i} - S_{growth,i}$$

$$\frac{d(\rho Z_i)}{dt} = S_{nuc,i} + S_{growth,i}$$

$$\frac{dN}{dt} = J_{nuc} - J_{coag} - J_{evap}$$

Mechanisms & assumptions:

- Nucleation: Classical **multicomponent nucleation theory** (Arstila et al.), no tuning parameters
- Growth: Standard Condensation (and Evaporation) theory (Friedlander)
- Coagulation: Coagulation theory for polydisperse aerosols (Lee & Chen)
- Assume log-normal size distribution with fixed geometric standard deviation

Aerosol formation in a laminar pipe flow

Dibutyl phthalate (DBP) aerosol formation and growth in a laminar cooled pipe flow (Nguyen)

Inlet: laminar pipe flow of initially dry and clean carrier gas

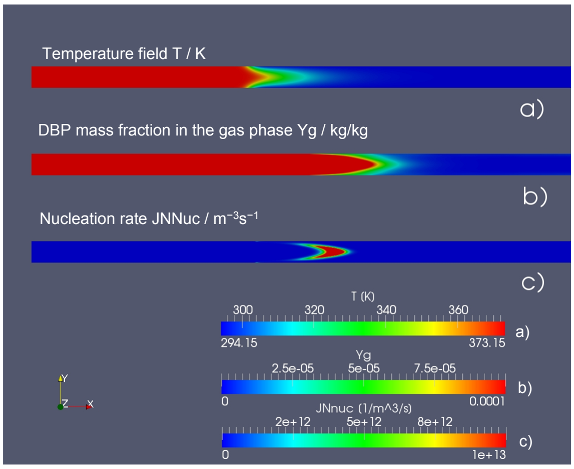
Saturator: reach saturation with dibutyl-phthalate (DBP)

Hot zone: reach uniform temperature

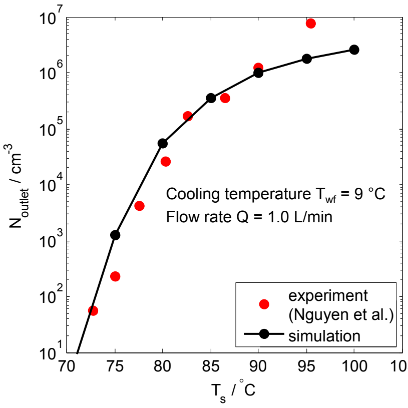
Cooling zone: sharp temperature drop, supersaturation and nucleation

Outlet: Sampling of aerosol and measurement of size distribution

Model validation



Snapshots from a laminar flow simulation of dibutyl phthalate (DBP)



Particle/droplet number density measured at outlet N_{outlet} as function of saturator temperature T_s

Model verification and validation:

- Convergence studies for single and multi-component systems
- Sensitivity to temporal and spatial resolution for CFD coupled simulations
- Various flow rates and cooling temperatures

Concluding remarks

Conclusions:

- Aerosol model with very small set of variables
- Integration of the model into CFD simulation platform
- Good reproduction of experimental results without tuning parameters

Outlook:

- Ongoing analysis of efficiency improvement by sub-time-step model
- Validation and application to multicomponent aerosol formation systems
- Influence of turbulence on aerosol generation and evolution

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