Influence of mixing and cooling on aerosol formation and evolution in backward-facing step flow

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Background

Goals

- controlled aerosol generation from oversaturated vapors
- understand formation and evolution of aerosols
- identify parameters which influence physical/chemical aerosol characteristics at given conditions
- develop numerical methods for prediction of aerosol behavior

Main challenges

- vapor: multi-species mixtures
- aerosol: small droplets at high density
- flow: unsteady and density-varying (large temperature gradients)

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CFD approach

Flow modeling

- low-Mach number approach
- in-house code based on OpenFOAM®: numerics & parallelization
- collocated mesh with PISO pressure-velocity coupling

Aerosol modeling

- Euler-Euler approach (one-way coupling)
- homogeneous nucleation
- condenstation/evaporation
- coalescence

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Aerosol modeling

Development approach

- aerosol formation: single-species[1] $\Longrightarrow$ multi-species[2]
- validation: pipe flow[3] $\Longrightarrow$ backward-facing step
- accuracy: PISO extension, TVD schemes, space-time refinement[4,5]

References

1. Efficient second-order time integration for single-species aerosol formation and evolution, C. Winkelmann, M. Nordlund, A.K. Kuczaj, S. Stolz, B.J. Geurts, International Journal for Numerical Methods in Fluids, 74 (5), 2014
2. Multispecies aerosol formation due to rapid cooling of alcohol mixtures, C. Winkelmann, A.K. Kuczaj, M. Nordlund, B.J. Geurts, submitted to JAS
3. Extension of compressible PISO algorithm to single-species aerosol formation and transport, E.M.A. Frederix, M. Stanic, A.K. Kuczaj, M. Nordlund, B.J. Geurts, to be submitted
4. Capturing aerosol droplet nucleation and condensation bursts using PISO and TVD schemes, E.M.A. Frederix, A.K. Kuczaj, M. Nordlund, B.J. Geurts, this conference
5. Solution-adaptive space-time refinement for multispecies aerosol formation, B.J. Geurts, E.M.A. Frederix, A.K. Kuczaj, M. Nordlund, this conference

Multispecies flow dynamics

Navier-Stokes flow:

$$
\begin{aligned}
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0 \\
\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) &= -\nabla p + \nabla \cdot (\mu \boldsymbol{\tau}) \\
c_p \partial_t (\rho T) + c_p \nabla \cdot (\rho T \mathbf{u}) &= \nabla \cdot (k \nabla T) + \mu \boldsymbol{\tau}(\nabla \mathbf{u}) + D_t p + S_h \\
\partial_t (\rho Y_i) + \nabla \cdot (\rho Y_i \mathbf{u}) &= \nabla \cdot (\rho D_i \nabla Y_i) + S_i^{l \to v}; i = 1, \ldots, n \\
\partial_t (\rho Z_i) + \nabla \cdot (\rho Z_i \mathbf{u}) &= -S_i^{l \to v} \\
\partial_t N + \nabla \cdot (N \mathbf{u}) &= S_N
\end{aligned}
$$

Assumptions:

- Mass fractions in gas Y_i and liquid Z_i state: $\sum_{i=1}^{n} (Y_i + Z_i) = 1$
- Dalton law for partial pressures of ideal gas: $p = \sum_{i=1}^{n} p_i^v; p_i^v = \rho k T \frac{Y_i}{m_i}$ (m_i - molecular mass of species)
- Soret, Dufour effects and diffusion of liquid droplets excluded
- Binary diffusion with Fick law and Fuller method to approximate diffusion constant D_i
- Aerosol droplet density N with fixed mean log-normal distribution

Aerosol formation and evolution

Multispecies aerosol dynamics

- Heat flow rate due to phase change $^{(l \to v)}$ related to heat of evaporation:
  $S_h = -\sum_{i=1}^{n} \Delta h_i^{vap} S_i^{l \to v}$
- Liquid-vapor mass transfer due to nucleation, evaporation and condensation:
  $S_i^{l \to v} = -S_i^{nuc} + S_i^{e-c}$
- Rate of change of droplet density number due to nucleation, coalescence and evaporation:
  $S_N = J_N - J_c - J_{ev}$

Homogeneous nucleation

Classical nucleation theory

- Nucleation mass flow rate based on nucleation rate J_N of molecules number N_i with mass twice that of the critical cluster: $S_i^{nuc} = 2 J_N N_i m_i$
- Nucleation rate $J_N = R_{av} Z c_{eq}$: average growth rate $\times$ Zeldovich factor $\times$ equilibrium concentration
- Average growth rate R_{av} based on the condensation rate (Ref. [1]) extended for multispecies mixture
- Zeldovich factor Z characterizes contribution of Brownian motion to the formation of critical cluster (Ref. [1])
- Equilibrium concentration of critical cluster (related to Gibbs free energy barrier to form an interface at the boundaries of a new phase) takes into account 'self-consistent' normalization (Ref. [2])

References:

1. H. Arstila, P. Korhonen, M. Kulmala, Ternary nucleation: kinetics and application to water-ammonia-hydrochloric acid system, Journal of Aerosol Science, 30, 1999
2. G. Wilemski, B. Wyslouzil, Binary nucleation kinetics, I. Self-consistent size distribution, J. Chem. Phys. 103, 1995

Condensation-evaporation

Mass flow rate due to evaporation/condensation S_i^{e-c}

- Separate treatment for each component (Ref. [1]):
  $S_i^{e-c} = 2\pi D_i \overline{d} \rho Y_i^s f(\overline{d}, \lambda) \left(E_i - \frac{S_i}{W_i} \right) N$
- $f(\overline{d}, \lambda)$ - Fuchs factor (Knudsen correction) (Ref. [2])
- $\overline{d}$ - count mean diameter computed from diameter of average mass through Hatch-Choate conversion equation (Ref. [2])
- E_i - equilibrium saturation takes into account Kelvin effect (Ref. [3])
- S_i, W_i - saturation of species and mole fraction in the liquid phase (Raoult's law used)

References:

1. S. Friedlander, Smoke, Dust and Haze, Wiley, New York, 1977
2. W. Hinds, Aerosol Technology, Wiley-Interscience, New York, 1999
3. M. Wilck, F. Stratmann, A 2-D multicomponent modal aerosol model and its application to laminar flow reactors, Journal of Aerosol Science, 28, 1997

Rate of change of droplet density number

$$S_N = J_N - J_c - J_{ev}$$

Coalescence rate J_c

- Binary collision mechanism: $J_c = \overline{K} N^2$
- Proportionality coefficient K based on the theory for polydisperse aerosols (Ref. [1])

Evaporation rate J_{ev}

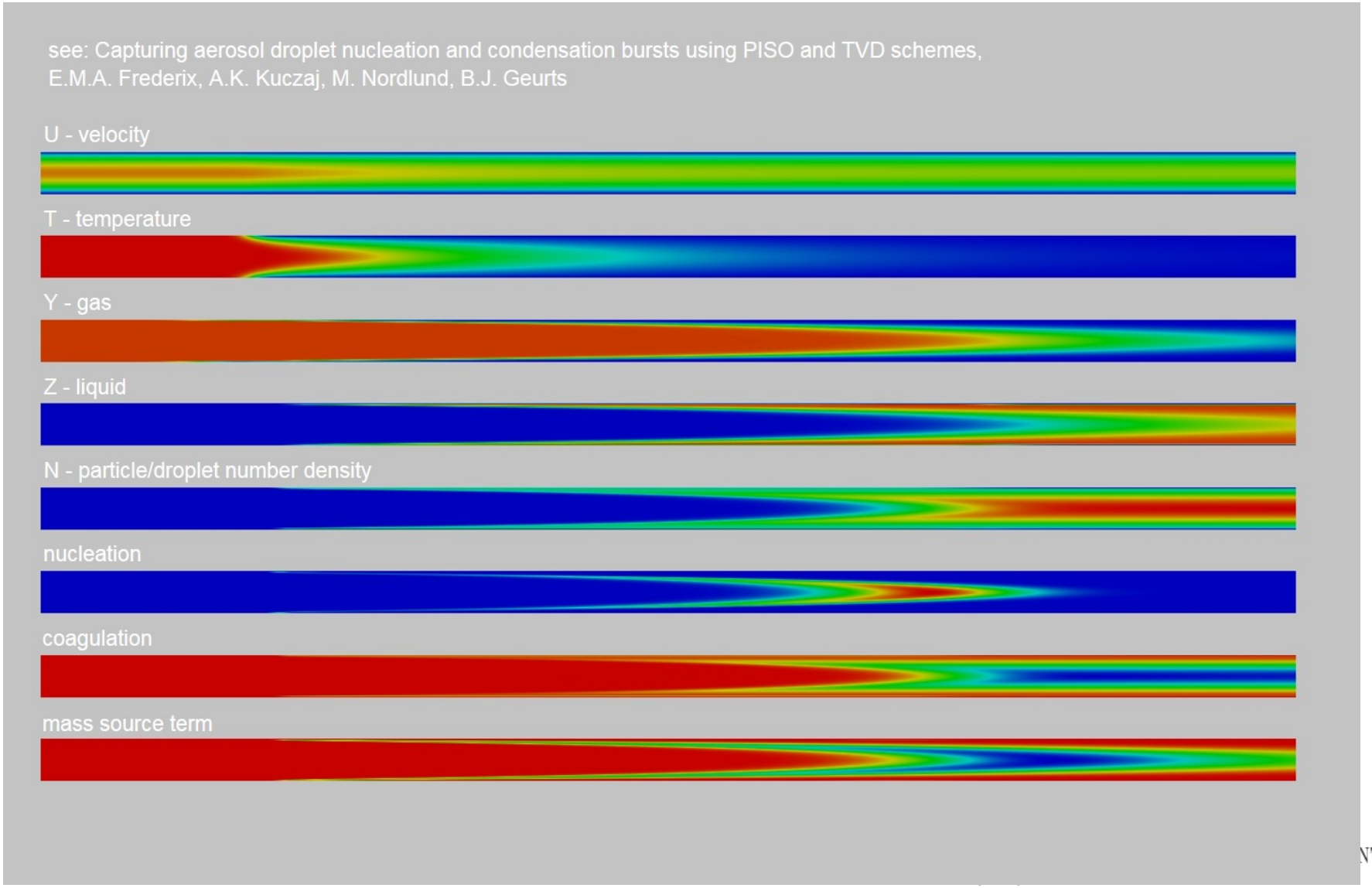
- Complete droplets evaporation based on the consideration of mass balance
- Critical droplet diameter is computed
- Based on log-normal distribution, the droplets with size smaller than critical diameter are eliminated

References:

1 K. Lee, H. Chen, Coagulation rate for polydisperse particles, Aerosol Science and Technology, 3, 1984

Single-species aerosol model validation

Laminar flow diffusion chamber (LFDC)

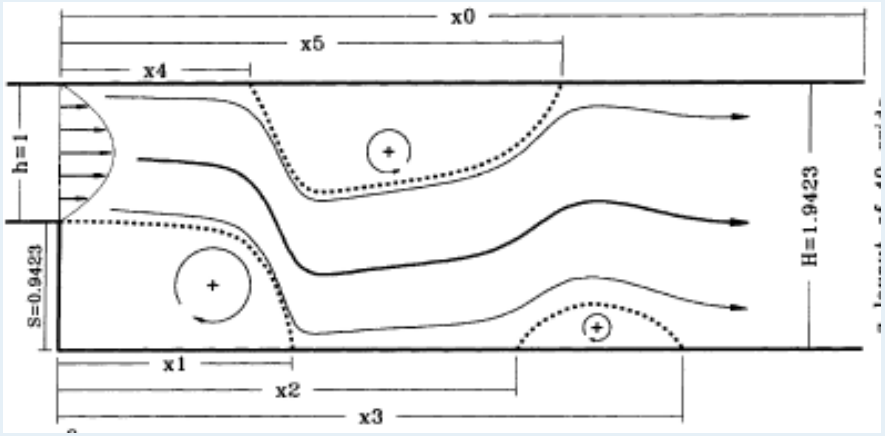


Backward-facing step flow

Motivaton

- Canonical flow case
- Wide range of application: laminar-transition-turbulent
- More complex flow than in laminar flow diffusion chamber
- Shear layer - mixing layer: various ways to utilize
- Mixing (geometry, Re) and cooling (wall temperature) can be studied

Flow behavior



T.P. Chiang, T.W.H. Sheu, C.C. Fang, Numerical investigation of vortical evolution in a backward-facing step expansion flow, Applied Mathematical Modeling, 23, 1999

B.F. Armaly, F. Durst, J.C.F. Pereira, B. Schoenung, Experimental and theoretical investigation of backward-facing step, J. Fluid Mech., 127, 1983

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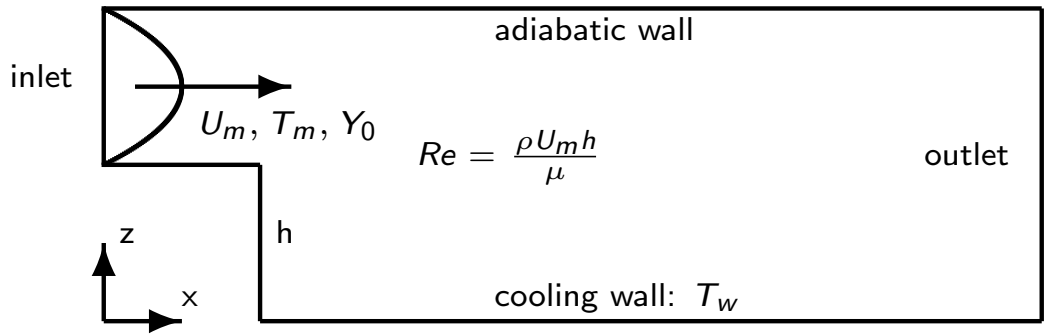
Backward-facing step



- Domain length based on the highest computed Re ($4 \times x_1$)
- Vapor mixture at saturated conditions at inlet
- Cooling wall T_w set constant
- Step-wall and upper wall with adiabatic conditions
- Laminar flow profile at the inlet

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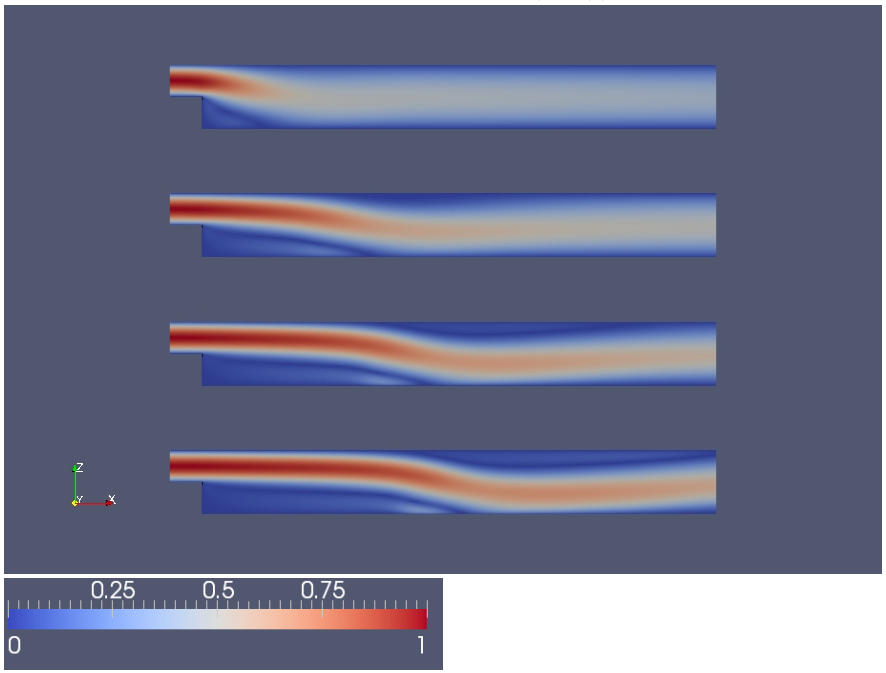
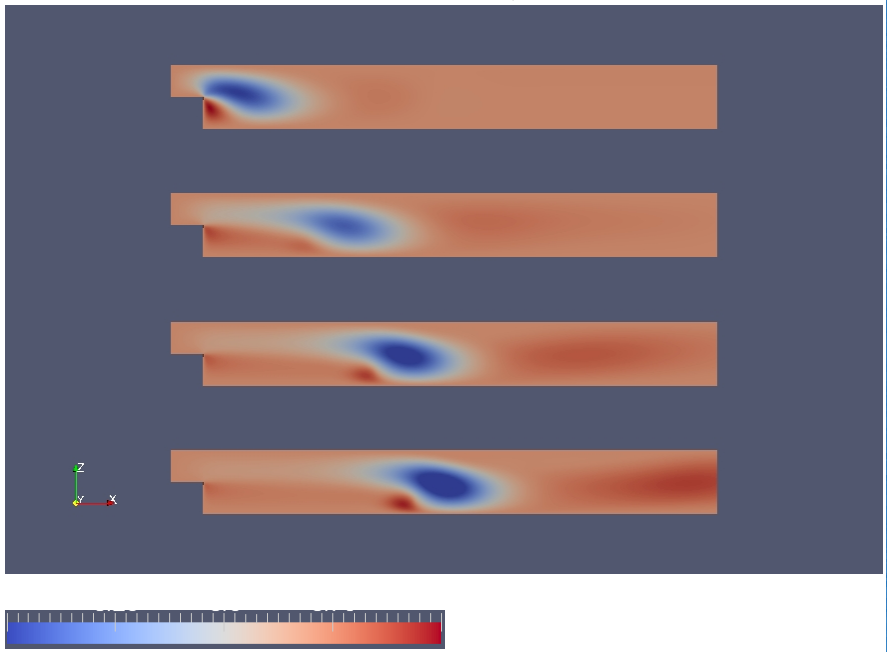
Flow - Re = 100 (top), 500, 1000, 1500 (bottom)

Velocity magnitude: $|\mathbf{u}|/U_m$



Vertical velocity: u_z/U_m



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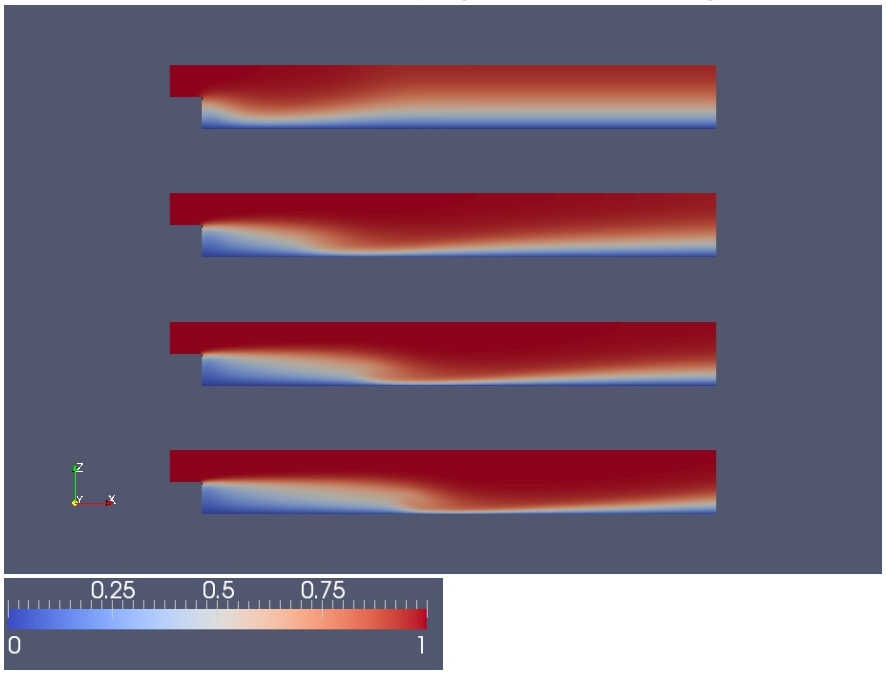
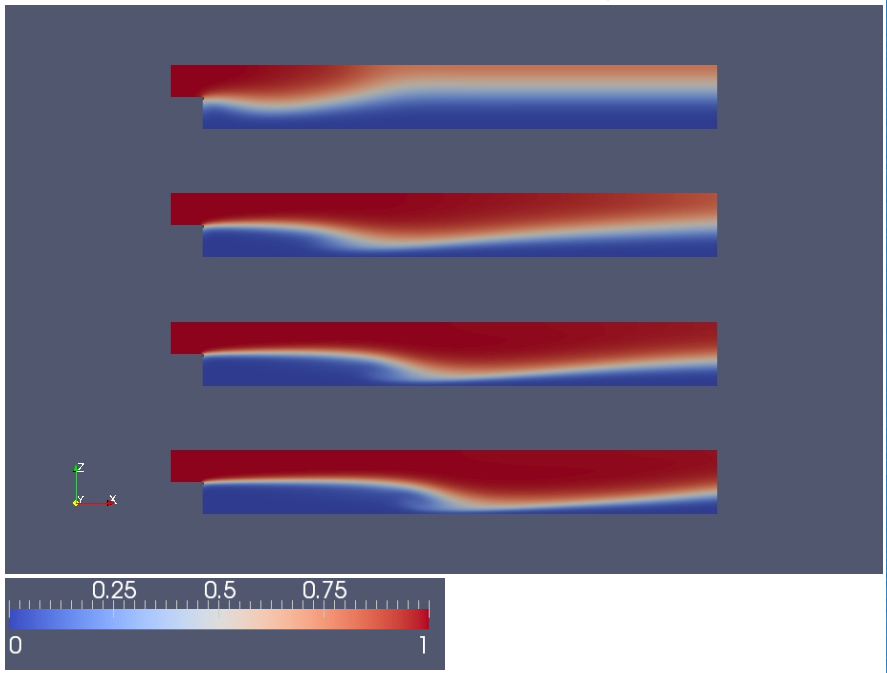
Temperature and vapor mass fraction

Temperature: $T/(T_m - T_w)$



Vapor mass fraction: Y/Y_0



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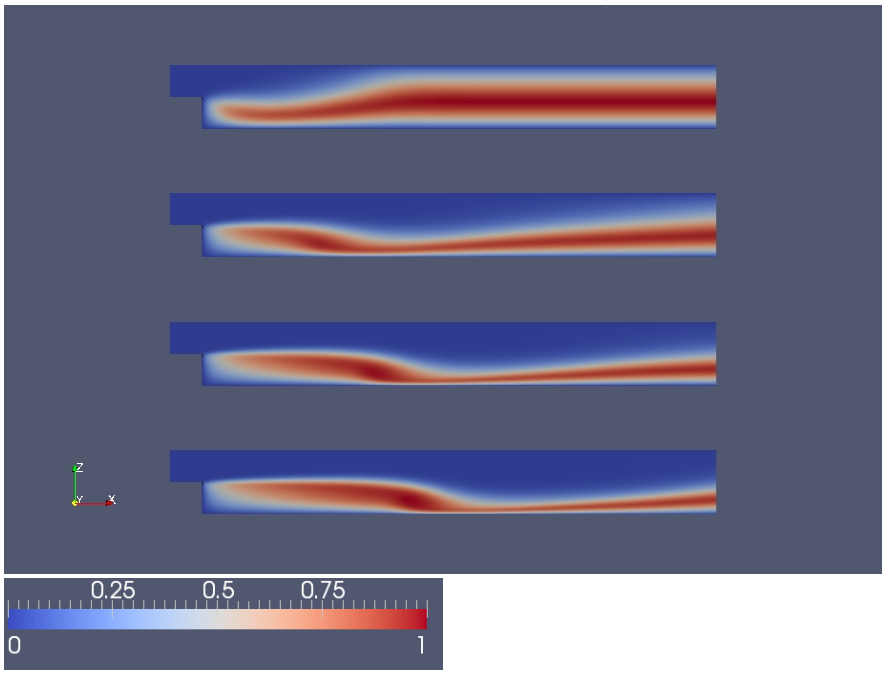
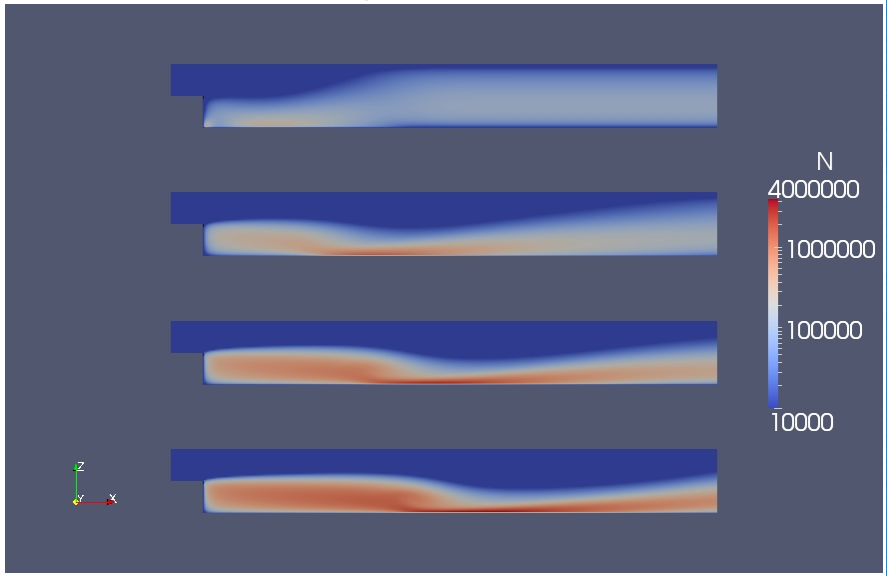
Liquid mass fraction and droplet density number

Liquid mass fraction: Z/Y_0



Droplet density number: N



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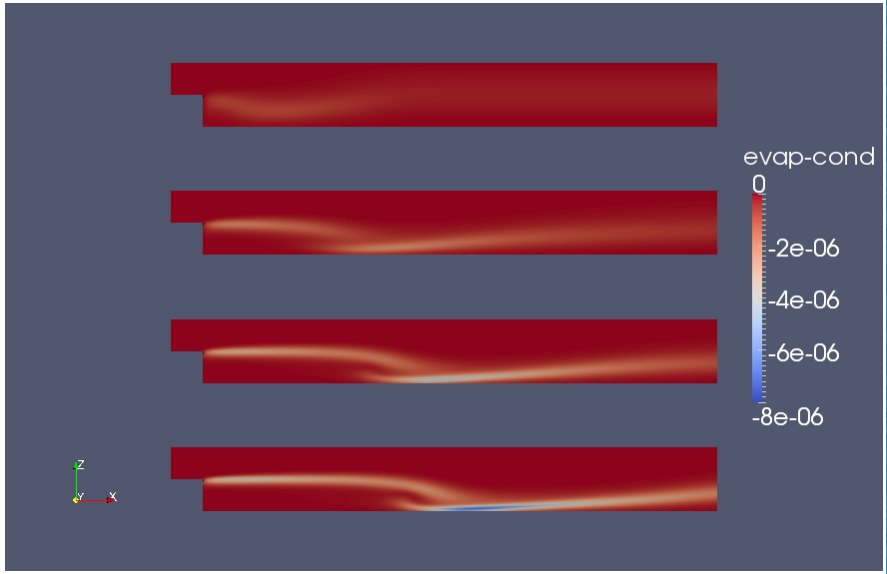
Nucleation and condensation/evaporation rate

Droplet nucleation rate

Condensation/evaporation rate



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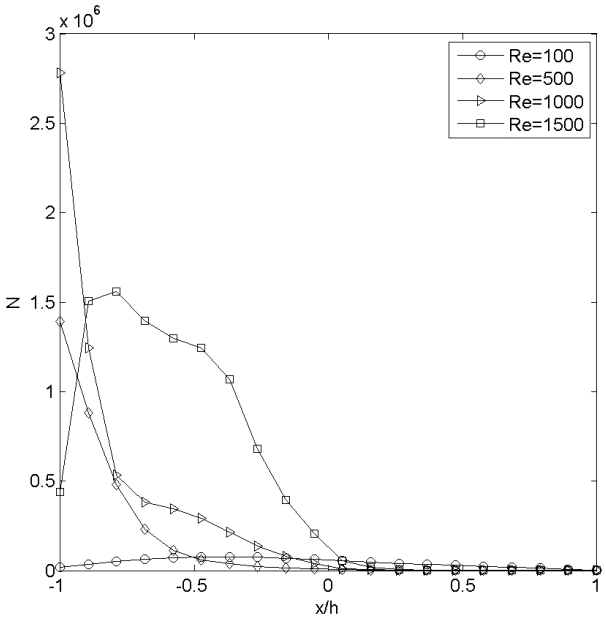
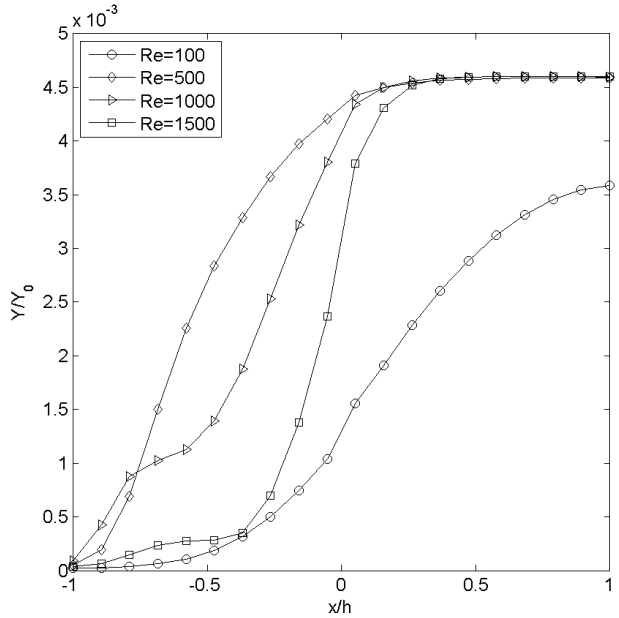
Quantification - example

Droplet number density profile at $x = 6h$



Mass fraction of gas species profile at $x = 6h$



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Summary

- Multispecies aerosol model in Euler-Euler framework developed
- Backward-facing step adopted for study of aerosol formation and evolution
- Quantification of aerosol formation and evolution possible (droplet number density, droplet size, amount of vapors turned into liquid droplets
- Future: Extensive parameter study for benchmarking the system at various conditions

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