Towards Large-Eddy Simulation of Primary Atomization

M.Sc. Sebastian Ketterl and Prof. Dr.-Ing. habil. Markus Klein
Institute for Numerical Methods in Aerospace Engineering
Werner-Heisenberg-Weg 39, 85577 Neubiberg

Universität der Bundeswehr München

Introduction

Problem:

- Multi-scale atomization is extremely challenging since liquid breakup includes turbulence, surface tension, interfaces large density ratios and a wide range of scales
- Direct numerical simulation of liquid atomization is restricted to moderate Reynolds numbers due to immense demand on computational resources
- Large eddy simulation provides promising tool to calculate primary atomization but requires the modeling of subgrid scale dynamics
- Tryggvason [2]: "Development of next generation models for large scale multiphase flows using input from DNS results is one of the most urgent challenges."

Objectives: Development of a large-eddy simulation based computation tool for the simulation of primary breakup

- Enhance understanding of physical mechanism leading to liquid breakup
- Modeling LES subgrid scale effects in multiphase flows
- Enable computation for Reynolds and Weber number relevant for technical applications

Direct Numerical Simulation

The one-fluid formulation of isothermal, incompressible, variable-density Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\, \mathbf{u}) = 0 \tag{1}$$

$$\frac{\partial \rho\, \mathbf{u}}{\partial t} + \nabla \cdot (\rho\, \mathbf{u} \otimes \mathbf{u} + \rho\, \mathbf{I} - \mu\, \mathbf{S} - \rho\, \mathbf{g} - \sigma\, \mathbf{n}\, \kappa\, \delta_S) = 0 \tag{2}$$

describe the dynamics of multiphase flows where $\mathbf{S} = \nabla \mathbf{u} + \nabla^T \mathbf{u}$ is the deformation rate. The phase interface is captured by a geometrical Volume-of-Fluid (VOF) method with PLIC interface reconstruction. A scalar volume faction field α is tracked by the transport equation

$$\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla \alpha = 0 \tag{3}$$

which determines the the physical properties in Eqn. (1) (2) to

$$\rho(\alpha) = \alpha\, \rho_l + (1-\alpha)\, \rho_g, \qquad \mu(\alpha) = \alpha\, \mu_l + (1-\alpha)\, \mu_g. \tag{4}$$

The multi-scale problem is fully resolved to the smallest turbulent structures in the dissipation range of the Kolmogorov scale. A databasis of very large DNS computations for different density and viscosity ratios, ρ_l/ρ_g respect. μ_l/μ_g, as well as Reynolds and Weber $Re \approx We \approx \mathcal{O}(10^4)$ is generated and serves as numerical experiments for the derivation of LES models. Insights from DNS will allow an identification of the most impacting subgrid-scale parameters and provide helpful knowledge for modelling the dynamics of small scale effects.

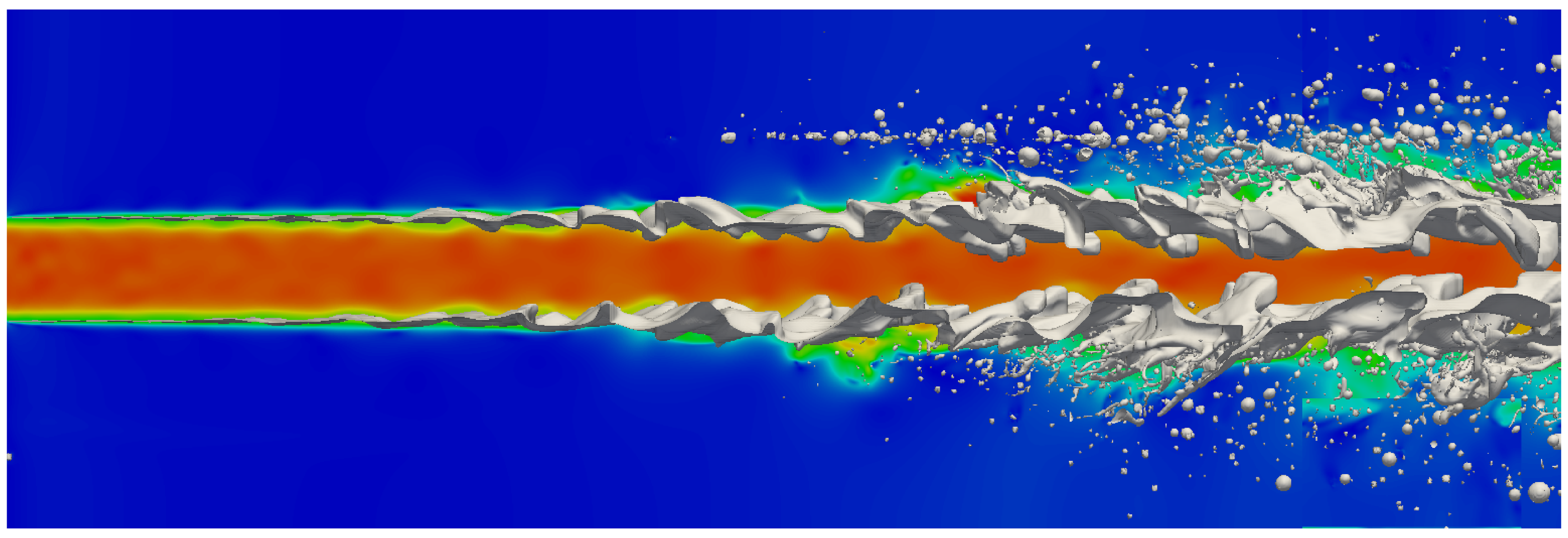

Figure 1 : DNS of a spatially developing liquid sheet with for $Re = 3500$, $We = 3000$ and $\rho_l/\rho_g = \mu_l/\mu_g = 40$ based on Klein [4]. Displayed is the $\alpha = 0.5$ isosurface, the axial velocity field and pressure field at the inlet. Inflow data generation is based on Klein [1].

Statistical moments, on the interface amplified wavelengths with growth rates and the size of primary droplets will be extracted from DNS data for validation purposes of the LES based computation tool.

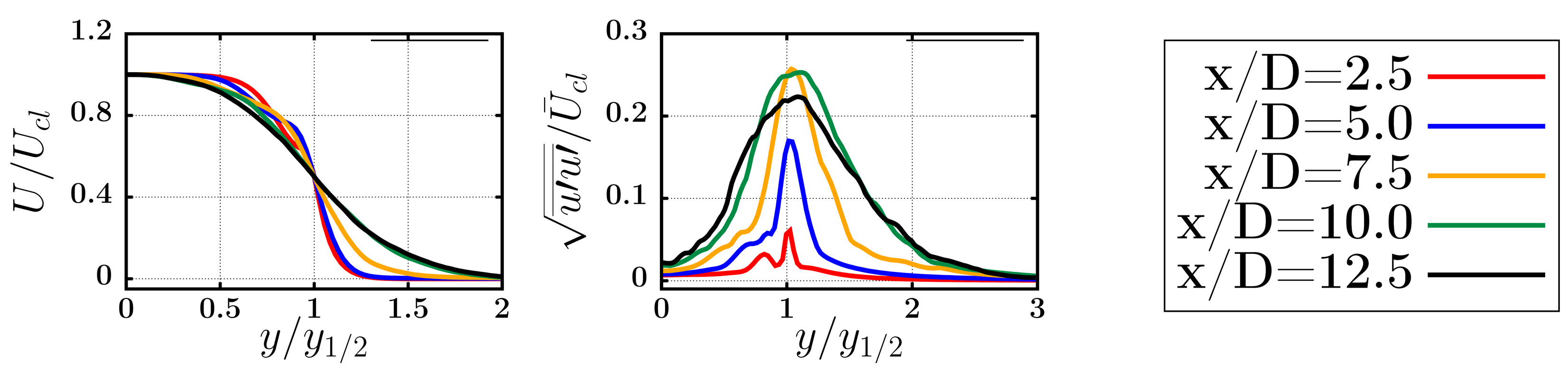

Figure 2 : Mean axial velocity (left) and axial velocity fluctuations (right) plotted in lateral direction for different axial locations. Statistics averaged over 14 through flow times corresponding to 340 independet samples

Large-Eddy Simulation framework

A LES-VOF formulation is derived by applying a LES low pass filter combined with a Favre filter

$$\overline{\psi}(\mathbf{x}) = G \star \psi(\mathbf{x}) = \int_{-\infty}^{\infty} \psi(\mathbf{y})\, G(\mathbf{x}-\mathbf{y}, \mathbf{x})\, \mathrm{d}y, \qquad \tilde{\psi}(\mathbf{x}) = \frac{\overline{\rho\, \psi}}{\bar{\rho}} \tag{5}$$

to the Navier-Stokes equations (1),(2),(3). Expressed in terms of filtered quantities the LES-VOF equations state

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho}\, \tilde{\mathbf{u}}) = 0 \tag{6}$$

$$\frac{\partial \bar{\rho}\, \tilde{\mathbf{u}}}{\partial t} + \nabla \cdot \left(\bar{\rho}\, \tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}} + \bar{\rho}\, \mathbf{I} - \bar{\mu}\, \tilde{\mathbf{S}} - \bar{\rho}\, \mathbf{g} - \sigma\, \bar{\mathbf{n}}\, \bar{\kappa}\, \delta_S \right) = -\nabla \cdot \left(\boldsymbol{\tau}_{\rho\mathbf{uu}} + \boldsymbol{\tau}_{\mu\mathbf{S}} \right) + \boldsymbol{\tau}_{\mathbf{nn}} \tag{7}$$

$$\frac{\partial \bar{\alpha}}{\partial t} + \tilde{\mathbf{u}} \cdot \nabla \bar{\alpha} = \boldsymbol{\tau}_{\mathbf{u}\alpha} \tag{8}$$

containing four unclosed subgrid scale contributions appearing due to the LES filter

$$\boldsymbol{\tau}_{\rho\mathbf{uu}} = \overline{\rho\, \mathbf{u} \otimes \mathbf{u}} - \bar{\rho}\, \tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}} \tag{9}$$

$$\boldsymbol{\tau}_{\mu\mathbf{S}} = \overline{\mu\, \mathbf{S}} - \bar{\mu}\, \tilde{\mathbf{S}} \tag{10}$$

$$\boldsymbol{\tau}_{\mathbf{nn}} = \overline{\sigma\, \mathbf{n}\, \kappa\, \delta_S} - \sigma\, \bar{\mathbf{n}}\, \bar{\kappa}\, \delta_S \tag{11}$$

$$\boldsymbol{\tau}_{\mathbf{u}\alpha} = \tilde{\mathbf{u}} \cdot \nabla \bar{\alpha} - \overline{\mathbf{u} \cdot \nabla \alpha} \tag{12}$$

which are unknown and need to be modelled in order to include the dynamics of small, unresolved scales in LES simulations. The tensor $\boldsymbol{\tau}_{\rho\mathbf{uu}}$ is the subgrid tensor known from single phase flows whereas $\boldsymbol{\tau}_{\mu\mathbf{S}}, \boldsymbol{\tau}_{\mathbf{nn}}$ and $\boldsymbol{\tau}_{\mathbf{u}\alpha}$ arise due to the multiphase nature of immiscible fluids. A-priori analysis of detailed DNS fields allow the exact evaluation of the subgrid contributions. This knowledge is used to derive subgrid-scale models adapted for multiphase flows representing the effects of unresolved small scales.

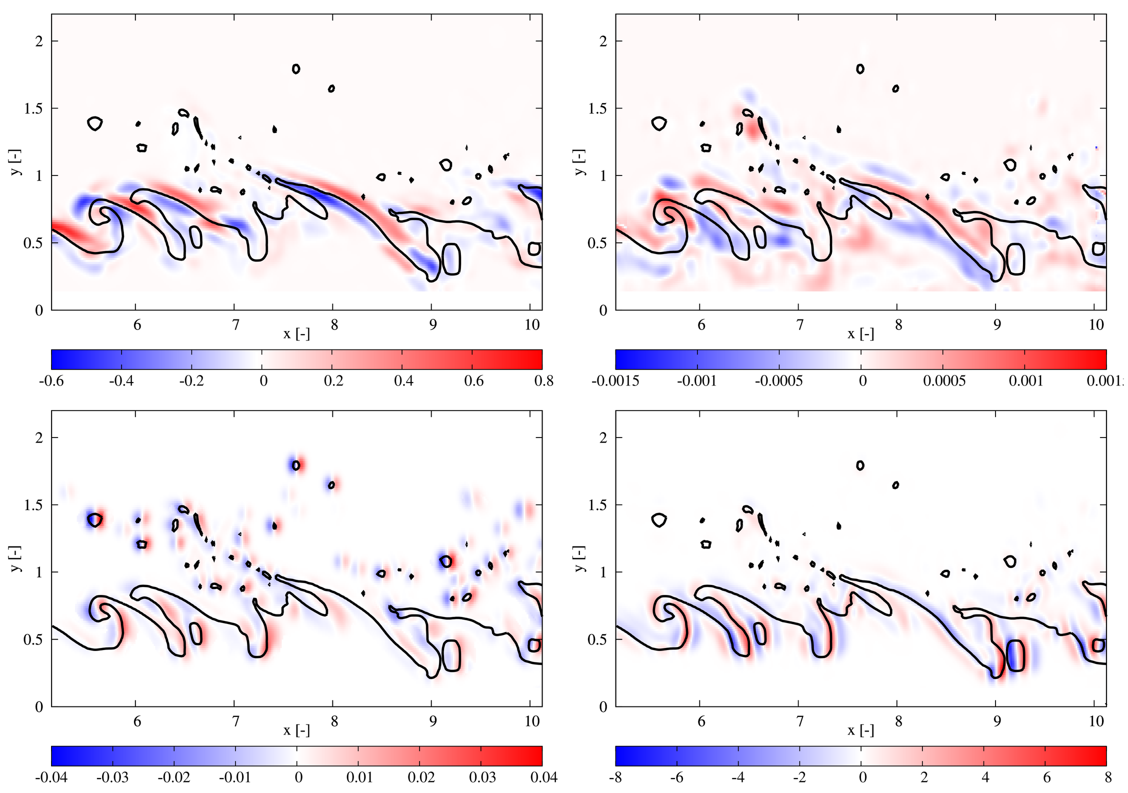

Figure 3 : Two-dimensional fields of $(\nabla \cdot \boldsymbol{\tau}_{\rho\mathbf{uu}})_x$ (top left), $(\nabla \cdot \boldsymbol{\tau}_{\mu\mathbf{S}})_x$ (top right), $\boldsymbol{\tau}_{\mathbf{nn},x}$ and $\boldsymbol{\tau}_{\mathbf{u}\alpha}$ in lateral *xy*-plane for $z = 0$.

Outlook

- Step 1: Derivation of subgrid scale models adapted to multiphase flow to model dynamics of small unresolved scales
- Step 2: Develpment of LES based computation tool $\rightarrow$ implementation of subrid models in flow solver
- Step 3: A-posteriori analysis: LES compuations on relatively coarser grids in order to check numerical stability and validate the quality by a comparison to detailed DNS data
- Step 4: LES computation of primary atomization of liquids for *Re* and *We* relevant for engineering devices

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