Modelling turbulent fluid-, thermo-, and droplet dynamics in the Leipzig Aerosol Cloud Interaction Simulator (LACIS-T)

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Leibniz Institute for Tropospheric Research

Outline

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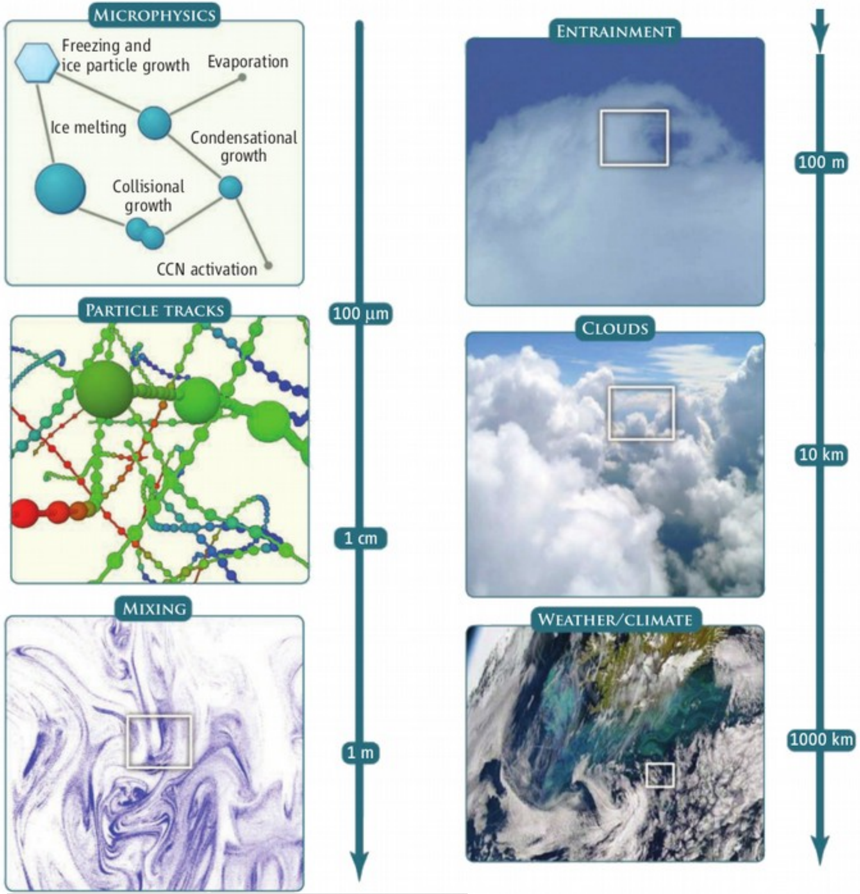
1 Introduction

1 Introduction – Clouds

- Play a huge role in long term climate predictions as wells as in short term weather forecasts
- Hard to investigate
  - Transient, turbulent, intermittent, inhomogeneous
  - Wide range of spatial and temporal scales
  - Usually hard to reach

➔ Set up of a facility able to simulate clouds under reproducible conditions



Source: Bodenschatz, E., Malinowski, S. P., Shaw, R. A., & Stratmann, F. (2010). Can we understand clouds without turbulence?. Science, 327(5968), 970-971.

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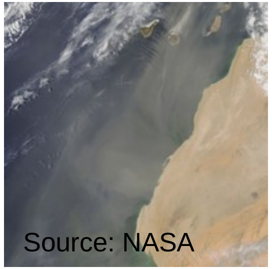
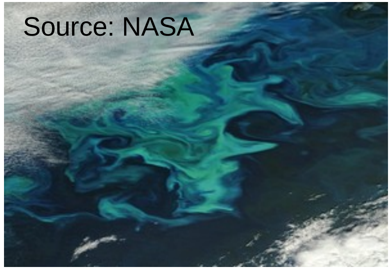
1 Introduction – Clouds

- Formed by water vapour, condensing at **c**loud **c**ondensation **n**uclei
- CCNs: Dust, black carbon, sulfate, phytoplankton, sodium chloride, …





- Size range ~0.1µm
- Condensation determined by material, particle and ambient physical properties (especially temperature and water vapour content)

➔ How much do turbulent fluctuations of ambient properties influence particle and droplet microphysics?

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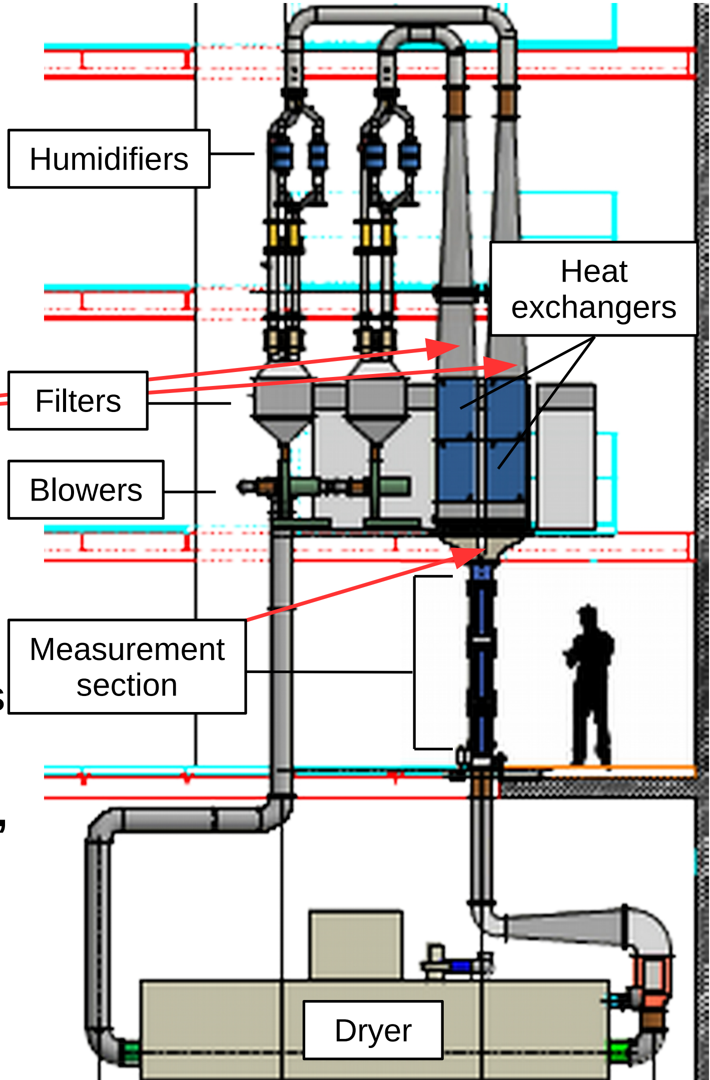
1 Introduction – LACIS-T

- Turbulent Leipzig Aerosol Cloud Interaction Simulator (LACIS-T)
- Closed-loop (Göttingen-type) wind tunnel
- Two branches, each with up to 5000 L/min
- Precisely defined thermodynamic and flow conditions
  - Velocity: up to 1.5m/s
  - Temperature and dew point: -40°C … 25°C
- Injection of well defined particles between the branches

Are we able to simulate the flow, the thermodynamics, and particle/droplet behaviour inside LACIS-T?

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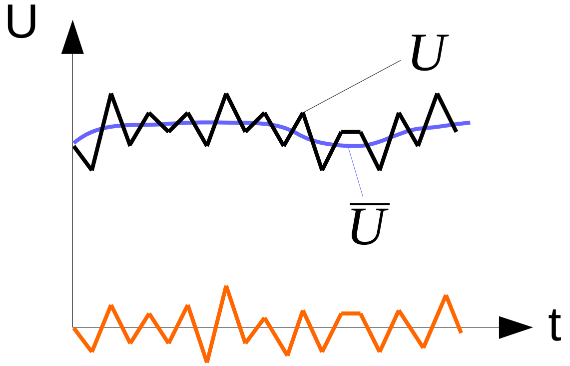
2 Fluid and thermodynamics

- Fields of instantaneous, mean and root mean square (RMS) values necessary for correlations between thermodynamic fluctuations and particle microphysics
- Measurement → Usually limited insight in flow and particle properties

➔ Simulation

- Exact knowledge of thermodynamic conditions necessary to simulate particle behaviour, including
  - Velocity and turbulence
  - Temperature
  - Humidity

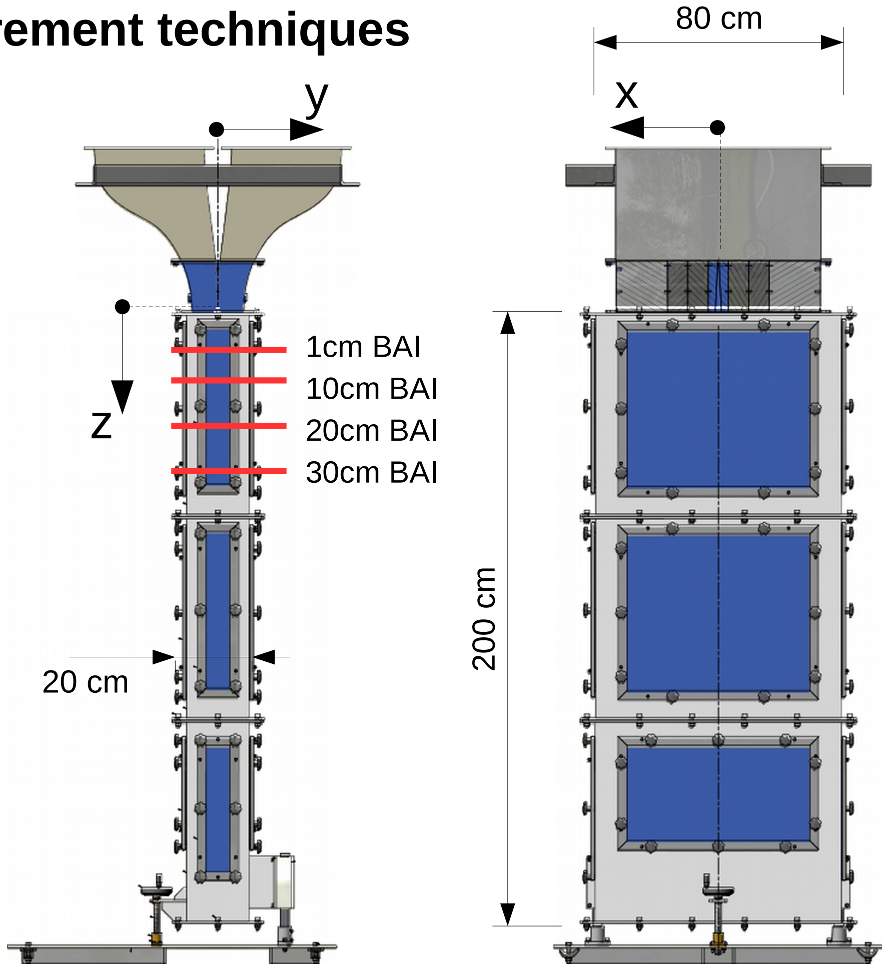


$$u' = U - \overline{U}$$

2 Fluid and thermodynamics – Measurement techniques

- Point probes:
  - Hot wire anemometer (velocity)
  - Cold wire (temperature)
- On points along lines in y-direction in different heights **b**elow **a**erosol **i**nlet (BAI) (z-axis)
- High frequency measurements (3kHz)

→ Analysis gives mean and RMS value profiles



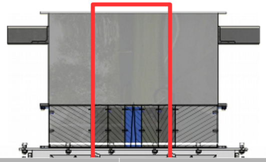
2 Fluid and thermodynamics – Numerical methods

- Finite volume method with OpenFOAM
- Solving transient, incompressible Navier-Stokes-Equations
- PIMPLE-algorithm (merged PISO[1)] and SIMPLE[2)]), allowing larger time steps
- Solver “pimpleFOAM”
- Simulation of temperature with Boussinesq approximation and humidity as passive scalar
- 2nd order schemes (except divergence of k and ν_t → limiter towards 1st order upwind)
- Considering turbulence with Large Eddy model (“dynamic k-equation”)
- Calculated 2.5s real time
- Statistics done for time after 0.5s (quasi steady flow reached)

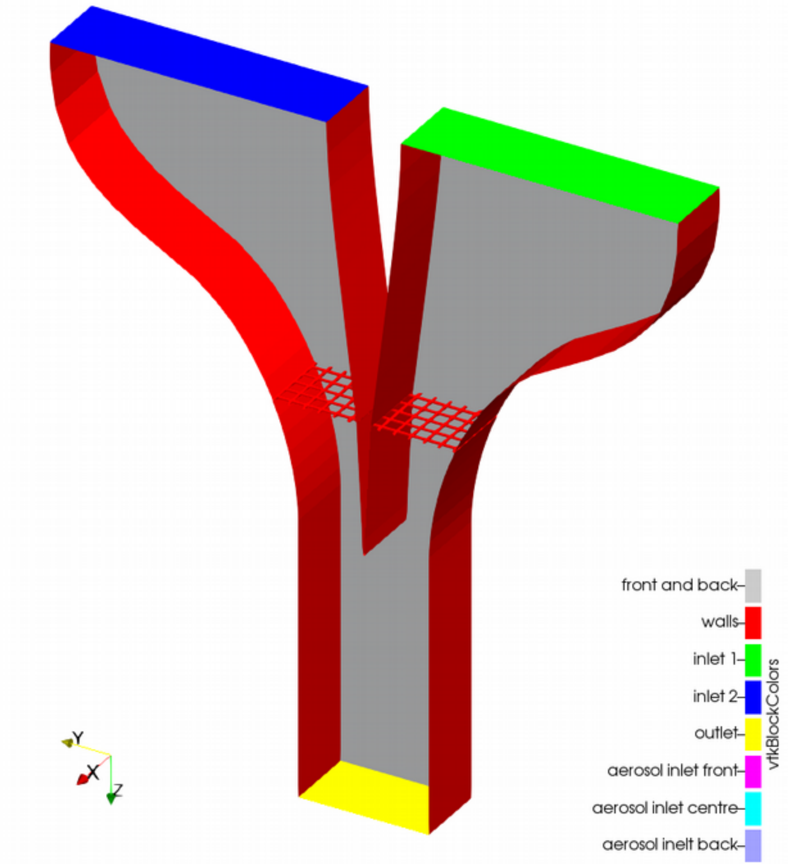
[1)] Pressure Implicit Split Operator (transient)
[2)] Semi Implicit Method of Pressure Linked Equations (steady state)

2 Fluid and thermodynamics – Domain & Boundary Conditions

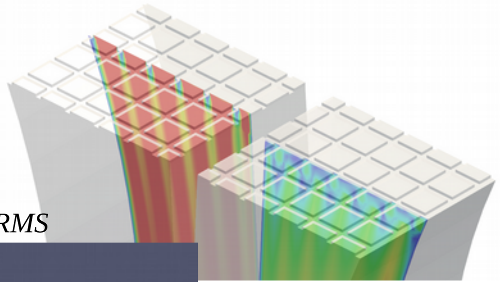
- Wind tunnel is modelled only partially
- Hex mesh, ~7.5M cells
- Boundary conditions:



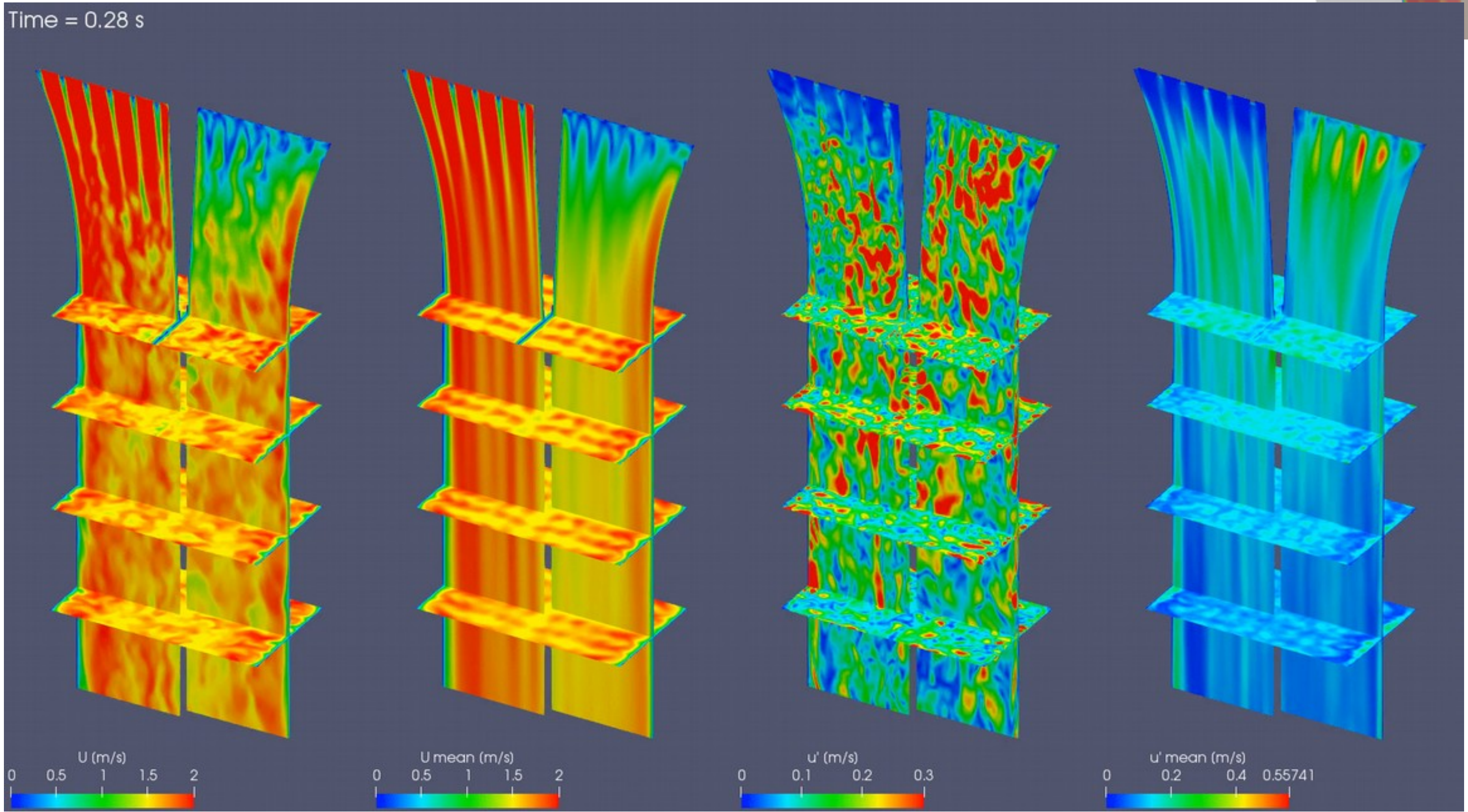
	U	p	T & H
Inlet 1 / Inlet 2	$\begin{pmatrix} 0 \\ 0 \\ 0.39 \end{pmatrix}$	Zero gradient	Fixed value
Walls	0	Zero gradient	Fixed value
Outlet	Zero gradient	0	Zero gradient
Aerosol inlets	0	Zero gradient	Fixed value
Front and back	cyclic	cyclic	cyclic



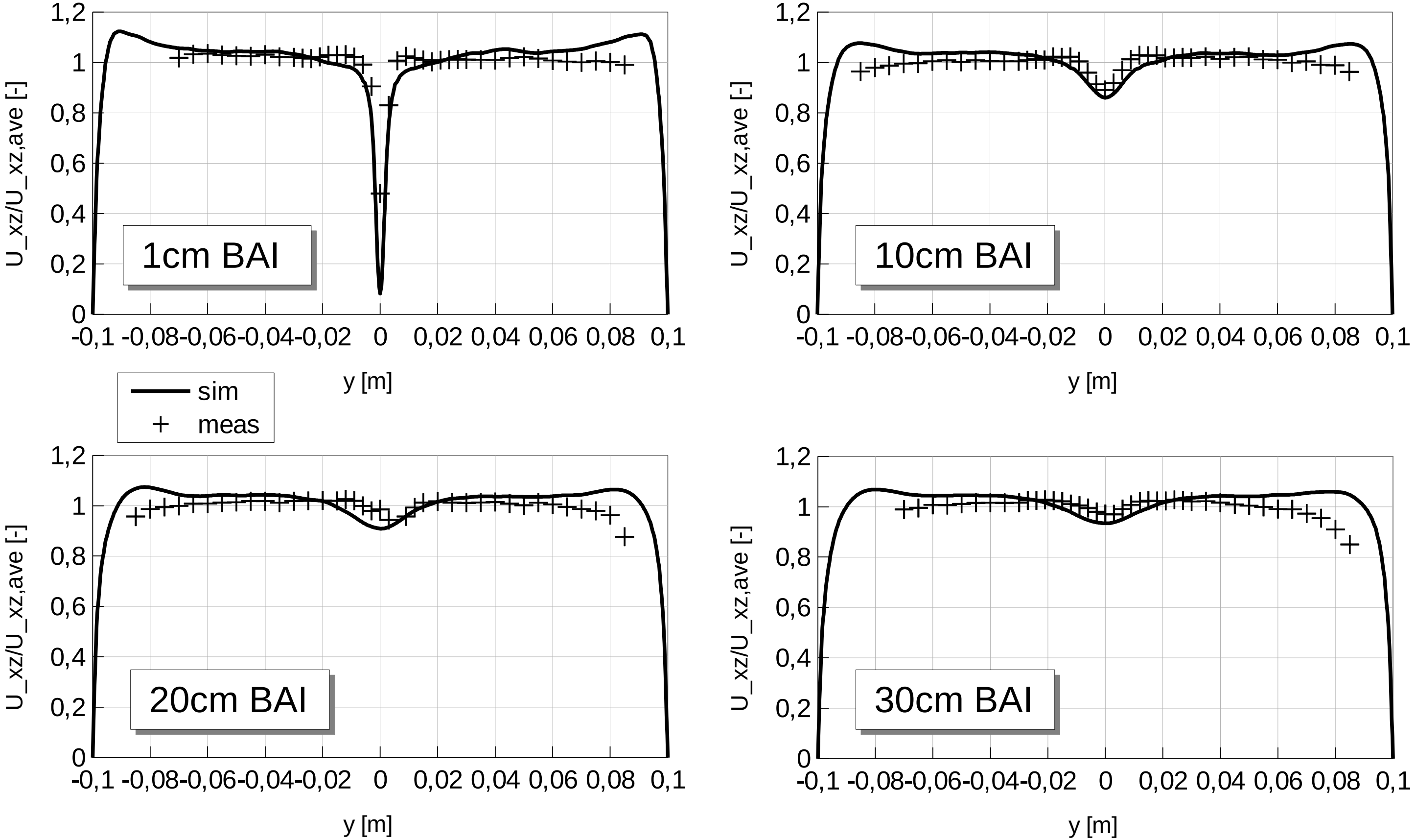
2 Fluid and thermodynamics – Results – Velocity

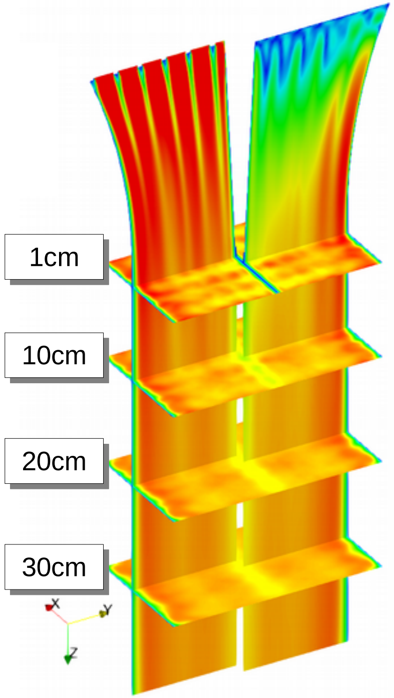


U_{inst} $\overline{U}$ $u' = U_{inst} - \overline{U}$ u'_{RMS}



2 Fluid and thermodynamics – Results – Velocity





2 Fluid and thermodynamics – Results – Turbulence

- Visualisation of turbulent structures with Q-iso-surfaces

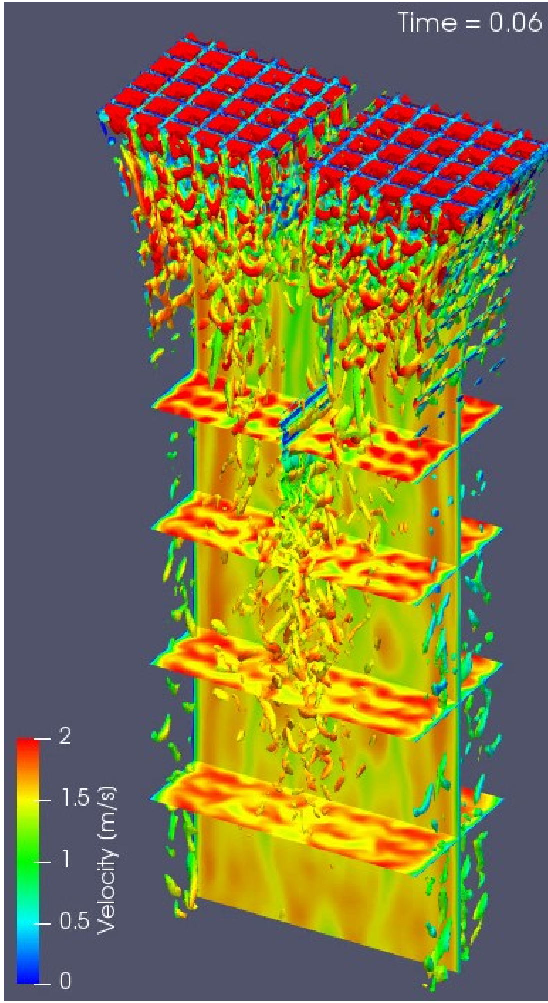
$$Q=\frac{1}{2}\left[\left(tr\left(\nabla \boldsymbol{U}\right)\right)^2-tr\left(\nabla \boldsymbol{U}\cdot\nabla \boldsymbol{U}\right)\right]$$

- Comparison to measurements with turbulent intensity

$$Tu=\frac{u'_{RMS}}{\overline{U}}=\frac{\left(\overline{U}-U\right)_{RMS}}{\overline{U}}$$

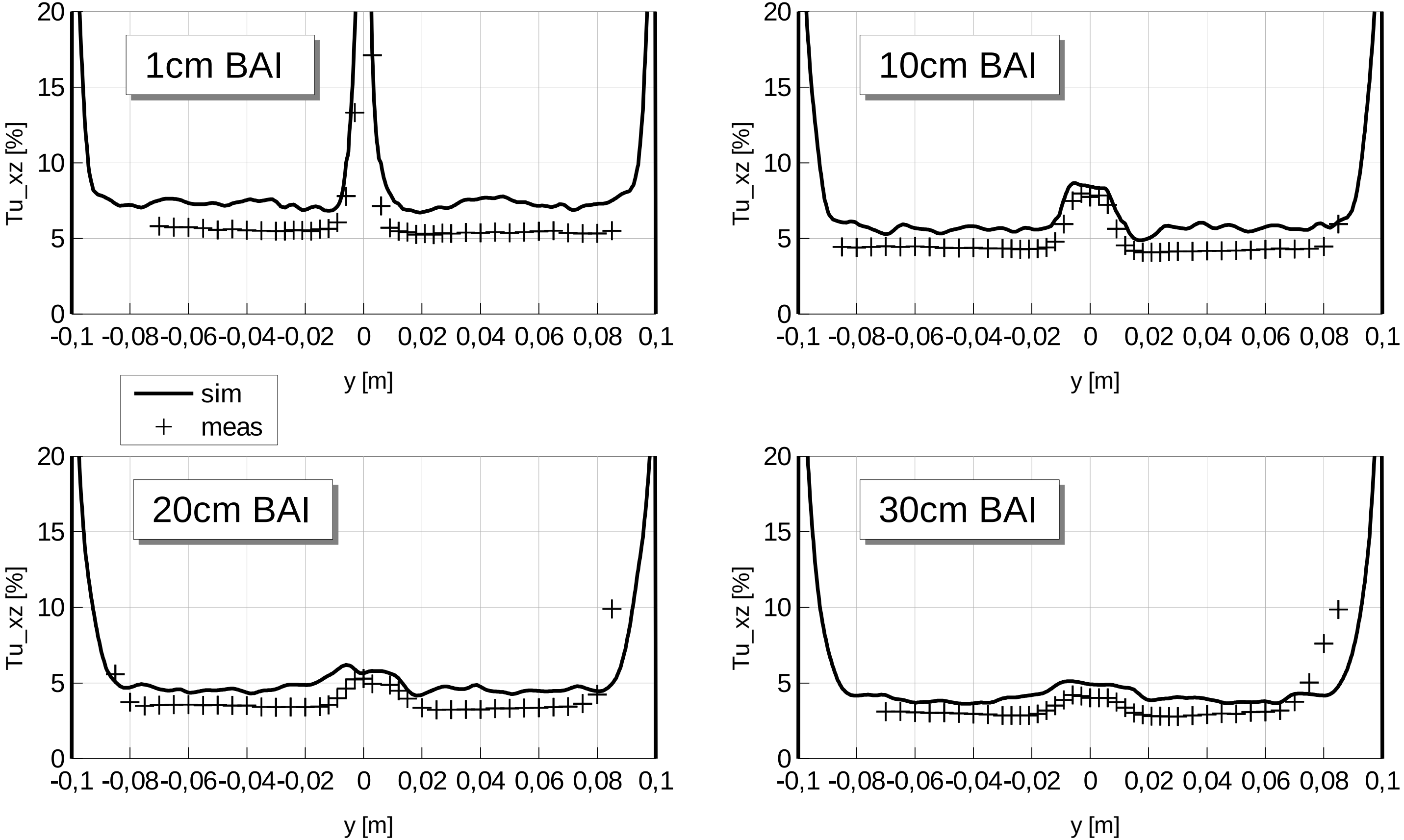
- Hot wire measures only two components, thus

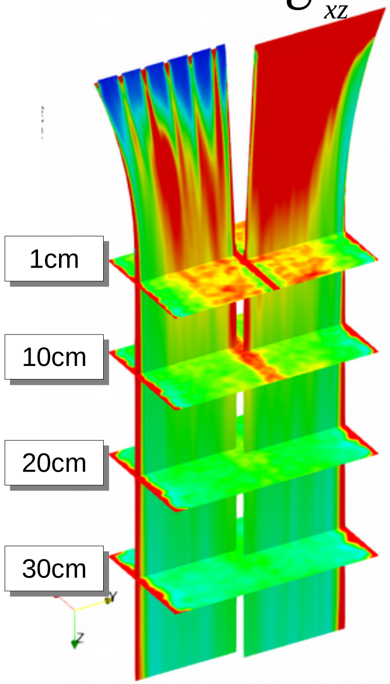
$$Tu=Tu_{xz}=\frac{u_{xz}'_{RMS}}{\overline{U}_{xz}}=\frac{\left(\overline{U}_{xz}-U_{xz}\right)_{RMS}}{\overline{U}_{xz}}$$



2 Fluid and thermodynamics – Results – Turbulence

$$Tu_{xz} = \frac{u_{xz}'_{RMS}}{\overline{U}_{xz}}$$





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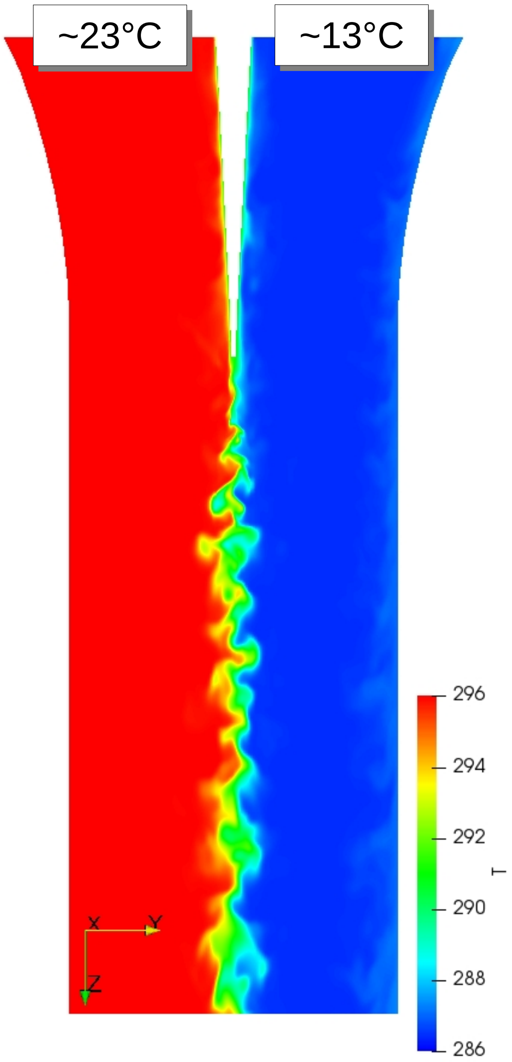
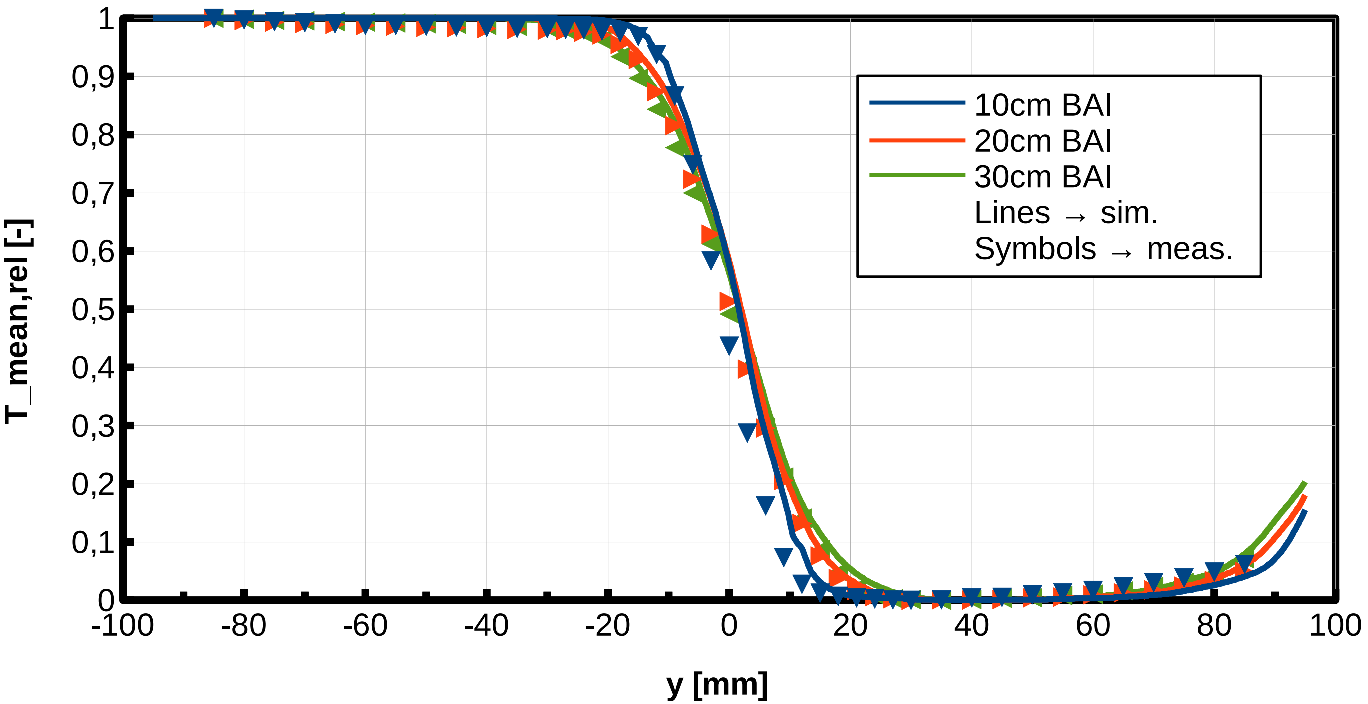
2 Fluid and thermodynamics – Results – Temperature

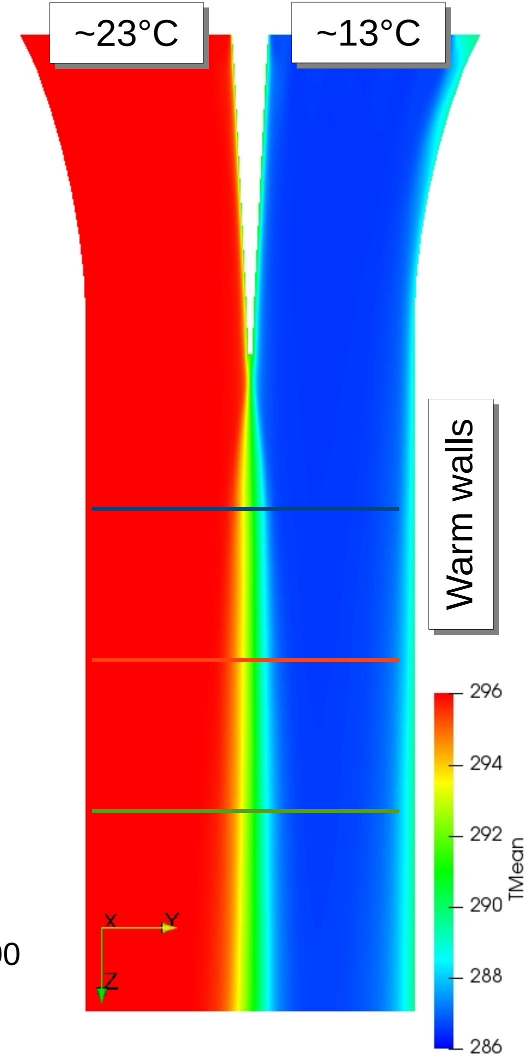
- Example: Mixing of warm and cold air below aerosol inlet



2 Fluid and thermodynamics – Results – Temperature

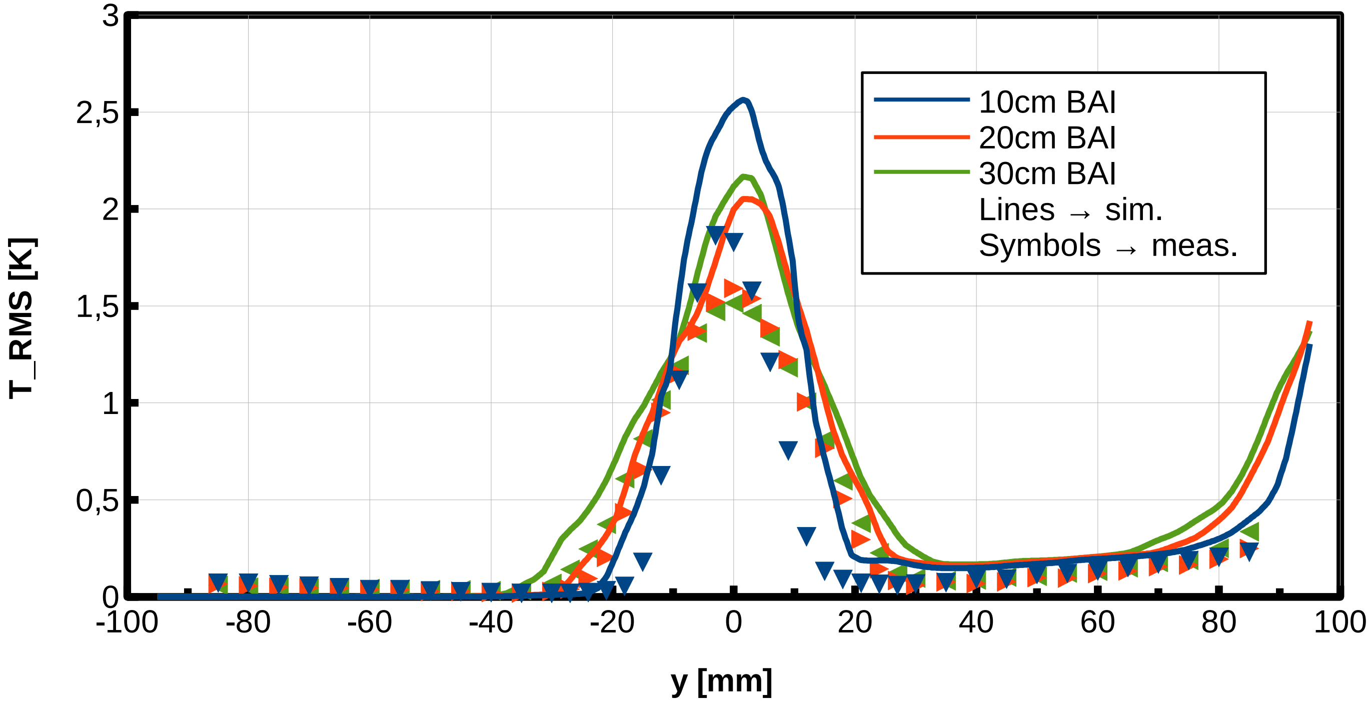
$$T_{mean,rel} = \frac{T_{mean} - min(T_{Mean})}{max(T_{Mean}) - min(T_{Mean})} \rightarrow 0 \triangleq T_{min}, \quad 1 \triangleq T_{max}$$

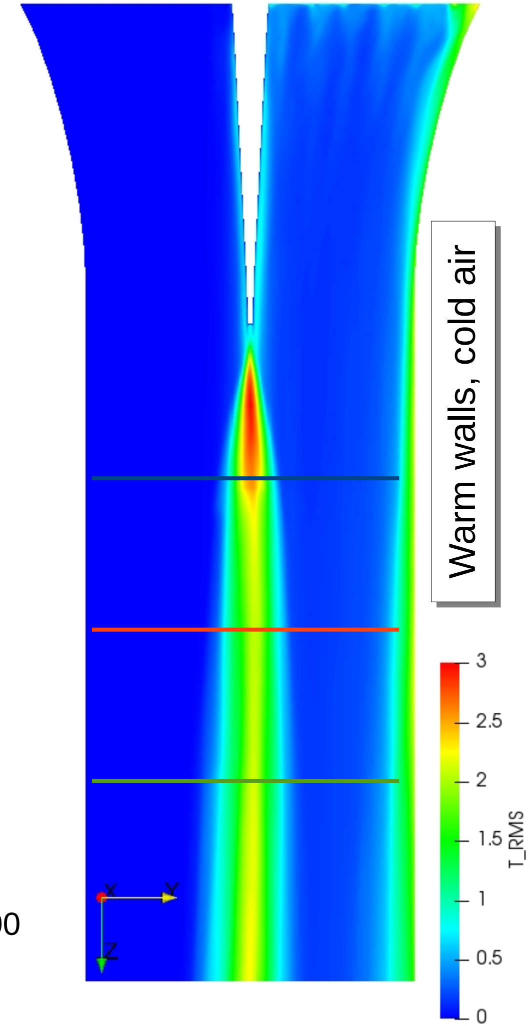




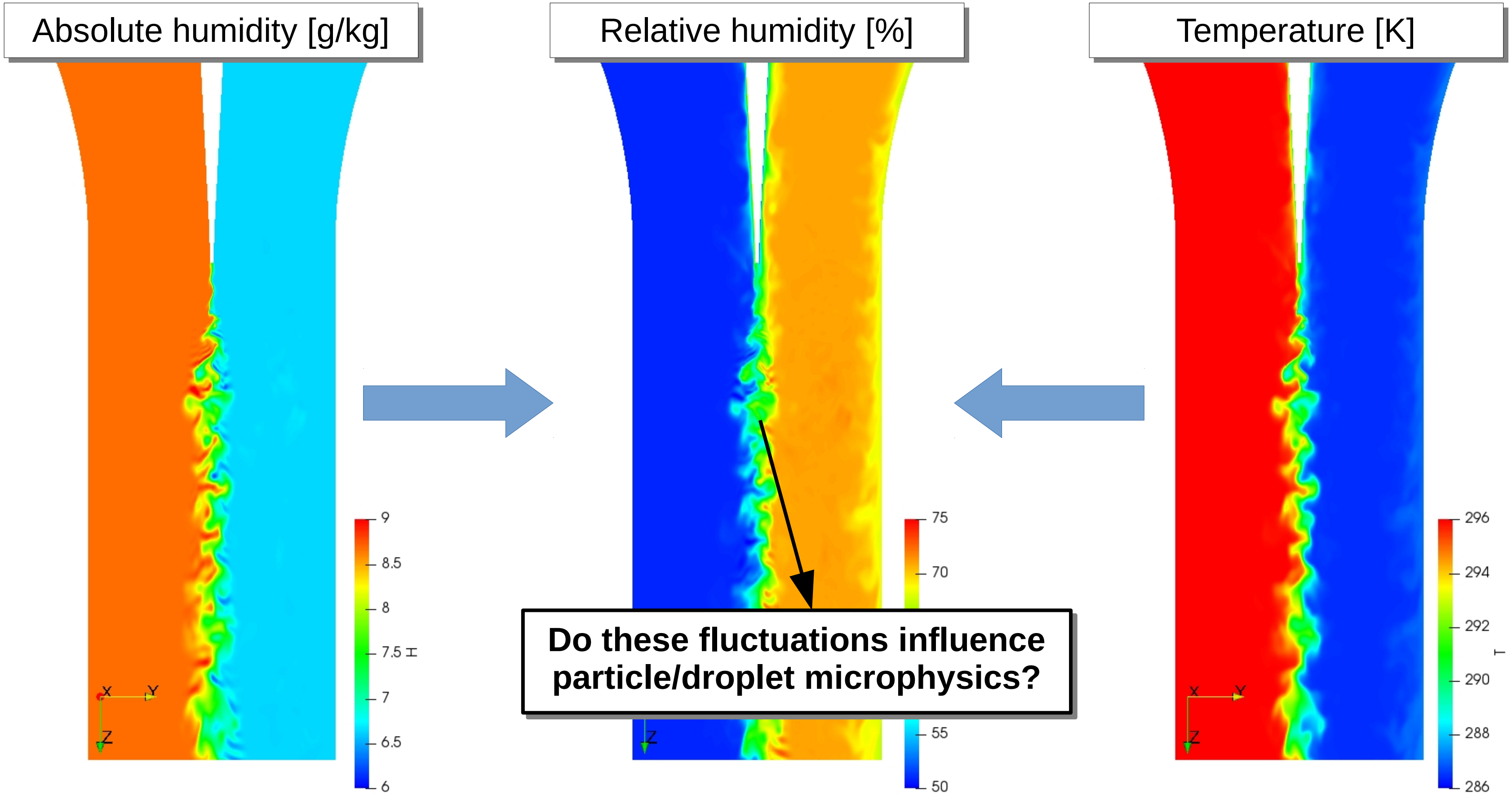
2 Fluid and thermodynamics – Results – Temperature

$$T_{RMS} = \sqrt{\overline{(T - T_{Mean})^2}}$$





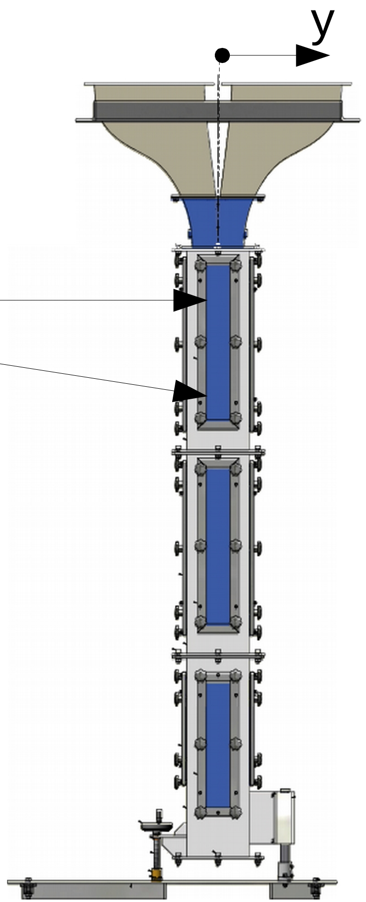
2 Fluid and thermodynamics – Results – Humidity



3 Particle and droplet dynamics – Measurement technique

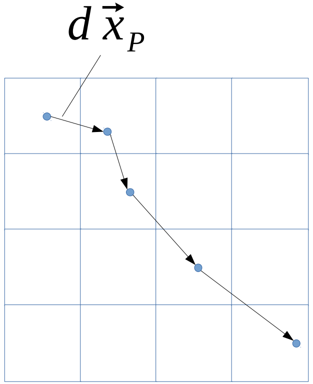
- Usage of white light spectrometer WELAS from PALAS
- Measurement heights ~10cm BAI or ~35cm BAI
- Measuring particle diameter for 20 minutes

→Particle size distribution



3 Particle and droplet dynamics – Numerical method

- Tracking of individual particles (Lagrangian reference frame) through flow field (Eulerian reference frame)



- Assumption: point-mass-particles

  → Models for interactions with carrier fluid, other particles, electric fields, ...

- Particles usually approximated as spheres

- Particle size << size of control volume

- Trajectory calculation through 3 ODEs:

$$\frac{d\vec{x}_P}{dt} = \vec{u}_P$$

$$m_P \frac{d\vec{u}_P}{dt} = \sum_i \vec{F}_i$$

$$\left(I_P \frac{d\vec{\omega}_P}{dt} = \sum_i \vec{T}_i \right)$$

3 Particle and droplet dynamics – Models

- Only drag force considered here
- Additional models:
  - Injection model (defining particle properties like position, size, and velocity at injection)
  - Growth/Mass transfer model

$$\frac{dm}{dt} = 2\pi d_p \rho_{v,sat} \left(S - S*\right) f_{mt}$$

➔ Mass transfer from gas phase to particles driven by gradient of water vapour saturation between particle surface and gas phase

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Fluid data (fixed for Lagrangian time step):

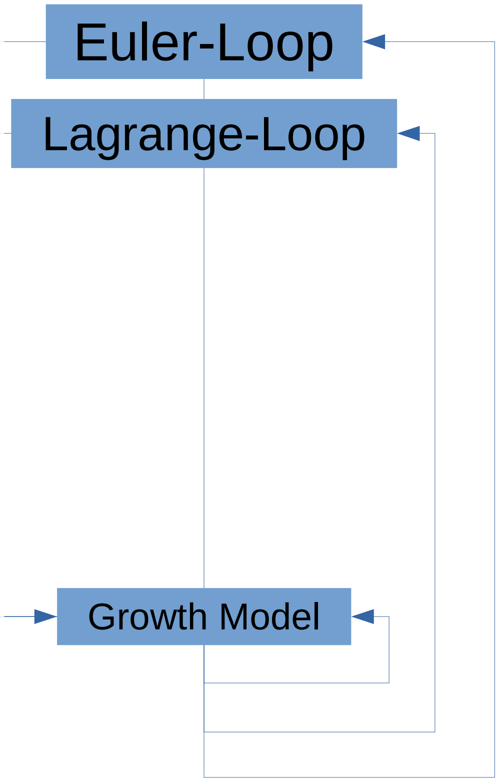
- p Ambient pressure [Pa]
- T Ambient temperature [K]
- T_C Ambient temperature [°C]
- H Mixing ratio [kg/kg]

Particle data:

- Variable:
  - d_p Particle diameter [m]
  - dt Lagrangian time step [s]
  - m_l Mass of liquid content [kg]
- Fixed:
  - m_s Mass of solid content [kg]
  - ρ_s Density of solid content [kg m^{-3}]
  - ρ_l Density of liquid content [kg m^{-3}]
  - sf Shape factor [-]

Model data (fixed):

- $dmRatio_{max}$ Maximum mass change ratio [-]
- D Vapour diffusivity in air [m^2 s^{-1}]
- M_l Molar mass of liquid content [kg mol^{-1}]
- M_s Molar mass of solid content [kg mol^{-1}]
- M_{dryAir} Molar mass of dry air [kg mol^{-1}]
- R Gas constant [J mol^{-1} K^{-1}]
- σ_l Surface tension of liquid [N m^{-2}]



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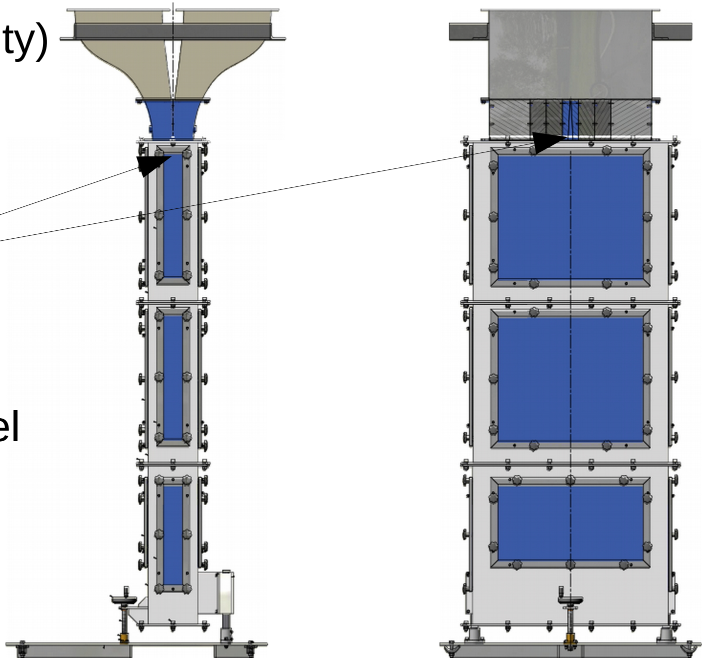
3 Particle and droplet dynamics – Boundary conditions

- Two cases considered (high and medium relative humidity)
- Properties of sodium chloride particles
- Diameter of 320nm (mass euqivalent to measurement)
- Injected at aerosol inlet between two branches
- Tracking time ~0.5s
- Sub time steps for Lagrangian tracking and growth model chosen automatically

$$Co_P \leq 0.5$$

$$\frac{dm_P}{m_P} \leq 0.2$$



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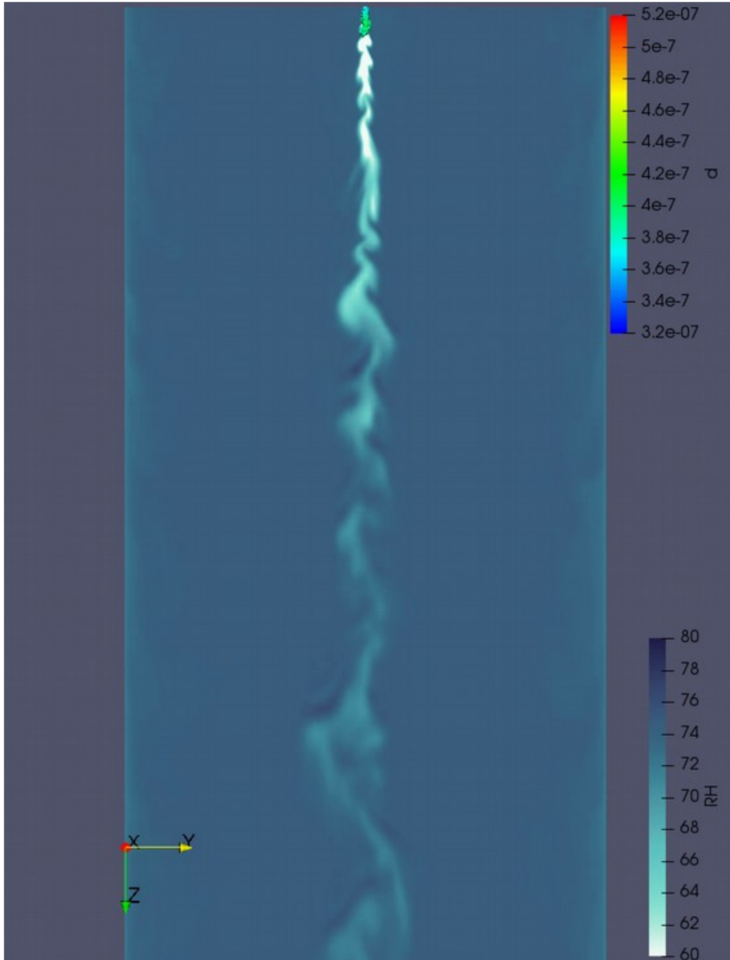
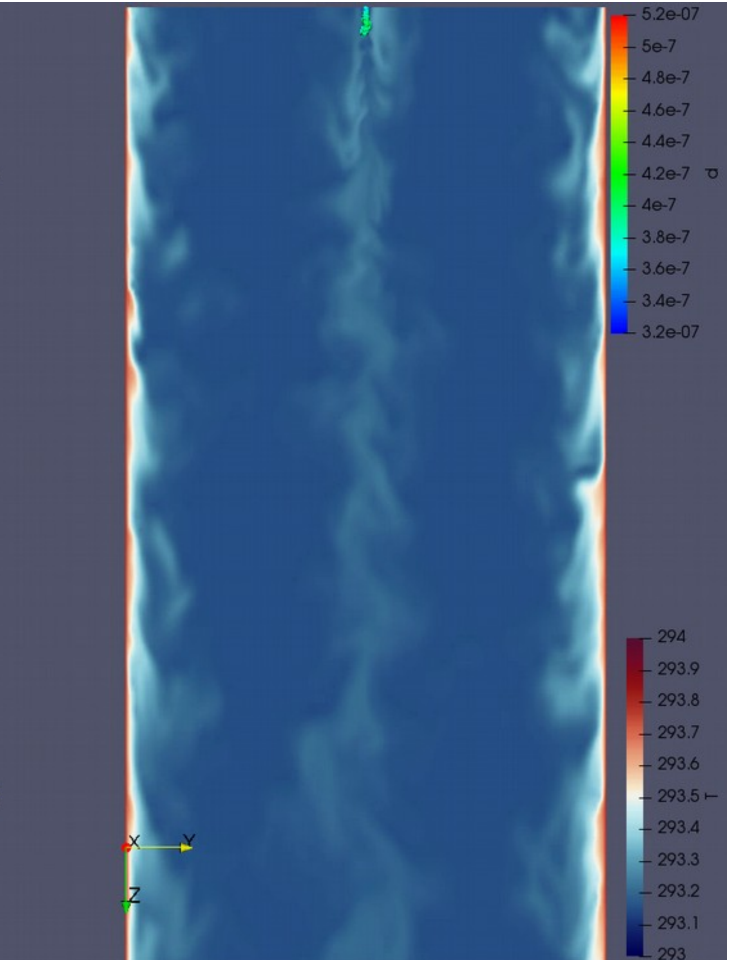
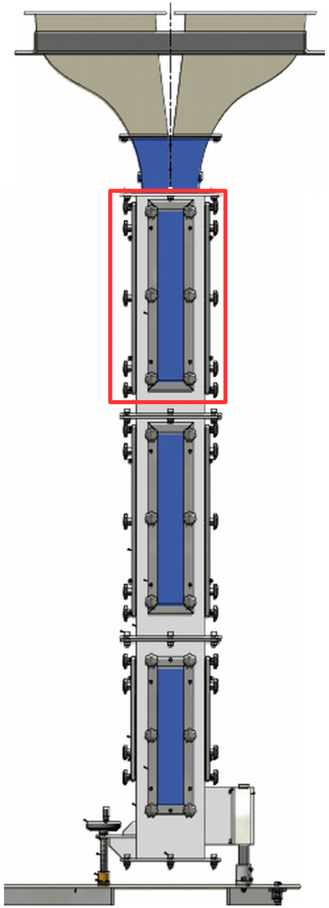
3 Particle and droplet dynamics – Results – Medium humidity

Relative humidity [%]

Temperature [K]







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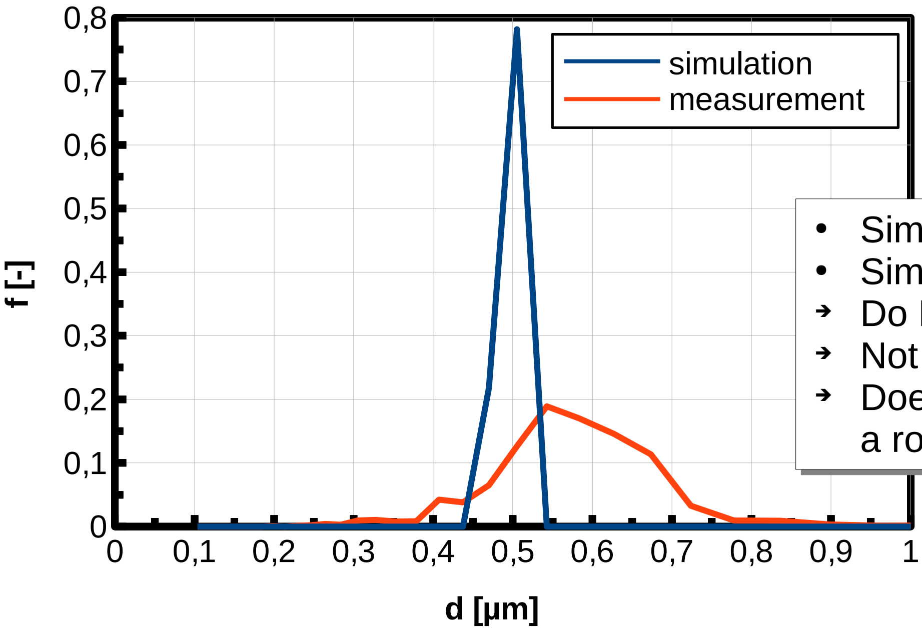
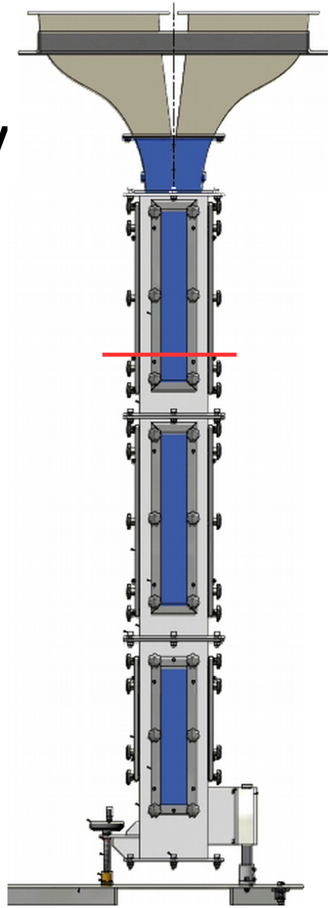
3 Particle and droplet dynamics – Results – Medium humidity

- Comparison of particle size distribution 35cm BAI



- Simulated diameter too small
- Simulated distribution too narrow
- ➔ Do BCs meet real conditions?
- ➔ Not enough time for statistics?
- ➔ Does subgrid scale turbulence play a role?



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3 Particle and droplet dynamics – Results – High humidity

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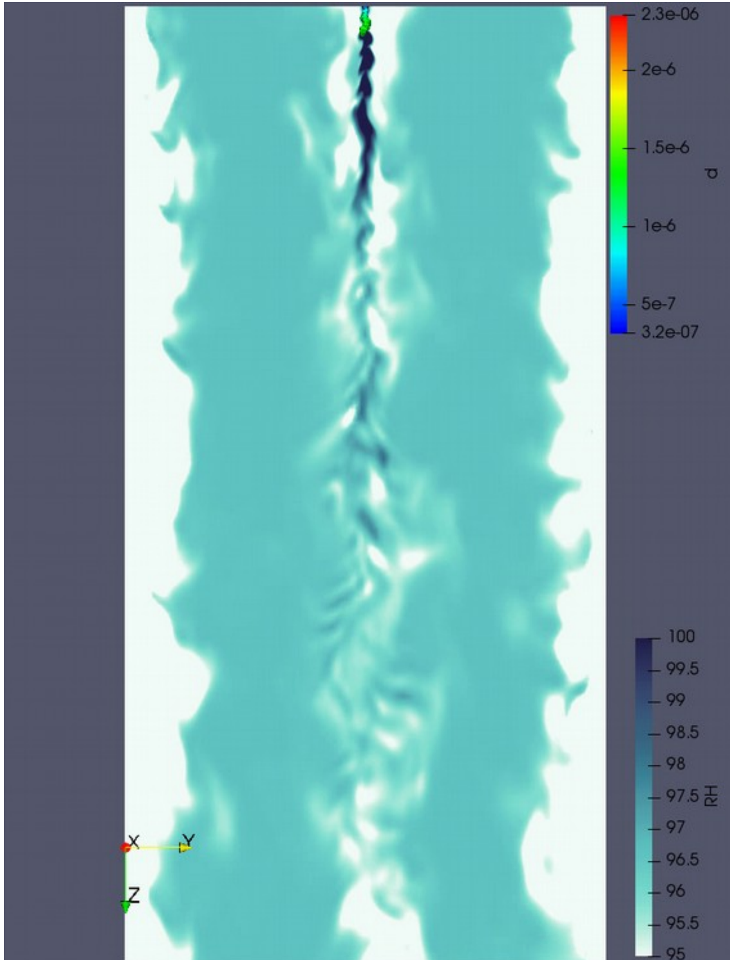
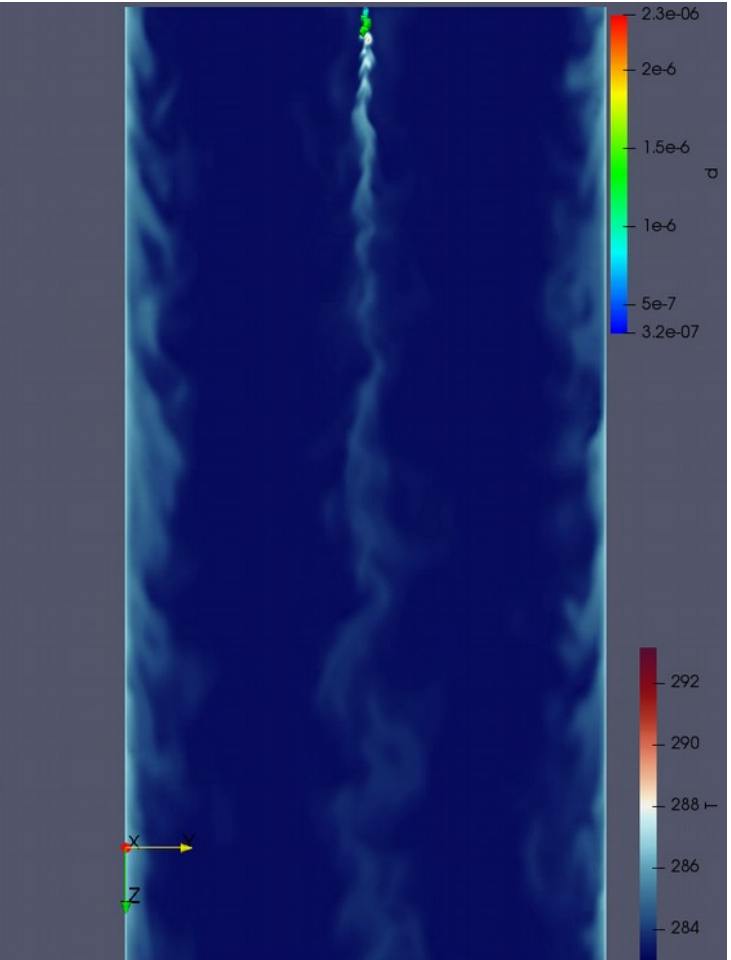
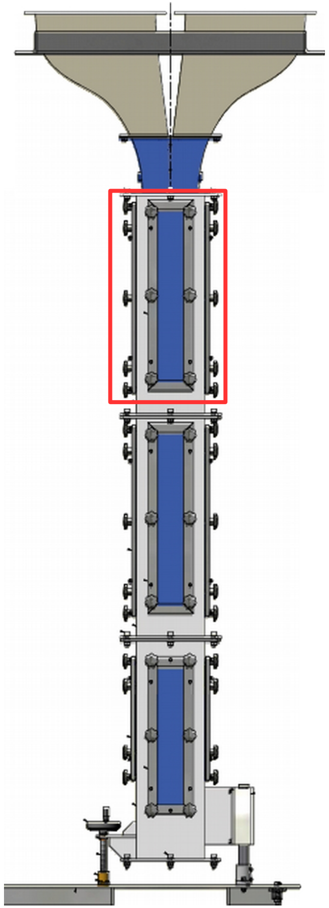
Relative humidity [%]

Temperature [K]







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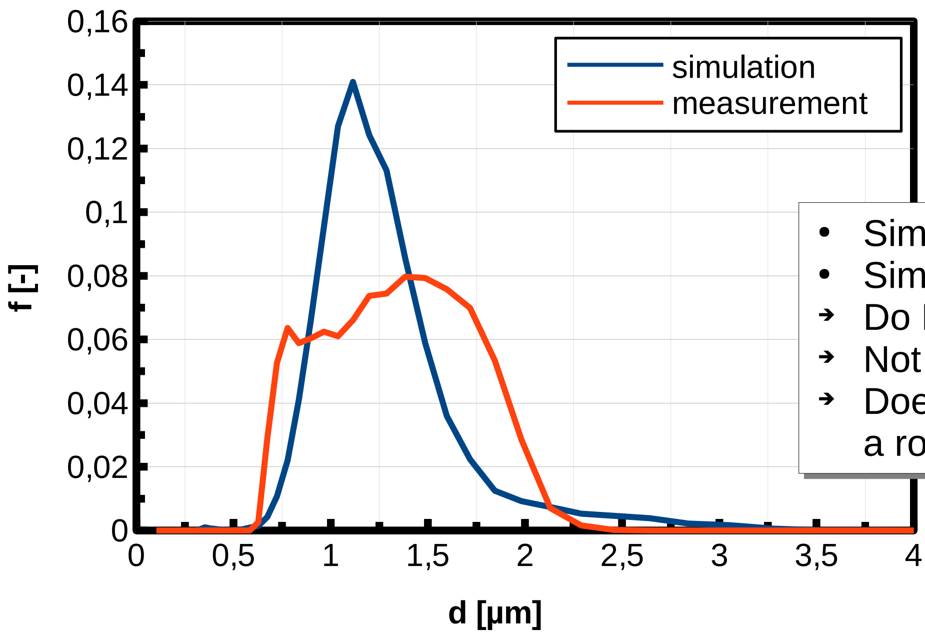
3 Particle and droplet dynamics – Results – High humidity

- Comparison of particle size distribution 10cm BAI



- Simulated diameter okay
- Simulated distribution too narrow
- ➔ Do BCs meet real conditions?
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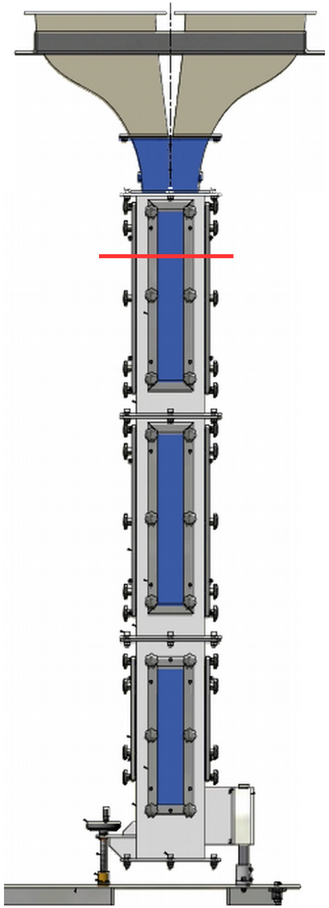

4 Summary and outlook

Summary

- Simulation of flow and thermodynamics inside LACIS-T with Large Eddy Simulations
- Results agree well with measurements
- Implementation of particle growth model in OpenFOAM’s Lagrangian module
- First particle simulations look promising, but have discrepancies to measurements

Outlook

- Implementation of sub grid scale turbulence dispersion for particles
- Further simulations for other conditions & longer time
- Further measurements, e.g. in lower regions of measurement section
- Long term: Correlations between turbulence and droplet/particle behaviour
- Improvements at LACIS-T (insulation, sealing) and particle measurements

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Thank you for your attention!