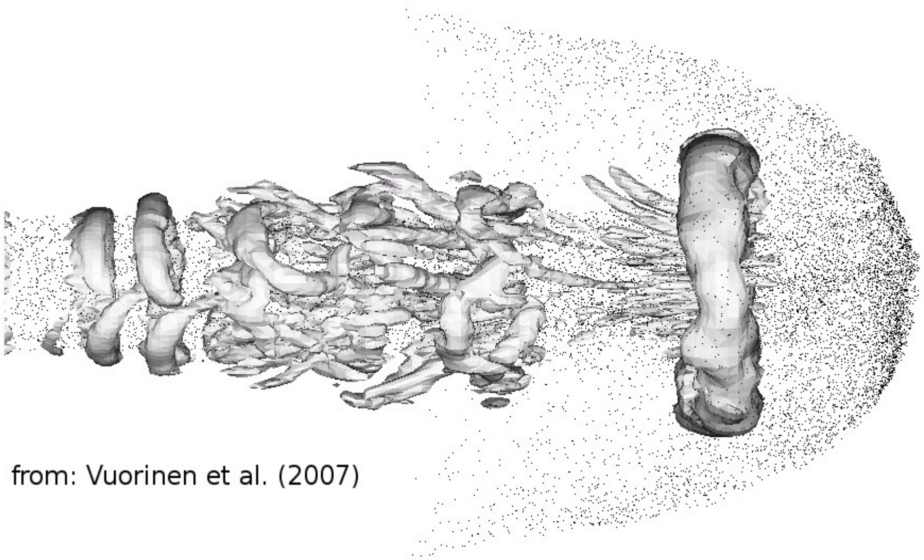
Recent Progress in Implicit Large-Eddy Simulation of Fuel Sprays with Focus on Droplet Size Effects



from: Vuorinen et al. (2007)

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About This Presentation

- The presentation summarizes part of the work done by the authors during the period 2007-2008
- Based on the papers
  - Vuorinen, Larmi, Fuchs, *Large-Eddy Simulation of Spray-Originated Turbulence Production and Dissipation*, ICMF-2007, Leipzig, (2007).
  - Vuorinen, Larmi, Fuchs, *Large-Eddy Simulation of Droplet Size Distribution Effects on Turbulence in Sprays*, AIAA-2008, Grand Sierra Resort, Reno (2008).
  - Vuorinen, Larmi, Fuchs, *Large-Eddy Simulation of Droplet Size Distribution on Mixing of Passive Scalar in a Spray*, SAE-Paper 2008-01-0933, (2008).

Contents

- Background on Particles in Multiphase Flow and Objectives
- Assumptions on the Particulate Phase
- Problem Setup
- Large-Eddy Simulation (LES)
- Results
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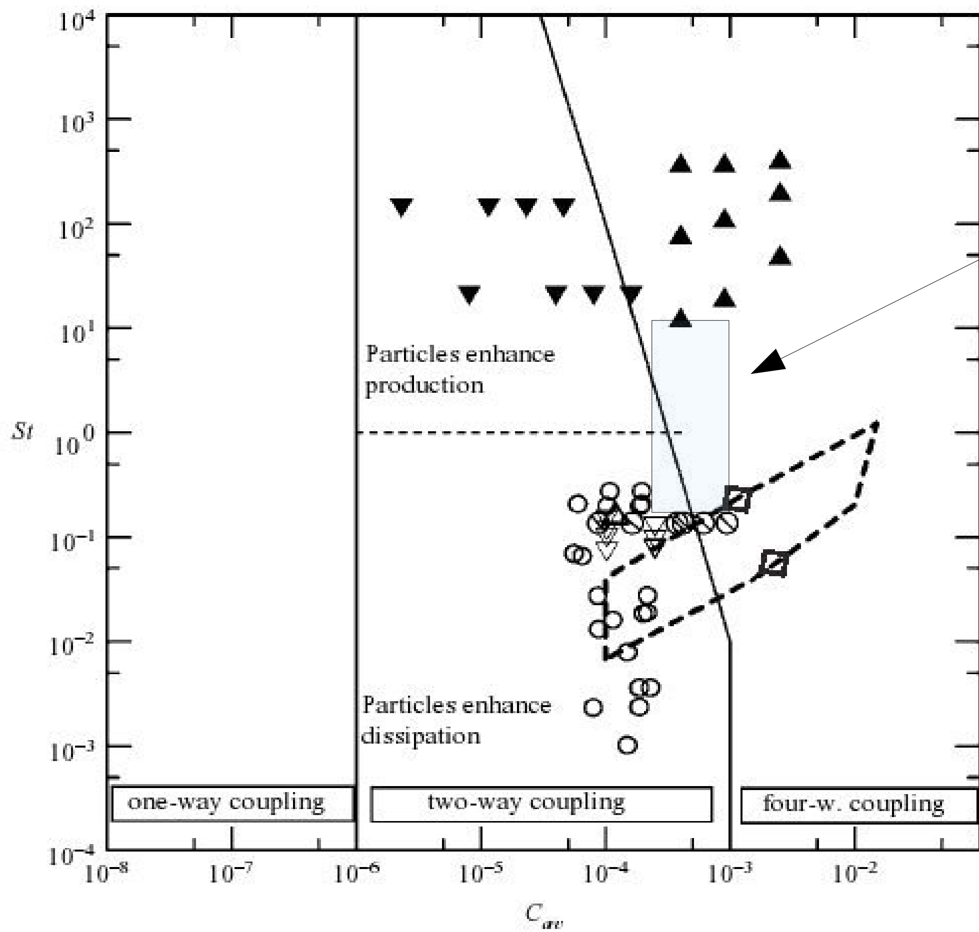
Background: Particles in Turbulence

- the characterization by Elgobashi (1994) on 'generic' particle laden flows: particle size and volume fraction determine turbulence dissipation/production.

Particle Stokes number:

$$St_p = \tau_p \frac{U}{\delta}$$



this study

size

volume fraction

Particle Momemtum relaxation time:

$$\tau_p = \frac{\rho_p d^2}{18 \rho_g \nu}$$

These definitions imply that small particles may follow a range of time frequencies.

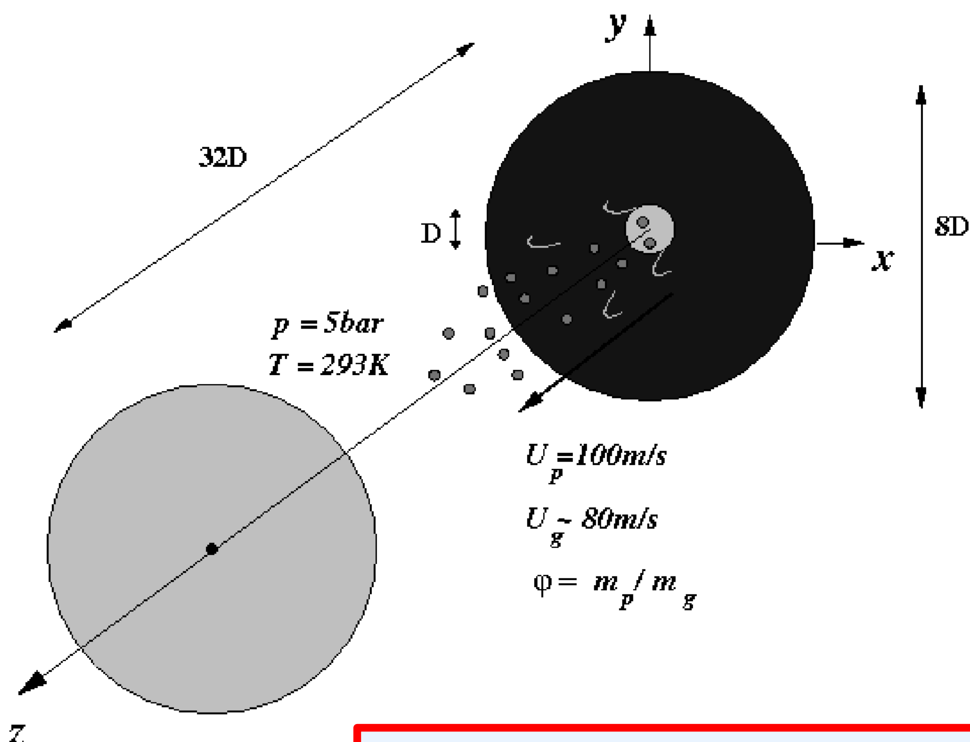
Objectives

- Discuss the role of droplet size in forming the spray dynamics
- Discuss the connection between small scale interactions and large scale observations and point out that the PDF's of droplet velocity and slip velocity explain the spray behavior
- Look at flow structures and preferential concentration
- Discuss the characteristics of turbulent diffusivity in particle laden flows

Assumptions on Particulate Phase

- the Lagrangian Particle Tracking approach (**LPT**)
- particles do not displace fluid
- particles are spherical and do not break
- particles do not interact (two way coupling)
- the stochastic “parcel” concept
- parcels couple to flow field via slip velocity
- gaseous phase is affected by the forces the parcels exert in each computational cell
- the gas velocity “seen” by parcel computed by linear interpolation to the parcel position

Problem Setup



$$\varphi = \frac{m_f}{m_g} = \frac{injected\ spray\ mass}{injected\ gas\ mass}$$

mass loading ratio

- Particles enter a gas jet
- slip velocity $+0.25U_{exit}$
- two mass loadings (i.e. 0.3 and 0.6) studied corresponding to strong and very strong two way coupling (i.e. 0.001 and 0.002 volume fractions)
- particles are distributed according to a size distribution
- injection time = 1.5ms
- inlet diameter D=2mm

Large-Eddy Simulation (LES)

- the full compressible Navier-Stokes is solved by a numerical algorithm (2nd order accurate in space, 1st order time)

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial}{\partial x_j}(-p\delta_{ij} + \sigma_{ij}) + \mathcal{M}_{spray}$$

$$\mathcal{M}_{spray} = -C_D(u_i - u_{d,i})|u_i - u_{d,i}|\delta_{r,r_d}$$

- “implicit LES”: filtering done by the discretization scheme
- an additional transport equation is solved for a passive scalar
- gaseous phase receives momemtum from the particle phase via **the slip velocity** $\delta W = u_{particle} - U_{gas}$

Parallel Simulations

- simulations carried out with OpenFOAM open source control volume code
- mesh contains 3.5M cells – cell resolution as small as 30um in the shear layer and center of the jet
- decomposition onto 32 processors
- one simulation takes about 4 days
- CFL < 0.12
- further details in the referred manuscripts

Some Simulated Cases

Stokes number as referred to SMD

Case	SMD	SMD/D	φ	distribution	V_p/V_g	St_{SMD}	$N_{p,SMD}$
A1	$2.0\mu m$	0.001	0.3	monodisp.	0.001	0.1	125
A2	$3.5\mu m$	0.00175	0.3	polydisp.	0.001	0.25	23
A3	$7.0\mu m$	0.0035	0.3	polydisp.	0.001	1	3
A4	$10.0\mu m$	0.005	0.3	polydisp.	0.001	2	1
B1	$2.0\mu m$	0.001	0.6	monodisp.	0.002	0.1	250
B2	$3.5\mu m$	0.00175	0.6	polydisp.	0.002	0.25	46
B3	$7.0\mu m$	0.0035	0.6	polydisp.	0.002	1	6
B4	$10.0\mu m$	0.005	0.6	polydisp.	0.002	2	2

mass loading 0.3

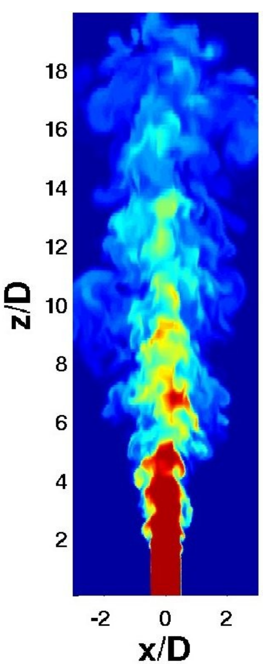
mass loading 0.6

4 different particle mean diameters

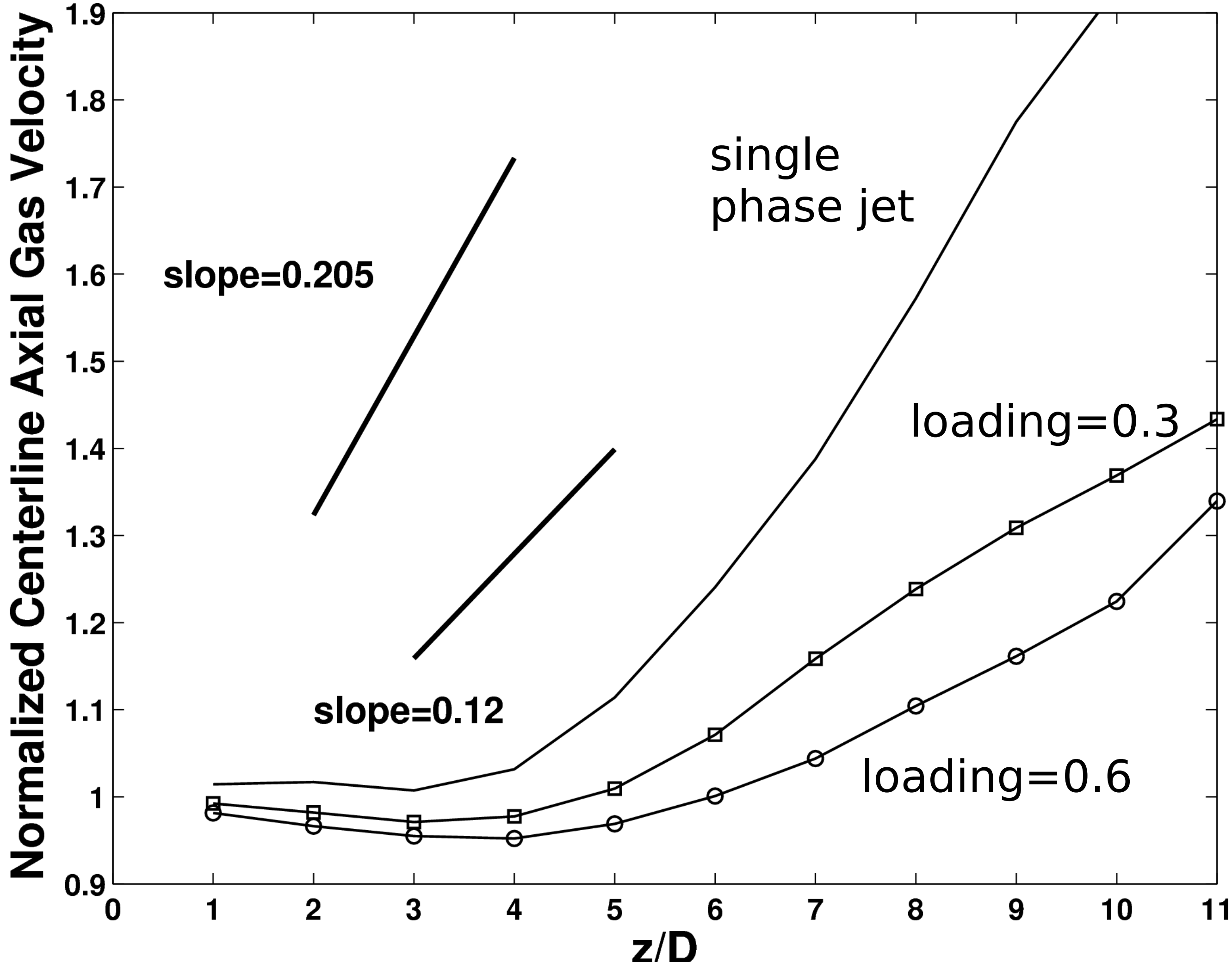
monodisperse = single size drops
polydisperse = droplet size distribution

- Altogether 8 simulations + 1 “single phase jet” simulation with negligible mass loading of small d=2μm tracer particles

Effect of Mass Loading on the Length of the Potential Core



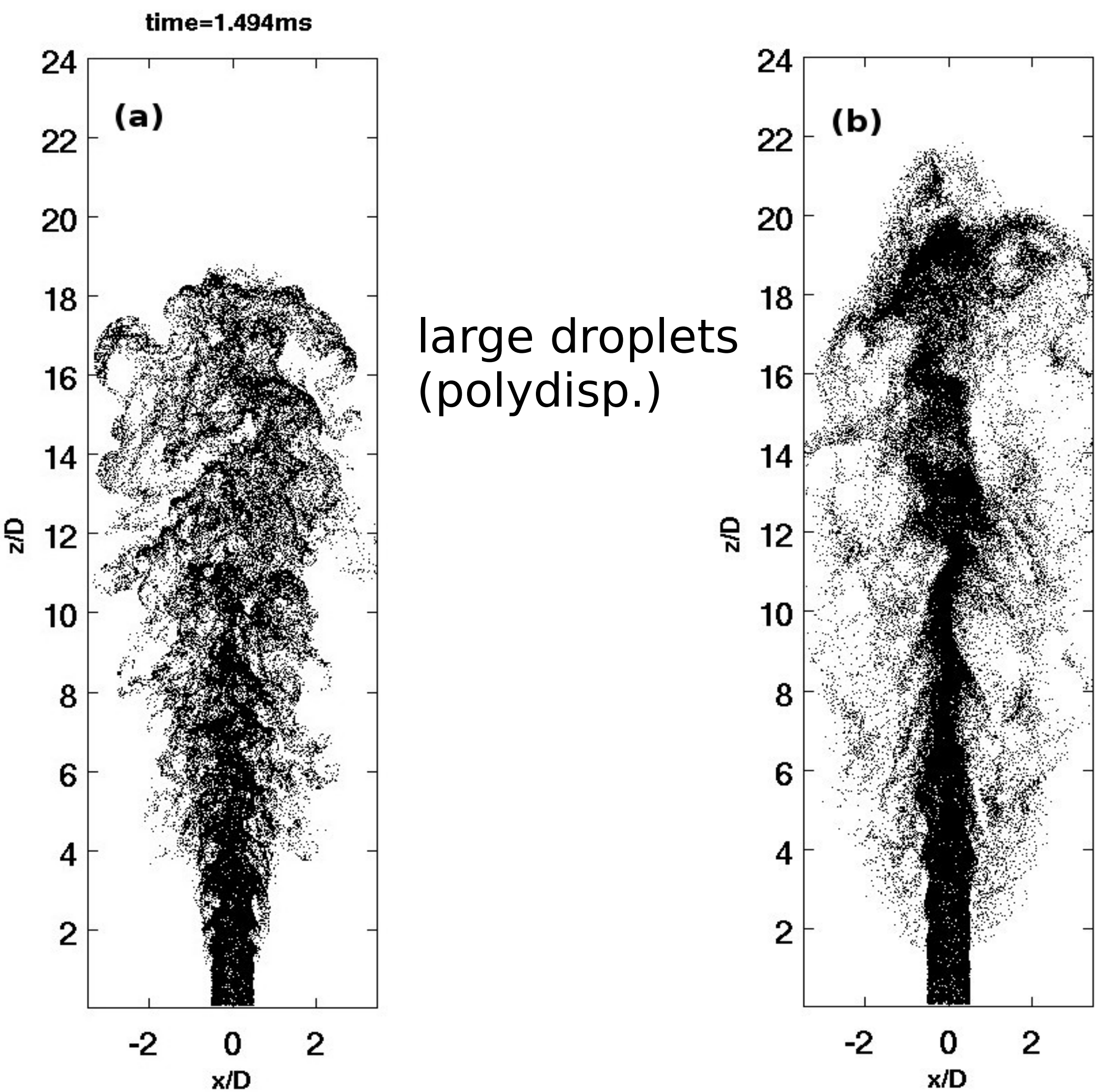
potential
core: laminar
interactions



Different Spray Cloud Shapes

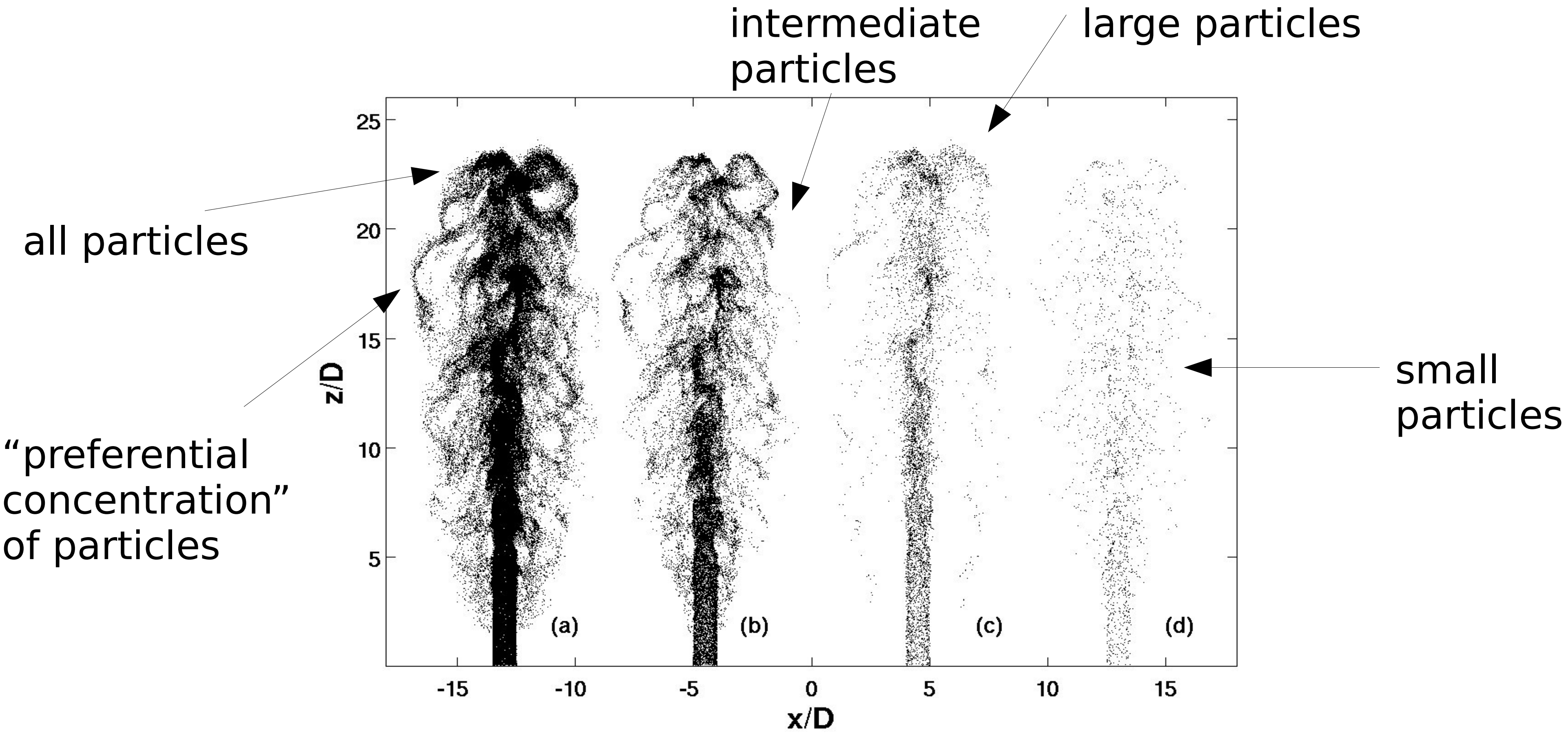
small droplets
(monodisp.)

large droplets
(polydisp.)



Superposition of Clouds with Different Stokes Numbers

- Particle Stokes number dominates the trajectory: large Stokes number indicates large inertia and that particle stays close to center

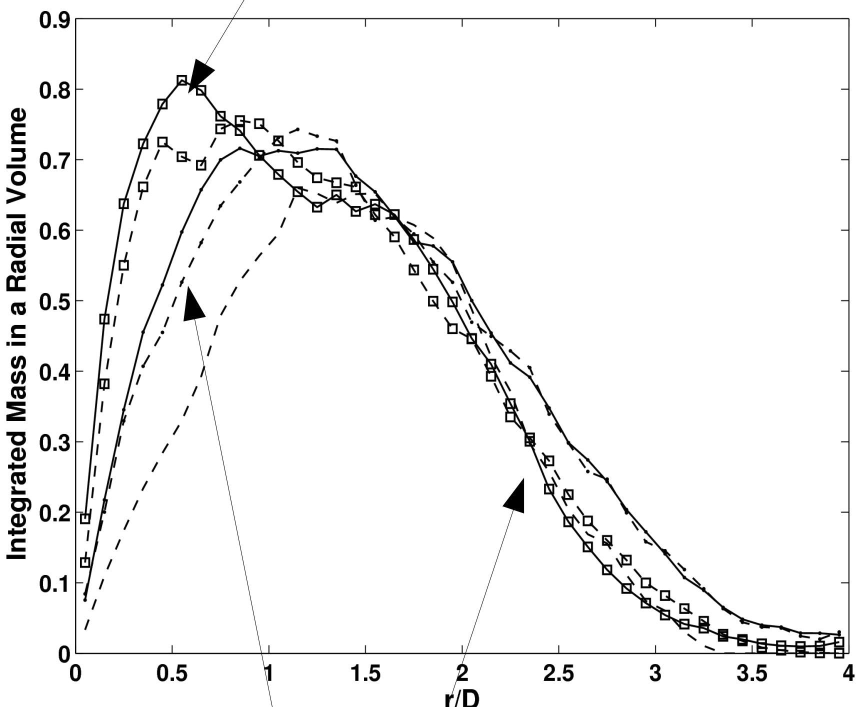


Mass Transfer and Mixing

large particles
stay near center

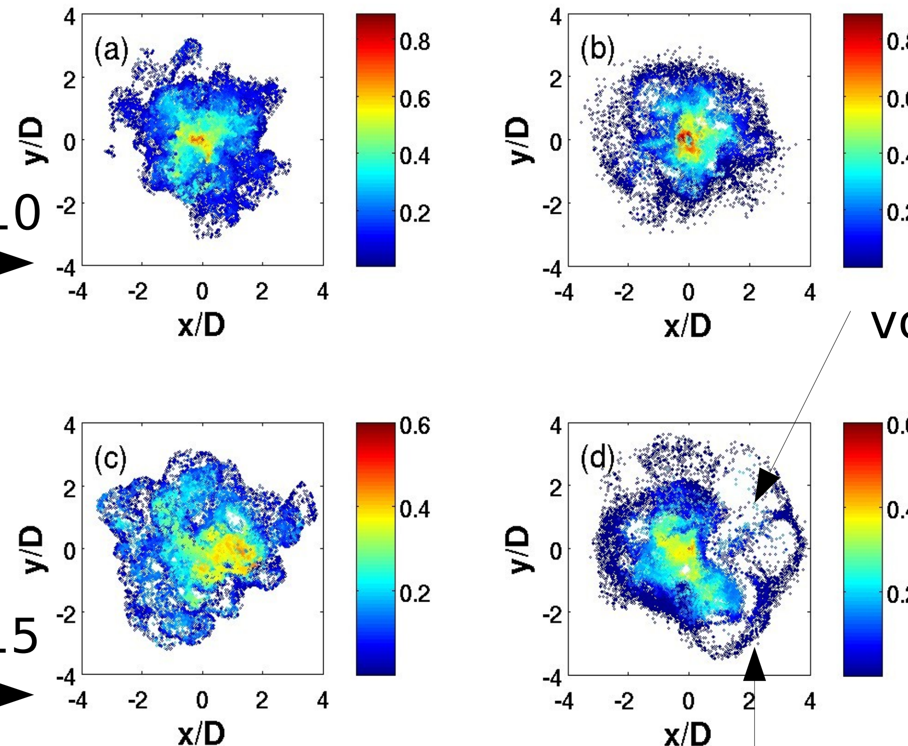
a&c small particles

b&d large particles



z/D=10

z/D=15

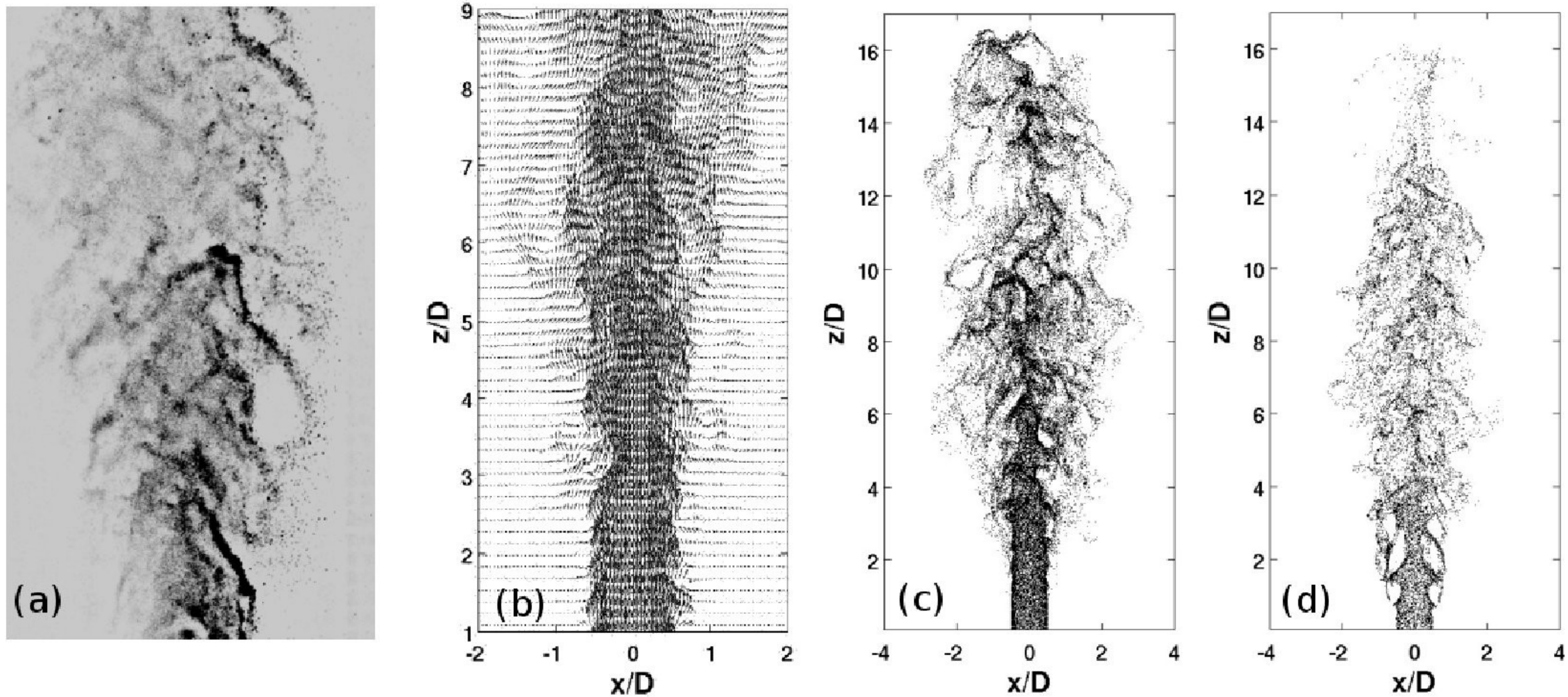


voids

small particles may
disperse better due to random fluctuations

preferential
concentration

Qualitative Comparison of LES and PIV



a) PIV

b) LES: velocity vectors

c) LES: fuel spray

d) LES: gas jet+ tracers

Gradient vs Counter Gradient Diffusion

- An often used closure model in turbulence models is the Gradient Diffusion Model (GDM) which associates turbulent fluxes with eddy diffusivity and mean concentration gradient.

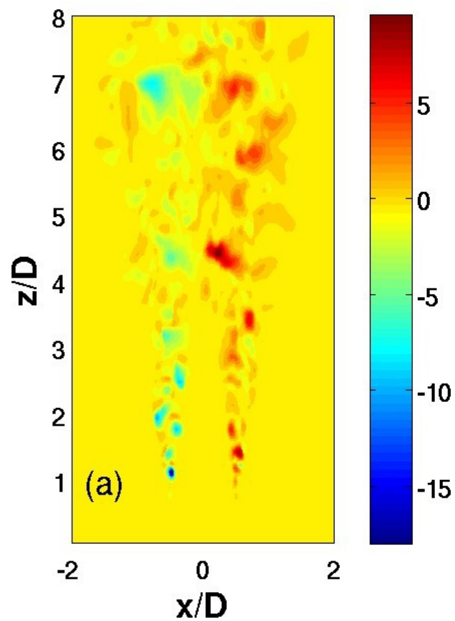
$$\overline{u'_j c'} = -\frac{\nu_t}{Sc_t}\frac{\partial C}{\partial x_j}$$

- The eddy diffusivity can then be solved for:

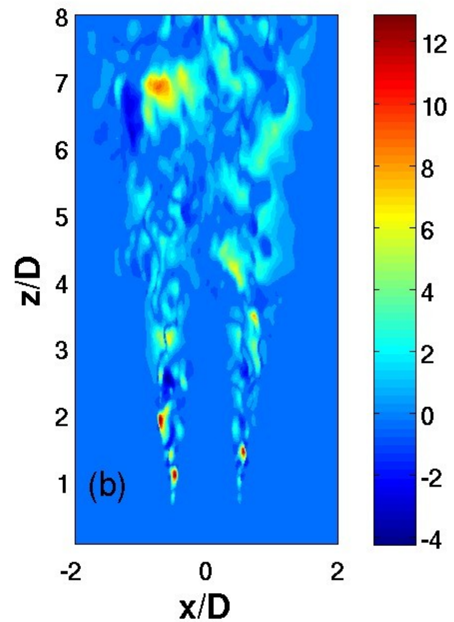
$$D_{tj} = \frac{-\overline{u'_j c'}}{\frac{\partial C}{\partial x_j}}.$$

- According to this D_{tj} should be strictly positive which can be checked for by computation of instantaneous turbulent concentration fluxes.

Counter Gradient Diffusion is Observed



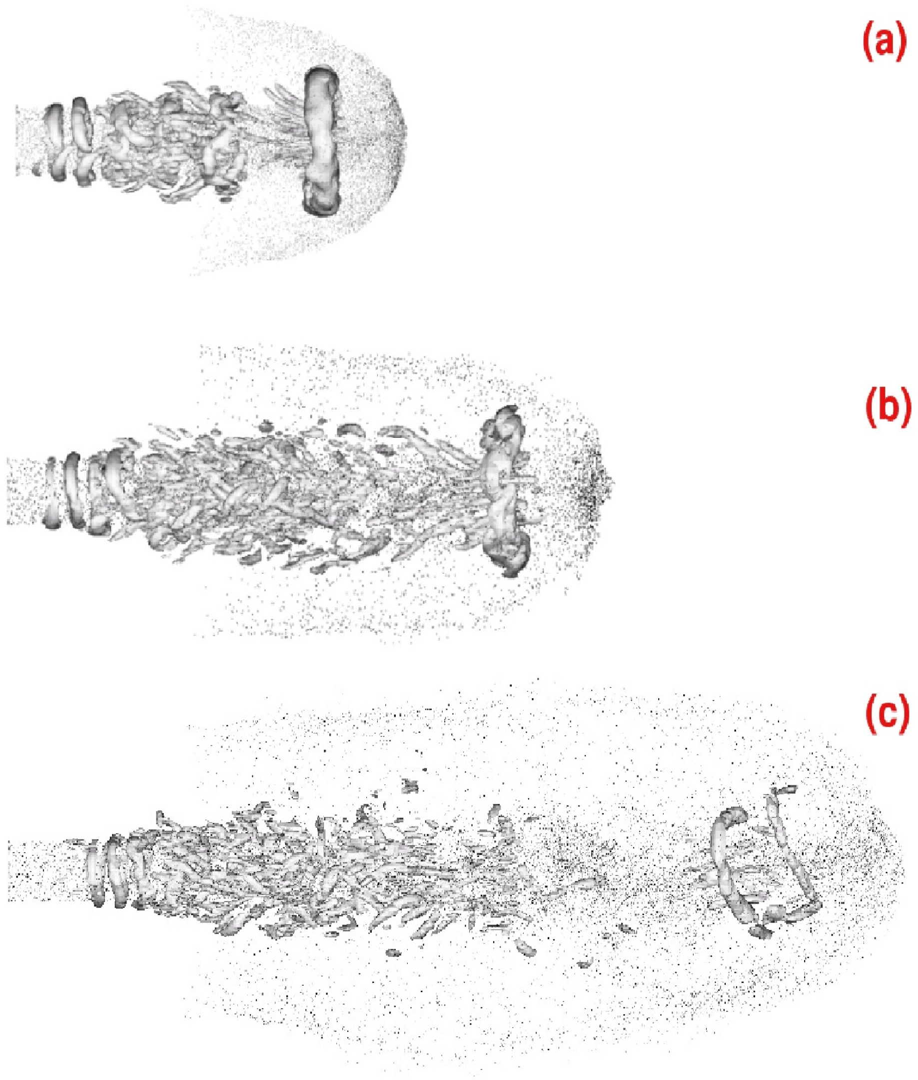
D_{tx}



D_{tz}

- The eddy diffusivity changes sign from + to -
- Thus the nature of turbulent diffusion is quite different from molecular diffusion and the GDM is not valid in particle laden free shear flows
- Counter gradient diffusion observed for large and small particles and mass loadings

Look at the Coherent Structures



- Example from Vuorinen et al. (2007): small mass loading of large particles
- Large doughnut shaped tip vortex observed
- Axially oriented vortices in the center
- Breakup of the tip vortex later downstream

Vuorinen, Larmi, Fuchs, *Large-Eddy Simulation of Spray-Originated Turbulence Production and Dissipation,*ICMF-2007, Leipzig, (2007).

Conclusions

- Spray cloud shape is explained by mean diameter of the droplet distribution and characteristic Stokes numbers – the results are generally in line with several earlier observations on sprays and jets
- Small particles -> follow the fluid motions closely
- Large particles -> particle clustering, high particle concentrations in the center, voids etc…
- Effect of increased mass loading: longer potential cores.
- The GDM-assumption could be most problematic in the shear layer
- Large tip vortex and shear layer vorticity are noted and their appearance seems to be sensitive to the droplet size, mass loading and boundary conditions in general.

Thank you for your attention!