CFD Modelling of Turbulent Mass Transfer in a Mixing Channel

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Overview

- Objectives
- Flow Configuration
- PIV/PLIF Experiment
- Governing Equations
- Turbulence and Micromixing Models
- Numerical Results
- Conclusions

Objectives

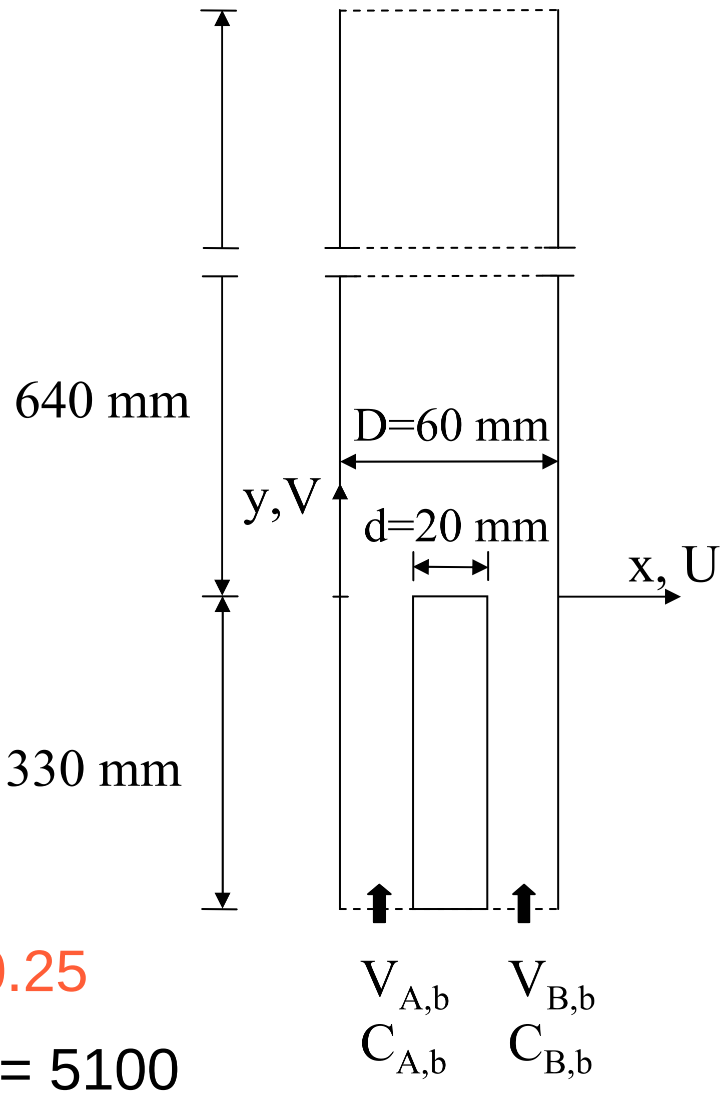
Objectives of current project

- PIV/PLIF measurements of mass transfer and chemical reactions in turbulent liquid flows
  - pure mixing/mass transfer
  - acid-base chemical reaction (Poster presentation)
- CFD modelling of mass transfer and chemical reactions (Poster presentation) in turbulent liquid flows

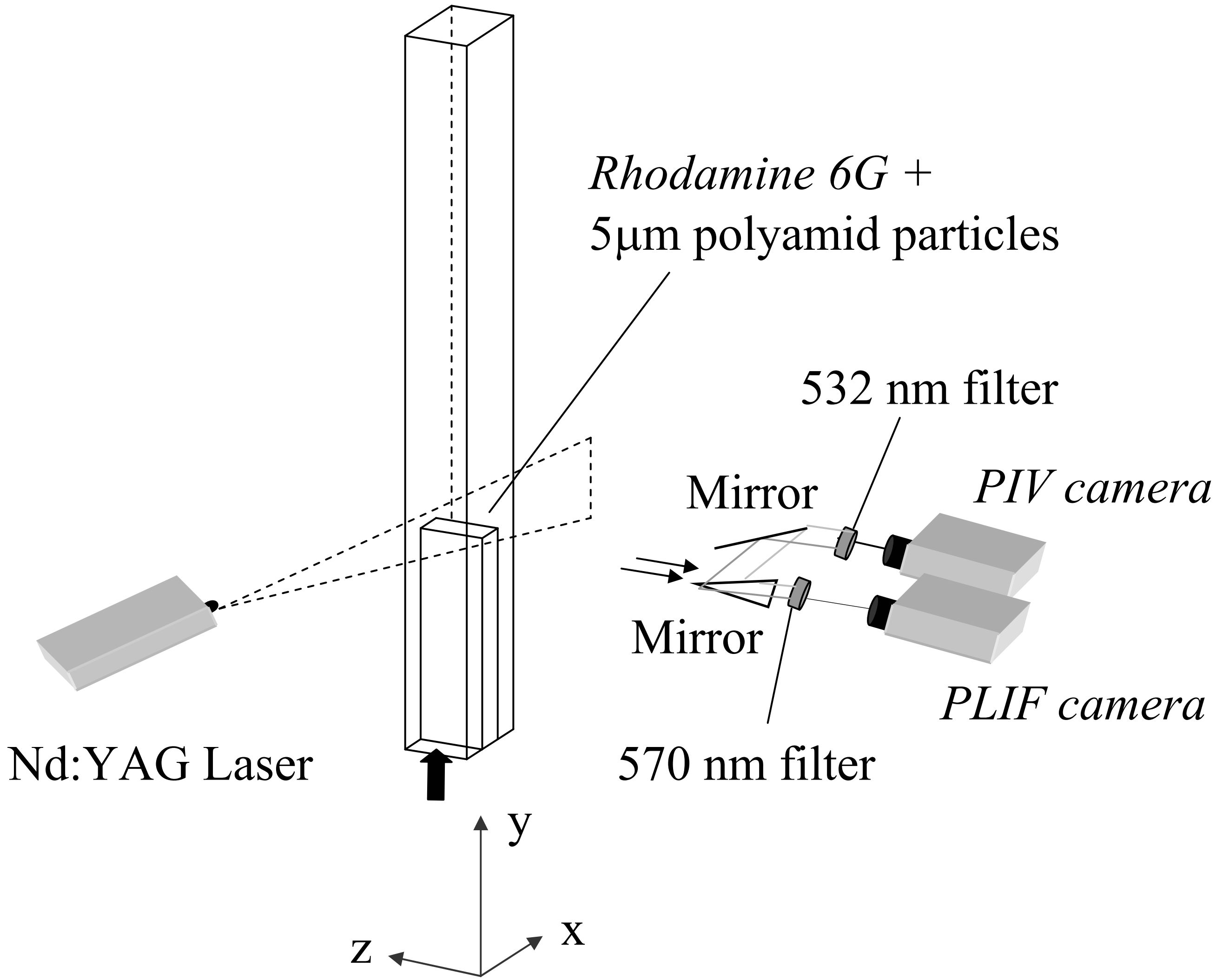
Flow Configuration

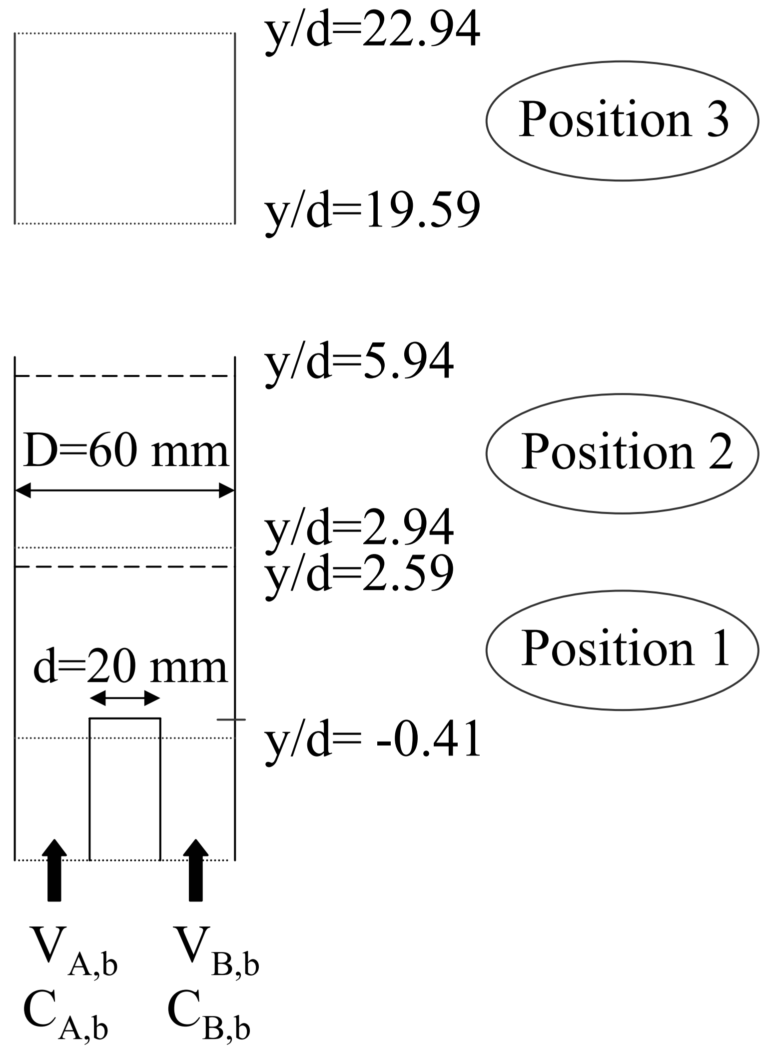
Confined wake flow

- Channel dimensions
  - Mixing channel
    - – Length 640 mm
    - – Cross-section 60 mm x 60 mm
  - Feed channel
    - – Length 330
    - – Cross-section 20 mm x 60 mm
- Flow conditions
  - Fluid : Water
  - Feed channel A : $V_{A,b}/ V_{B,b}$= 1, 0.5 , 0.25
  - Feed channel B : $Re_B = \rho\, V_{B,b}\, D_{h,B}/\mu = 5100$



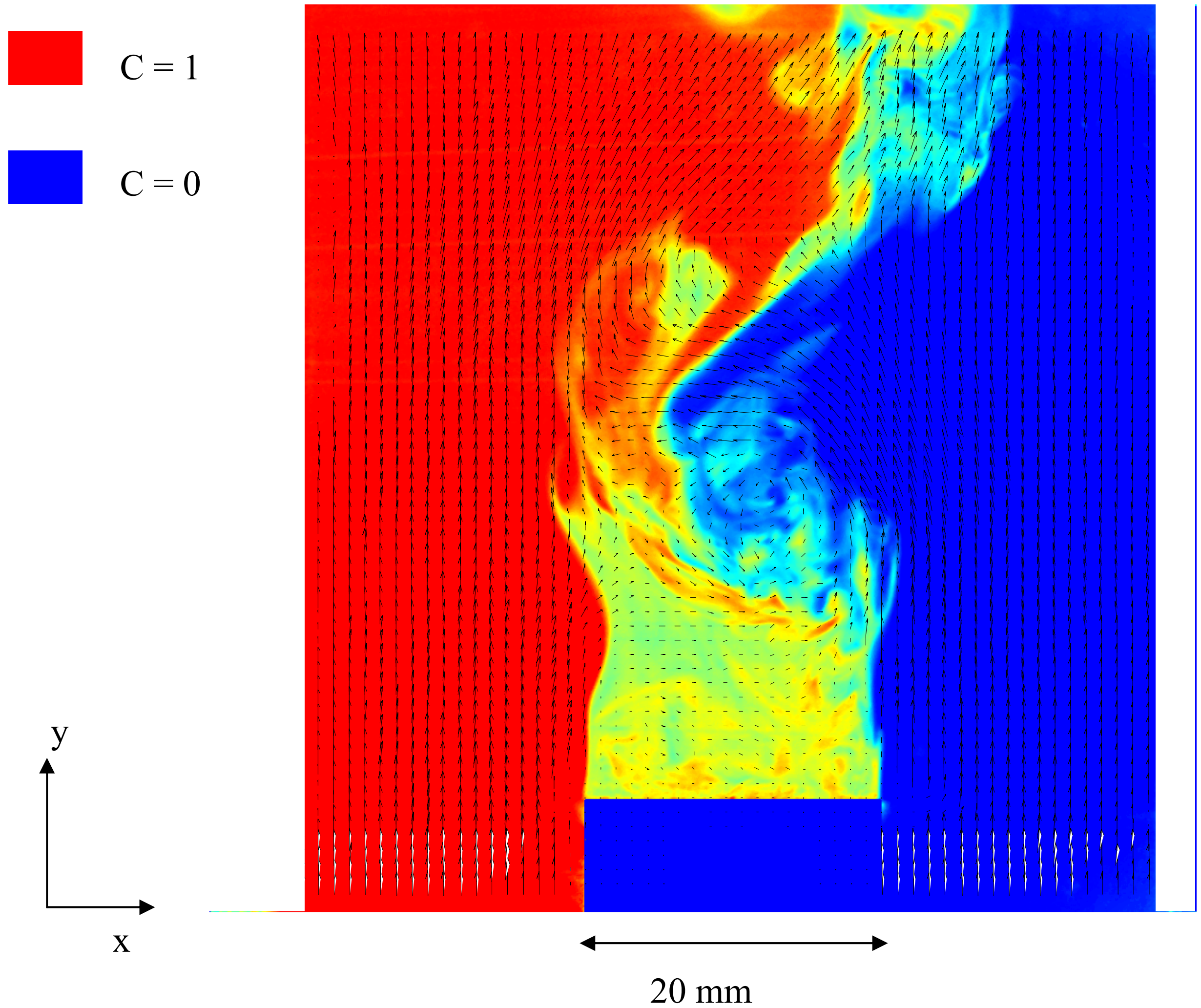
PIV/PLIF System



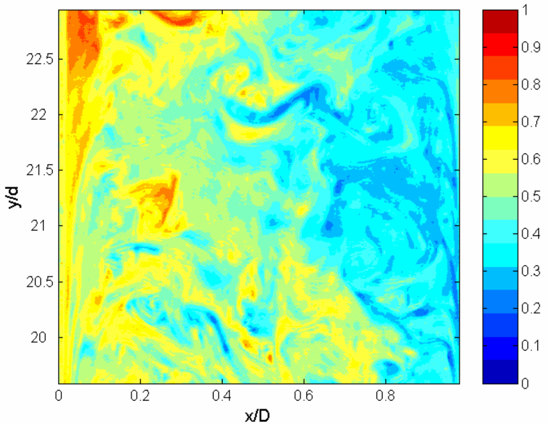


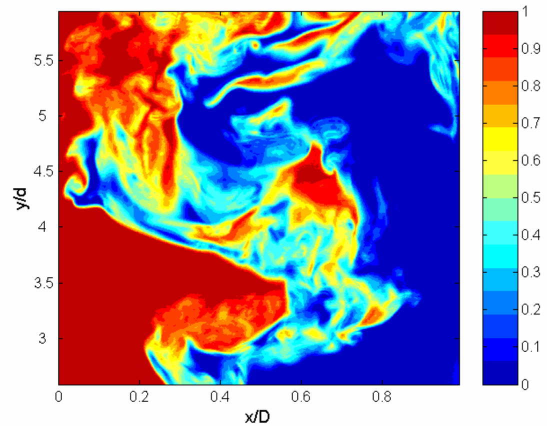
PIV/PLIF Measurements (1)

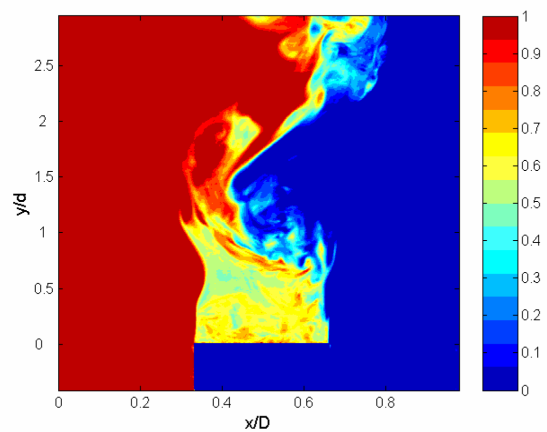
Instantanous velocity and concentration



PIV/PLIF Measurements (2)



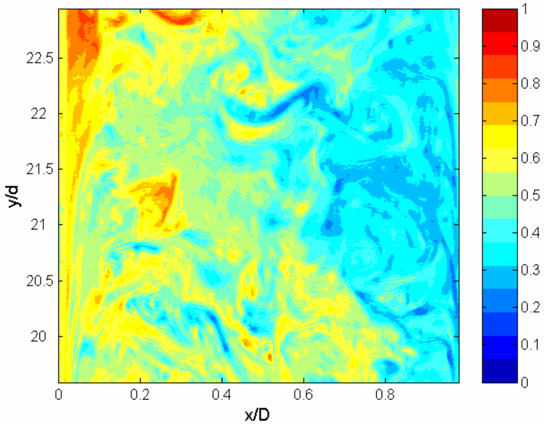


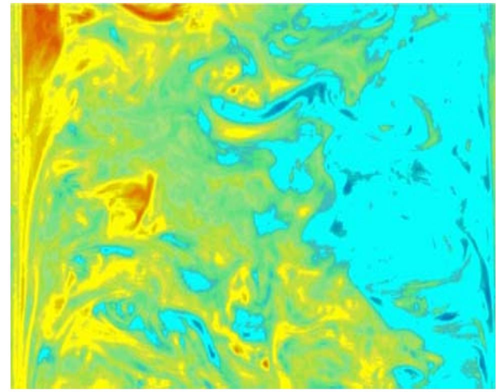


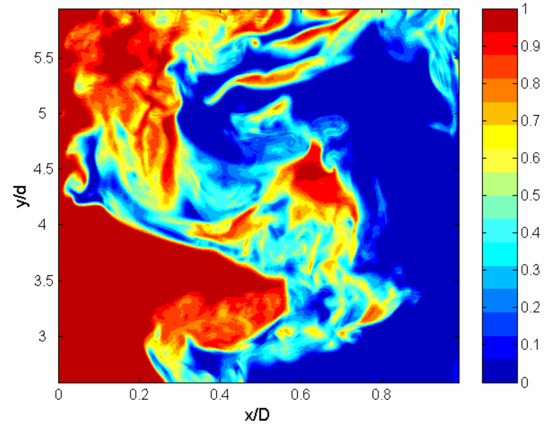
C = 1

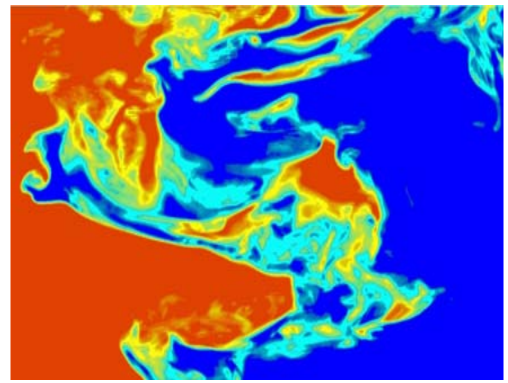
C = 0

- Pure mixing experiment
  - Concentration of species A
    – High concentration (C=1) red
    – Low concentration (C=0) blue
- Instantaneous images at three different heights
- Note heterogeneous structures
- Averages produced using 200 images


y/d
22.5
22
21.5
21
20.5
20
x/D
0
0.2
0.4
0.6
0.8
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

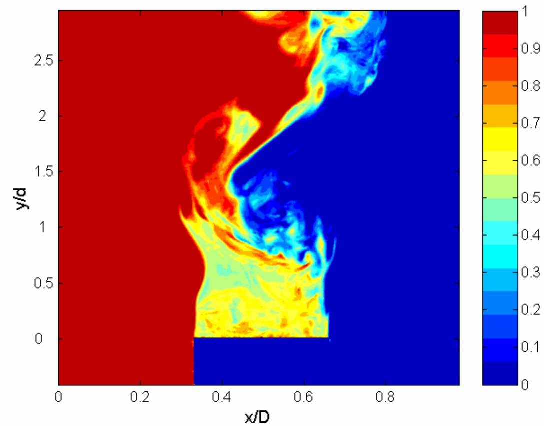


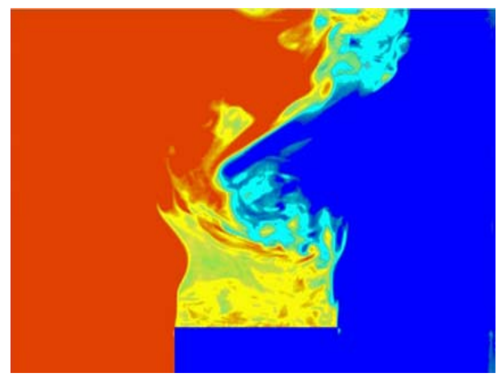

y/d
5.5
5
4.5
4
3.5
3
x/D
0
0.2
0.4
0.6
0.8
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

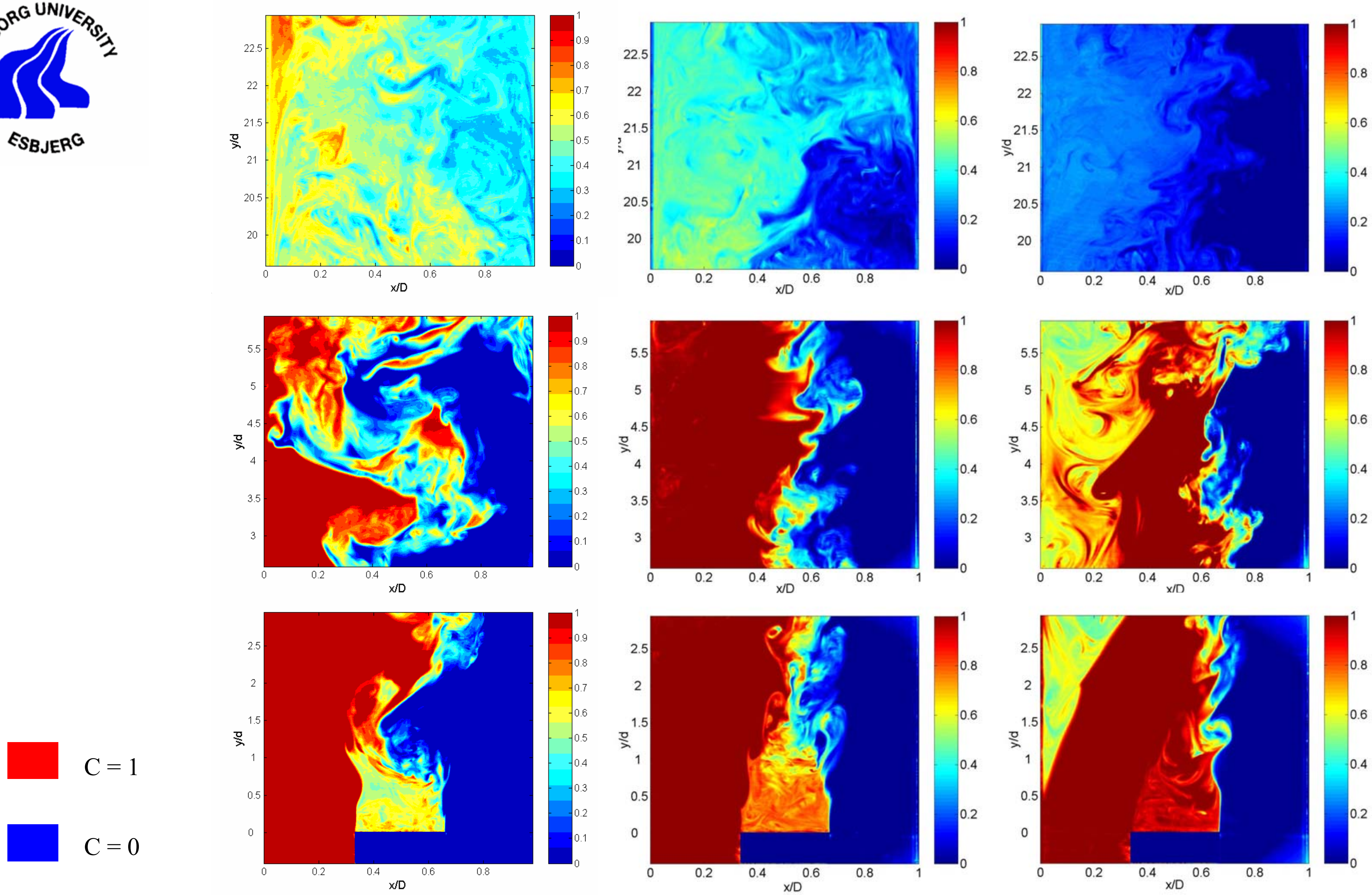


C = 1

C = 0


y/d
2.5
2
1.5
1
0.5
0
x/D
0
0.2
0.4
0.6
0.8
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

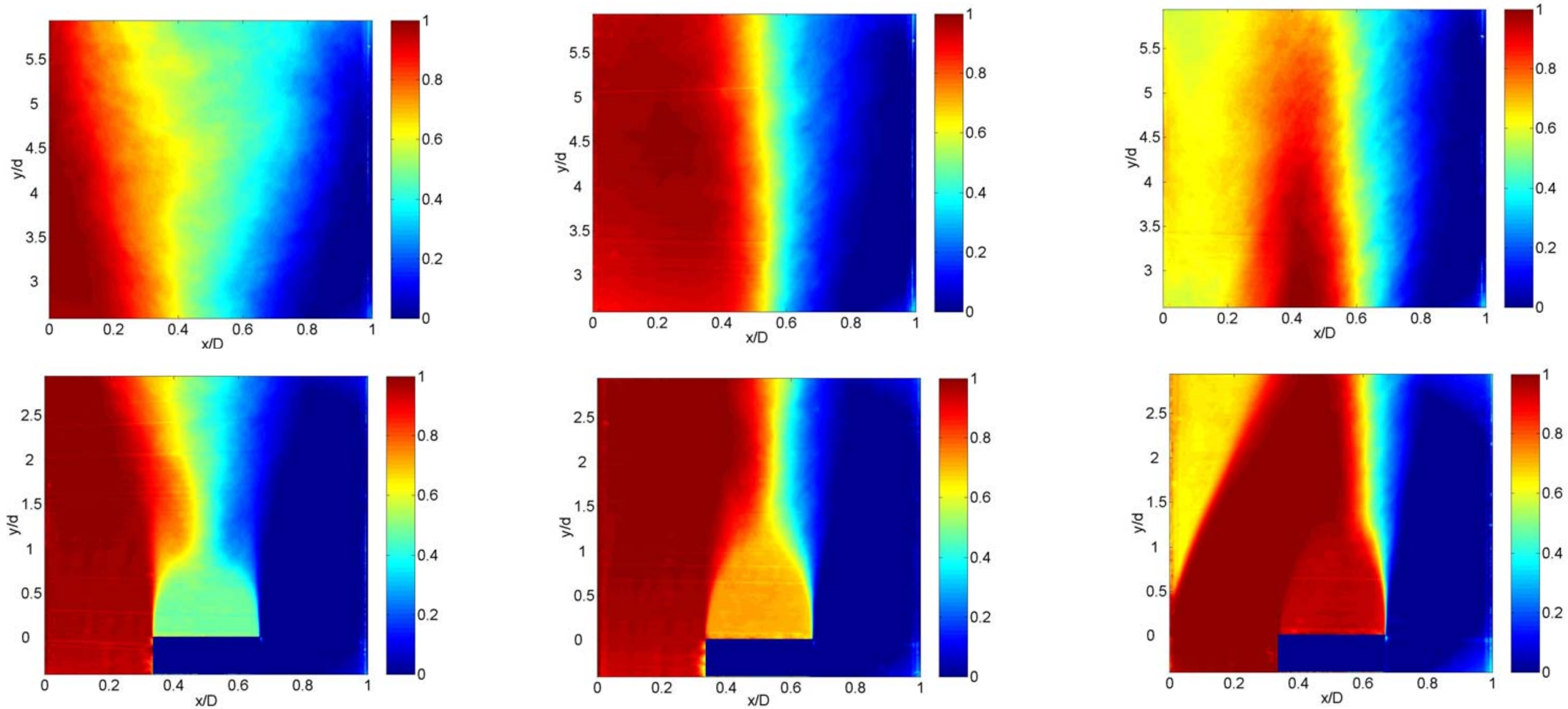




1:1 0.5:1 0.25:1

PIV/PLIF Measurements (3)

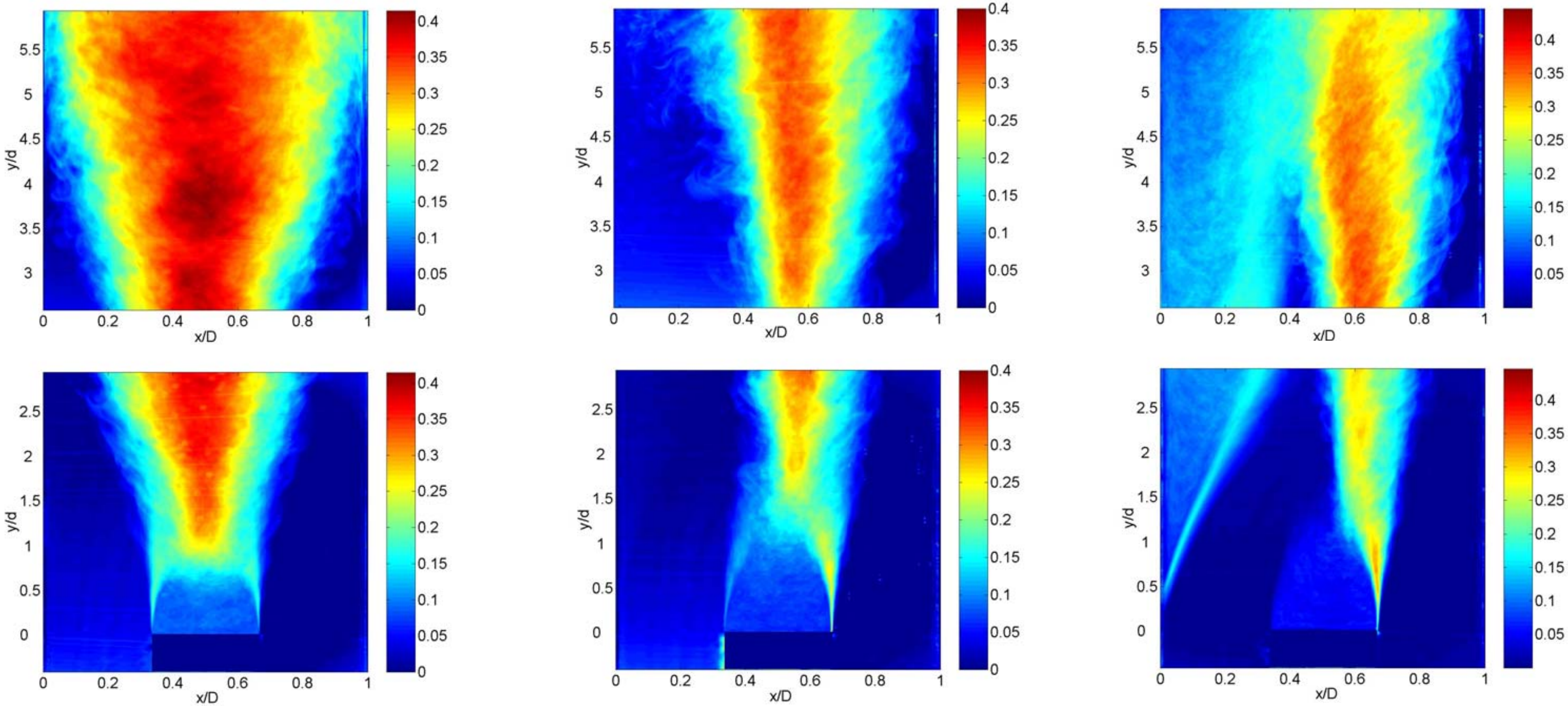
Mean concentrations



1:1 | 0.5:1 | 0.25:1

PIV/PLIF Measurements (4)

RMS concentrations



1:1

0.5:1

0.25:1

Conservation Equations

Mass

$$\frac{\partial U_j}{\partial x_j} = 0$$

Momentum

$$\frac{\partial}{\partial x_j}\left(\rho U_j U_i\right) = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j}; \qquad \tau_{ij} = (\mu + \mu_T)\cdot\left[\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right] - \frac{2}{3}\delta_{ij}\cdot\rho k$$

Mixture fraction

$$\phi = C / C_{A,b}$$

$$\frac{\partial}{\partial x_j}\left(\rho U_j \phi\right) = \frac{\partial}{\partial x_j}\left(\Gamma_\phi \frac{\partial \phi}{\partial x_j}\right); \qquad \Gamma_\phi = \frac{\mu}{Sc_\phi} + \frac{\mu_T}{Sc_T}$$

Turbulence and mixing models

Turbulence Models

- Standard *k*-ε model
- *RNG k*-ε model
- Chen-Kim *k*-ε model

Micromixing model

- Multi-peak presumed PDF model (Fox 1998)

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Multi-Peak PDF Model (1)

Presumed PDF

$$f_{\phi}(\psi;x,t)=\sum_{n=1}^{N_p} p_n(x,t)\,\delta\left(\psi-\phi_n(x,t)\right)$$

Transport equation for probability p_n

$$\frac{\partial}{\partial t}(\rho\, p_n)+\frac{\partial}{\partial x_j}(\rho\, U_j\, p_n)=\frac{\partial}{\partial x_j}\left(\Gamma_T\,\frac{\partial p_n}{\partial x_j}\right)+G_n(p)$$

Transport equation for probability-weighted concentration s_n

$$\frac{\partial}{\partial t}(\rho\, s_n)+\frac{\partial}{\partial x_j}(\rho\, U_j\, s_n)=\frac{\partial}{\partial x_j}\left(\Gamma_T\,\frac{\partial s_n}{\partial x_j}\right)+M_n(p,s)$$

- Conservation relations $\sum_{n=1}^{N_p} p_n=1;\quad \sum_{n=1}^{N_p} G_n=0;\quad \sum_{n=1}^{N_p} M_n=0$

Multi-Peak PDF Model (2)

Local concentration in environment/peak *n*

$$\phi_n = \frac{s_n}{p_n}$$

Mean concentration

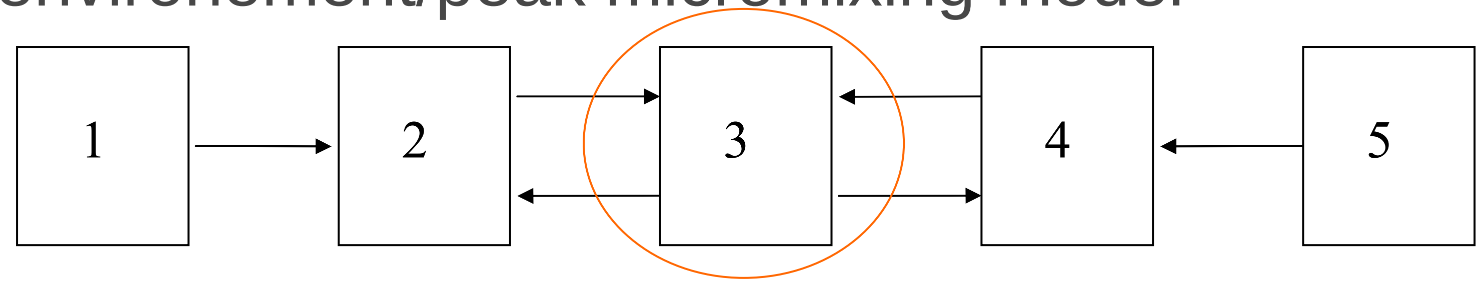
$$\langle \phi \rangle = \sum_{n=1}^{N_p} p_n \phi_n = \sum_{n=1}^{N_p} s_n$$

Variance of concentration fluctuations

$$\langle \phi'^2 \rangle = \sum_{n=1}^{N_p} p_n \phi_n^2 - \langle \phi \rangle^2$$

Multi-Peak PDF Model (3)

Five environement/peak micromixing model



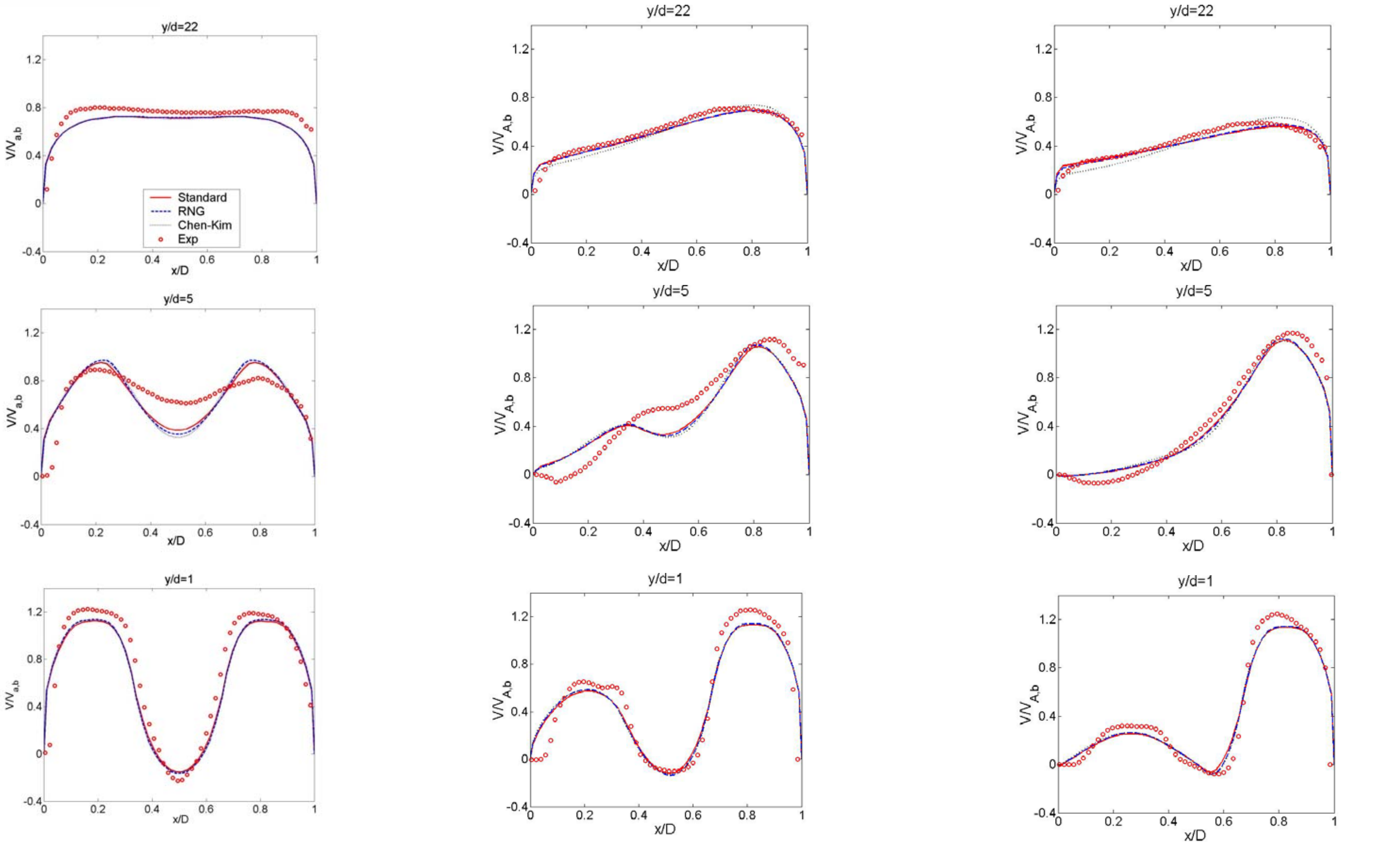
Inlet stream 1:				**Inlet stream 2:**
$\phi_1 = 1$	$\phi_2 < 1$	$1 > \phi_3 > 0$	$\phi_4 > 0$	$\phi_5 = 0$
$p_1 = 1$				$p_5 = 1$

Typical modelling of G_n and M_n for environment/peak 3

$$G_3 = r_2 + r_4 - 2r_3; \qquad M_3 = r_2\,\phi_2 + r_4\,\phi_4 - 2r_3\,\phi_3$$

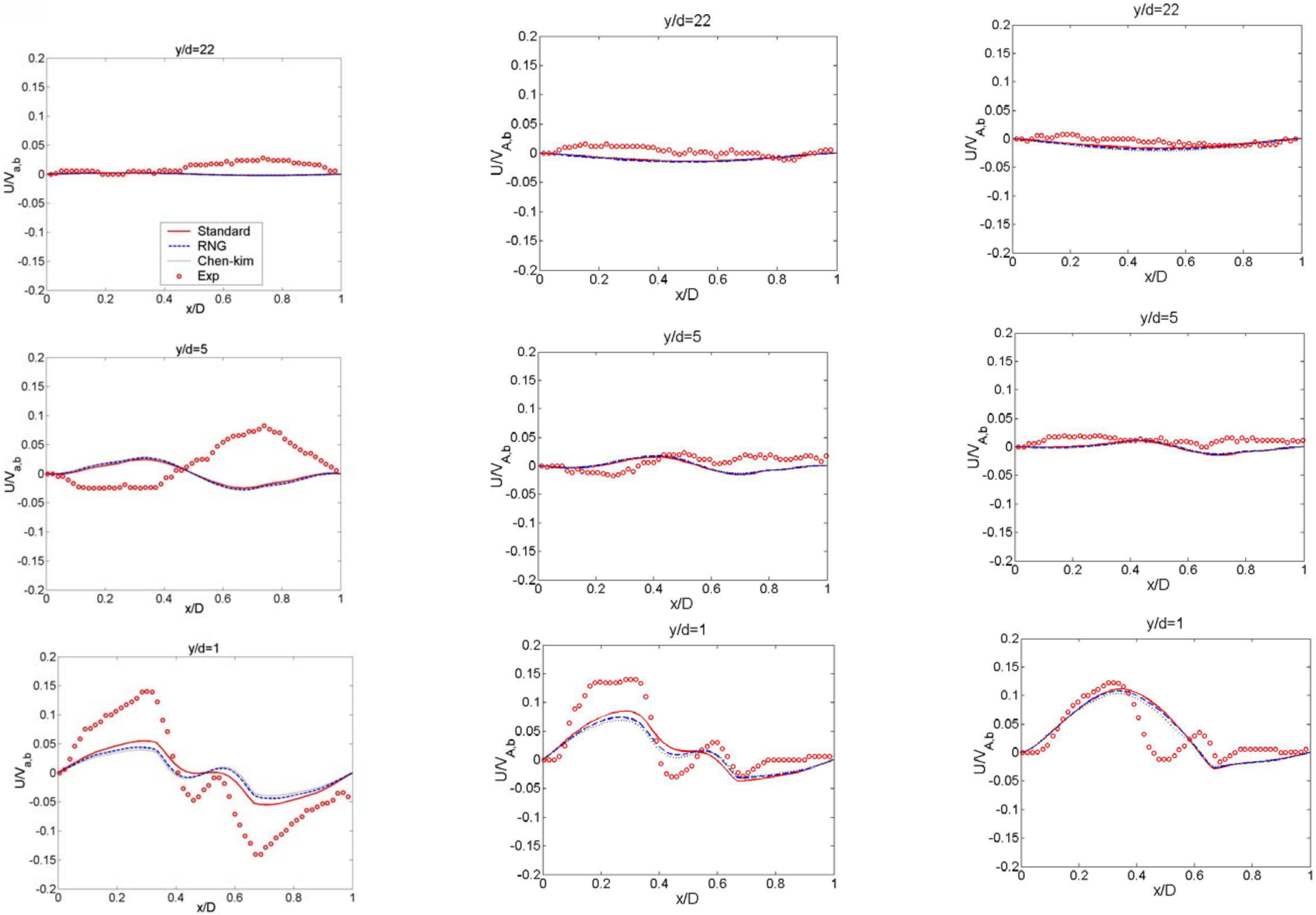
- Probability fluxes $\quad r_n = \gamma\ p_n$
- Rate of micromixing $\gamma = \dfrac{1}{\tau_m}; \qquad \tau_m = \dfrac{1}{C_\phi}\dfrac{k}{\varepsilon}; \quad C_\phi = 1.0$

Mean Axial Velocity (V)



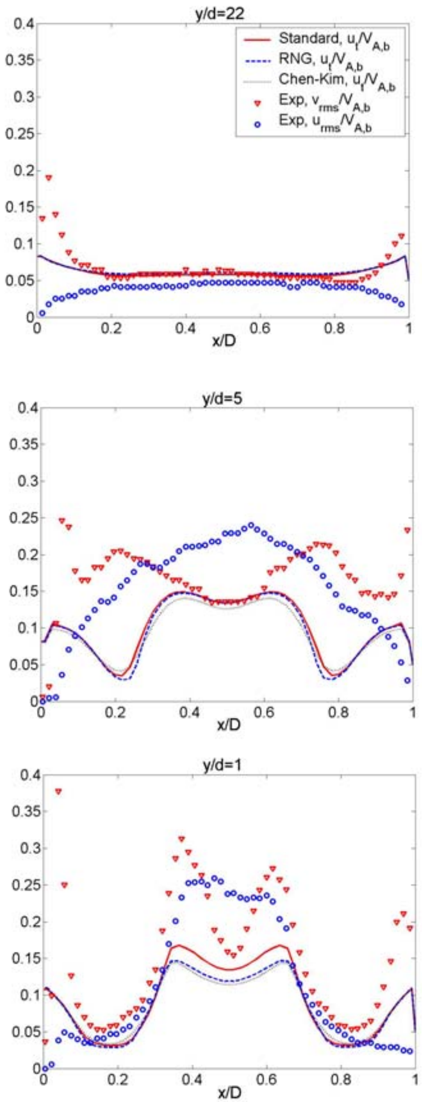
1:1 0.5:1 0.25:1

Mean Transverse Velocity (U)

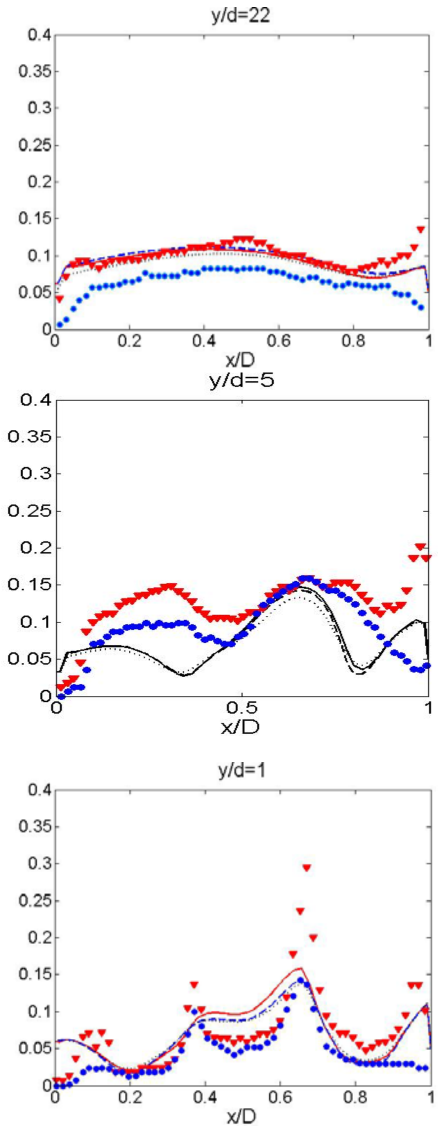


1:1 0.5:1 0.25:1

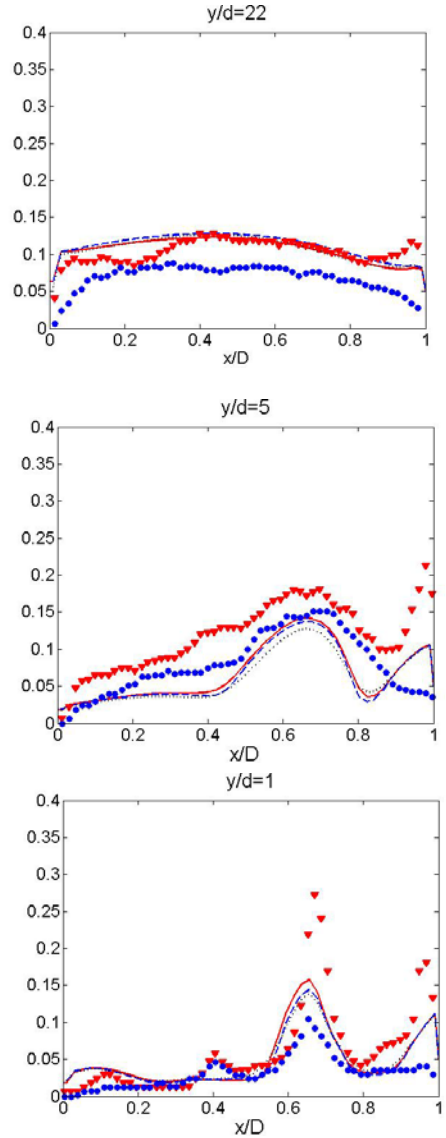
Turbulence Velocities



1:1



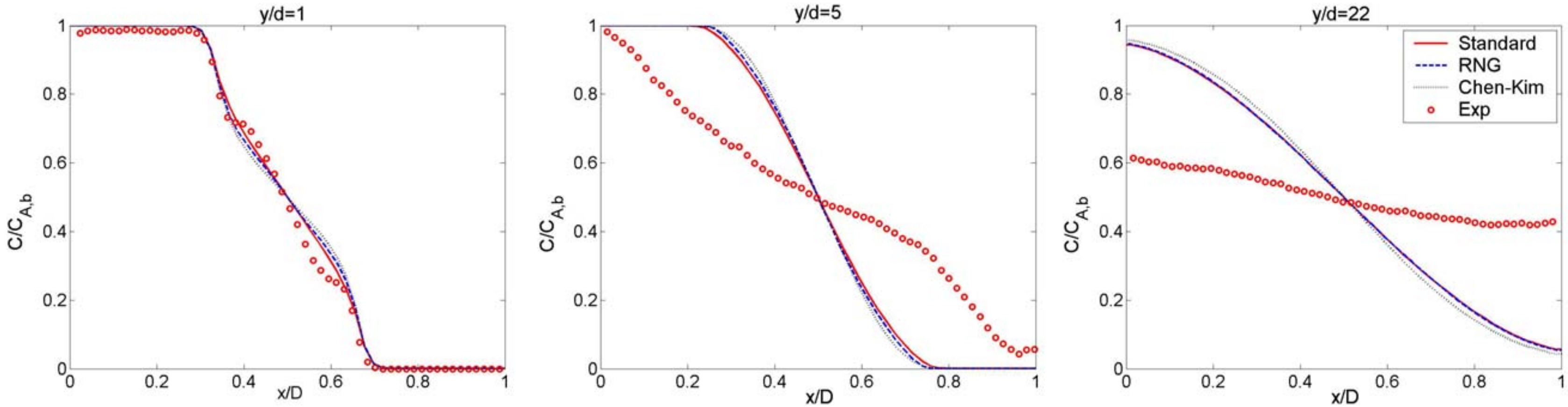
0.5:1



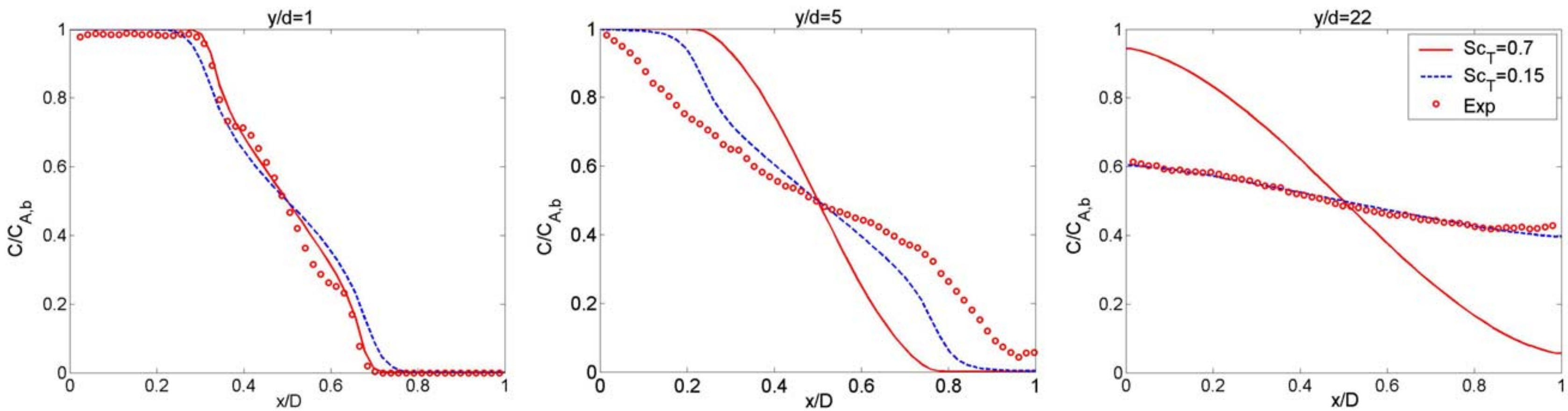
0.25:1

Mean Concentration

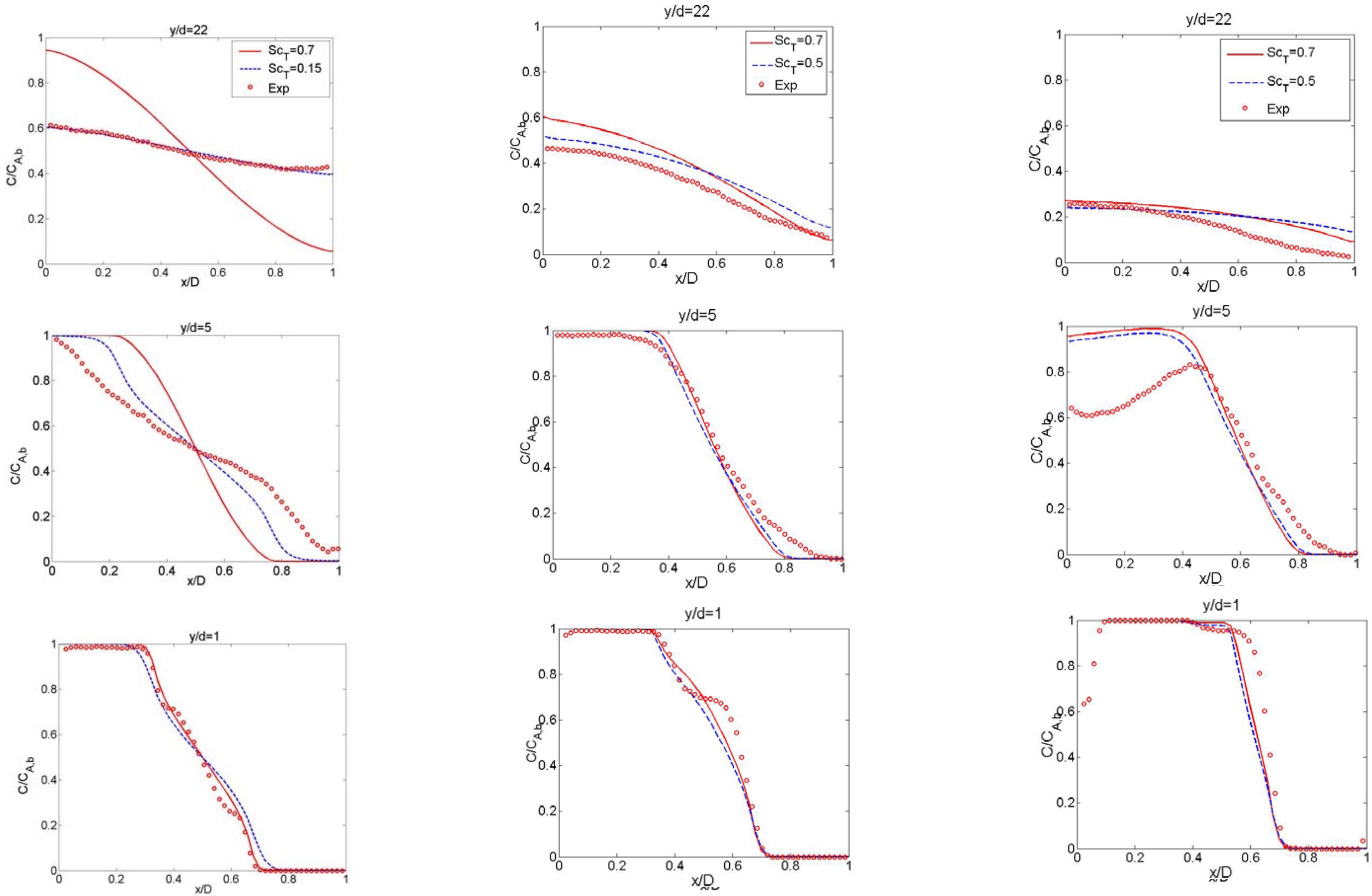
Turbulence models; 1:1 case



Turbulent Schmidt number; 1:1 case

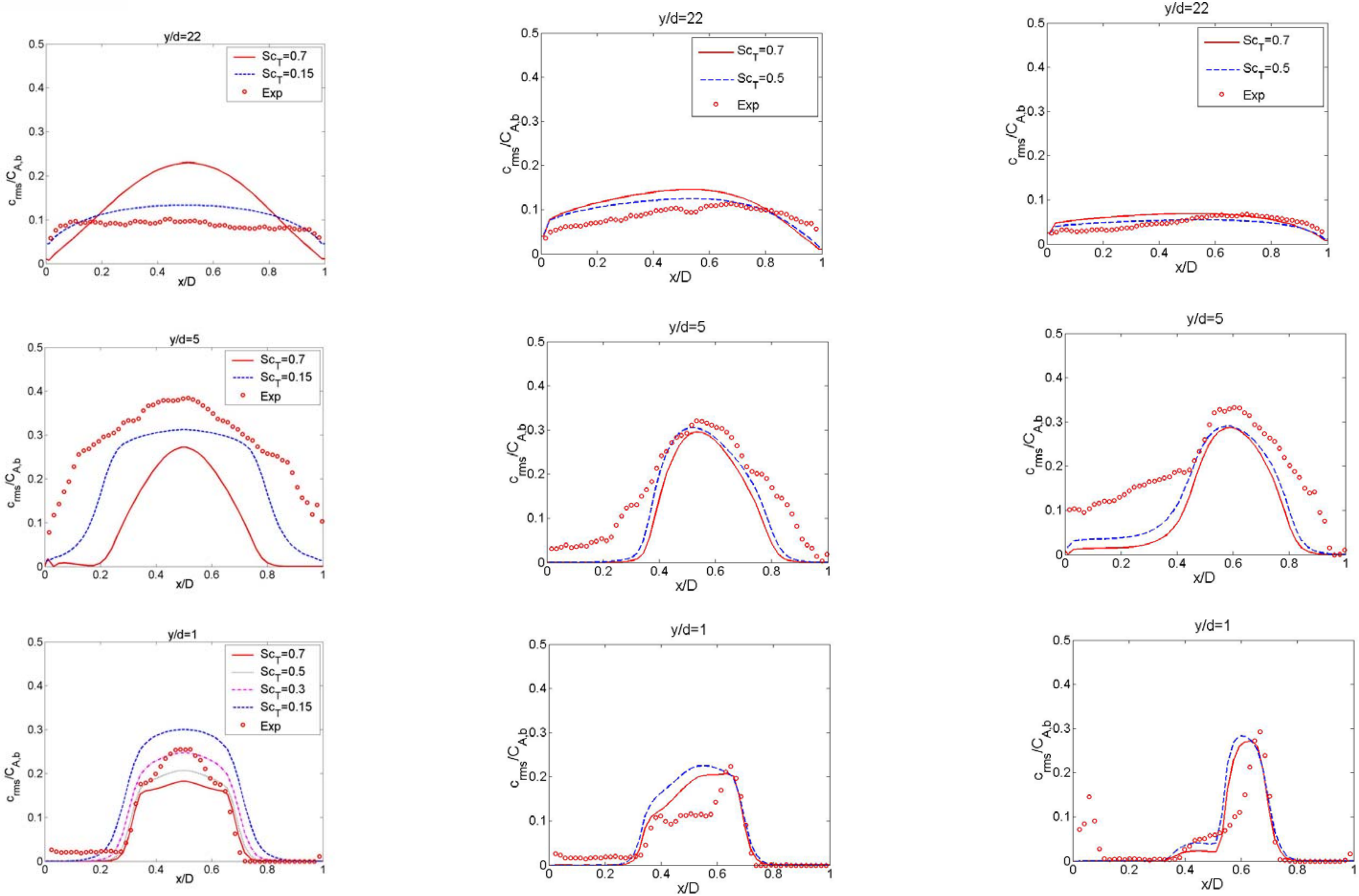


Mean Concentration



1:1 | 0.5:1 | 0.25:1

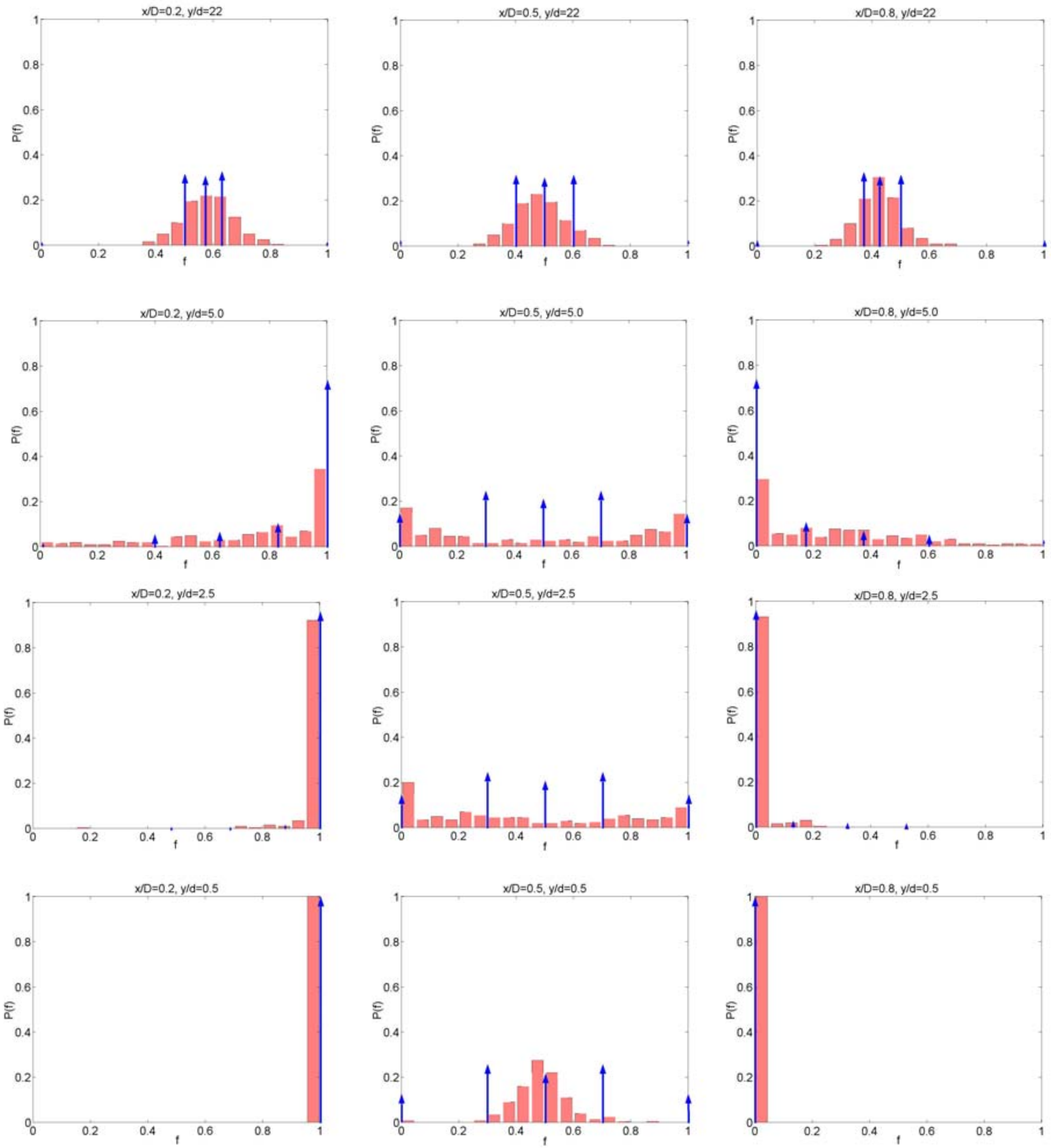
Concentration Fluctuations



1:1 0.5:1 0.25:1

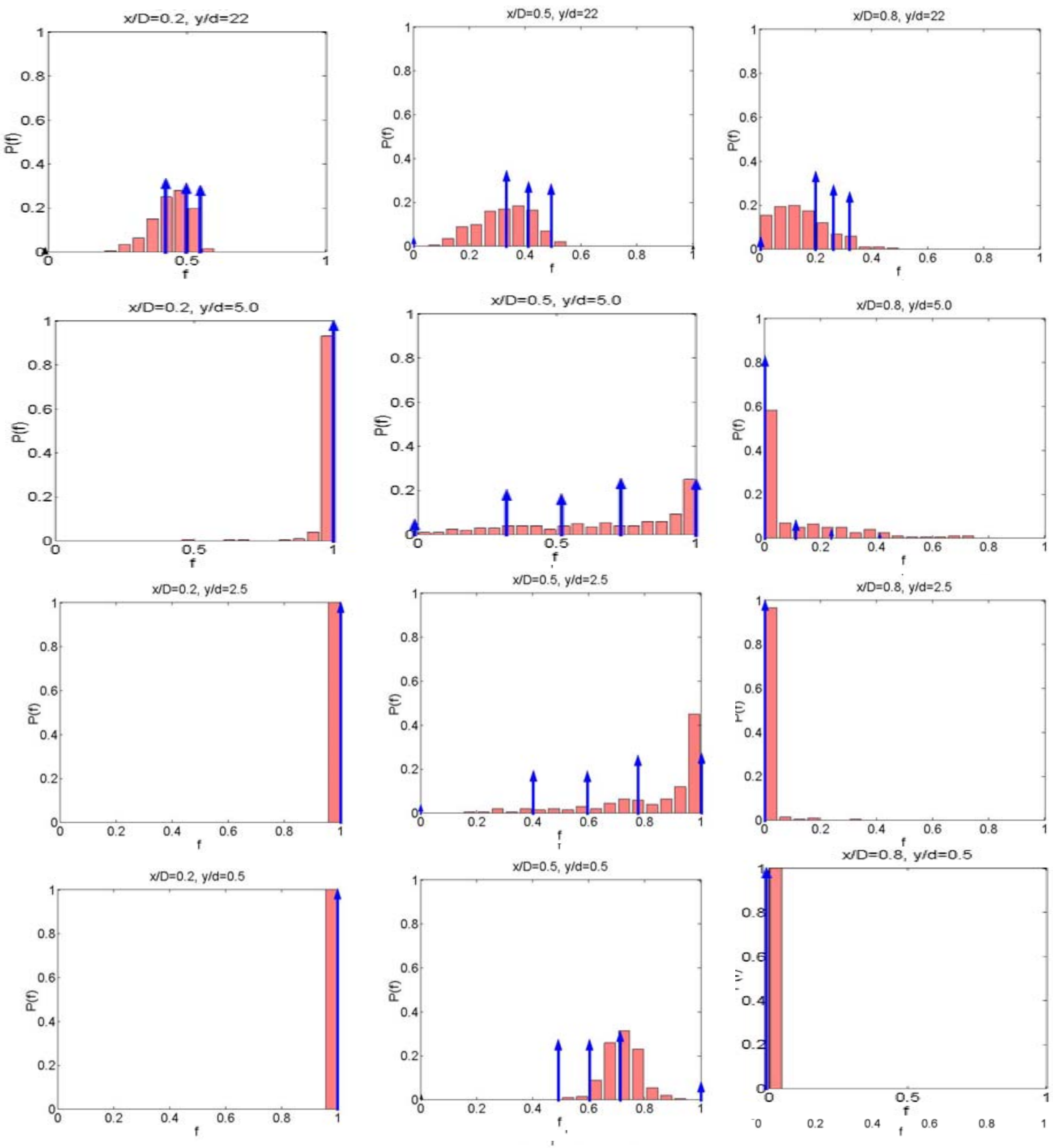
Five-peak presumed PDF model 1:1

Probability Density Functions



Five-peak presumed PDF model 0.5:1

Probability Density Functions



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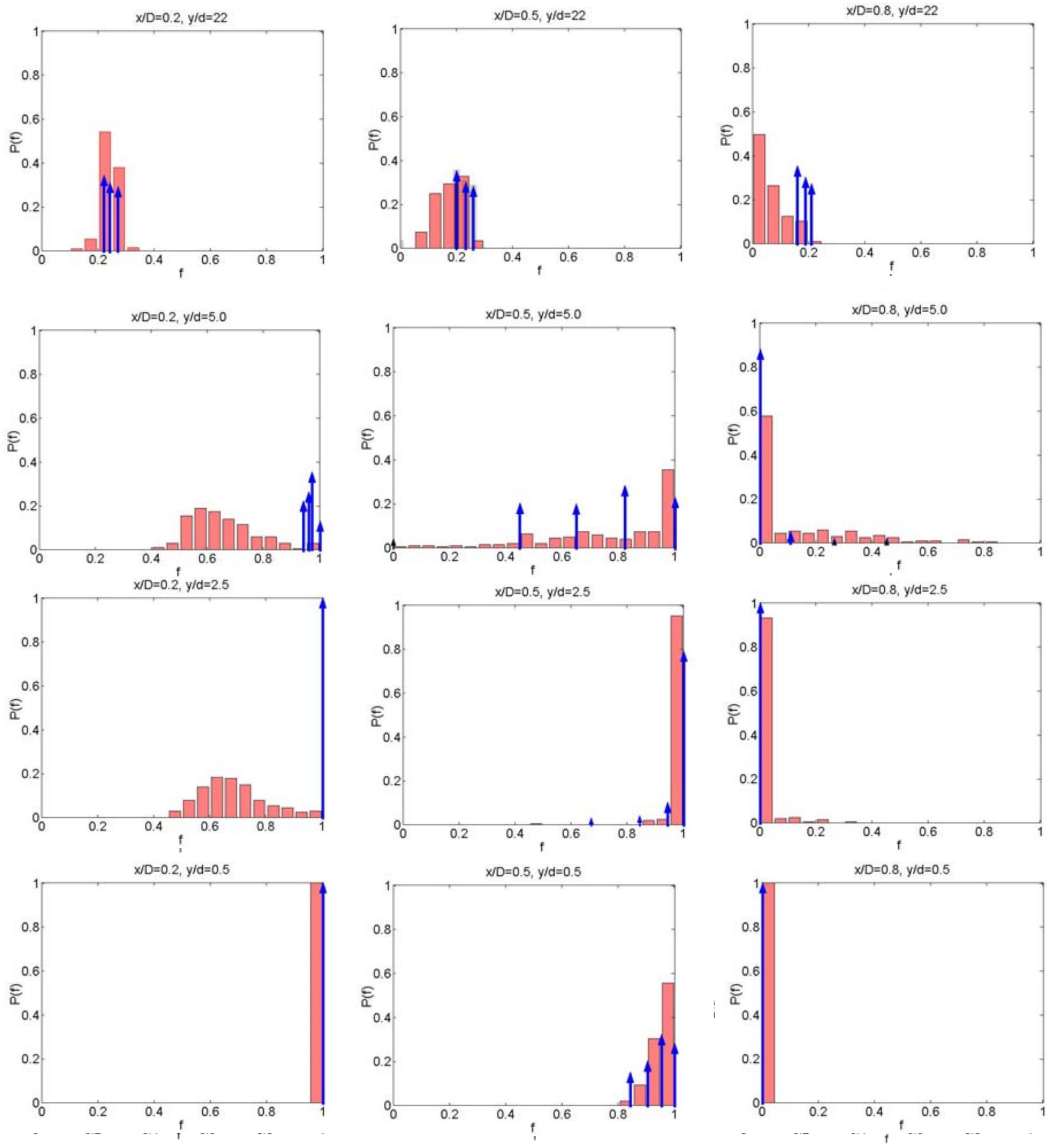
Five-peak presumed PDF model 0.25:1

Probability Density Functions



Overall mixing characteristics

- Coefficient of variation => Measure of macromixing

$$\mathrm{CoV} = \frac{\sqrt{\dfrac{\sum_{i=1}^{N}\left(C_i - \langle C\rangle_A\right)^2}{\mathrm{N}-1}}}{\langle \mathrm{C}\rangle_{\mathrm{A}}}$$

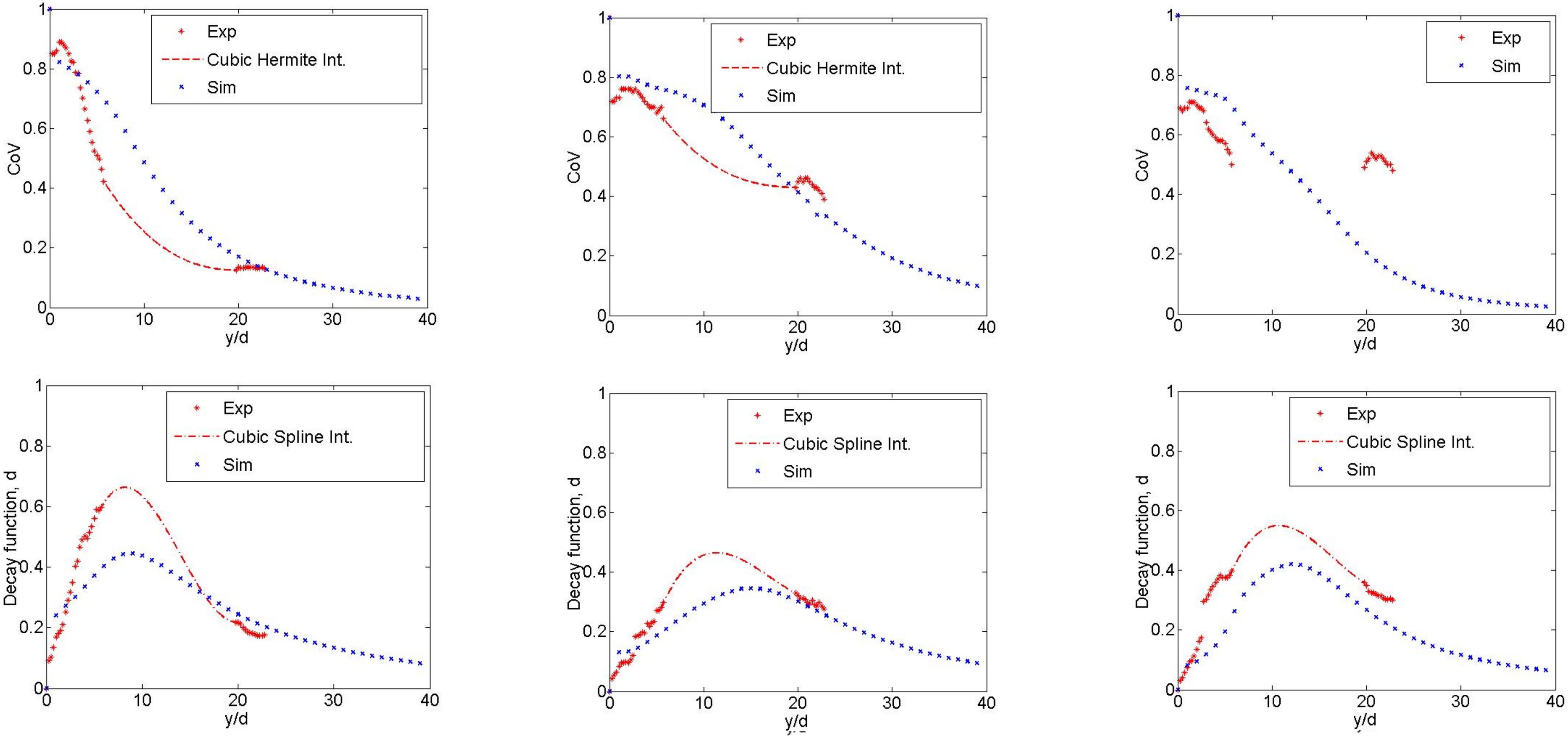
$A\text{–}area$

- Decay function => Measure of micromixing

$$d = \frac{\langle c_{rms}\rangle_A}{\langle C\rangle_A}$$

Coefficient of variation (CoV) and decay function (d)

1:1 | 0.5:1 | 0.25:1



Concluding remarks (1)

- The different k-ε turbulence models do not manage to capture the correct recovery from wake to channel flow, especially for the 1:1 case
- The defects in the flow modelling also transfers to the mixing predictions
- A reduction of the turbulent Schmidt number (0.15 for 1:1 case and 0.5-0.7 for the other) is needed to achieve good predictions of both mean and rms concentrations
- The five-peak presumed PDF model predicts the streamwise decay of micromixing reasonably correct

Concluding remarks (2)

- The concentration PDF's are reasonably predicted by the five-peak presumed PDF model
- The overall mixing characteristics (CoV and decay function) are reasonably predicted
- A LES turbulence model is probably required to improve the flow modeling
- Solution of the multi-peak PDF method should use the direct quadratic method of moment (DQMOM) technique