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 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: \( \frac{V_{A,b}}{V_{B,b}} = 1, 0.5, 0.25 \)
  - Feed channel B: \( \text{Re}_B = \rho \frac{V_{B,b} D_{h,B}}{\mu} = 5100 \)
PIV/PLIF System

Nd:YAG Laser
570 nm filter

PLIF camera
532 nm filter

PIV camera

Rhodamine 6G + 5\(\mu\)m polyamid particles

Position 1: y/d= -0.41
Position 2: y/d=2.59
Position 3: y/d=22.94

D=60 mm

v_A,b
C_A,b
v_B,b
C_B,b
PIV/PLIF Measurements (1)

Instantaneous velocity and concentration

- **C = 1**
- **C = 0**

20 mm
PIV/PLIF Measurements (2)

- 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
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

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

Mixture fraction

\[ \phi = \frac{C}{C_{A,b}} \]

\[ \frac{\partial}{\partial x_j} \left( \rho U_j \phi \right) = \frac{\partial}{\partial x_j} \left( \Gamma_\phi \frac{\partial \phi}{\partial x_j} \right); \quad \Gamma_\phi = \frac{\mu}{Sc_\phi} + \frac{\mu_T}{Sc_T} \]
Turbulence and mixing models

Turbulence Models

- Standard $k-\varepsilon$ model
- RNG $k-\varepsilon$ model
- Chen-Kim $k-\varepsilon$ model

Micromixing model

- Multi-peak presumed PDF model (Fox 1998)
Multi-Peak PDF Model (1)

Presumed PDF

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

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 environment/peak micromixing model

Inlet stream 1:
\[ \phi_1 = 1 \quad \phi_2 < 1 \quad 1 > \phi_3 > 0 \quad \phi_4 > 0 \quad p_1 = 1 \]

Inlet stream 2:
\[ \phi_5 = 0 \quad p_5 = 1 \]

Typical modelling of \( G_n \) and \( M_n \) for environment/peak 3

\[ G_3 = r_2 + r_4 - 2r_3; \quad M_3 = r_2 \phi_2 + r_4 \phi_4 - 2r_3 \phi_3 \]

- Probability fluxes
\[ r_n = \gamma p_n \]

- Rate of micromixing
\[ \gamma = \frac{1}{\tau_m}; \quad \tau_m = \frac{1}{C_\phi \varepsilon}; \quad C_\phi = 1.0 \]
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
Five-peak presumed PDF model 1:1
Five-peak presumed PDF model 0.5:1
Five-peak presumed PDF model 0.25:1
Overall mixing characteristics

- Coefficient of variation $\Rightarrow$ Measure of macromixing

\[
\text{CoV} = \sqrt{\frac{\sum_{i=1}^{N} (C_i - \langle C \rangle_A)^2}{N - 1 \langle C \rangle_A}}
\]

- Decay function $\Rightarrow$ 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 $k-\varepsilon$ 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 transfer 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