Introduction to CFD, Modelling of turbulence

Simon Lo
CD-adapco
Trident House, Basil Hill Road
Didcot, OX11 7JH, UK
simon.lo@cd-adapco.com

Contents

- Conservation equations
- What is CFD
- Solution method
- CFD grids and boundary types
- Turbulence models
- Boron dilution transient
- Pressure drop in spacer grid
- Thermal stripping in T-junction
Conservation of mass

- Conservation of mass, often called “Continuity”, in Cartesian tensor notation:

\[
\frac{\partial \rho}{\partial t} + \sum_{j} \frac{\partial}{\partial x_j} (\rho u_j) = \dot{m}
\]

\(\rho\) = density,
\(u\) = velocity,
\(\dot{m}\) = mass injection rate.

Conservation of momentum

- Conservation of momentum:

\[
\frac{\partial}{\partial t} (\rho u_i) + \sum_{j} \frac{\partial}{\partial x_j} (\rho u_j u_i - \tau_{ij}) = -\frac{\partial p}{\partial x_i} + \rho g_i + M
\]

\(p\) = pressure,
\(g\) = gravity vector,
\(\tau\) = stress tensor,
\(M\) = momentum sources, external forces.

\[M = F_{ext} + \dot{m}u_{inj}\]
Stress tensor

• The stress tensor in the momentum equation is:
  \[ \tau_{ij} = \mu S_{ij} - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} - \bar{\rho} u'_i u'_j \]

• The rate of strain tensor:
  \[ S_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \]

• Kronecker delta:
  \[ \delta_{ij} = 1 \quad \text{when} \quad i = j ; \quad \delta_{ij} = 0 \quad \text{when} \quad i \neq j \]

• Reynolds stresses due to turbulent motion: \( \bar{\rho} u'_i u'_j \)

Conservation of energy

• Conservation of thermal energy:
  \[ \frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_j} \left( \rho u_j h - \lambda \frac{\partial T}{\partial x_j} + \bar{\rho} u'_j h' \right) = Q \]

  \( h \) = enthalpy,

  \( \lambda \) = thermal conductivity,

  \( T \) = temperature,

  \( Q \) = external heat sources.

• Diffusional heat flux due to turbulent motion = \( \bar{\rho} u'_j h' \)
**What is CFD**

- CFD stands for Computational Fluid Dynamics.
- For a given set of boundary conditions at A & B we can calculate the mean flow velocity between A & B using the momentum equation.
- A simplified momentum equation could be:
  \[ P_A - P_B = K \frac{1}{2} \rho U^2 \]

**A simple solution method**

1. Guess \( P_C \).
2. Calculate \( U_1 \) and \( U_2 \) using the momentum equation.
3. Check mass balance: \( (\rho A U)_1 = (\rho A U)_2 \)
4. Stop if mass balance is achieved, if not continue.
5. Adjust \( P_C \) in order to change \( U_1 \) and \( U_2 \) such that mass balance is achieved:
   - If inflow is higher than outflow then increase \( PC \).
   - If inflow is lower than outflow then decrease \( PC \).
6. Repeat calculation from Step 2.

? Change \( P_C \) by how much?
Pressure correction method

- The exact mass balance equation: \((\rho A U)_1 - (\rho A U)_2 = 0\).
- Velocities \(U^*_1\) and \(U^*_2\) obtained from the momentum equation may not satisfy mass balance exactly. \((\rho A U^*_1) - (\rho A U^*_2) = \epsilon\).
- Correction to velocities to achieve mass balance is:
  \[
  (\rho A U^*_1) - (\rho A U^*_2) = -\epsilon \quad U = U^* + U'
  \]
- Velocity correction in terms of pressure correction:

  \[
  \left(\rho A \frac{\partial U}{\partial P} P'\right)_1 - \left(\rho A \frac{\partial U}{\partial P} P'\right)_2 = -\epsilon \quad P = P^* + P' \quad U' = \frac{\partial U}{\partial P} P'
  \]

Multi-dimensional CFD

- Generalise the solution method to 2 and 3 dimensions for arbitrary geometry and include the time dependent term.
A CFD solution procedure

1. Guess pressure.
2. Calculate velocity using the momentum equation.
3. Solve pressure correction equation according to mass balance.
4. Adjust pressure and velocity.
5. Repeat calculation from Step 2 until convergence (i.e. all residuals reached acceptable level).

- Residual is typically the sum of absolute error ($\varepsilon$) of all cells.
- $\varepsilon = \text{abs}(\text{LHS}-\text{RHS})$ of equation.

**CFD grids**

- Tetrahedral
- Trimmed hexahedral
- Polyhedral
### CFD boundary types

- **Inlet**
  - All boundary values are specified.
  - A negative velocity would mean outflow (suction).
- **Outlet**
  - Outflow only.
- **Pressure**
  - Outflow and inflow are allowed (fully developed flow).
- **Wall**
  - Slip or no-slip, stationary or moving.
- **Symmetry**
  - Plane or axis.
- **Periodic plane**
  - Works in pair.

### 2D asymmetric model of vertical pipe

- **Water + steam**
- **Sub-cooled water**
- **Heated wall**
- **Symmetry plane**
- **Symmetry axis**
- **Void**
- **Outflow**
- **Inflow**
- **Pipe axis**
CFD today

- Typical CFD model today has order of 100,000 to 1 million computational cells.

- We solve conservation equations for mass (1 eqn), momentum (3 eqn) and energy (1 eqn) for each cells.
  - For 1 million cells model we have 5 million equations to solve simultaneously!

- We need to add additional equations to represent the physics, for examples:
  - Turbulence models.
  - Heat transfer and mass transfers.
  - Non-Newtonian fluids.
  - Multiphase flows.
Turbulence:

Eddy viscosity model (momentum)

- Recalling the shear stress term in the momentum equation:
  \[ \tau_{ij} = \mu S_{ij} - \frac{2}{3} \mu \frac{\partial u_k}{\partial x_k} \delta_{ij} - \bar{\rho} \bar{u}_i \bar{u}_j \]

- Model the Reynolds stress as:
  \[ -\bar{\rho} \bar{u}_i \bar{u}_j = \mu_s S_{ij} - \frac{2}{3} \left( \mu_t \frac{\partial u_k}{\partial x_k} + \rho \kappa \right) \delta_{ij} \]

- Turbulent kinetic energy:
  \[ k = \frac{u_i u_j}{2} \]

- Turbulent eddy viscosity:
  \[ \mu_t = \frac{c_\mu \rho k^2}{\varepsilon} \]

Eddy viscosity model (energy)

- Recalling the energy equation:
  \[ \frac{\partial}{\partial t} (\rho h) + \frac{\partial}{\partial x_j} \left( \rho u_j h - \lambda \frac{\partial T}{\partial x_j} + \bar{\rho} \bar{u}_j \bar{h}' \right) = Q \]

- Model the turbulent heat flux as:
  \[ \bar{\rho} \bar{u}_j \bar{h}' = -\frac{\mu_t}{\sigma_h} \frac{\partial h}{\partial x_j} \]
**k-ε model**

- The most commonly used turbulence model is the k-ε model.
- Equation for turbulent kinetic energy:
  \[
  \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} \left[ \rho u_j k - \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] = \mu_t P - \frac{2}{3} \left( \mu_t \frac{\partial u_i}{\partial x_j} + \rho k \right) \frac{\partial u_i}{\partial x_j} - \rho \varepsilon
  \]
- Equation for dissipation rate of turbulent kinetic energy:
  \[
  \frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_j} \left[ \rho u_j \varepsilon - \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] = C_{\varepsilon 1} \frac{\varepsilon}{k} \left[ \mu_t P - \frac{2}{3} \left( \mu_t \frac{\partial u_i}{\partial x_j} + \rho k \right) \frac{\partial u_i}{\partial x_j} \right] - C_{\varepsilon 2} \rho \varepsilon^2
  \]

**k-ε model (2)**

- Production term: \( P = S_{ij} \frac{\partial u_i}{\partial x_j} \)
- Model constants: \( C_\mu = 0.09 \)
  \[ \sigma_k = 1 \]
  \[ \sigma_\varepsilon = 1.22 \]
  \[ \sigma_h = 0.9 \]
  \( C_{\varepsilon 1} = 1.44 \)
  \( C_{\varepsilon 2} = 1.92 \)
Anisotropic $k$-\( \epsilon \) model

- Eddy-viscosity models:

\[
\rho \overline{u_i u_j} = \frac{2}{3} \left( \mu_i \frac{\partial u_i}{\partial x_k} + \rho k \right) \delta_{ij} - \mu_i S_{ij}
\]

- Anisotropic $k$-\( \epsilon \) model

\[
\rho \overline{u_i u_j} = \frac{2}{3} \left( \mu_i \frac{\partial u_i}{\partial x_k} + \rho k \right) \delta_{ij} - \mu_i S_{ij}
\]

\[
+ C_i \mu_i \left[ S_{ij} S_{ij} - \frac{1}{3} \delta_{ij} S_{ii} S_{ii} \right] + C_i \mu_i \left[ \Omega_{ij} - \frac{1}{3} \delta_{ij} \Omega_{ii} S_{ii} \right] + C_i \mu_i \left[ \Omega_{ij} - \frac{1}{3} \delta_{ij} \Omega_{ii} S_{ii} \right]
\]

Reynolds stress model

- Reynolds stress model solves directly for the Reynolds stresses:

\[
\frac{\partial}{\partial t} \left( \rho \overline{u_i u_j} \right) + C_{ij} - D_{ij} = P_{ij} + \Phi_{ij} - \rho \varepsilon_{ij}
\]
Boron Dilution transients

- A decrease of the boron concentration in the core leads to a reactivity increase and may result in a power excursion ➔ a so-called boron dilution transient.

- Slugs of under-borated coolant can be formed in the primary circuit, e.g. due to a malfunction of the chemical and volume control system, or due to an SBLOCA with partial failure of the safety injection system.

International Standard Problem (ISP) No. 43

Scaled down model of a Babcock & Wilcox (B&W) PWR with height ratio of 1:4.

Simplified model of PWR [ROCOM]

- 4 Loops PWR model, with perforated drum.


Internal components

Fuel channels
Perforated drum
Flow and boundary conditions

<table>
<thead>
<tr>
<th></th>
<th>Inlet 1</th>
<th>Inlet 2</th>
<th>Inlet 3</th>
<th>Inlet 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow [m³/h]</td>
<td>185</td>
<td>185</td>
<td>185</td>
<td>185</td>
</tr>
<tr>
<td>Mixing Scalar f(t):</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

Scalar mixing transient
### Downcomer flow mixing

<table>
<thead>
<tr>
<th>Model</th>
<th>Image</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard k-ε</td>
<td><img src="image1.png" alt="Standard k-ε" /></td>
</tr>
<tr>
<td>Anisotropic k-ε</td>
<td><img src="image2.png" alt="Anisotropic k-ε" /></td>
</tr>
<tr>
<td>RSM</td>
<td><img src="image3.png" alt="RSM" /></td>
</tr>
</tbody>
</table>

![Graph showing scalar concentration](image4.png)

### Transient scalar mixing

And better scalar mixing in the inlet region
Models comparison

- Standard k-ε
- Anisotropic k-ε
- RSM

Lower Plenum Mixing

- The perforated drum homogenizes the flow.
- The influence of “turbulence modeling” is reduced.
International Benchmark - OECD T junction

T-junction Benchmark Results - Blind test

normalized flow profiles at 1.6 diameters downstream of the mixing zone
normalized flow profiles at 2.6 diameters downstream of the mixing zone

S.T. Jayaraju, E.M.J. Komen: Nuclear Research and Consultancy Group (NRG), Petten, The Netherlands
• Conservation equations of mass, momentum and energy
• What is CFD
  - Solution method
  - Grids and boundary types
• Turbulence models
  - Eddy viscosity model
  - k-ε turbulence model
  - Anisotropic turbulence models
• Boron dilution transient
  - Effect of turbulence modelling on mixing
• Thermal stripping
  - Modelling flow instability