

# COMPUTATIONAL FLUID DYNAMICS

ENCH 355

Lecture : 3  
Tutorial : 1  
Practical : 0

Year : III  
Part : II

## Course Objectives:

The objective of this course is to familiarize students with the governing equations of fluid flow, heat transfer, and mass transfer that form the foundation of computational fluid dynamics (CFD). It teaches to solve appropriate numerical methods used in CFD.

- 1 Introduction (6 hours)**
  - 1.1 Definition and scope of CFD
  - 1.2 CFD in chemical engineering: applications and industrial relevance
  - 1.3 CFD versus analytical and experimental approaches
  - 1.4 CFD process: Pre-processing, Solving, Post-processing
  - 1.5 Overview of CFD software tools
  - 1.6 Advantages, limitations, and challenges of CFD
  - 1.7 Governing equation of mass, energy and momentum
  
- 2 Discretization and Numerical Methods (12 hours)**
  - 2.1 Overview of Finite Difference Method (FDM), Finite Element Method (FEM), and Finite Volume Method (FVM)
  - 2.2 Control Volume formulation
  - 2.3 FVM Basics: Discretization of 1D steady-state diffusion equation, Discretization of the 1D unsteady convection-diffusion equation
  - 2.4 Spatial Discretization Schemes: Central differencing Scheme (CDS), upwind differencing scheme (UDS), numerical diffusion and stability diffusion issues (Courant number)
  
- 3 Grid Generation and Mesh Quality (6 hours)**
  - 3.1 Structures versus unstructured mesh
  - 3.2 Mesh quality parameters
  - 3.3 Grid independence study
  - 3.4 Boundary layer meshing (Inflation layers)
  
- 4 Solvers and Algorithms (6 hours)**
  - 4.1 Pressure velocity coupling
  - 4.2 SIMPLE algorithm (Semi implicit method for pressure linked equation)

- 4.3 SIMPLEC, PISO algorithms
- 4.4 Linear equation solvers: Gauss Siedel, TDMA (Tri-diagonal matrix algorithm)
- 4.5 Residuals and convergence criteria

**5 Turbulence Modelling (5 hours)**

- 5.1 Nature of turbulence
- 5.2 Reynolds averaging
- 5.3 Reynolds-Averaged Navier-Stokes (RANS) models ( $k-\epsilon$  turbulence models)

**6 Multiphysics in Chemical Engineering (10 hours)**

- 6.1 Heat transfer (Conduction, convection)
- 6.2 Species transport and reactions
- 6.3 Multiphase flow: Eulerian-Eulerian, Eulerian-Lagrangian

**Tutorial (15 hours)**

1. Turbulence model comparison: Simulate flow separation in a sudden expansion and compare different RANS turbulence models to see their predictions difference
2. Conjugate heat transfer: Model a double pipe heat exchanger and solve both fluid flow and heat conduction in the solid at the same time
3. Species Transport and Mixing: Simulate mixing of two fluid streams in a T-junction to understand turbulence and diffusion-driven species transport
4. Reacting Flows: Combine turbulence and chemical reactions using the Finite Rate/Eddy Dissipation Model to simulate a simple Arrhenius reaction in a cylindrical reactor
5. Multiphase Flow: Simulate a cyclone separator to track particle motion and calculate how efficiently particles are collected

**Final Exam**

The questions will cover all the chapters in the syllabus. The evaluation scheme will be as indicated in the table below:

Chapter	Hours	Mark distribution*
1	6	8
2	12	16
3	6	8
4	6	8
5	5	8
6	10	12
<b>Total</b>	<b>45</b>	<b>60</b>

\* There may be minor deviation in marks distribution.

## References

1. Versteeg, H. K., Malalasekera, W. (2007). An introduction to computational fluid dynamics: The finite volume method. Pearson Education.
2. Anderson, J. D. (1995). Computational fluid dynamics: The basics with applications (Latest edition). McGraw-Hill.
3. Ranade, V. V. (2002). Computational flow modeling for chemical reactor engineering. Academic Press.
4. Patankar, S. V. (1980). Numerical heat transfer and fluid flow. Taylor & Francis. (Latest edition)