GUJARAT TECHNOLOGICAL UNIVERSITY

Program Name: Master of Engineering
Level: PG
Branch: Chemical Engineering
Subject Code: ME02030071
Subject Name: Computational Fluid Dynamics

w. e. f. Academic Year:	2024-25
Semester:	2
Category of the Course:	Professional Elective Course

Prerequisite:	Numerical Methods
Rationale:	To be able to model and simulate all the mass, momentum, and energy transport processes in chemical engineering using the generalized conservation equations. Students will understand the governing equations of fluid dynamics and their derivation from laws of conservation. To develop a good understanding in computational skills, including discretisation, accuracy and stability. To acquaint the students with a process of developing a mathematical and geometrical model of flow, applying appropriate boundary conditions and solving system of equations.

Course Outcome:

After Completion of the Course, Student will able to:

No	Course Outcomes
01	Develop governing equations for a given fluid flow system
02	Apply finite difference method for fluid flow and heat transfer problems
03	Solve computational fluid flow problems using finite volume techniques
04	Get familiarized to modern CFD software used for the analysis of complex fluidflow systems

Teaching and Examination Scheme:

Teaching Scheme(in Hours)			Total Credits L+T+ (PR/2)	Assessment Pattern and Marks				Total Marks
				Theory		Tutorial / Practical		
L	T	PR	C	ESE (E)	PA / CA (M)	PA/CA (I)	ESE (V)	
3	0	2	4	70	30	20	30	150

Course Content:

Unit No.	Content	No. of Hours	% of Weightage
1.	**Introduction to Fluid Dynamics:** Concepts of Fluid Flow, Pressure distribution in fluids, Reynolds transport theorem, Integral form of conservation equations, Differential form of conservation equations, Different Types of Flows, Euler and Navier Stokes equations, Properties of supersonic and subsonic flows, Flow characteristics over various bodies. Philosophy of CFD, Governing equations of fluid dynamics and their physical meaning, Mathematical behavior of governing equations and the impact on CFD simulations, Simple CFD techniques and CFL condition. Numerical Methods in CFD: Finite Difference, Finite Volume, and Finite Element, Upwind and downwind schemes, Simple and Simpler schemes, Higher order methods, Implicit and explicit methods, Study and transient solutions	**10**	**22**
2.	**Grid Generation:** Basic theory of structured grid generation, Surface grid generation, Mono block, multi block, hierarchical multi block, Moving and sliding multi-block, Grid clustering and grid enhancement. Basic theory of unstructured grid generation, advancing front, Delaunay triangulation and various point insertion methods, Unstructured quad and hex generation, grid based methods, various elements in unstructured grids, Surface mesh generation, Surface mesh repair, Volume grid generation, Volume mesh improvement, mesh smoothing algorithms, grid clustering and quality checks for volume mesh. Adaptive, Moving and Hybrid Grids, Need for adaptive and, moving grids, Tet, pyramid, prism, and hex grids, using various elements in combination	**10**	**22**
3.	**Turbulence and its Modeling:** Transition from laminar to turbulent flow, Effect of turbulence on time averaged Navier-Stokes equations, Characteristics of simple turbulent flows, Free turbulent flows, Flat plate boundary layer and pipe flow, Turbulence models, Mixing length model, the k-e model, Reynolds stress equation models, Algebraic stress equation models	**10**	**22**
4.	**Chemical Fluid Mixing Simulation:** Stirred tank modeling using the actual impeller geometry, Rotating frame model, The MRF Model Sliding mesh model, Snapshot model, Evaluating Mixing from Flow Field Results, Industrial Examples	**8**	**18**
5.	**Post-Processing of CFD results:** Contour plots, vector plots, and scatter plots, Shaded and transparent surfaces, Particle trajectories and path line trajectories, Animations and movies, Exploration and	**7**	**16**

	analysis of data.		
	Total	**45**	**100**

Suggested Specification Table with Marks (Theory):

Distribution of Theory Marks					
R Level	**U Level**	**A Level**	**N Level**	**E Level**	**C Level**
7	12	35	10	6	0

Where R: Remember; U: Understanding; A: Application, N: Analyze and E: Evaluate C: Create (as perRevised Bloom's Taxonomy)

References/Suggested Learning Resources:

(a) Books:

1. Computational Fluid Dynamics: The Basics with Applications by Anderson John D., McGraw Hill, 1995
2. Computational Flow Modeling for Chemical Reactor Engineering by Ranade V.V., Process Engineering Science, Volume 5, 2001
3. Fundamentals of Grid Generation by Knupp Patrick and Steinberg Stanly, CRC Press, 1994.
4. Turbulence Modelling for CFD by Wilcox D.C., 1993
5. An Introduction to Multigrid Methods by Wesseling Pieter, John Wiley & Sons, 1992
6. Numerical Grid Generation: Foundations and Applications by Thompson J.F., Warsi Z.U.A. and Mastin C.W., North Holland, 1985
7. Numerical Heat Transfer and Fluid Flow by Patankar S.V., McGraw-Hill,1981
8. Simulation and Modelling of Turbulent Flows by Gatski Thomas B., Hussaini M. Yousuff and Lumley John L., Oxford University Press, 1996
9. Computational Gas Dynamics by Laney, C. B., Cambridge Uni. Press, 1998.

(b) Open source software and website:

1. OpenFOAM (https://www.openfoam.com/)
2. ANSYS/Fluent (https://www.ansys.com/en-in/products/fluids/ansys-fluent)
3. Star-CD (https://mdx.plm.automation.siemens.com/star-cd)
4. Star-CCM+ (https://mdx.plm.automation.siemens.com/star-ccm-plus)
5. COMSOL Multiphysics
6. CFDTool (https://www.cfdtool.com/)
7. MATLAB
8. C/C++/Python based tutorials

Suggested Course Practical List:

1. Evaluation of matrix format of conservation equation
2. Grid generation for Ideal CSTR and PFR reactors
3. Grid generation technique for fluidized bed
4. Application of grid refinement on PID of chemical plant
5. Simplification of momentum balance to derive bernoulli's equation
6. Comparison of solution methods for various CFD softwares
7. Evaluation of heat loss using CFD software
8. Evaluation of fluid dynamics in water hammer effect using Open FOAM
9. Setting up the modeling equation for simultaneous heat, mass and momentum transfer application.

List of Laboratory/Learning Resources Required:

- Computer lab

Suggested Project List:

- Study Pressure drop and heat transfer in packed bad for exothermic reaction.
- Simulate fluid flow and optimize impeller design for improved mixing.
- Investigate gas liquid interactions and bubble dynamics.
- Study solid liquid interactions and pressure drops.
- Study mass transfer enhancement due to microbubbles.

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