Indian Institute of Technology, Kanpur

Proposal for a New Course

1. Course No: ChE 6XX

2. Course Title: CFD-Based Simulation of Transport Phenomena in Chemical Engineering

3. Per Week Lectures: 3 (L), Tutorial: x (T), Laboratory: x, Additional Hours[0-2]: x

   Credits (3*L+2*T+P+A): 9 Duration of Course: Full Semester

4. Proposing Department/IDP: Chemical Engineering

   Other Departments/IDPs which may be interested in the proposed course: NA

   Other faculty members interested in teaching the proposed course: NA

5. Proposing Instructor: Prof. Nishith Verma, ChE
6. Course Description:

A) Objectives:

Transport Phenomena is one of the core subjects in Chemical Engineering and traditionally relies on analytical solutions of the governing equations of momentum, heat and mass transfer. While these classical solutions provide valuable physical insight, modern engineering practice increasingly employs Computational Fluid Dynamics (CFD) for analysing transport processes encountered in industrial equipment and processes.

This course aims to complement the traditional analytical treatment of Transport Phenomena by introducing CFD as a learning and analysis tool. Students will simulate classical transport problems using ANSYS Fluent and compare the numerical predictions with available analytical or semi-analytical solutions. Emphasis will be placed on physical understanding of transport phenomena, model development, mesh generation, specification of boundary conditions, solution convergence, validation and interpretation of simulation results rather than on the mathematical formulation of CFD algorithms.

Upon successful completion of the course, students will be able to:

- Develop CFD models for classical Chemical Engineering transport problems.
- Generate suitable computational meshes and prescribe appropriate boundary conditions.
- Simulate momentum, heat and mass transfer using ANSYS Fluent.
- Validate CFD predictions against analytical solutions and established correlations.
- Critically interpret simulation results and apply CFD as an engineering tool for solving transport problems encountered in Chemical Engineering practice.

B) Contents (*preferably in the form of 5 to 10 broad titles)*:

1. Introduction to CFD in Chemical Engineering (2 Lectures)
   - Governing equations of transport
   - CFD workflow
   - ANSYS Fluent environment
2. Geometry, Mesh Generation and Boundary Conditions (4 Lectures)
   - Computational domain
   - Mesh generation and quality
   - Boundary conditions
   - Grid independence
   - Convergence criteria
   - Mesh independence
   - Comparison with analytical solutions
   - Interpretation of CFD results

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3. Simulation of Momentum Transport (4 Lectures)
   - Laminar pipe flow; Start-up flow (isothermal)
   - Flow through porous and packed beds
4. Simulation of Heat Transfer (5 Lectures)
   - Constant wall temperature
   - Constant wall heat flux
   - Brinkman problem (viscous heating)
   - Natural convection in a liquid storage tank with/without external heating
5. Simulation of Mass Transfer (8 Lectures)
   - Species transport in channels or tubes with catalytic/non-catalytic reactions (homogenous and heterogeneous)
   - Mass transfer in packed beds with/without chemical reactions
   - Hydrogen storage systems with/without mechanical stresses in walls.
   - Abrupt liquid-gas (NH_3/SO_2) 2-phase release from a storage tank or vessel.
   - Coupled heat and mass transfer in a CVD reactor
6. Simulation of Electrochemical Systems (5 Lectures)
   - Species transport in a fuel cell
   - Species transport in a microbial fuel cell

C) Pre-requisites, if any: ChE 611 (Transport Phenomena)

D) Short summary for including in the Courses of Study Booklet:
Develop CFD models for classical Chemical Engineering transport problems; Generate suitable computational meshes and prescribe appropriate boundary conditions; Simulate momentum, heat and mass transfer using ANSYS Fluent: Validate CFD predictions against analytical solutions and established correlations; Critically interpret simulation results and apply CFD as an engineering tool for solving transport problems encountered in Chemical Engineering practice.

7. Recommended books:

Textbooks**:** 1. Bird, Stewart and Lightfoot, Transport Phenomena, Wiley. 2. Deen, Analysis of Transport Phenomena, Oxford University Press. 3. Versteeg and Malalasekera, An Introduction to Computational Fluid Dynamics: The Finite Volume Method.

Reference Books: ANSYS Fluent User's Guide and Theory Guide.

8. Any other remarks: All CFD simulations will be performed by the students on their personal laptop, or PCs available and free to use in their research laboratories. Fluent Ansys license is available from the Institute (CC).

Dated: July 13, 2026 Proposer: Prof. Nishith Verma

Dated: Jul 13, 2026 DUGC/DPGC Convener:

The course is approved / not approved

Chairman, SUGC/SPGC

Dated:_____