Course Chemical Process Modeling

Basic Information

Course «Chemical Process Modeling» will provide you with the advanced knowledge and skills to training in use of modelling and simulation approaches, and their application to practical problems of relevance to chemical and refinery industries.

This is a course, which contributes to MSc award in Petroleum Chemistry and Refining

Title of the Academic Program	Master's Degree Programs in English "Petroleum Chemistry and Refining"
Type of the course	core /mandatory
Course period	From December 1st till December 31st, 1 semester (5 weeks)
Study credits	4 ECTS credits
Duration	144 hours
Language of instruction	English
Academic requirements	– BSc degree in Petroleum Engineering, Engineering, Chemistry , , Environmental Sciences or equivalent (transcript of records), – good command of English (certificate or other official document)

Course Description

The course of «Chemical Process Modeling» provided a curriculum of master's program 04.04.01.10 «Petroleum chemistry and refining».

Chemical Process Modeling considers a systematic approach to the creation of information systems of modeling and design of complex chemical-technological processes. The students are introduced to the methods of computer simulation of engineering systems as used within the chemical and refinery industry, for the prediction of the (steady-state) behavior and performance of various technology processes such as separation processes, heat transfer and chemical conversions.

Special Features of the Course (module)

Chemical Process Modeling deals with the overall system behavior and how the individual units should be combined to achieve optimal overall performance. Important topics are multi-scale process modelling, operation and control, design and synthesis, simulation, statistics and optimization.

The course covers the application parts in various core chemical engineering courses such as chemical engineering thermodynamics, fluid mechanics, material and energy balances, mass transfer operations, reactor design, computer applications in chemical engineering,

Mastering of this course will be useful in master thesis and for industrial applications in a variety of fields, including oil and gas production, refining, chemical and petrochemical processes.

In addition, this course uses the advanced practices of "interactive learning" through computer-based simulation exercises with the use of mathematical and chemical engineering CAD software's such as Excel, Mathcad, Matlab, Aspen tech etc.

Course Aim

- To provide a systematic introduction to the concepts, principles, methods, and related software tools for mathematical modelling and simulation of chemical process systems;
- To improve and expand chemistry and chemical engineering knowledge;
- To learn to use soft wares to engineering calculations.

Course Objectives

- To study the types of various mathematical models of engineering processes;
- To provide an overview of the possibilities of process simulation as a tool for computer systems analysis, which minimizes risks and costs in experimentation.
- To familiarise students with the techniques of modeling of engineering processes and of the developed models optimization;
- To introduce students to different commercial softwares to simulate the chemical processes from the design stage to the control and optimization;
- To provide the background needed by the chemical engineers to carry out computer-aided analyses of large-scale chemical processes.

Learning Outcomes of the Course

By the end of the course, students will be able to:

- To calculate the different physicochemical and thermodynamic properties chemicals;

- To understand the physico-chemical laws of Oil & Gas processing operations: flash separation, compression, expansion, heating or cooling, mixing, pumping, etc.;
- To describe chemical engineering processes in mathematical form and create simulation models of various types;
- To apply simulation techniques to solve complex system issues and to select feasible, if not optimum, solutions and configurations amongst competing designs;
- To implement optimization process and chemicals.

Teaching and Learning Methods

The course includes lectures and hands-on computer works in a computer laboratory of «General chair of chemistry and technology of natural energy resources and carbon materials» with the use of engineering CAD software's such as Mathcad, Matlab, Aspen Plus, Hysys, etc.

Each topic starts with a description of the physical problem in general terms. Then those general terms are put into a mathematical context so the student can to process the data using computer technologies. Next, the course covers several examples in which typical problems are solved, providing step-by-step instructions. Sometimes, the same problem is solved using different programs for demonstration the advantages of each program.

Course (module) Structure

Learning Activities	**Hours**
Lectures	10
Practice sessions / Seminars,	26
Self-study Assignments	72
Final Exam (including preparation)	36
Total study hours	**144**

Course Outline

Week	Lectures	Practice sessions / Seminars	Assignments	Hours[1]
Topic / Course Chapter 1 « Basics of modeling and simulation chemical engineering processes»				
1	Lecture No 1: Simulation methods of physical and mathematical modeling. Analytic and Empirical Methods for modeling process. The main types of mathematical models of chemical processes. Steps in model building	Lab No 1: Introduction to Softwares to model chemical engineering processes	Home assignment No 1; Test No 1	16
Topic / Course Chapter 2 « Fundamental laws for modeling chemical engineering processes»				
1-2	Lecture No 2: Continuity Equations. Energy Equation. Equations of Motion. Transport Equations. Equations of State Equilibrium. Chemical Kinetics Problems.	Lab No 2: Solving equations of state using computer programs; Lab No 3: Calculation of physical properties of matter; Lab No 4: Solution equations of vapor- liquid equilibria using computer programs	Home assignment No 2; Test No 2	20
Topic / Course Chapter 3 «Modeling of separation processes»				
2-3	Lecture No 3: Mass transfer models: such as liquid-liquid extraction, distillation, multicomponent separation, multicomponent steam distillation, absorption, steady state gas absorption with heat	Lab No 5: Simulation of technological schemes of compressor and gas turbine ; Lab No 6: The model of the evaporator; Lab No 7: Building a model of the regeneration column;	Home assignment No 3; Test No 3	22

[1] Hours designed for Classroom sessions, Web-sessions, Home Assignments etc.

	effects, evaporator. The main steps in model building of separation equipment	Lab No 8: Multicomponent distillation with shortcut methods		
Topic / Course Chapter 4 « Modeling of heat transfer processes »				
3-4	Lecture No 4: Major types of available heat-exchange equipment. Boilers and Condensers. Shell-and-tube heat exchangers. Required Heat Duty. Heat Transfer Coefficients. The main steps in model building of heat-exchange equipment	Lab No 9: Building a model of the Boiler; Lab No 10: Building a model of the Condenser	Home assignment No 4; Test No 4	18
Topic / Course Chapter 5 «Modeling of chemical reactors »				
4-5	Lecture No 5: Chemical reactions. Reaction stoichiometry. Direction of a reaction. Entropy, Enthalpy and Gibbs free energy of reaction system. Chemical reactions and equilibrium. Equilibrium constant (K). Activities. Laws of Mass Action. The Temperature Dependence of K (van’t Hoff Eq.). Reaction Rate. Type of Reactors: Batch Reactor, Continuous Stirred-Tank Reactor (CSTR), Plug Flow Reactor (PFR). Basic Mole Balance for different chemical reactors. Principles of reactor modelling	Lab No 11: Modelling and optimization of the Gibbs reactor Lab No 12: Modelling and optimization of the plug-flow reactor; Lab No 13: Modelling and optimization of the continuous-stirred tank reactor	Home assignment No 5 Test No 5 Final test	32
5	**Final Exam**			**36**

Course Instructor(s) and Tutor(s), Contact information

Nina V. Deryagina

Senior Lecturer at School of Petroleum and Natural Gas Engineering, Siberian Federal University

(room 315) 82/6, Svobodny prospect, Krasnoyarsk, Russia.

Tel: +7(391) 2-062-879; +7 (923) 306-97-79

E-mail: NGavgolenko@sfu-kras.ru

Assessment

Grade policy for both home assignments and the final exam is:

- A (excellent work) 91–100 points
- B (above average work) 81–90 points
- C (average work) 71–80 points
- D (below average work) 50–70 points
- F (failed work) < 50 points

Students are assessed by results of practical laboratory work, tests, and a final exam. Progress assessment:

- 25% home assignments;
- 25% reports of the laboratory work;
- 25% intermediate test
- 25% written examination

Students should be able to:

- describe model's classification, model properties and suggest modeling tools for individual case (50 points maximum);
- write an answer on 2 questions: to use balance laws and thermodynamics to formulate simple models for process systems; to use kinematics and kinetics to write down equations of motion for simple processes (50 points maximum).

Attendance Policy

Students are expected to attend and participate in classes and should notify lecturer of excused absences in advance, where possible. Students who have an excused absence are expected to make arrangements with lecturer for alternative assignment.

Every topic has a home assignment work that should be done. The final mark will be made by the same grade policy as for a final exam.

Web page of the course

The webpage of the course _ https://e.sfu-kras.ru/course/view.php?id=8586 is available through E-learning SibFU web site: www.e.sfu-kras.ru. You must be logged in to access this course. Course Guide and all accompanying materials are also available at the course web-page.

Core reading

The main book for this course is Modeling and simulation of catalytic reactors for petroleum refining by J. Ancheyta. It contains all information that is required for study in a more extensive manner. It will help students to reach a deeper understanding of modeling engineering processes.

The book Handbook of Petroleum Processing Steven A. Treese, Peter R. et al is also recommended for studying the basic petroleum chemistry that will be used during the course.

Almost all Labs include the column apparatuses modeling (the main devices for separation and chemical processes realization in petroleum industry). The book Modeling of Column Apparatus Processes will be extremely helpful in order to understand the essence of distillation column work mode.

Facilities, Equipment and Software

The implementation of the course provides for the availability of lecture rooms, as well as a computer class (personal computers, printers, copier, projector, demonstration materials) with access to webpages of the E-learning SibFU through web site: www.e.sfu-kras.ru.

The training process for this course uses standard Microsoft Office programs and specialized software MathCAD, Matlab, Aspen Tech.