Product and Process Design Courses

Department of Chemical & Biochemical Engineering

Technical University of Denmark

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Process design: Principles & methods

MSc-level course

10 ECTS points course

14 weeks course; 8 hours per week plus additional time in working on the process design project

More information (lecture slides, exercise problems, etc., can be obtained from Rafiqul Gani (rag@kt.dtu.dk)

Course 28350 (Spring 2010)
Process Design: Principles and Methods
(Chemical and Bio-chemical)

Textbook: Systematic *Methods of Chemical Process Design (Biegler, Grossmann & Westerberg)* plus **Notes**

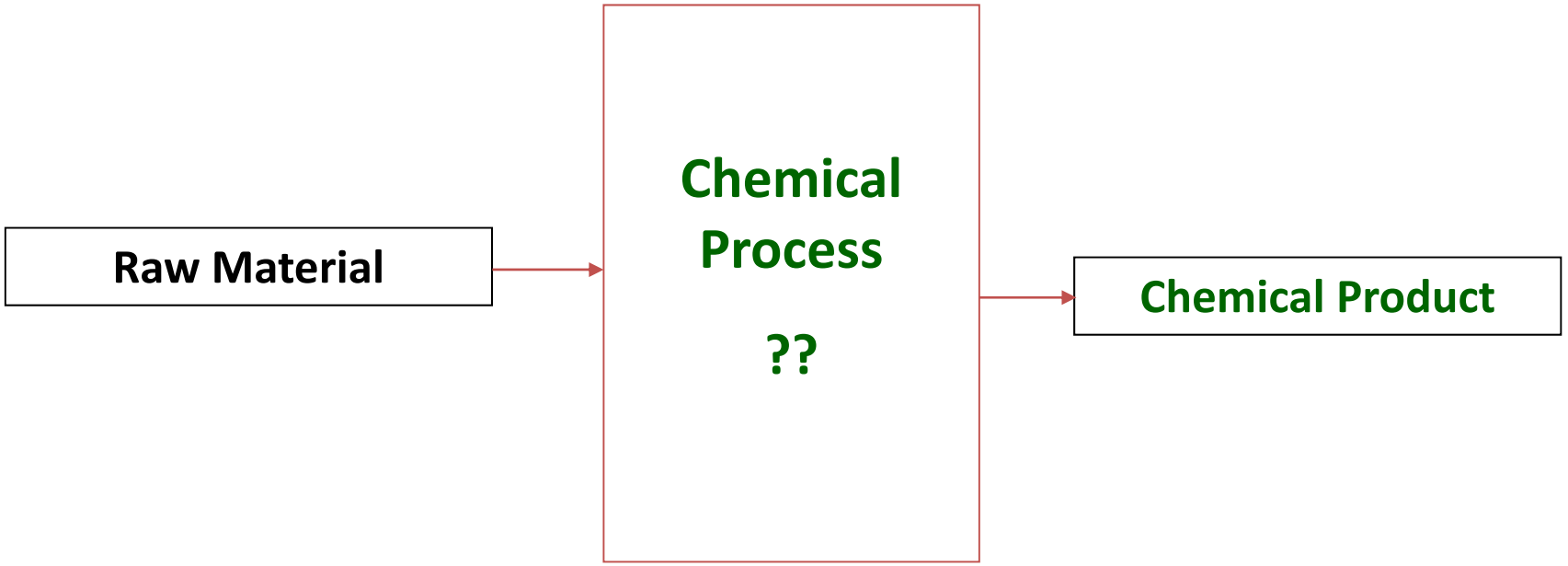
Lecture Plan: 12 lecture periods (4 hours per week) plus tutorials and exercises (4 hours per week) covering a 14-week period (February-May)

Exam: Design project report, oral presentation of the design project, and 3 exam problems

Design Project: Design project is given at the start of the course and must be delivered on or before the specified deadline (last day of the course)

Grading: Based on submitted design project report, exam problems, and oral presentation of the design project (7-scale system)

Definition of Chemical Process Design



Chemical process design is about finding a sustainable process that can convert the raw materials to the desired chemical products

Sustainable: Economic, low environmental impact, low waste, efficient operation, correct raw material, …..

Chemical Process Design: Important Issues

- **Process design is about making design decisions (which decisions, when & how?), verifying if they are acceptable, and if not, improve the design with better decisions**
- **The process design problem starts with the identification of a chemical product that needs to be made from a selected raw material**
- **Process simulators should not be used for blind trial and error but for fast evaluation of design decisions**
- **Process design is iterative by nature but if a systematic procedure is followed, better results can be obtained faster**
- **Use everything (knowledge) that has been learnt from other courses**

Methods & tools used: Conceptual design methods; ICAS, PROII; .....

Chemical Process Design: Organization of the work

Process design work is divided into 12 hierarchical tasksand the students are encouraged to follow the tasks.

The lectures are organized to highlight the tasks and how to perform them.

The students are encouragced to make partial reports for each task and later combine them to form the full design project report.

Students work in groups of 2-3 and are encouraged to follow a strict time-table.

Process Design Tasks 1-6

- **Task 1**: Collect information about the product and the raw materials that could be used to make it
- **Task 2**: Collect information on the path to convert the raw material to the desired product (that is, an idea of the process)
- **Task 3**: Generate (and/or select) preliminary process flowsheet
- **Task 4**: Decide process conditions (such as reaction conversion, separation factor, purge, etc.) and perform a preliminary mass balance on the selected flowsheet
- **Task 5**: Based on the results from above, set temperatures and pressures on the process flowsheet
- **Task 6**: Based on the results from above, perform a preliminary mass & energy balance

Process Design Tasks 7-12

- **Task 7**: Perform detailed process simulation – convert each of the simple models with the more rigorous option, one at a time, until all simple models have been converted.
- **Task 8**: Based on the simulation results from task 7, perform equipment sizing and costing calculations
- **Task 9**: Based on the results from tasks 1-8, perform an economic evaluation, using the current design as the "base case"
- **Task 10**: Investigate if opportunities for heat and mass transfer exist. If yes, apply them and check by how much the cost of operation can be further reduced?
- **Task 11**: Perform environmental impact analysis
- **Task 12**: Investigate how the current design can be further improved by formulating & solving an appropriate process optimization problem

Computer Aided Chemical Product Design

MSc-level course

7.5 ECTS points course

14 weeks course; 4 hours per week; case study approach using computer aided methods & tools

More information (lecture slides, exercise problems, etc., can be obtained from Rafiqul Gani (rag@kt.dtu.dk)

Special PhD-Course (also taken as a special course at MSc-level): Computer-Aided Chemical Product Design

- 2 weeks intensive course based on the case study approach (plus exam problem for another two weeks)
- Course involves lectures and tutorials
- Methods and tools needed to solve some features of chemicals based product design problems are highlighted through case studies
- Exam problems cover similar products discussed in the case studies
- 7.5 ECTS points
- Grading: Based on submission of report of exam problems
- Time: January-February 2011
- To be given by Prof Rafiqul Gani, DTU-Chemical Engineering

Special PhD-Course: Computer-Aided Chemical Product Design

Part I

- Molecular design (**solvents, refrigerants, process fluids, ...**) – CAMD
- Binary mixtures (**solvent mixtures, non-azeotropes; azeotropes; ....**) – CAMD
- Polymer design (**repeat unit design**) – CAMD
- Active Ingredient (**backbone**) design – ProPred, CAMD, Database

Part II

- Mixture (**blend**) design – graphical method and mixture design tool
- Product performance verification (**controlled release, AI-uptake, ...**) – CAMD, MoT, Virtual Product-Process Design
- Formulation design (**virtual experiments**) – vPPD-lab
- Integrated product-process design – PropRed, CAMD, ICAS, Database

Two MSc-level courses were presented in this lecture (process design & computer aided product design)

- **Courses on process control, introduction to product and process design and hazards-safety are also given at the BSc- & MSc-levels**

- **Courses on computer-aided modelling, modelling under uncertainty, process-tools integration, and, advances in PSE are also given at PhD-level**