Course XXXXX

Process Design: Principles and Methods (Chemical and Bio-chemical)

Course Plan: 2017

Lecture Plan:	12 lectures (see appendix 2 for lecture schedule) plus tutorials and exercises (can be given in 2 weeks intensive, 6 weeks or 12 weeks). Lecture: 12 lectures on specified dates from 08.30 – 11:40 (see lecture schedule) Tutorial: Every afternoon after the morning lectures from 13:30 – 17:00
Exam:	Submission of design project, presentation of design project in a seminar and 3 take-home exam problems
Design Project:	Design project will be given at the start of the course and must be delivered on or before the specified deadline
Grading:	Based on submitted design project, exam problems, and oral presentation of the design project
Teachers:	Professor Rafiqul Gani (responsible teacher)

Textbook:

Lorenze T. Biegler, Ignacio E. Grossmann and Arthur W. Westerberg: Systematic *Methods of Chemical Process Design*, Prentice Hall, 1997.

Other Useful Books:

Warren D. Seider, J. D. Seader, Daniel R. Lewin, *Process Design Principles: Synthesis, Analysis and Evaluation*, John Wiley & Sons Ltd, 2004 (edited copies of 4^{th} Edition in print will be supplied)

Max S. Peters and Klaus D. Timmerhaus, *Plant Design and Economics for Chemical Engineers*, 4th Edition, McGraw-Hill, 2003.

Robin Smith, *Chemical Process Design and Integration*, John Wiley & Sons, Ltd, 2005.

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Appendix 1

Textbook:

Lorenze T. Biegler, Ignacio E. Grossmann and Arthur W. Westerberg: Systematic *Methods of Chemical Process Design*, Prentice Hall, 1997.

Other Useful Books:

Warren D. Seider, J. D. Seader, Daniel R. Lewin, S. Widegado, Rafiqul Gani, Ka M. Ng *Process Design Principles: Synthesis, Analysis and Evaluation*, John Wiley & Sons Ltd, 2016 (4th Edition). Electronic version now available in online bookshops.

Max S. Peters and Klaus D. Timmerhaus, *Plant Design and Economics for Chemical Engineers*, 4th Edition, McGraw-Hill, 2010.

Robin Smith, *Chemical Process Design and Integration*, John Wiley & Sons, Ltd, 2005.

Design Concept

Process design involves the solution of open-ended problems. The design problem is first defined and then broken down into a set of sub-problems (tasks) that are solved in a specified sequence. In each task, a set of design decisions are made, analyzed and verified. Therefore, the final process design and the path to achieve it depend on the design decisions taken in each of the design tasks. This means that there could be many process designs for the defined design problem.

In this course, the process design problem solution is broken down into 12 design tasks, to be performed in a specific sequence. The design tasks and the sequence in which they are to be performed have been developed through a combination of experience, process (design) insights and the use of a systems approach to manage the complexity of the problem (managing data from different sources, different models, and different software tools).

A brief overview of the design tasks are given below. A more detailed list can be found in the "process design document" that will be supplied during the first week of the course.

• Task 1: Identify (through a search of publicly available information) details about your chemical product. Collect useful information about your product – for example, why is the product important? What are its uses? What are its characteristic properties? Who are the biggest producers? See also chapter 1 of textbook plus the supplied notes (if any given).

• Task 2: Collect as much information you can find for the process you have chosen (based on the reaction steps) to make your product. You need to decide about the additional details of the raw material (that should be used) and the product quality – check also the process design document for additional (specified) details about the product and the raw material. See also chapter 2 plus notes.

• Task 3: Use the hierarchical method for process synthesis to complete the preliminary details of your process flowsheet. You may also use this method to verify that the process flowsheet you have selected from publicly available information satisfies the rules given in the hierarchical method for process synthesis. See also chapter 2.

• Task 4: Perform a mass balance on the process flowsheet you have selected and verified in Task 3. Note that before you can complete a mass balance, you will need to make a number of design decisions and you will need a model for performing mass balance calculations (you can develop the model yourself and/or you can use a process simulator). Use the process simulation results to verify your design decisions. See chapter 3 plus notes on PROII, the commercial process simulator that will be used in this course.

• Task 5: Using the results of task 4 as the basis, make decisions on the process stream conditions. For example, decide about the state (vapor or liquid or solid or some combination of them) of the stream, the pressure and/or temperature. Verify the design decisions using calculations and/or analysis. See chapter 3 plus notes.

• Task 6: Using the results from task 5 as the basis, perform mass and energy balances using the simple process model from task 4, but now expanded to cover mass and energy balances. Determine the heat added or removed from each unit operation, which will again verify if your earlier design decisions are acceptable.

• Task 7: Replace each of the component stream calculator (used to model a separation unit) with their corresponding rigorous model, one at a time, and perform the mass and energy balances for the total process flowsheet using the PROII simulator. See chapters 3, 7-8.

• Task 8: Using the results from Task 7, perform equipment sizing and costing calculations for all equipment in the process flowsheet. See also chapter 4. A number of new design decisions need to be taken here. The sizing and costing values will indicate if the earlier decisions need to be changed, and previous steps (tasks) need to be repeated.

• Task 9: Using the results from Task 8, perform an economic evaluation of the design process. Here you will need to use data you collected before on costs, as well as new data that will need to be obtained. The results will indicate if the decisions taken previously are still reasonable. If yes, then you have an acceptable "base case" design. See chapter 5 plus notes.

• Task10: Investigate if the base case design at the end of Task-9 can be further improved. Formulate a process optimization problem to improve the profit further. Analyze the process carefully to target the part of the process where the largest improvement can be achieved.

• Task11: Using the results of Task 10, investigate if opportunities for heat and mass integration exist. If yes, apply them. This will reduce the operating (manufacturing) cost and therefore, the process economics will improve. See chapters 10 & 16. Note – tasks 10 and 11 can be interchanged.

• Task 12: Using the updated process (design) flowsheet from Tasks 10-11 as the basis, perform environmental impact and sustainability calculations to verify if your design decisions are also acceptable from an environmental point of view. See supplied notes for environmental impact analysis.

Tasks 1-7 should be finished by 40% of the course time

Important Issues to Note

Process design means making design decisions to generate process flowsheet alternatives that satisfy the given process specifications.

The design decisions (reactor conversion, separation factors, equipment type, stream state, etc.) are based on theory, knowledge, rules, heuristics, and experience.

Process simulators are only used to verify/validate decisions/design and not to make the design decisions by trial and error by performing blind simulations.

Design decisions are made considering the potential environmental impact and sustainability or “green” engineering issues.

Software will be used to help generate information (data) so that design decisions can be made (for example, if the stream should be a saturated liquid, what is the temperature at a selected pressure?).

Software will be used to perform some equipment design calculations (distillation, flash, crystallizer, heat exchangers, reactors, ….) – it will be up to the individual group members to decide if they want to use the software. Also, to perform mass and energy balances, use of an appropriate solver will reduce the time and resources.

Software will be used for environmental impact calculations.

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<u>Appendix 2: Lecture (Tuesday 08.30-12.00) & Tutorial (Friday 13.00 – 17.00)</u>

Lecture	**Date**	**Topic**	**Remarks**	
1		Introduction to chemical- & bio-process design (chapter 1 + notes) plus review of property estimation; also concept of "Green Engineering" *Overview of chemical and biochemical process design needs to be given* *This will be introduction to chemical (and bio-chemical) process design with additional comments on Green Engineering" issues and "Sustainability" issues.*	Highlight design tasks 1-12	RaG
		Introduction to course software; Design project (Tasks 1-2)	ICAS & PROII	RaG
2		Process Flow Diagrams – Synthesis (generation of process flowsheet) (chapter 2 + notes) *This lecture will cover mainly topics on how to generate a chemical (and bio) process flowsheet? It will be mainly the downstream separations that are needed after the reactor and the recycle of the unreacted material (which usually is not important for bio-processes)* *For chemical process flowsheet synthesis, chapter 2 + my notes cover the topic.* *For bio-process flowsheet generation, additional notes will be supplied*	Lecture plus Exercise	RaG
		Design project tasks 1-3; software training	Tutorial	RaG

3		Mass balance (chapter 3, 7, 8) *Special features for bioprocesses needs to be given* *This is simple mass balance for the generated flowsheet. Because the problem is large, hand calculations are not feasible. The lecture will cover on how to set-up the simple mass balance models, perform flowsheet decomposition and select solution strategy*	Lecture plus exercise (highlight design task 4)	RaG
		Design project task 4: Mass balance for the process	Tutorial	RaG
4		Energy balance (chapter 3, 7, 8) plus property estimation (enthalpy, heat of reaction, …)	Lecture plus exercise (highlight design task 5-7)	RaG
		Design project tasks 5-7: Perform energy balance for the Process	Tutorial	
5		Reactor design, sizing, selection, …(notes + parts of chapter 4) *Cover chemical reactors and bio-reactors* *This is going to be more a review of reactor design, necessary for this course. Given the reaction that is going to take place and the kinetic model (if the reaction is kinetically controlled), it is necessary to decide on the temperature and pressure of the reactor (and therefore, calculate the conversion), select the reactor type (CSTR, plug flow, etc.) and then fix the important equipment size parameters (volume, area, length, etc.)*	Lecture plus exercise Exam problem 1	RaG/NN
		Design project tasks 7-8: Detailed reactor design and Sizing	Tutorial	

6		Separation process design, sizing, selection, …. (notes + parts of chapter 4, 7) *Include separation techniques typically used in bio-processes (chromatography, crystallization, centrifuge, …)* *This lecture will cover mainly the design issues related to the most common separation processes – flash tanks, evaporation/crystallization, distillation, absorption, …. The idea is that given the flowrates and compositions that have already been calculated from the simple mass balance,* *how can one design the corresponding separation process that will match the mass balance. For* *example, in a flash, one needs to find out the T and/or P, in a distillation column, the* *number of stages, reflux ratio, etc. In the case of solvent-based separation, selection of* *solvents is also important*	Lecture plus exercise (highlight design task 7-9)	RaG
		Design project tasks 7-8: Separation process design & Sizing	Tutorial	All
7		Design, sizing of pumps, compressors, heat exchangers, … (chapter 4 plus notes) *Once the reactors and separation units have been placed, the heating/cooling requirements as well as pressure (increase/decrease) requirements are established. Therefore, based on this data, the heat exchangers, pumps, refrigeration cycles, etc., can be design. (chapter 4 of the textbook plus notes can provide a good background).* Plus Lecture on costing& economic analysis (chapter 5)	Lecture plus exercise As notes for heat exchanger calculations, the book by Peters & Timmerhaus to be used	RaG
		Design project tasks 7-9: Miscellaneous equipment design & sizing	Tutorial	

8		Process Flowsheet Optimization (chapter 9) *This lecture will give an overview of the non-linear optimization methods and show how process optimization problems are formulated and solved. (note that this is task 12)*	Lecture plus exercise Exam problem 2	RaG
		Design project tasks 7-9: Costing & economic evaluation	Tutorial	
9		Heat/mass integration (chapter 10 plus notes) *For bio-processes, mass integration would be more useful.* *At this moment, the process flowsheet will be known together with all the equipment and their design.* *Therefore, economic analysis can be performed and based on these first estimations, opportunities for operating cost reduction can be evaluated through heat integration.*	Lecture plus exercise	RaG
		Design project tasks 7-10: Opportunities for heat/mass integration	Tutorial	
10		Synthesis of HEX Networks (chapter 16) plus mass-exchange network *This lecture will cover more detailed heat integration using optimization techniques.*	Lecture plus numerical exercise Exam problem 3	RaG
		Design project tasks 7-11: Heat/mass integration	Tutorial	

11-12		Process analysis – environmental impact, sustainability, …. *This will be new topics related to methods used to calculate environmental impacts, sustainability indicators, etc. There are standard rules for them and notes will be supplied on how to calculate them. The objective would be to see that the environmental impacts are lower than the boundary value set by regulations and that the sustainability indicators are as low as possible.* Synthesis of Reactor Networks (chapter 13) *This lecture will cover some additional aspects of reactor design – attainable region, the network of reactors that can achieve this, etc.* *Bioreactors with multiple reactions will benefit from this chapter (own reading)*	Lecture plus exercise Numerical exercise	RaG
		Design project tasks 7-12: Perform environmental impact analysis and investigate how to improve the base case design – formulate & solve process optimization problems	Tutorial	
12		*Oral presentations*		
		Design project		

- Submission of the final design report: before the end of the course
- Date for oral presentation of design project (15 min presentation per group; each group consisting of maximum 2 students). All students will need to participate and each group will present their design project. Coffee/tea will be provided.
- Additional own reading: Chapters 7-8, 11, 14, and 17 (from textbook).