Course: Chemical Product Centric Sustainable Process Design

Objective

The objective of this graduate-level course is to give the participants a view of chemical product design and the important process design issues related to their development (product-centric sustainable process design). The course will highlight how to define the needs of a chemical product; how to identify the candidate chemicals and/or mixtures of chemicals and how to quickly evaluate the important process design issues so that decisions related to product development can be made in the early stages of product development. The objective is also to highlight the currently available methods and tools that can be applied to solve various types of problems associated with product-process design in a systematic and integrated manner. Different case studies will be used as application examples.

Background

In chemical product design and development, one first tries to find a candidate product that exhibits certain desirable or targeted behaviour and then tries to find a process that can manufacture it with the specified qualities. The candidate may be a single chemical, a mixture, or a formulation. For the later product type, additives are usually added to an identified active ingredient (molecule or mixture) to significantly enhance its desirable (target) properties. Examples of chemical products, such as functional chemicals (solvents, refrigerants, lubricants, etc.), agrochemicals (pesticides, insecticides, etc.), pharmaceuticals & drugs, cosmetics & personal care products, home and office products, etc., can be found everywhere. The workshop will only cover chemicals based products and cover issues related to their design, development (includes also process design) and analysis (product performance).

Even though it is possible to identify many chemicals or their formulations as potential chemical products, only a small percentage actually becomes one. Finding a suitable process that can sustainably (that is, reliably, efficiently and economically) manufacture the identified chemical with the desired product qualities as well as evaluating product performance during application and analyzing market trends play important roles in product design and development. From a process point of view there are products where the reliability of the quality of the manufactured chemical may be the deciding factor (for example, drugs & agrochemicals), while there are others where the cost of manufacturing the product is at least as important as the reliability of the product quality (solvents, refrigerants, lubricants). This means that product-centred sustainable process design is important because identifying a feasible chemical product is not enough. To make it sustainable, the process needs to be efficient, reliable, economically feasible and environmentally acceptable. Also, while in the case of functional chemicals, the identified molecule or mixture is the final product, in the case of chemicals based consumer products (drugs, cosmetics & personal care products, etc.), they are intermediate products from which the final products are obtained through additional processing. Therefore, the performance of the manufactured product, when applied, needs to be tested and validated. For some functional chemical products (such as solvents and

refrigerants) this may be straight forward, but for some consumer products (such as drugs and food-products), it may not be so straight forward.

Course Description

The course will introduce to the participants, the concepts involved and the methods and tools (including software) that can be used to obtain product centric sustainable process designs. These methods and tools assist the process engineers in the decision-making to generate, develop, evaluate and identify candidate products and their sustainable design alternatives in a systematic and efficient manner. In the tutorial sessions, participants will be introduced to specialized software such as ICAS, SustainPro and commercial process simulators (depending on availability).

The first day of the course will introduce the concepts (such as sustainability, driving force, reverse targeted design and product centric process design); definition and solution of a class of chemical product design problems; and definition and solution of targeted product centric process design problems. The second day of the course will introduce methods for sustainable process design and explain with examples, the main features of the sustainable process method; introduce the role of modeling in product-process design. The use of computer-aided tools to further improve (make more sustainable) and optimize the process design alternatives in terms of clean and energy efficient process design will be illustrated through examples.

References

- Achenie, L.E.K, Gani, R., Venkatasubramanian, V., 2003 "Computer-Aided Molecular Design: Theory and Practice", CACE-12, Elsevier, The Netherlands.
- Ng, K. M., Gani, R., Dam-Johansen, K., "Chemical Product Design: Toward a Perspective through Case Studies", CACE-23, Elsevier, The Netherlands.
- Carvalho, A., Gani, R., Matos**,** H**.,** 2008, Design of sustainable chemical processes: Systematic retrofit analysis generation and evaluation of alternatives, *Process Safety and Environmental Protection*, 86 (5), 328-346.
- Bek-Pedersen, E., Gani, R., 2004, Design and synthesis of distillation systems using a driving-force-based approach, *Chemical Engineering and Processing*, 43(3), 251-262.
- Jaksland, C. A., Gani, R., Lien, K. M., 1995, Separation process design and synthesis based on thermodynamic insights, *Chemical Engineering Science*, 50(3), 511-530.
- Tula, A K, Eden, M R, Gani, R, 2015, Process synthesis, design and analysis using a process-group contribution method, *Computers & Chemical Engineering*, 81, 245-259
- Zhang, L, Babi, D K, Gani R, 2016, New vistas in chemical product-process design, *Annual Review of Chemical and Biomolecular Engineering*, 7, 557-582
- Tula, A. K, Babi, D K, Bottlaender, J, Eden, M, Gani, R. 2017, A computer-aided tool for sustainable process synthesis-intensification, *Computers & Chemical Engineering*. 105, 74-95

Course Organizer & Contact

The course is organized by ???? (different location and organizer).

Course Schedule

Date	Time	Topic
(Day 1)	0800 – 0830	Welcome and introduction
	0830 – 0930	Definition of concepts (such as, chemical product design; sustainable process design; reverse design); Introduction to product centric process design; general problem definition & solution approaches - RaG
	0930-1000	Break
	1000 – 1230	Computer aided product (molecules & mixtures) design – RaG • Computer aided molecular design • Computer aided mixture (formulation) design • Introduction to ICAS software: Solvent, refrigerant and process fluid design (tutorial)
	1230 – 1400	Lunch
	1400 – 1700	Computer aided product (polymer; coatings) design – RaG • Polymer design • Solvent design • Case study (tutorial): polymer design, solvents for organic synthesis, formulations design
	16:45 – 1700	Review of day 1

Date	Time	Topic
	0800 – 0930	Introduction to sustainable process design - RaG
	0930-1000	Break
	1000-1230	Targeted reverse process design & concept of process group based flowsheet synthesis – AKT • Driving force based separation process design • Solvent-based environmentally acceptable process design Case study (tutorial): Application of the reverse design technique for sustainable process design (AKT)
	1230 – 1400	Lunch
	1400 – 1530	Introduction to Computer Aided Chemical Product Design, ProCAPD – RaG
	1530 - 1645	Introduction to computer aided sustainable process design – AKT
	1645 – 1700	Review of day 2 and final review of course

Course Lecturer

The course lecturers will be given by Dr Rafqul Gani (RaG) and Dr. Anjan K Tula (AKT)

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