

Forces Shaping the Future of Design and Design Education

Jeffrey J Siirola

Davidson School of Chemical Engineering, Purdue University, West Lafayette, Indiana, USA

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CHEMICAL PROCESS DESIGN

All ABET-accredited engineering programs mandate a culminating major design experience based on knowledge and skills acquired in earlier course work and incorporating realistic appropriate engineering standards and multiple realistic constraints. Some chemical companies organize their Manufacturing Innovation Process into a sequence of stages which typically include Need Identification, Product Design, Basic and Detailed Chemistry, Process Design, Equipment Design, Plant Design, Detailed Engineering and Vendor Specifications, Component Acquisition, Plant Construction Planning and Execution, Operating Procedure Development, Plant Commissioning and Start-up, and Production Planning, Scheduling, and Operation. Each of these stages involve the solution of many "design" problems that could be the subject of the culminating undergraduate chemical engineering design experience.

Most chemical engineering programs historically have chosen Process Design and Equipment Design for the capstone design experience as these aspects incorporate more of the science and engineering principles (mass and energy conservation, classical, solution, and reaction thermodynamics, transport phenomena, kinetics, separations, unit operations, control, safety, etc.) and computational tools (equation solvers, physical property prediction, process and fluid dynamics simulators, etc.) taught within undergraduate chemical engineering curricula. However, some programs have chosen instead a Product Design experience, especially if the product is itself a process (like an analytical instrument, oxygen concentrator, etc.) or if product fitness-for-use depends on its performance in a process (a solvent, mass separating agent, refrigerant, membrane, catalyst, etc.) or user experience (microstructured consumer products, etc.). Other aspects of the innovation process (e.g., Needs Identification, Basic and Detailed Chemistry, Plant De-

sign, Vendor Specification, Construction Planning, Operating Procedure Development, Production Planning and Scheduling, etc.), while certainly interesting, typically have not been used as the capstone design experience either because they require more specialized mathematics, chemistry, biology, materials science, etc. knowledge than most undergraduates are exposed to, or because they require prerequisite Process and Equipment Design.

Process Design at Purdue

At Purdue our chemical engineering senior design experience has focused on Conceptual Process Design and Economic Evaluation with some aspects of Plant Design, Plant Wide Control, and Process Safety. This includes Equipment Design at different levels of detail appropriate for conceptual economic evaluation and sometimes for vendor specification. Our subject processes may be of any scale, usually continuous but can be batch, and of a complexity that can be reasonably solved by teams of four or five students within one semester. We expect this course scope to continue into the future.

We teach a design paradigm (using terminology appropriate for Process Design, but applicable in general to many design problems within the innovation process) involving Formulation, Synthesis, Analysis, Evaluation, and Optimization.

As might be expected, we have a somewhat greater emphasis on Process Synthesis (generation of process flowsheet alternatives by identifying tasks required to achieve objectives, phenomena to be exploited to accomplish these tasks, equipment and utilities required to implement these tasks, and interconnections among those equipment) than most process design courses or textbooks. We describe three basic approaches to Process Synthesis: Evolutionary Modification (alteration of existing flowsheets), Superstructure Optimization (simultaneous selection of equipment, equipment interconnections, and operating conditions with a purported optimizing simulator), and Systematic Generation

(hierarchical specification of property difference resolving tasks between raw materials and desired products). We make a specific distinction between the Tasks that must be completed in a process and the Equipment in which these tasks will be accomplished. We teach both goal-oriented and constraint-oriented (largely the result of nonideal solution thermodynamics) strategies for identifying process tasks as well as patterns of interconnected tasks that have previously found applicability in specific situations, for example for breaking homogeneous and heterogeneous azeotropes. Our process design approach is specifically task-oriented rather than equipment-oriented. We further take the position that process designs have Primary Objectives (make the right stuff, in the right amount, fit for use - not too difficult; even a computer can do it) while at the same time optimizing as best as possible Secondary Objectives (economics, environmental impact, safety, controllability, sustainability, societal impact, etc. - the real challenge). We note that the relative importance of some of these secondary objectives are currently changing, and new emphasis especially on the environment is the principal challenge impacting the future of chemical process design.

Our approach to Process Analysis and Evaluation is fairly conventional, involving computer-simulation-assisted heat and material balancing about each proposed task in the synthesized flowsheet, choosing operating parameters and finding annual utility requirements and costs for each task, and flows and other properties of the interconnecting streams among the tasks to meet the Primary Design Objectives. Then an initial assumption is made that each task can be implemented in a single piece of equipment after which that equipment is designed at an appropriate conceptual level of detail using (sometimes computer-assisted) methods learned throughout the curriculum just sufficient to estimate a preliminary acquisition and installation cost. Then these equipment capital costs are combined with utility and other annual operating costs in an appropriate way to produce an economic Figure of Merit, initially simple Total Annual Cost (or Levelized Cost) and later Net Present Cost better accounting for variable cash flow timing and financing, depreciation, and income tax implications,

At this point we turn our attention to Optimization of the Secondary Design Objectives. Students first start with Design Heuristics (published results of previous equipment selection and parameter optimization experience) for example, best equipment type selection in particular situations, optimum approach temperatures, operating number of stages and reflux ratios, multistage compression pressure ratios, economic pipe velocities, etc. These will be starting points for more detailed model-based parameter optimizations with realistic objective functions typically economic considering both capital and annual operating costs, but other objectives including

improved safety or environmental impact minimization may also be appropriate. Preliminary safety studies such as Failure Modes and Effects Analysis are also performed early, especially since proposed response to identified critical issues may involve changes to the process structure or operating conditions.

In addition to Design Parameter Optimizations, we also consider what we call Structural Parameter Optimizations. These are based on consideration of some sixty thought-provoking ideas we have accumulated related to reaction path, input-output-recycle structure, heat and power management and thermodynamic efficiency (including heat and power integration algorithms and process condition adjustment to increase the opportunities for such integration), alteration of phase, solution, or reaction equilibria or rate- (and size-) determining mechanisms (classical process intensification), changing the order of tasks and the relationship between tasks and the equipment used to execute them (another form of process intensification), advantaged scale-up or scale-down, cost reduction, and improved safety, operability, controllability, and maintainability. This broader consideration of structural parameter optimization all involves synthesizing local alternatives (for example, a proposed heat integration, or compressor staging with intercoolers, or enhanced heat transfer device, or alternative solvent, or combined reaction and separation, etc.) with selection then based on capital and operating cost economic evaluation or other appropriate criteria. Finally, development of equipment layout, plot plans, and a plant-wide control strategy complete our process design approach. Although not required for conceptual capital cost estimation and more appropriate for vendor specification, sometimes more detailed design of selected equipment such as shell-and-tube heat exchangers or distillation columns using more of the methods described in textbooks and handbooks is performed for the learning experience.

WHAT IS CHANGING

Not too long ago, after not discovering any new large oil or gas fields for a few decades, there was prediction of "peak oil" and a time when we would run out of finite fossil reserves not only for fuels but also as organic chemical industry feedstocks exacerbated by higher prices as worldwide demand approached known productive capacity. While some suggested a return to coal (whose reserves appeared to be an order of magnitude greater than those of oil and gas), others advocated a switch to "renewable" (recently alive biological) feedstocks ultimately derived from continuing photosynthesis. As these renewable materials, for example cellulose, starch, lignin, triglycerides, etc., are compositionally different from traditional coal, petroleum, or natural gas, it was thought that entirely new processes would need to

be developed, or entirely new products more appropriate to renewable raw materials would need to be developed to meet society's needs (especially for fuels, but other products as well). As these renewable raw materials were created by biological reactions, it was assumed that biological reactions may also be important in their transformation to products. As a result, biochemistry was added to the scientific foundation in many chemical engineering curricula and fermentation was added to the list of unit operations studied. While the process design paradigm remained applicable essentially unchanged, the chemistries and products to which it could be applied in practice and in the classroom were significantly expanded.

Then, with the successful development of directional drilling, logging-while-drilling, slickwater hydraulic fracturing, and microseismic monitoring technologies to extract fossil hydrocarbons from impermeable shale formations, shale resources became included within exploitable reserves expanding them to more than a century of projected demand. Peak oil never happened, and prices fell (and in the case of natural gas, to half its historical ratio compared to oil). Access to hydrocarbon feedstocks for both fuels and chemicals no longer appears to be an immediate problem.

Carbon Dioxide Emissions

However, continued emission of carbon dioxide to the atmosphere is. These emissions principally come from burning carbonaceous fuels for heating, power (electricity production), transportation, and from certain chemistries (notably the smelting of ores, limestone decomposition, and the production of hydrogen). These emissions are measurably increasing the concentration of CO₂ in the atmosphere which in turn is causing deleterious climate change. Carbon dioxide emissions, and not feedstock availability, is the real sustainability issue facing society in general and the processing industries in particular.

If the carbon source resulting in CO₂ emissions were biological ("renewable"), then some would consider such a process to be "carbon neutral" just recycling CO₂ back to where it came, although others would argue that such a process should not be considered carbon neutral until the biological feedstock is actually regrown.

If CO₂ emissions are from a stationary source like an electricity-producing power plant boiler, utility steam boiler, furnace, fired heater, lime kiln, etc., in principle they could be captured, separated from other things with which they may be admixed, and permanently sequestered from the atmosphere, for example by injection into a suitable capped porous geological formation, dissolution in a deep saline aquifer, or reaction with an appropriate alkaline geologic material such as basalt. This is not widely done at present, but to do so does not involve any new process design paradigm.

If CO₂ emissions are from a mobile source, carbon capture may not be practical. Either some other non-CO₂-emitting process must be used, or the emitted amount of CO₂ must be captured from the atmosphere (true for any CO₂-emitting process). CO₂ must also be captured from the atmosphere if it is desired to reduce atmospheric concentrations from existing levels.

Process Electrification

Since most CO₂ emissions are currently from the combustion of carbonaceous fuels for heat and power (space heating, industrial heating, electricity generation, and transportation), there is interest in substituting carbon-emissions-free electric power in as many of these applications as possible. Carbon-emissions-free electricity does exist from nuclear, hydroelectric, wind, photovoltaic, and geothermal sources (and stationary fossil-fired power plants might also be included if the resulting CO₂ were captured and sequestered). Electricity is already widely used for space heating and also increasingly for short distance transportation. Until now because of cost, electricity is not much used for heating in the process industries, with the exception of electric arc furnaces in steel production. That is about to change, and that will be one of the biggest factors affecting the future of the process industries.

Hydrogen

Hydrogen is a major chemical mostly used for desulfurization in petroleum refineries and for ammonia and methanol production. It is now also being considered as a carbon-emissions-free fuel for all sorts of heating applications in furnaces, for power production, and for transportation. Currently, hydrogen is usually made from high temperature endothermic steam reforming of a carbonaceous feedstock (methane, light naphtha, coal, etc.) resulting in significant CO₂ coproduction. Although not yet much practiced, this CO₂ could be captured and sequestered ("blue hydrogen"), or hydrogen could be made by water electrolysis with carbon-emissions-free electricity using a number of different electrolyzer technologies ("green hydrogen").

Direct Air Capture

If to offset CO₂ emissions to the atmosphere an equal amount of CO₂ is removed from the atmosphere (Direct Air Capture), then how should this CO₂ be captured, and what should be done with this captured atmospheric CO₂? Both biological (agricultural, silvicultural, aquicultural, etc.) and technical (absorption, adsorption, etc.) carbon capture processes are possible. Then after capture, this CO₂ could be sequestered or it could be converted into the very products that resulted in CO₂ emissions to the atmosphere, although this latter choice would generally involve chemical reduction, likely with carbon-emissions-free hydrogen (a new demand for

hydrogen).

THE FUTURE OF PROCESS DESIGN

What does all this likely mean for the future of process design?

First, many new processes, using new chemistries, and involving new raw materials (possibly biological where that may make sense) will be developed. But not necessarily any new theory of process design.

Second, energy will become more expensive (because of carbon capture and sequestration or CO₂ emissions avoidance). That may lead to even more consideration of energy-saving structural optimizations involving heat integration and process intensification. Even so, it is not necessarily certain that there will be a fundamental shift in the ratio of operating costs to capital costs, since historically as process energy costs have risen (for whatever reasons), so too soon thereafter have process capital costs (because energy is the major economic input in producing the material for process equipment).

Third, carbon-free electricity will replace fossil fuel combustion for space heating and short distance transportation throughout society. This will approximately double total electricity demand requiring a corresponding increase in total electrical generation and distribution capacity (with any fossil-fired capacity either retired or retrofitted with carbon capture and sequestration).

Fourth, the process industries will become electrified for heat as they already have increasingly become for work. Electric heating will be implemented in numerous ways including resistive heating, inductive heating, dielectric (microwave) heating, plasma heating, arc heating, etc. Much of this detail will be new to chemical process and equipment designers. Electricity may be used to boil steam (so that chemical processes heated by steam condensation remain unchanged), or to directly heat equipment (perhaps more precisely) including replacement of fired heaters and furnaces for temperatures greater than steam.

Fifth, chemical processes are unique in that many kinds of operations like distillation and absorption both require heat at higher temperature and reject nearly the same quantity of heat at lower temperature. These situations may be appropriate for electricity-powered heat pumps moving heat from the lower temperature source to the higher temperature requirement (generally more efficient than straight electrical heat itself) which heretofore have been practically limited to the distillation of close-boiling mixtures but whose applicability may be much expanded given CO₂ emission elimination considerations.

Sixth, hydrogen will be more in demand both as a chemical reducing agent and as a carbon-emissions-free fuel for both mobile and stationary applications. It remains to be seen whether that hydrogen is best

produced by carbon-free electrolysis or carbon-free electrically-powered carbon-captured fossil reforming.

Seventh, powerful oxidants oxygen and chlorine are already produced by electrically powered air separation and chloride electrooxidation. Reductant hydrogen will either be made by water electrolysis or electrically powered fossil reformation (with carbon capture). Given these reagents, it is not yet clear if chemical electrosynthesis will find other major advantaged applications.

While process design theory may not change, the future overarching emphasis on carbon dioxide emissions elimination, atmospheric CO₂ concentration reduction, and process electrification will have a significant impact on Structural Optimization objectives in addition to traditional economics, safety, waste minimization, and controllability. This inevitably will result in new and different process flowsheets, product costs different from current experience, and many new problems and case studies for undergraduate design courses. However, our students will be prepared and will be up to the challenge.

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