CACHE GUIDE TO TEACHING DESIGN WITH INTERNET LINKS

Paper for CACHE Learning Resource Center[1][2]
Edited by
Warren D. Seider, University of Pennsylvania
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ABSTRACT

This paper is intended to provide a framework of materials for teaching design available on the CACHE Learning Resource Center, an Internet web site (http://cache.org/teaching-resources-center). Guidance is provided for teaching product and process design, with Internet links to recommended materials from many sources including textbooks, monographs, completed design case studies, design problem statements, design software, POWER POINT lectures, and related materials prepared by design instructors[3]. Instructors are requested to make us aware of additional links.

The framework provides materials in several areas, with the area editor(s) in parentheses:

Product Design (Warren D. Seider)
Process Flowsheet Synthesis (Rafiqul Gani, Warren D. Seider)
Process Simulation (Chau-Chyun Chen, Warren D. Seider)
Process Integration (Mahmoud El-Halwagi)
Equipment Design (Gavin Towler)
Environment and Sustainability (David Shonnard)
Safety (Dan Crowl)
Optimization – Process Synthesis and Flowsheet Optimization (Lorenz T. Biegler and Ignacio Grossmann)
Process Modeling (Rafiqul Gani)
Design Case Studies and Design Problem Statements (Ignacio Grossmann, Joseph Shaeiwitz, Richard Turton)

The latest contributions from the area editors are presented in each section. This initial Guide is being installed on the CACHE Learning Resource Center website in August 2011. Note that some overlap exists among the sections; e.g., links to case studies appear in several sections.

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[1] Initially, this Guide is being prepared for instructors that use the CACHE Learning Resource Center. When completed, CACHE will notify ChE Department chairs and design instructors. As the article is completed, we will decide whether it can be adopted for *Chem. Eng. Educ.* and possibly for the broader *CEP* audience.
[2] To introduce this guide, a workshop has been proposed for the 2012 ASEE Summer School for ChE faculty.
[3] Also, eventually, the links may be organized to guide students and practitioners, in addition to design instructors, in finding Internet links to answer their questions and locating instructional materials in various areas. We may seek to translate common key words into more useful terms; e.g., “agitators” rather than “mixers” when carrying out equipment design.

Note, also, three additional sections are in preparation in the Batch Process Design, Computational Fluid Dynamics, and Energy areas.

INTRODUCTION

The principal objective of each section is to provide design instructors with Internet links to quality materials available for teaching product and process design in specific areas. Each area editor has prepared the text that introduces the links. In many cases, the text is organized into well-recognized sub-areas to assist instructors in locating materials more easily.

PRODUCT DESIGN (Warren Seider)

Innovation Map

When carrying out product design, it is important to link customer needs to various new technologies under development. For this purpose, it helps to prepare an *innovation map*, which is described and illustrated by:

Seider, W. D., J. D. Seader, D. R. Lewin, and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, 3rd Ed., Wiley 2009 – Chapter 1

http://www.wiley.com/WileyCDA/WileyTitle/productCd-EHEP000024.html

An example innovation map is illustrated for the design of a lab-on-a-chip for screening clopidogel resistance prior to coronary surgery - as shown on pages 4 and 5 of:

http://repository.upenn.edu/cgi/viewcontent.cgi?article=1009&context=cbe_sdr

Product Design Strategies

Often systematic strategies for designing new products are used in practice. These include the Stage-Gate Product Development Process (SGPDP), which is described and illustrated by:

Cooper, R. G., *Winning at New Products: Accelerating the Process from Idea to Finish*, 3rd Ed., Perseus Publ., Cambridge, MA, 2002.

http://www.stage-gate.net/pdi/pc/viewCategories.asp?idCategory=37

Cooper, R. G., *Product Leadership: Pathways to Profitable Innovation*, Basic Books, 2nd Ed., Cambridge, MA, 2004.

http://www.stage-gate.net/pdi/pc/viewCategories.asp?idCategory=36

Similar strategies are presented by:

Cussler, E. L., and G. D. Moggridge, *Chemical Product Design*, Second Edition, Cambridge University Press, 2011.

http://www.cambridge.org/gb/knowledge/isbn/item5979168/Chemical%20Product%20Design/?site_locale=en_GB

Wei, J., *Product Engineering*, Oxford University Press, 2007.

http://ukcatalogue.oup.com/product/9780195159172.do?keyword=Wei&sortby=bestMatches

Concept Stage: In this first stage of product design, it is important to obtain the voice-of-the-customer and to make technical specifications based upon perceived customer needs. Then, to satisfy these specifications, methods for generating ideas for new products are needed. These are illustrated for many potential products by:

Cussler, E. L., and G. D. Moggridge, *Chemical Product Design*, Second Edition, Cambridge University Press, 2011.

http://www.cambridge.org/gb/knowledge/isbn/item5979168/Chemical%20Product%20Design/?site_locale=en_GB

Given the most promising product concepts, a business case (using simple profitability measures) and of an intellectual property (IP) patent search are needed to assess the potential for product concept, as described by:

Seider, W. D., J. D. Seader, D. R. Lewin, and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, 3rd Ed., Wiley 2009 – Chapter 2

http://www.wiley.com/WileyCDA/WileyTitle/productCd-EHEP000024.html

Examples of the implementation of the concept stage can be found in the following product design case studies. These include:

> Software Product for the Design and Control of Deposition Reactors using Stochastic Models. This senior design study implemented kinetic Monte Carlo techniques to simulate deposition thickness and roughness. See:
>
> http://repository.upenn.edu/cgi/viewcontent.cgi?article=1007&context=cbe_sdr
>
> Software Product for Chemicals-based Liquid Formulation Design - The Virtual Product Process Design Lab (VPPDL). Examples covering the design of chemicals-based consumer products like hair-sprays and liquid insect repellents are available as case studies. See
>
> http://www.capec.kt.dtu.dk/documents/software/PPD-Lab_Formulation_Tutorials.pdf

Molecular Structure Design

Often molecular structure design is used to identify chemical products having the properties required by customers. This is often a key part of generating the most promising product concepts in the Concept Stage. Techniques for molecular structure design, with examples, are presented by:

> Wei, J., *Product Engineering*, Oxford University Press, 2007.
> http://ukcatalogue.oup.com/product/9780195159172.do?keyword=Wei&sortby=bestMatches
>
> Seider, W. D., J. D. Seader, D. R. Lewin, and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, 3rd Ed., Wiley 2009 – Chapter 3
> http://www.wiley.com/WileyCDA/WileyTitle/productCd-EHEP000024.html

Achenie, L. E. K., R. Gani, and V. Venkatsubramanian, Computer-Aided Molecular Design: Theory and Practice, Computer Aided Chemical Engineering, 12, 2003 http://www.elsevier.com/wps/find/bookdescription.cws_home/699785/description#description

Extensive teaching materials are available that use the ProCAMD software developed at the Denmark Technical University (DTU). ProCAMD carries out molecular structure design using the group-contribution concept and includes an extensive thermophysical property database and a large collection of property estimation methods. The user specifies the desired property values, with upper and lower bounds, and other desired properties (e.g., the candidate molecules should not form azeotropes with specified compounds and/or should be totally miscible with them). ProCAMD solves mixed-integer nonlinear programming problems using a decomposition-based solution approach to locate the candidate molecules. The teaching materials and software are available from Professor Rafiqul Gani. See:

<http://www.capec.kt.dtu.dk/documents/software/tutorials/chemical-product-design-tutorial-document-1.pdf> for integrated chemical product design

<http://www.capec.kt.dtu.dk/documents/software/tutorials/solvent-selection-cam10-2010.pdf> for solvent design and selection through CAMD

<http://www.capec.kt.dtu.dk/documents/software/tutorials/PPD-Lab_Formulation_Tutorials.pdf> for liquid formulation design

In addition, DTU provides teaching materials for the design of polymer repeat units that satisfy user specifications of properties such as the glass transition temperature, solubility parameters, refractive index, density, and viscosity. For this purpose, the ProPred software package has been created. These teaching materials and ProPred are available from Professor Rafiqul Gani:

<http://www.capec.kt.dtu.dk/documents/software/tutorials/Overview_of_ICAS.pdf> overview of ICAS (Integrated Computer Aided System) and its tools

http://www.capec.kt.dtu.dk/documents/software/tutorials/pure-prop-with-propred.pdf for pure component property prediction through ProPred http://www.capec.kt.dtu.dk/Software/ICAS-Tutorials/ICAS-Tutorials-Workshops

Product-Design Case Studies

Numerous product design case studies are available beginning with:

Cussler, E. L., and G. D. Moggridge, *Chemical Product Design*, Second Edition, Cambridge University Press, 2011.

http://www.cambridge.org/gb/knowledge/isbn/item5979168/Chemical%20Product%20Design/?site_locale=en_GB

Collections of case studies are presented in books, including:

Ng, K. M., R. Gani, and K. Dam-Johansen, *Chemical Product Design: Towards a Perspective Through Case Studies*, Elsevier, 2007.

http://www.elsevier.com/wps/find/bookdescription.cws_home/708653/description#description

Brockel, U., W. Meier, and G. Wagner, *Product Design and Engineering*, Vols. 1 and 2, Wiley VCH, 2007.

http://www.wiley.com/WileyCDA/WileyTitle/productCd-3527315292.html

Achenie, L. E. K., R. Gani, and V. Venkatsubramanian, Computer-Aided Molecular Design: Theory and Practice, Computer Aided Chemical Engineering, 12, 2003

http://www.elsevier.com/wps/find/bookdescription.cws_home/699785/description#description

Software for Product Design

As mentioned under Molecular Structure Design, the DTU packages, ProCAMD and ProPred, are available from Professor Rafiqul Gani:

http://www.capec.kt.dtu.dk/Software/ICAS-and-its-Tools/

http://www.capec.kt.dtu.dk/documents/software/tutorials/workshop-capec-2011-propred.pdf

A commercial package, SLEEK^{TM}, is provided by Clear Water Bay Technologies to construct phase diagrams for solid-liquid equilibria (SLE) by regressing experimental data. This package, which can be helpful in designing crystallization processes for generating solid products (e.g., pharmaceuticals), is described at:

http://www.cwbtech.com/SLEEK.html

Lecture – Tutorial Material (Workshops)

Lecture notes with worked-out examples are available at:

http://www.capec.kt.dtu.dk/Courses/Workshops/Workshop-on-Product-Design

PROCESS FLOWSHEET SYNTHESIS (Rafiqul Gani and Warren D. Seider)

When carrying out process design and/or simulation, an important first step is process flowsheet synthesis, also known as process flowsheeting. That is, given the raw materials and the product specifications, what is the process flowsheet that can convert the raw materials into the desired products? The process flowsheet provides the list of operations and the sequence in which they should be performed to obtain the final products. However, to perform process simulation, a minimum number of variables for each operation must also be specified; for example, the temperature and pressure in reactors; the number of stages, feed location, reflux ratio, and product recoveries in distillation columns; the outlet pressures in pumps; the outlet temperatures in heat exchangers, and many more. Therefore, process flowsheeting is closely linked with process design and process simulation. Also, process flowsheeting is closely linked with energy issues, water consumption, process economy, control-operability, and sustainability.

Methods to Generate and Evaluate the Process Flowsheet

One of the earliest strategies for process synthesis was introduced in the first textbook on process synthesis:

> Rudd, D. F., G. J. Powers, and J. J. Siirola, *Process Synthesis*, Prentice-Hall, 1973.
> http://books.google.com/books/about/Process_synthesis.html?id=89hkGwAACAAJ

To summarize, their five-step strategy involved:

1. Eliminating differences in molecular types – using chemical reaction operations
2. Distributing the chemicals by matching *sources* and *sinks* – using mixing operations
3. Eliminating differences in composition – using separation operations
4. Eliminating differences in temperature, pressure, and phase – using temperature, pressure, and phase change operations
5. Integrating tasks: that is, combining operations into unit processes

At each step, it is common to consider alternative operations, often using heuristics, that is, rules of thumb, to specify key variables; for example, temperatures, pressures, and flow ratios.

Such a strategy was utilized to synthesize a process to hydrodealkylate toluene to benzene in the classic textbook:

Douglas, J. M., *Conceptual Design of Chemical Processes*, McGraw-Hill, 1988.
http://books.google.com/books?id=M6JTAAAAMAAJ&source=gbs_similarbooks
also:
http://www.alibris.com/search/books/qwork/1268430/used/Conceptual%20Design%20of%20Chemical%20Processes

Subsequently, other design textbooks introduced similar examples. For the synthesis of a continuous process to manufacture vinyl-chloride monomer and a batch process to manufacture the pharmaceutical, tissue plasminogen activator (tPA), see:

Seider, W. D., J. D. Seader, D. R. Lewin, and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, 3rd Ed., Wiley 2009 – Chapter 4.
http://www.wiley.com/WileyCDA/WileyTitle/productCd-EHEP000024.html

Similarly, for the manufacture of vinyl-chloride monomer, see:

Peters, M. S., K. D. Timmerhaus, and R. E. West, *Plant Design and Economics for Chemical Engineers*, 5th Ed., McGraw-Hill, 2003 – Chapter 4.
http://highered.mcgraw-hill.com/sites/0072392665/

And, for the synthesis of a process to manufacture ethanol from ethylene, see:

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*. Prentice Hall, New Jersey (1997) – Section 2.4.
http://www.pearsonhighered.com/educator/product/Systematic-Methods-of-Chemical-Process-Design/9780134924229.page

Software

Few software packages are dedicated solely for process flowsheeting. Most are linked with process simulators. Several are listed below in various categories.

Process Flowsheeting

ICAS-CAPSS (for process flowsheeting using a combination of the hierarchical approach and thermodynamic insights)
http://www.capec.kt.dtu.dk/Software/ICAS-Tutorials/ICAS-Tutorials-Workshops

Expert system based flowsheet synthesis software called Prosyn ^{TM}. See:
http://www.process-design-center.com/2.1.1-technology.htm

Separation Process Synthesis

ICAS-PDS (for synthesis of separation processes based on vapor-liquid equilibrium)
http://www.capec.kt.dtu.dk/documents/software/tutorials/pds-manual.pdf

ICAS-PDS (for synthesis of reaction-separation systems)
http://www.capec.kt.dtu.dk/documents/software/tutorials/workshop-2011-pds.pdf

Conceptual Design of Distillation Systems by Michael F. Doherty and Michael F. Malone
http://www.mcgraw-hill.co.uk/html/0072488638.html

Heat-Exchange Networks

See the section on Process Integration.

Flowsheet Optimization

See the section on Optimization – Process Synthesis and Flowsheet Optimization

Lecture – Tutorial Material

Lecture notes with worked-out examples are available at:

http://www.capec.kt.dtu.dk/Courses/MSc-level-Courses/Computer-Aided-Process-Engineering-supplement-to-Course-28350-Process-Design2

PROCESS SIMULATION (Chau-Chyun Chen and Warren D. Seider)

The major process simulators, including ASPEN PLUS, Aspen HYSYS, UNISIM, CHEMCAD, and PRO/II, have materials to introduce chemical engineers to the basics of process simulation. Most design courses focus on the simulation of process flowsheets in the steady state, the subject of this first section. Because most instructors and students need guidance on the selection of estimation methods for thermophysical properties and the regression of physical property data, teaching materials for this purpose are introduced in a second brief subsection. For the past decade, most of the process simulation packages have the capability to perform dynamic simulations of process flowsheets including their control systems – see links to the teaching materials in the third subsection. Finally, teaching materials for specialized applications such as polymerization process simulation and the simulation of fossil energy conversion processes are presented in the fourth subsection.

To varying extents, process flowsheet simulation is included in the design textbooks – as virtually all process design courses involve student solutions using the process simulators, either to solve homework exercises or to carry out design projects. The textbooks have many examples and homework exercises – many of which are solved in their Solution Manuals.

Steady-State Process Simulation

An excellent source of introductory material on the usage of ASPEN PLUS for the solution of many kinds of process engineering problems is provided by Bruce Finlayson in his book: *Introduction to Chemical Engineering Computing*. Many simple examples are provided as well as Chapter 7 on Process Simulation and Appendix C, Hints When Using ASPEN PLUS. See:

> Finlayson, B. A., *Introduction to Chemical Engineering Computing*, Wiley, 2006.
> http://www.wiley.com/WileyCDA/WileyTitle/productCd-0471740624.html

Since 1994, teaching materials for ASPEN PLUS and HYSYS have been prepared at the Technion and the Univ. of Pennsylvania. These have been titled *Using Process Simulators in Chemical Engineering: A Multimedia Guide for the Core Curriculum* – which focuses on steady-state simulation. Individual modules, presented in encyclopedic form, present instruction in the following areas:

Principles of Flowsheet Simulation
Separators
Heat Exchangers
Pumps, Compressors, and Expanders
Chemical Reactors
Physical Property Estimation

Brief introductions with text and voice are provided and examples using ASPEN PLUS and HYSYS show the specifics of carrying out solutions. Also, tutorials are provided showing how to complete full simulations using ASPEN PLUS and HYSYS.

These instructional materials can be downloaded from the website associated with the textbook:

> Seider, W. D., J. D. Seader, D. R. Lewin, and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, 3rd Ed., Wiley 2009.
> http://www.wiley.com/WileyCDA/WileyTitle/productCd-EHEP000024.html

Instructors can access the multimedia package from the Instructor Companion Site by clicking on the bullet: Using Process Simulators in Chemical Engineering Software. Note that by clicking on the bullet, Solution Manual, instructors can obtain solutions to all of the simulation exercises using ASPEN PLUS, HYSYS, and CHEMCAD.

In addition, for the ASEE Summer School for Chemical Engineering Faculty, in Boulder, CO, in 2002, Workshop 12 was entitled "Simulators for Design Across the Curriculum." A 112-page handout was provided for instructors in the following core courses:

Material and Energy Balances
Thermodynamics
Heat Transfer
Separation Principles
Reactor Design

It recommends self-paced instruction sequences, to be followed by students, using the multimedia instructional materials, and problem statements and solutions for class exercises and projects using process simulators for each of these courses. A copy of a 112-page handout, entitled "Materials for Participants – Module Instruction Sequence and Problem Statements by Core Course" can be downloaded from:

http://www.seas.upenn.edu/~dlewin/FOCAPD_2004/Workshop%2012.pdf

At the Technion, a one-credit Simulation Laboratory course has been taught during the second semester of the junior year. The students use the self-paced instructional modules to learn simulation techniques and solve problems in all of the core course areas. A description of the Simulation Laboratory is available:

http://www.seas.upenn.edu/~dlewin/FOCAPD_2004/Simulation%20Laboratory%20-%20054330.pdf

At Bucknell University, a self-paced instructional manual to teach freshmen and seniors to use the AspenTech HYSYS Process Simulator has been prepared. Also, an introductory manual on material balances, phase equilibria, and energy balances supports the HYSYS manual. Both can be downloaded from the following web addresses as read-only files:

http://www.departments.bucknell.edu/chem_eng/cheg200/HYSYS_Manual/a_BlueHYSYS.pdf
http://www.departments.bucknell.edu/chem_eng/cheg200/CinChE_Manual/a_whiteCinChE.pdf

Paper copies of these two manuals can be purchased at https://www.createspace.com/3655451 (beginning in August 2012) and https://www.createspace.com/3574827 (beginning in August 2011), respectively.

More recently, an introductory book on ASPEN PLUS has been published:

Schefflan, R., *Teach Yourself the Basics of Aspen Plus*, Wiley-AIChE, 2011.

http://www.amazon.com/Teach-Yourself-Basics-Aspen-Plus/dp/0470567953

Finally, using PRO/II, a simulation of a vinyl-chloride monomer process has been prepared at the University of California, San Diego. See:

http://chemelab.ucsd.edu/CAPE/

Thermophysical and Transport Properties

Most students (and some instructors) need guidance on the selection of property estimation methods for various chemical mixtures – especially when working on product and process design projects. Also, in many cases, the physical property databases don't include data records for specific chemicals. For these chemicals, it becomes necessary to estimate the constants for their pure-component data records (e.g., critical temperature, critical pressure, normal boiling point, liquid density at 25°C, ...). Also, for many mixtures, the databases don't include interaction coefficients for binary pairs to compute vapor-liquid or liquid-liquid equilibria. In these cases, it is often necessary to regress VLE and/or LLE data.

In *Using Process Simulators in Chemical Engineering: A Multimedia Guide for the Core Curriculum* (referred to in Steady-State Simulation above), under ASPEN PLUS or HYSYS, click on Physical Property Estimation to obtain recommended methods. Under ASPEN PLUS, follow the path, Physical Property Estimation → Property Package Selection to obtain guidance on the selection of property estimation methods. Also, follow the paths Physical Property Estimation → Equilibrium Diagrams → Estimation Parameters for Pure Species and Physical Property Estimation → Equilibrium Diagrams → Property Data Regression to obtain the details of estimating constants for pure-component data records and for regressing VLE or LLE data. Under HYSYS, follow the path, Physical Property Estimation → Package Selection to obtain guidance on the selection of property estimation methods.

For use in senior design projects, especially, design instructors should be aware that Version 7.3 of ASPEN PLUS includes ~5 million experimental data points along with literature references for pure species and binary systems. All have been reviewed and approved by the National Institute of Science and Technology (NIST).

Finally, for the prediction of the thermophysical properties of feed oils (triglyceride mixtures) and product fuels (e.g., biodiesel – FAMEs), Professor Y. A. Liu at Virginia Tech provides an

EXCEL spreadsheet. Instructions are given for using the NIST Thermo Data Engine (TDE) data in ASPEN PLUS simulations of trans-esterification processes. See:

http://www.design.che.vt.edu

Then, select the Biodiesel Modeling option.

Dynamic Process Simulation

At some universities, process control and dynamics are taught at the junior level, prior to product and process design courses. When this is the case, some process design instructors cover plant-wide control with emphasis on the selection of control loops (pairs of manipulated and controlled variables) to achieve processing objectives. Excellent coverage of this subject is provided by:

Luyben, W. L., Tyreus, B. D., and M. L. Luyben, *Plantwide Process Control*, McGraw-Hill, 1998.

A McGraw-Hill link doesn't appear to be available. This book is available at most technical libraries.

Also, for introductory coverage and several process design examples, see Chapter 12, Plantwide Controllability Assessment, in:

Seider, W. D., J. D. Seader, D. R. Lewin, and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, 3rd Ed., Wiley 2009.

http://www.wiley.com/WileyCDA/WileyTitle/productCd-EHEP000024.html

After the selection of plant-wide control loops for promising process designs, dynamic process simulation is often used to evaluate the performance of tuned control loops in responding to typical disturbances and setpoint changes. Note that few design instructors teach dynamic simulation in their lecture courses. However, some senior design groups use dynamic simulation to evaluate the performance of their process designs with control loops.

Four excellent books show how to use ASPEN DYNAMICS and other computation packages (e.g., MATLAB) to permit design engineers to balance the optimization of steady-state process designs with the performance of their process control systems. Each provides step-by-step procedures for creating the steady-state simulations, tuning the controllers, and carrying out the dynamic simulations. The first focuses on general chemical processes:

Luyben, W. L., *Plantwide Dynamic Simulators in Chemical Processing and Control*, Marcel Dekker, 2002.
http://www.amazon.com/Plantwide-Simulators-Chemical-Processing-Industries/dp/0824708016/ref=sr_1_3/002-2942684-3565654?ie=UTF8&s=books&qid=1187723368&sr=1-3

The second focuses on distillation towers:

Luyben, W. L., *Distillation Design and Control Using Aspen Simulation*, Wiley, 2006.
http://www.wiley.com/WileyCDA/WileyTitle/productCd-0471778885.html

The third focuses on chemical reactors:

Luyben, W. L., *Chemical Reactor Design and Control*, Wiley, 2007.
http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470097701.html

And, the fourth focuses on reactive distillation:

Luyben, W. L., and C.-C. Yu, *Reactive Distillation Design and Control*, Wiley, 2008.
http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470226129.html

Yet another source of teaching materials that show how to carry out dynamic simulations using UNISIM to evaluate control loop performance for promising designs is the Chapter 12 supplement, *Flowsheet Controllability Analysis*, in:

Seider, W. D., J. D. Seader, D. R. Lewin, and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, 3rd Ed., Wiley 2009.
http://www.wiley.com/WileyCDA/WileyTitle/productCd-EHEP000024.html

On the Instructor Companion Site, click PDF files and select Chapter 12.

Turning next to the process control course, over the past three decades, Prof. William Svrcek has promoted an approach to teaching control without Laplace transforms and frequency-domain analysis. He uses HYSYS dynamic simulation of processes and their controllers. Note that Prof. Svrcek introduced HYSIM in the early 1980s which was followed by the dynamic flowsheet simulator, HYSYS. See:

> Svrcek, W. Y., Mahoney, D. P., and B. R. Young, *A Real-Time Approach to Process Control*, 2nd Ed., , Wiley, 2006.
> http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470025336.html

Specialized Simulations

Increasingly, senior design projects involve more specialized chemical processes – especially when these projects focus on product designs. In this brief section, two sources of teaching materials involving the process simulators are provided. Note, however, that most design instructors have insufficient time to offer lectures covering these specialized applications.

The first is a book that teaches the process simulation of step-growth polymerization processes and their product designs:

> Seavey, K., and Y. A. Liu, *Step-Growth Polymerization Process Modeling and Product Design*, Wiley, 2008.
> http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470238232,descCd-description.html

The second is a book that teaches the process simulation of fossil energy conversion processes:

> Fan, L. S., *Chemical Looping Systems for Fossil Energy Conversions*, Wiley, 2010.
> http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470872527.html

PROCESS INTEGRATION (Mahmoud El-Halwagi)

Definition and Classification of Process Integration

Process integration is a holistic approach to process design, retrofitting, and operation which emphasizes the unity of the process. Typically, process integration involves the following activities:

1. Task Identification
2. Targeting
3. Generation of Alternatives (Synthesis)
4. Selection of Alternative(s) (Synthesis)
5. Assessment of Selected Alternative(s) (Analysis)

Process integration activities and literature may be classified into the following three categories (arranged in order of their chronological development):

1. Energy integration
2. Mass integration
3. Property integration

Common Applications of Process Integration

1. Network synthesis (e.g., heat-exchange networks, mass-exchange networks, direct-recycle networks)
2. Sustainability applications (e.g., conservation of natural resources: raw materials, water, solvents, heat, reduction in GHG emission, simultaneous consideration of fossil and renewable energy)
3. Process enhancement (e.g., debottlenecking, yield enhancement)

Reading Materials

Several textbooks have covered the fundamentals and applications of process integration (e.g., El-Halwagi, 2011, 2006; Kemp, 2006; and Smith, 2005). The tools in these texts include graphical, algebraic, and optimization approaches. The incorporation of process synthesis and integration approaches in design is covered by Biegler et al. (1997), Douglas (1988), Seider et al. (2009), Towler and Sinnott (2008), and Turton et al. (2009). The text by Majozi (2010) addresses batch process integration. Process integration has been particularly effective in resource-conservation and sustainable-design applications. Tools and case studies can be found in (El-Halwagi, 2011, 2006, 1997; Klemes et al., 2010; Kemp, 2006, Smith, 2005; and Mann and Liu, 1999).

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*. Prentice Hall, 1997.
http://www.pearson.ch/HigherEducation/ChemicalEngineering/ChemicalEngineering/1471/9780134924229/Systematic-Methods-of-Chemical-Process.aspx

Douglas, J. M., *Conceptual Design of Chemical Processes*, McGraw-Hill, 1988.
http://www.alibris.com/search/books/qwork/1268430/used/Conceptual%20Design%20of%20Chemical%20Processes

El-Halwagi, M. M., *Sustainable Design through Process Integration: Fundamentals and Applications to Industrial Pollution Prevention, Resource Conservation, and Profitability Enhancement*, Butterworth-Heinemann/Elsevier, 2011.
http://www.elsevierdirect.com/ISBN/9781856177443/Sustainable-Design-Through-Process-Integration

El-Halwagi, M. M., *Process Integration*, Academic Press, 2006.
http://www.elsevier.com/wps/find/bookdescription.cws_home/707754/description#description

El-Halwagi, M. M., *Pollution Prevention through Process Integration: Systematic Design Tools*, Academic Press, 1997.
http://www.elsevier.com/wps/find/bookdescription.agents/700863/description#description

Kemp, I., *Pinch Analysis and Energy Integration: A User Guide on Process Integration for the Efficient Use of Energy*, Elsevier, 2006 http://search.barnesandnoble.com/Pinch-Analysis-and-Process-Integration/Ian-C-Kemp/e/9780750682602

Klemes, J., F. Friedler, I. Bulatov, and P. Varbanov, *Sustainability in the Process Industry: Integration and Optimization*, McGraw Hill, 2010. http://www.mhprofessional.com/mhhe_product.php?isbn=0071605541

Majozi, T., *Batch Chemical Process Integration: Analysis, Synthesis and Optimization*, Springer, 2010. http://www.springer.com/chemistry/book/978-90-481-2587-6

Mann, J. G., and Y. A. Liu, Industrial Water Reuse and Wastewater Minimization, McGraw-Hill, 1999. http://www.design.che.vt.edu/waterdesign/waterdesign.html

Seider, W. D., J. D. Seader, D. R. Lewin, and S. Widagdo, *Product and Process Design Principles: Synthesis, Analysis, and Evaluation*, 3rd Ed., Wiley, 2009. http://www.wiley.com/WileyCDA/WileyTitle/productCd-EHEP000024.html

Smith, R., *Chemical Process Design and Integration*, Wiley, 2005. http://www.wiley.com/WileyCDA/WileyTitle/productCd-0471486817.html

Towler, G. and R. Sinnott, *Chemical Engineering Design: Principles, Practice and Economics of Plant and Process Design*, Elsevier, 2008 http://www.elsevierdirect.com/product.jsp?isbn=9780750684231

Turton, R., C. Bailie, B. Wallace, B. Whiting, and J. A. Shaeiwitz, *Analysis, Synthesis, and Design of Chemical Processes*, 3rd Edition, Prentice-Hall, 2009. http://www.abebooks.com/9780135129661/Analysis-Synthesis-Design-Chemical-Processes-0135129664/plp

Additional Web Links

1. The Process Integration educational web site developed as part of the North American Mobility Program:

   http://www.polymtl.ca/namp/

It was developed by faculty and students from six universities in North America

2. The web site developed as part of the NSF curriculum reform project at Texas A&M:

   http://alcheme.tamu.edu/?page_id=2151

One of the modules is on mass integration.

3. The Water Design web site, which contains PC-based software for water-pinch analysis and synthesis in Chapters 1-7 of:

   Mann, J. G., and Y. A. Liu, *Industrial Water Reuse and Wastewater Minimization*, McGraw-Hill, 1999.
   http://www.design.che.vt.edu/waterdesign/waterdesign.html

4. The Hydrogen Pinch Analysis web site, which contains an EXCEL spreadsheet to minimize fresh hydrogen consumption while maximizing hydrogen recovery and reuse in petroleum refineries and petrochemical complexes:

   http://www.design.che.vt.edu/h2pinch/h2pinch.html

EQUIPMENT DESIGN (Gavin Towler)

Equipment design is an intrinsic part of process design. You can't design or cost a process without selecting, specifying and sizing equipment. Although detailed design of unit operations is often neglected in foundation courses, students must gain some proficiency in plant and equipment design to be able to complete a realistic capstone design project.

The teaching of equipment design can be challenging because of the wide range of operations encountered in the process industries, many of which involve proprietary designs and know-how. Students and novice engineers usually have no difficulty tapping into the wealth of equipment information that is available on the Internet, but may struggle with interpreting that information and using it to make sensible design decisions.

From a practical, as well as pedagogical, standpoint it is useful to divide equipment into two categories: proprietary and non-proprietary designs. Non-proprietary equipment includes those unit operations that are broadly enough understood that an operating company can complete their own design without requiring the involvement of a specialist vendor. Proprietary equipment, on the other hand, would be very difficult or very expensive to design and build without the involvement of a vendor. This could be because the design requires specialist know-how, involves patented parts, materials or operations, or requires proprietary manufacturing techniques. Table 1 gives some examples of unit operations that fall in each category; however, there is no sharp line between the groups. It is also important to note that operating companies very rarely have the ability to make their own equipment, so it is almost always necessary to involve an equipment vendor at some point in the design process.

Table 1: Examples of Proprietary and Non-proprietary Operations

Non-proprietary Equipment	Proprietary Equipment
Pressure vessels	Compressors
Heat exchangers	Centrifuges
Distillation columns	Crystallizers
Pumps	Membrane modules
Settlers	Mills and grinders
Tanks	Dryers
Conveyors	Continuous chromatography
Some reactors	Some reactors

From a teaching perspective, most design projects introduce the students to the design of at least three of the four most-commonly encountered types of non-proprietary equipment: reactors, separation columns, heat exchangers and pumps. Ideally, the students entering senior design would be familiar with these operations from their foundation classes; however, in many cases the students will have a theoretical understanding of the operation, but little idea of how to arrive at a practical design. The Internet can be helpful in broadening students' practical understanding of these operations. Some good web sites are:

www.uspto.gov The US Patent Office's free web site has a great collection of patents on different reactor designs. www.delphion.com is a subscription service that is much easier to search for patents.

www.knovel.com Knovel has many good chemical engineering books covering all kinds of unit operations available on-line. Knovel is free to AIChE members and AIChE membership is free to students, so this is probably the best bargain available to chemical engineers.

www.chemengg.com is a chemical engineering portal run out of India whose mission statement is "to be the largest and the most comprehensive human-edited directory in the area of Chemical Engineering on the web directing to the required info (about chemical engineering on the web) instead of searching through a large pile of sites thrown by search engines by culling out the irrelevant and useless and keeping only the best content". Some of the links from this site are good, but some more culling would make it more useful.

http://people.clarkson.edu/~wwilcox/Design/reacdesn.htm is a site set up by Professor W.R. Wilcox for his design course. It has a lot of links to other resources on reactor design.

http://www.distillationgroup.com/distill.htm has an excellent site on distillation with links to technical papers published by employees of The Distillation Group.

http://lorien.ncl.ac.uk/ming/distil/distil0.htm is a site set up by Dr. M.T. Tham at Newcastle University that gives a really good brief overview of distillation and includes a lot of pictures of column internals.

www.fri.org is the website of Fractionation Research Inc., the distillation research consortium. There's not much available for free on their web site, but you can view some very short clips from the legendary "Film A". At $400 for a DVD of the movie (unless you are an FRI member, in which case it's only $50), Film A is probably the most expensive movie you would ever buy, but it is the authoritative movie on distillation, as well as a classic of 1970s industrial cinema.

There are many excellent Internet sites on heat exchangers, mostly hosted by exchanger manufacturers. http://shell-tube.com/ from Southwest Thermal Technology has background information on shell and tube exchanger construction. http://www.rigginscompany.com/heat_exchangers.htm has lots of great pictures of shell and tube exchangers under construction. http://www.dhtnet.com/heat_exchangers.htm provides coils and plate exchangers as well as S&T exchangers, and has many good pictures on their site. http://www.alfalaval.com/showroom/en-us/ is the Alfa-Laval showroom, which has some nice pictures of plate and spiral exchangers. This is just a small sample and there are many other great exchanger sites.

One of the key gaps in students' ability to accurately design reactors and distillation columns is their lack of knowledge of pressure vessel specification and design. Pressure vessel design is covered in only a few design textbooks. There are several software vendors who provide free tools online, for example www.codeware.com, which has a trial version of the COMPRESS software and http://www.chempute.com/pvelite.htm, which has PVElite (not for free!) and some simpler free programs.

Some chemical engineering textbooks provide lecture slides for instructors who adopt the book. Details are usually given in the book or on the publisher's web site.

For proprietary equipment, the design instructor's task is made easier by the wide availability of excellent vendor web sites. Equipment vendors need to maintain a strong online presence to attract new business and establish their credentials and the capability of their products. Finding the good web sites can be difficult though. Table 2 shows the results of Google searches for some separation operations that are usually sourced from vendors. Table 2 also shows how many sites had details of equipment specifications, sizes or a design tool.

Table 2: Web sites for separation equipment vendors

Topic	Total Hits	Actual industrial-scale vendors in top 10 hits	Actual industrial-scale vendors in top 30 hits	Number of sites with spec sheets in top 30
Crystallizer	“about 231,000”	3	7	2
Reverse Osmosis	“about 2,650,000”	2	5	3
Pressure-swing adsorption	“about 136,000”	4	10	6
Gas separation membranes	“about 298,000”	1	4	2
Simulated moving bed chromatography	“about 29,900”	1	3	1

It can be seen from Table 2 that some patience is required in sifting through web sites to find vendor sites that have high quality information.

Internet searching is obviously more difficult when the search term is in common use. Searches for “filters”, “heaters”, “furnaces”, “dryers” and “mixers” yield a very low fraction of useful hits. The terms “size reduction” and “size enlargement”, long used in chemical engineering and particle technology to describe grinding and agglomeration operations, have acquired entirely different connotations online. For operations where the search term is in common use, it is better to use a specialized chemical industry or chemical engineering portal such as www.chemindustry.com, www.matche.com or www.cheresources.com.

ENVIRONMENT AND SUSTAINABILITY (David Shonnard)

Definition of Green Engineering

Green Engineering, an approach synonymous with environmentally-conscious design, is defined as the design, commercialization, and use of processes and products that prevent pollution at the source and reduce risk to human health and to the environment. The goal of green engineering is to inform engineering design of the environmental and human health impacts of chemical or biochemical processes or products over their entire life cycle through a number of considerations:

a) understanding of environmental issues and regulations,
b) environmental and toxicological properties of chemicals,
c) pollutant emission sources and release rates,
d) environmental fate and transport behavior of chemicals,
e) impact assessment for environmental and human health,
f) implications of materials and chemical reactions on design

A website dedicated to disseminating green engineering curriculum materials, including lecture modules and links to computer-aided green engineering tools, is at the US EPA green engineering homepage: http://www.epa.gov/oppt/greenengineering/

Definition of Sustainable Engineering

Engineers can design products, processes and technologies that are sustainable by integrating environmental, economic, and social factors in the evaluation of their designs. Sustainable designs meet the economic, environmental, and social performance needs of today, while taking into full account the needs of future generations.

Textbooks: Texts have been developed on green engineering and sustainable engineering with example problems, case studies, end of chapter problems, and solution manuals.

Allen, D.T. and Shonnard, D.R. (and other contributors), 2002, Green Engineering: Environmentally Conscious Design of Chemical Processes, Prentice-Hall, Upper Saddle River, NJ, 2002, pp. 552, ISBN 0-13-061908-6.

This text outlines a hierarchical design process where environmental assessments of increasing complexity and scope are implemented as the design engineer moves from early screening design activities up through detailed flowsheet simulation and assessments.

Allen, D.T. and Shonnard, D.R. (2012), Sustainable Engineering, Prentice-Hall, Upper Saddle River, NJ (in press).

Graedel, T.E. and Allenby, B.R., 2003, Industrial Ecology, 2nd Ed, Prentice-Hall

Bishop, P.L., 2000, Pollution Prevention: Fundamentals and Practice, McGraw-Hill

Allenby, B.R., 2011, Theory and Practice of Sustainable Engineering, Prentice-Hall, Upper Saddle River, NJ, 432 pages, ISBN-10: 0132127997.

Graedel, T.E., Allenby, B.R., 2011, Industrial Ecology and Sustainable Engineering, Prentice-Hall, Upper Saddle River, NJ, 352 pages, ISBN-10: 0136008062.

El-Halwagi, M. M., 2011, Sustainable Design through Process Integration: Fundamentals and Applications to Industrial Pollution Prevention, Resource Conservation, and Profitability Enhancement, Butterworth-Heinemann/Elsevier, SBN/9781856177443.

Klemes, J., F. Friedler, I. Bulatov, and P. Varbanov, 2010, Sustainability in the Process Industry: Integration and Optimization, McGraw Hill.

El-Halwagi, M. M., 1997, Pollution Prevention through Process Integration: Systematic Design Tools, Academic Press, 334 pages.

Software Tools and Websites:

Environmental and Toxicological Properties

EPI Suite (environmental properties – partitioning and fate),
http://www.epa.gov/opptintr/exposure/pubs/episuite.htm

ECOSAR (ecological toxicity estimation)
http://www.epa.gov/oppt/newchems/tools/21ecosar.htm

OncoLogic (carcinogenic potential of chemicals)
http://www.epa.gov/oppt/sf/pubs/oncologic.htm

Pollutant Emission Sources and Release Rates

Air CHIEF (emission factors for industrial sources),
http://www.epa.gov/ttnchie1/

ChemSTEER (environmental releases and worker exposure)
http://www.epa.gov/opptintr/exposure/pubs/chemsteer.htm

TANKS (emission estimation from storage tanks)
http://www.epa.gov/ttnchie1/software/tanks/

Environmental Fate and Transport Behavior of Chemicals

Mackay Level III Model (multi-media compartment environment model)
http://www.trentu.ca/academic/aminss/envmodel/models/VBL3.html

EPI Suite (environmental properties – partitioning and fate),
http://www.epa.gov/opptintr/exposure/pubs/episuite.htm

Impact Assessment for Environmental and Human Health

WAR-WAste Reduction Algorithm (flowsheet environmental assessment)
http://www.epa.gov/nrmrl/std/cppb/war/sim_war.htm

Life Cycle Assessment Software Tools

- SimaPro: http://www.pre.nl/simapro/
- EIO-LCA: http://www.eiolca.net/
- GREET: http://greet.es.anl.gov/
- GaBi: http://www.gabi-software.com/
- Umberto: http://www.umberto.de/en/

Implications of Materials and Chemical Reactions on Design

Green Chemistry Expert System: http://www.epa.gov/gcc/pubs/gces.html

PARIS II (computer-aided solvent design): http://www.epa.gov/nrmrl/std/mtb/paris.htm

PROCESS AND PRODUCT SAFETY (Daniel Crowl)

Definitions

Safety deals with accident prevention. Accidents in a chemical plant may cause injury or death to workers, damage to the environment, damage to equipment or facilities, and loss of production and inventory. This is frequently given the general title of loss prevention. For product design, additional consideration must be given to accidents that may occur due to use of the product by the consumer.

It is essential that safety be considered as early as possible in the design of a new chemical process or product. The cost to make changes later in the design increases dramatically and the options to make changes are reduced as the design nears completion.

Process and product safety requires the following steps:

1. Identification of the hazards associated with the chemicals, the process and the procedures to operate the plant. For product design, this step must also identify the hazards associated with the use of the product by the consumer.
2. Estimation of the risks associated with these hazards. Risk is the product of both probability and the magnitude of the consequences.
3. Application of inherently safer design methods to eliminate or reduce the hazard, and other methods to reduce either the probability of the accident or the magnitude of the consequence.

A website devoted to these issues is supported by the AIChE/CCPS Safety and Chemical Engineering Education (SACHE) web site at www.sache.org. This web site has dozens of instructional modules related to process safety. The modules have a variety of formats, including Powerpoints, videos, and problem sets. These modules can be found here:
http://sache.org/products.asp.

The modules are only available to faculty at U.S. institutions that are members of SACHE. Membership is provided free of charge. Each member university has a designated SACHE representative. A list of member universities and their SACHE representatives is found here:
http://sache.org/members.asp

In addition, the web site supports a growing number of certificate modules. For the certificate modules, the student studies the on-line materials, completes an on-line test, and then receives the certificate of completion directly from AIChE. The certificate modules include material on risk

assessment, dust explosion control, inherently safer design, runaway reactions, and reactive chemicals hazards. The content is delivered by Powerpoint, video and reference documents. In 2010, over 3,000 certificates were awarded to students. Students must be members of AIChE to complete the certificates – it is currently only available to students. The certificate program is found here: http://sache.org/student_certificate_program.asp
The SACHE web site also provides links to a lot of useful process safety resources. These links are found here: http://sache.org/links.asp

Textbooks:

Currently, there is only one textbook in process safety:

> D. A. Crowl and J. F. Louvar, *Chemical Process Safety, Fundamentals with Applications*, 2nd ed., Prentice Hall, Englewood Cliffs, NJ, 2002. A third edition will be available in the Spring of 2011.
> http://www.pearsonhighered.com/educator/product/Chemical-Process-Safety-Fundamentals-with-Applications/9780130181763.page

Reference Materials:

There are several excellent reference materials in process safety:

> D. W. Green and R. H. Perry, *Perry's Chemical Engineering Handbook*, 8th ed., Mc-Graw-Hill, NY, 2008. Section 23: Process Safety.
> http://www.mhprofessional.com/book.php?isbn=0071422943

> S. Mannan, ed., *Lee's Loss Prevention in the Process Industries*, Elsevier, 2004.

AIChE also has a large number of professional reference volumes related to process safety. A list of these monographs can be found here:

> http://www.aiche.org/Publications/PubCat/Categories/ProcessSafety.aspx

Many of these books are available on-line through www.knovel.com

Journals:

Two international journals are focused on process safety and loss prevention.

Process Safety Progress, published by the AIChE Safety and Health Division
http://onlinelibrary.wiley.com/journal/10.1002/(ISSN)1547-5913

Journal of Loss Prevention in the Process Industries, published by Elsevier.
http://www.elsevier.com/wps/find/journaldescription.cws_home/30444/description#description

Websites and Software:

www.knovel.com is a link to the Knovel online library of engineering reference materials. This site provides a large library of safety reference materials on-line. Membership in AIChE provides partial access to these materials.

www.csb.gov is a link to the U.S. Chemical Safety Board. This link provides a large library of videos related to chemical plant accidents. Accident investigation reports on specific accidents can also be found here.

http://www.cdc.gov/niosh/npg/ is a link to the National Institute for Occupational Safety and Health (NIOSH). This link provides either online or downloadable access to the NIOSH Pocket Guide to Chemical Hazards. This guide is intended as a source of general industrial hygiene information on several hundred chemicals/classes for workers, employers, and occupational health professionals. This is an excellent starting place to determine the hazardous properties of common chemicals.

www.osha.gov is a link to the U.S. Occupational Safety and Health Administration. This link provides access to all the regulations related to process safety, including 1910.119 Process safety management of highly hazardous chemicals. This includes permissible exposure limits (PEL) promulgated by OSHA.

http://www.internationalsafety.com/PDF/3M-2009-respirator-selection.pdf is a link to the 3M Respirator Selection Guide. This guide also provides hazardous properties for a large number of chemicals.

http://www.response.restoration.noaa.gov/ provides a link to the National Oceanic and Atmospheric Administration. Two free, downloadable software programs are available here:

1. Chemical Reactivity Worksheet: a program to chemical reactivity of substances or mixtures of substances. This program includes a database of about 5,000 chemicals.

2. CAMEO Program: consists of four core programs: CAMEO, CAMEO Chemicals, ALOHA, and MARPLOT. These programs are useful to estimate the consequences due to the release and atmospheric dispersion of chemicals.

http://www.chem.mtu.edu/org/aiches&h/links.html is a list of internet links related to process safety support by the AIChE Safety and Health Division. This includes a large number of government and professional links.

http://www.epa.gov/emergencies/index.htm provides government resources for emergency management. This includes regulations, publications, databases and tools.

http://toxnet.nlm.nih.gov/ is a toxicology data network provided by the U.S. National Library of Medicine. This includes free databases on toxicology, hazardous chemicals, environmental health and toxic releases.

http://www.cpsc.gov/ is a link to the U.S. Consumer Product Safety Commission. This is an excellent place to look for product safety information.

Specific Hazards:

Specific hazards that occur in chemical plants include toxic, flammable, and reactivity. Specific references on each type of hazard are available:

Toxic Hazards:

Crowl and Louvar, *Chemical Process Safety, Fundamentals with Applications*, 2nd ed., Prentice Hall, Englewood Cliffs, NJ, 2002. Chapter 2.

American Conference for Governmental Industrial Hygienists (ACGIH). www.acgih.org

NIOSH Pocket Guide to Chemical Hazards. This is a free database of chemical hazards. www.cdc.gov/niosh/npg/

Society of Toxicology. This is a professional organization of scientists from academic institutions, government and industry representing toxicologists. www.toxicology.org

TOXNET, Toxicology Data Network provided by the U. S. National Library of Medicine. This includes free databases on toxicology, hazardous chemicals, environmental health, and toxic releases. www.toxnet.nlm.nih.gov

U.S. Department of Labor, Occupational Safety and Health Administration. This includes all regulations and PEL values. www.osha.gov

Flammable Hazards:

Crowl and Louvar, *Chemical Process Safety, Fundamentals with Applications,* 2nd ed., Prentice Hall, Englewood Cliffs, NJ, 2002. Chapters 6 and 7.

Crowl, D. A. *Understanding Explosions*, John Wiley, Hoboken, NJ, 2003.
http://www.wiley.com/WileyCDA/WileyTitle/productCd-081690779X.html

D. W. Green and Robert H. Perry, editors, *Perry's Chemical Enginees' Handbook* 8th ed., McGraw-Hill, NY, 2008. See Section 23 on Process Safety.

Reed Welker, *Explosions*, 35 minute video prepared for SACHE.
http://sache.org/product_view.asp?id=51

Reed Welker, *Seminar on Fire*, Powerpoint presentation prepared for SACHE.
http://sache.org/product_view.asp?id=50

Fire Protection Guide to Hazardous Materials (2010), National Fire Protection Association (NFPA), www.nfpa.org

Reactivity (Stability) Hazards:

Crowl and Louvar, *Chemical Process Safety, Fundamentals with Applications,* 2nd ed., Prentice Hall, Englewood Cliffs, NJ, 2002. Chapter 8.

R. W. Johnson, S. W. Rudy and S. D. Unwin, *Essential Practices for Managing Chemical Reactivity Hazards,* John Wiley, Hoboken, NJ, 2003.
http://www.wiley.com/WileyCDA/WileyTitle/productCd-0816908966.html
Available for free download from www.knovel.com.

Chemical Reactivity Worksheet, National Oceanic and Atmospheric Administration (NOAA)
http://response.restoration.noaa.gov/

Brethericks Handbook of Reactive Chemical Hazards, P. Urben, ed.
(2006), Elsevier Publishers, www.elsevier.com

CHETAH: Computer Program for Chemical Thermodynamics and Energy Release Evaluation, American Society for Testing and Materials (ASTM). www.astm.org

OPTIMIZATION – PROCESS SYNTHESIS and FLOWSHEET OPTIMIZATION

(Lorenz T. Biegler and Ignacio E. Grossmann)

Optimization and its applications to flowsheet optimization and process synthesis are topics that are normally taught at the undergraduate level within the process design course. At the graduate level, they are taught as specialty courses, normally in those departments that happen to have faculty in Process Systems Engineering. At the undergraduate level, as opposed to in the past where the emphasis was to cover many optimization methods, the emphasis is currently to teach modeling using tools such as GAMS and only cover the basics of the major methods (e.g., simplex algorithm, successive quadratic programming). In courses at the graduate level, an in-depth analysis of the algorithms is presented, and also complemented with modeling, especially in mixed-integer programming and dynamic optimization.

Problems in process synthesis can be formulated as mixed-integer programming models, which involve discrete and continuous variables. The discrete variables are used to model the selection of units that are postulated in a superstructure of alternative flowsheets or process schemes. The continuous variables are used to model the selection of design parameters and operating conditions. Depending on the level of representation, synthesis problems can be models as mixed-integer linear programming (MILP) models at the simplest level, and as mixed-integer nonlinear programming (MINLP) problems when nonlinearities for process equations are included. Both MILP and MINLP techniques are readily available in modeling systems such as GAMS. There are also several libraries of mixed-integer programming models that are listed below. As for specific software for process synthesis, there are few packages available such as JACARANDA and THEN.

Flowsheet optimization combines elements of optimization algorithms and process simulation. With the widespread use of process simulation for design, the natural extension is to manipulate the design degrees of freedom in an efficient, automatic way to maximize process profit, minimize operating and capital cost, or achieve the best level of process performance. In practice, most flowsheet optimization problems are represented as nonlinear programming (NLP) problems and efficient gradient-based NLP solvers are typically applied. Note that simulation training materials can be found in the section on Process Simulation.

Process optimization techniques, models for flowsheet optimization and process synthesis, are described in several of the textbooks below. These provide descriptions of optimization concepts and algorithms, process optimization case studies, and extensive exercises on optimization problems. We also provide links for tutorials on optimization as well as libraries of optimization problems and models.

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*. Prentice Hall, 1997.
http://www.pearsonhighered.com/educator/product/Systematic-Methods-of-Chemical-Process-Design/9780134924229.page

Biegler, L. T., Nonlinear Programming: Concepts, Algorithms and Applications to Chemical Engineering, SIAM, Philadelphia, PA, 2010.
http://www.ec-securehost.com/SIAM/MO10.html

CACHE Chemical Engineering Optimization Models with GAMS
http://www.che.utexas.edu/cache/casestudy.html#vol6

Chinnek, J.W.: Gentle Introduction to Optimization
http://www.sce.carleton.ca/faculty/chinneck/po.html

Cyberinfrastructure site for Mixed-Integer Nonlinear Programming containing over 30 examples of MILP and MINLP problems with formulations and GAMS implementations.
http://www.minlp.org

Edgar, T., D. Himmelblau, and L. Lasdon, “Optimization of Chemical Processes,” McGraw Hill, 2nd Edition, 2001.
http://www.4shared.com/document/sbBIu5lp/Optimization_of_chemical_proce.html

GAMS model library
http://www.gams.com/modlib/modlib.htm

Pike, R.: Optimization Book
http://www.mpri.lsu.edu/bookindex.html

Virtual Library of Process Systems Engineering: Optimization and process synthesis modules containing lecture material, exercises, papers and GAMS input files
http://cepac.cheme.cmu.edu/pasi2005/slides/index.htm

West Virginia University Optimization Problems. These can be solved with EXCEL spreadsheets as described in Anderson, B. J., R. S. Hissam, J. A. Shaeiwitz, and R. Turton, "Optimization Problems," *Chemical Engineering Education*, **45** (2), 144-149 (2011).
http://www.che.cemr.wvu.edu/publications/projects/index.php

Applications of optimization to process synthesis can be found in:

Fraga, E.: JACARANDA: Conceptual Design Flowsheets and HEN Synthesis
http://www.homepages.ucl.ac.uk/~ucecesf/jacaranda.html

Grossmann, I.E: Mixed-integer programming models in process synthesis, planning, scheduling
http://newton.cheme.cmu.edu/interfaces/

To download HEN synthesis program THEN
http://www.mpri.lsu.edu/thenindex.html

The following links provide access to optimization software.

COIN-OR: Open source software for optimization (LP, NLP, MILP, MINLP, global)
http://www.coin-or.org/

GAMS link for downloading free demonstration software for LP, NLP, MILP and MINLP models.
http://www.gams.com/download

NEOS Server for information and access to optimization software
http://neos-server.org/neos/

Neumaier, A.: Website on Global Optimization
http://www.mat.univie.ac.at/~neum/glopt.html

PROCESS MODELING (Rafiqul Gani)

Mathematical models play a central role in the solution of many process engineering problems such as those related to process design. Generally, when enough data/information (knowledge) about the system and sub-systems are available, an appropriate design methodology is applied to find the new and/or optimal design. However, when the necessary knowledge (data/information) is not available, models can supplement the available information. For example, models predict the behavior of the process, evaluate the performance of the process, monitor and/or control the process, and many more. Furthermore, most algorithms for process design, analysis, control, planning, and the like, are model-based and the application range of the models defines the applicability and usage of the corresponding algorithm. The models, however, may be of different types (involving different types of equations to represent the system); scales (involving sub-systems requiring different size and time scales); complexity (involving large numbers of equations, high degrees of non-linearity, multiple dimensions, *etc.*) and simulation mode (steady state, dynamic, batch, identification, *etc.*).

Systematic Methods for Process Modeling

An excellent book describes the use of models in process engineering:

> Hangos, K.M. and I.T. Cameron (2001) *Process modelling and model analysis*. Academic Press, London.
> http://www.elsevier.com/wps/find/bookdescription.cws_home/675670/description#description

Next, consider the various modelling objectives it addresses. To manage processing and manufacturing systematically, the engineer brings together many different techniques and analyses to understand the interactions among various aspects of processes. For example, process engineers often apply models to perform feasibility analyses of novel process designs, to assess their environmental impact, and to detect potential hazards or accidents. To manage complex systems and enable process design, the behavior of systems is often reduced to simple mathematical forms. This book provides a systematic approach to the mathematical development of process models and explains how to analyse those models. In addition, it provides a comprehensive bibliography for further reading, a question and answer section, and an accompanying web site with additional data and exercises.

Another book covers product and process modelling using a case-study approach:

> Cameron, I., and R. Gani, *Product and Process Modelling: A Case-Study Approach*, Elsevier, 2011.
> http://www.elsevierdirect.com/product.jsp?isbn=9780444531612

This book addresses a wide range of modelling applications with emphasis on modelling methodology and the subsequent in-depth analysis of mathematical models to gain insights using structural aspects of the models. These approaches are described in the context of life-cycle modelling, involving multiscale and multiform modelling, which are increasingly prevalent in the 21st century. The book commences with a discussion of modern product and process modelling theory and practice followed by a series of case studies drawn from a variety of process industries, ranging from the traditional petroleum and petrochemical industries to biotechnology applications, food, polymer, and human health applications. Emphasis is placed on the importance of modern product and process modelling in decision-making processes across the life cycle, providing an important resource for students, researchers, and industrial practitioners.

Modeling Software

Several software packages are available to assist in process modeling:

ICAS-MoT and ICAS-ModDev: developed at CAPEC-DTU (2011), Computer Aided Process Engineering Center

http://www.capec.kt.dtu.dk/Software/ICAS-and-its-Tools/ICAS-Toolboxes2, accessed February 27, 2011.

gPROMS: developed by Process Systems Enterprise, London, UK http://www.psenterprise.com/gproms/index.html, accessed February 27, 2011.

Daesim: developed at Daesim Dynamics, Brisbane, Queensland, Australia http://www.daesim.com/software/daesim/dynamics/, accessed February 27, 2011.

Aspen Custom Modeler: developed by Aspen Technologies, Cambridge, MA, USA. http://www.aspentech.com/products/aspen-custom-modeler.aspx accessed February 27, 2011.

MATLAB: Mathworks http://www.mathworks.com/products/matlab/ accessed February 27, 2011.

Courses Workshops and Notes

Course lecture notes for graduate level courses on advanced computer-aided process modelling are available from Professor Rafiqul Gani, including a library of models. See also:

http://www.capec.kt.dtu.dk/Courses/Workshops/Workshop-on-modelling

DESIGN CASE STUDIES AND DESIGN PROBLEM STATEMENTS

(Ignacio Grossmann, Richard Turton, and Joe Shaeiwitz)

One of the major components in undergraduate process and product design courses are the design projects. A major challenge for the instructor of these courses is the need to define such projects and the organization of the design groups. A first major question is whether to supply a single project to the class, or different projects, possibly one for each group. The advantage of a single project is that the instructor only has to worry about one single problem. The potential disadvantage is when the project does not lend itself to having many design alternatives as then most groups will produce very similar designs which defeats the purpose of exposing them to open-ended problems. The advantage of offering multiple projects is having greater diversity of problems, but the obvious disadvantage is that it requires a very significant effort by the instructor. Either way, selecting design projects is a real challenge, particularly for the process design course.

Process Design Project

In the case of a process design project, the common approach is to ask the students to develop a preliminary design of a process flowsheet for producing a specified amount of given product. Traditionally, the products have been large-scale commodities (e.g., methanol) while more recently the trend has been towards biofuels, as well as deciding their plant capacity and their geographic location. A process design project usually requires a greater level of detail and knowledge than a product design project since students have to select a process technology, synthesize a process flowsheet, perform material and heat balance, size the units, and perform a fairly comprehensive economic evaluation. This also means that the instructor has to supply to the students basic information on the process technology and design alternatives, as well as support the course through process simulators, reactor models, etc. Retired individuals from industry, who increasingly teach the process design course, have an easier task in selecting the design project compared to tenure track faculty member, particularly, when they have limited background in Process Systems Engineering. In the past it was more common for industry to provide design projects. Unless the instructor has such an industrial contact, the most common source nowadays is to rely on published case studies. These include the series of case studies by CACHE, selected books (e.g. Dimian and Bildea, 2008), the AIChE Student Contest design problems, EURECHA. See the links below.

Product Design Project

A product design project is commonly performed at a more general level than the process design project since it involves identifying a need and its potential market, conceiving a conceptual solution in the form of a product or device, and performing a preliminary economic evaluation without detailed analysis. One approach that is used is to ask design groups to define their own project since in many ways this fits one of the goals of product design which is to identify a need for which they have to propose developing a new product. Furthermore, since there is no need to perform a detailed analysis, the instructor need not worry as much about providing much information and support as is needed in the process design course. Nevertheless, case studies for product design can still provide a useful guide to an instructor on how to organize such a course, especially since it is still not taught at many universities. Currently, there are very few product design case studies that have been published (e.g., Gani et al., 2007).

In the remainder of this section, we present links to both design case studies and design problem statements without solutions. First, the links focus on the case studies (problem statements and solutions). Then, we focus on problem statements without solutions.

Design Case Studies

Below we list links to basic references for process and product design case studies that include solutions and material for the instructor:

Biegler, L.T., Process Design Case Study: Nitrogen from Air
http://www.cheme.cmu.edu/course/06302/airsep2/

Biegler, L. T., I. E. Grossmann, and A. W. Westerberg, *Systematic Methods of Chemical Process Design*. Prentice Hall, New Jersey (1997).
http://www.pearsonhighered.com/educator/product/Systematic-Methods-of-Chemical-Process-Design/9780134924229.page

CACHE Design Case Studies
http://www.che.utexas.edu/cache/casestudy.html

Dimian, A.C. and C.S. Bildea, *Chemical Process Design: Computer-Aided Case Studies*, Wiley-VCH, Weinheim (2008).
http://www.wiley.com/WileyCDA/WileyTitle/productCd-3527314032,descCd-description.html

Case studies can be downloaded from:
http://www.elsevier.com/wps/find/bookdescription.editors/708653/description#description

http://ebookee.org/download/?file=Chemical+Process+Design%3A+Computer-Aided+Case+Studies

EURECHA Student Contest Projects
http://atom.uni-mb.si/~ukeeur004/competition.html

Ng, K.M, R. Gani and K.M. Johansen (Editors), *Chemical Product Design: Towards a Perspective through Case Studies*, Elsevier B.V., Amsterdam (2007).

University of Notre Dame. Environmenta;l design problems:
http://www.nd.edu/~enviro/design/design.html

Scott, R. and N. Macleod , Product and Process Design Case Studies, IChemE, UK (1992).

Seay, J. and J. Gish, “Educational Module: A Sustainable Design Project for the Process Separations Class”
http://www.ce.cmu.edu/~cse/modules/10-21_Seay.pdf

Seider, W.D., J.D. Seader, D.R. Lewin: Product and Process Design Principles: Synthesis, Analysis, and Evaluation, Wiley (2009)
http://www.seas.upenn.edu/~dlewin/index_students.htm

Design Problem Statements

There are several resources available providing examples of process design project statements that have been used successfully. These differ from the case studies discussed elsewhere, because these are only project statements; no solutions are provided. Solutions may be available from the author's of the web sites.

A comprehensive library of design project statements is available at a web site prepared at the West Virginia University:

http://www.che.cemr.wvu.edu/publications/projects/index.php.

Project statements are included for the capstone experience and for companion projects throughout the curriculum. Troubleshooting and retrofitting projects for existing processes are also provided. This web site is updated every year with new project statements.

A similarly extensive web site contains design project statements with an environmental flavor, created at the University of Notre Dame:

http://www.nd.edu/~enviro/design/design.html

This web site appears not to be updated regularly.

Yet, another source is the textbook, Towler, G., and R. Sinnott, *Chemical Engineering Design*, Elsevier, 2008, pages 1,135-1,192:

http://www.elsevierdirect.com/product.jsp?isbn=9780750684231

For 71 design problem statements mostly prepared by industrial consultants at the University of Pennsylvania, in a 132-page PDF file, see the web site:

http://bcs.wiley.com/he-bcs/Books?action=index&itemId=0470048956&bcsId=4801

Click PDF files, then Appendix II. The problems are organized in several areas: petrochemicals, petroleum products, gas manufacture, foods, pharmaceuticals, biomedical, polymers, electronic materials, environment (air quality, water treatment, soil treatment, renewable fuels and chemicals).

A source of design project statements from the recent academic year is available at:

http://www.seas.upenn.edu/~seider/2010_2011Projects.pdf

Design project synopses from the last several years are available at:

http://www.stevens.edu/ses/cems/undergrad/design.html

http://www.expo.mtu.edu/expo2002/report.html

http://www.engin.umich.edu/students/involvement/teamprojects.html;

although, the latter site's projects do not include much chemical engineering.

A good web site that does not provide specific design project statements, but does provide excellent resources for those teaching design and doing design projects is available at:

http://people.clarkson.edu/~wwilcox/Design/refs.htm.

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