

CACHE NEWS ARTICLE

GUIDE TO TEACHING DESIGN WITH INTERNET LINKS

In the early 2000's, Prof. Thomas F. Edgar, CACHE Executive Officer, created the CACHE Learning Resource Center, which contains Internet links to teaching materials in 28 areas of chemical engineering. At his request, Prof. Warren D. Seider, Univ. of Pennsylvania, prepared a website in the area of Process and Product Design. Brief introductory statements preceded links to teaching materials in several categories: Course Materials, Optimization Websites, Discussion Groups, and Software. Approximately 50 links were provided – unfortunately, most of which were no longer functioning in 2011 – as no vehicle was established for regular maintenance and updating of the links.

Nearly a decade later, in the summer of 2010, several CACHE Trustees decided to try a new approach involving experts in 10 areas of Product and Process Design who agreed to serve as area editors – with the areas and editors listed below:

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)

All agreed to write text introducing links to be maintained annually – checking links, adding new links as appropriate, and removing outdated links.

It was decided to create a [*Guide to Teaching Design with Internet Links*](#). Guidance would be 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. Instructors, who would use the *Guide*, would be requested to make the area editors aware of new links as they were encountered.

Initially, it was decided the *Guide* would be prepared for instructors that use the CACHE Learning Resource Center. When completed, it might be adopted for *Chem. Eng. Educ.* and possibly for the broader *CEP* audience. To introduce this *Guide*, it was decided to plan a workshop for the 2012 ASEE Summer School for ChE Faculty. Also, eventually, it was thought the links might be organized to guide students and practitioners, in addition to design instructors, in finding Internet links to answer their questions and to locate specific instructional materials. In so doing, common key words might be translated into more specific terms; e.g., “mixers” to “agitators” when carrying out equipment design.

During this first organizational year, the area planned their contributions in the early Fall, met at the Salt Lake City Meeting of the AIChE, submitted their text to the overall editor, Prof. Warren D. Seider, and gradually upgraded their text and links through interactions among themselves. The resulting initial *Guide*, which is being installed on the CACHE Learning Resources Center in August 2011, is comprised of nearly 50 pages of text that introduce over 180 Internet links to specific teaching materials.

Often, links are provided to the sections, chapters, pages, ..., of textbooks that have unique coverage of a subject. For example, the innovation map in product design, to our knowledge, is covered in just one textbook (Seider et al., 2009). Other links are provided to software packages; for example, the ProCAMD package for molecular structure design at the Denmark Technical University. Yet other links are to design case studies, prepared either by instructors or students; for example, a book of product design case studies (Ng et al., 2007). Some links are to lecture notes with worked out examples. Others are to multimedia self-paced instructional materials; for example, to teach the usage of the process simulators, ASPEN PLUS and HYSYS.

To those that teach design, it is well-recognized that even the most comprehensive textbooks don't cover many subjects – with most design instructors assembling materials that supplement

the book(s) they adopt. Our *Guide* is a great source of supplemental materials – sufficiently broad to permit design instructors to formulate easily custom-made curricula for their courses.

As anticipated, with so many sections and area editors, overlap among the sections cannot be avoided; for example, links to case studies appear in the last section and in several other sections. When searching for case studies, especially, instructors are advised to check specific sections in which case studies are likely to appear. For example, case studies on molecular structure design can be found in the Product Design section.

Again, to instructors that use our *Guide*, we ask you to make us aware of other sources and links. For some sources, links can be created when appropriate. Please address these to the area editors or to the overall editor, Prof. Warren D. Seider (seider@seas.upenn.edu). Feel free to suggest new sources, or even new areas – perhaps you would be willing to consider being an area editor. Note, however, that three sections are currently being prepared: Batch Process Design (G. V. Reklaitis), Computational Fluid Dynamics (Charles Petty), and Energy (Mahmoud El-Halwagi and Jeffrey J. Sirola).

As you will see, various techniques are employed by our area editors to cover their subjects and introduce their links. As an example, for this news article, the section on Process Simulation by Dr. Chau-Chyun Chen and Prof. Warren D. Seider appears next.

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.createpace.com/3655451> (beginning in August 2012) and <https://www.createpace.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>