ASPEN PLUS® IN THE ChE CURRICULUM

Suitable Course Content and Teaching Methodology

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ASPEN Plus® software represents the standard in the chemical process industries (CPI) for process simulation. This software serves industries such as refining, oil and gas, chemicals and petrochemicals, polymers, pharmaceuticals and specialty chemicals, power and utilities, consumer goods, food and beverage, and engineering and construction. It is used by forty-six of the world's fifty largest chemical companies, twenty-three of the world's twenty-five largest petroleum refiners, eighteen of the world's twenty largest pharmaceutical companies, and seventeen out of the world's twenty largest engineering and construction firms that serve the CPI. This popularity is also evidenced in the academic community, where ASPEN Plus continues to be the simulator of choice for studying process design and simulation.[5-17] As such, providing undergraduates with a strong background in ASPEN Plus is a desirable program trait for many chemical engineering (ChE) departments, and is a recruiting consideration to many employers of ChE graduates.

This paper does not attempt to teach the software, nor does it contain teaching materials for use by instructors. Lecture resources drawn from numerous sources[1-4] are available online on the homepage of the author on the Chemical Engineering Department's web server at New Mexico State University <chemeng.nmsu.edu>. Demonstration files can be obtained from the author as well as from the Knowledge Base of the ASPENTech website <www.aspentech.com>.

INCORPORATING ASPEN PLUS INTO THE CURRICULUM

The topic of chemical process simulation is taught as a computing laboratory integrated with a senior-level design course at New Mexico State University. The ASPEN Plus simulator is taught as a one-credit hour laboratory that is taken concurrently with a three-credit lecture on process design during the first semester of the senior year. Students must demonstrate competency with the simulator in their last semester by providing an independently worked solution to a chemical plant design problem.

It has been found that the fundamental ASPEN Plus education is best taught through a watch-and-do method, using a short discussion of a concept, followed by a live application. Consequently, lectures become a forum for demonstration. The homework assignments associated with each lecture are then slightly modified, requiring the students to follow the same keystrokes as they observed during the lecture. In doing so, students learn to navigate the location of the major features of the software, while interpreting the response of the software.

The design project(s) for the course (and subsequent courses) are designed to compel the students to demonstrate a more advanced level of understanding of these features than the laboratory homework. Whenever possible, it is recommended that previously built examples be used to demonstrate new concepts. Homework should also be designed around this principle.

DEFINING BASIC SKILL SETS IN ASPEN PLUS

Because of the many levels of complexity associated with

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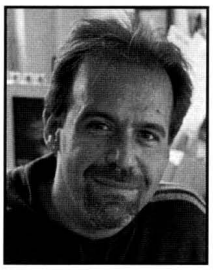

ASPEN Plus, preparing to teach the tool in an undergraduate curriculum can be as intimidating as preparing to learn the software in that same environment. Preparation of a reasonable curriculum that builds upon knowledge learned in previous lessons is critical in the training of students to begin using the software independently. Such a program of study must teach students to

- Specify unit operations in rating and design modes
- Manipulate physical property models and estimate physical property parameters
- Access variables to perform sensitivity analyses and variable optimizations, or to specify design criteria
- Insert user-specified code
- Work with non-conventional materials, pseudocomponents, electrolytes, and solids
- Understand the interoperability of ASPEN Plus

Weekly computation laboratories permit fourteen topics for a standard semester-based program (one of the fifteen three-hour sessions is used for student presentations). Each week gives the opportunity to build up on the concepts of the previous week.

TABLE 1
Weekly Topic Summary

Week	*Topic*
1.	Graphical User Interface, Basic Unit Ops
2.	Distillation Models, Rating Mode
3.	Distillation Models, Design Mode
4.	Stoichiometric Reactor Models
5.	Kinetic Reactor Models
6.	Physical Property Methods
7.	Property Constant Estimation System
8.	Accessing Variables: Sensitivity Analysis
9.	Accessing Variables: Design Specs
10.	Accessing Variables: FORTRAN
11.	Electrolytes
12.	Non-Conventional Solids and Substreams
13.	Optimization and PFD Customization
14.	Interoperability

HOMEWORK SUBMISSIONS

While the students should be aware of the information that can be included in an ASPEN Plus report file, and how to modify such content, it is unnecessary (and a waste of paper) for students to submit a lengthy report for grade evaluation. Most of the simulations in this semester course can be evaluated from a three-page document that includes copies of the flowsheet, the stream table, and the input file. Consequently, it is worthwhile for the instructor to learn to interpret a simulation from the input file. In addition, the input summary generates a header that contains time/date/user information that is unique for each user and file generated. This information is useful in assuring that each student is submitting a unique document.

SUBJECT TOPIC SCHEDULE

The basic schedule of topics discussed in this course (see Table 1) can be categorized into five groups:

(1) Specifying unit operations
(2) Manipulating physical properties
(3) Accessing variables
(4) Specifying nonstandard components
(5) Applying advanced features

Specifying Unit Operations • Early in the course, topics of discussion center on specification of the most important unit operations: the RADFRAC distillation column and the reactor blocks. While these primary units are discussed, units of lower complexity (such as the simple HEATER heat exchanger block) are included in demonstrated process flow diagrams, and are thus also learned. The student becomes comfortable with graphical user-interface (GUI) during these discussions, and is prepared for the more difficult concepts that follow.

Manipulating Physical Property Information • Having established students as "users" of the software, the next step is to demonstrate the methods by which the software treats physical property models and data. In two sessions, the students are shown how ASPEN Plus obtains physical property data, where the information is located within the GUI, and how to generate parameters for components not present in the database. Students initially make property comparisons and generate parameters in the stand-alone mode, then convert their files to simulations.

Accessing Variables • Once students have learned the basics of building a flowsheet, specifying unit operations, and manipulating physical properties, they are ready to begin learning to access and manipulate variables within the software. The ability to create managed objects based on accessed variables is a necessary skill for students to derive from the program of study. Without an understanding of how to access variables, one is unable to perform a sensitivity study, converge process design specifications, or insert user-defined code into a simulation. Thus, the fundamentals of accessing variables in ASPEN Plus is the most important concept beyond flowsheet construction and requires a minimum of three sessions to complete. Tear stream convergence is also considered during these sessions.

Nonstandard components • By this point, students are capable of preparing a relatively sophisticated flowsheet of a *traditional* chemical process in the sense that it contains only conventional database components. Undoubtedly, students have sought to perform simulations of processes that contain aqueous salt systems, non-conventional components, or solids. While performing a simulation with such components is not difficult, specifying such components differs from and is slightly more difficult than simply selecting a species from the database, as is done with standard conventional components. Consequently, it is important that examples and prob-

lems to this point in the course only include conventional components.

The first feature covered in this section is the inclusion of electrolytes in a simulation. The *Electrolyte Wizard* GUI makes this the simplest of the concepts in this section to apply, yet greatly expands the students capabilities within ASPEN Plus.

In the second discussion, *non-conventional solids* and *solid substreams* are introduced, affording the student the capability of including heterogeneous solids in a simulation. This discussion leads quickly to the ability to specify *Solids* separation unit operations.

Advanced User Features • Students have now become proficient in applying the simulator, and many have developed the confidence to explore and apply some of the advanced features on their own. The final two sessions supplement the students' simulation capabilities by presenting them with options for fine tuning their programs, and enhancing the presentation of their works. In the first session, the *optimization* and *constraint* capabilities are demonstrated. These features are contained with the *sensitivity analysis* feature in the *model analysis tools* folder, thus students already know of their existence, and some have likely used these attributes. Customization of the PFD is also considered.

In the final session, students learn of the software interoperability, with emphasis on integrating the numerical results of the simulation with a spreadsheet. The spreadsheet can be designed to perform subsequent equipment sizing and economic calculations.

Advanced Elective Content • The described fundamental education in ASPEN Plus prepares the student for an elective course containing advanced simulator concepts, including: specifying pseudocomponents; working with the MULTIFRAC multiple column model; minimizing utilities with MHeatX, rating exchangers with the HeatX block, writing ActiveX code to run the simulator in the background of a spreadsheet, and ultimately, preparing a USER2 block based on FORTRAN code and seamlessly integrating the block into the software.

Demonstration Lecture Details

❒ *Week 1: Graphical User Interface, Basic Unit Ops*

The introductory session should be informative, entertaining, and, most importantly, not intimidating. The instructor should open the software and build the first flowsheet from a blank page, rather than start with the program opened to a completed flowsheet. It is critical that the first example be simplistic, with the emphasis of the first session more on becoming familiar with navigating the software than with the details of the unit operations. A suggested protocol for this session is

1. Discuss the need for chemical process simulation.
2. Explain the origin of ASPEN Plus (Advanced Simulator for Process Engineering).
3. Discuss good flowsheeting practices (build large flowsheets a few blocks at a time to facilitate troubleshooting; check that units for input data match values entered; ensure inputs are reasonable; check that results are consistent and reasonable).
4. Navigate through the key features of the software, including such items as the menu bar, tool bars, process flowsheet window, model library, the "Next" button, and the reporting functions.
5. Demonstrate common operations, such as switching between the data browser and the process flowsheet window. Perform these common operations by using the toolbar and by using the menu, thereby allowing each user to determine their individual preference, rather than forcing them to use those of the presenter.
6. Establish the variety of unit operations available in the software by scrolling through the items in the module library. Comment on those that will be used regularly, pointing out when each will be covered in the curriculum.
7. Build and solve a simple material and energy balance flowsheet employing only simple unit operations, such as the Heater, Pump, and Flash2 blocks. Use the "Next" button to fill in data upon completing construction of the flowsheet.
8. Specify which property package to use without justification, noting that later sessions will cover physical properties in greater detail.
9. Prepare a report file and manipulate the content of the report file.
10. Demonstrate to the students how to access the input summary for purposes of preparing the submitted documentation of their simulation.
11. Assign a flowsheet identical to the one prepared in class, but request the material and energy balances be performed for a different set of operating conditions associated with the unit operations (*i.e.,* the heat exchanger and flash units operate at different temperatures than used in class).

❒ *Weeks 2 and 3: Distillation Models*

The rigorous distillation model RADFRAC is the workhorse of the separation models in ASPEN Plus. The number of options and capabilities associated with the RADFRAC block are tremendous. Consequently, it should be introduced early in the course to give the student as much time as possible to become comfortable with using it. Each use of the block should be directed toward specific goals to avoid over-

whelming the student, however.

RADFRAC simulations can be performed in *design* or *rating* modes. In *design* mode, the simulation determines the value of operating parameters to achieve specified product criteria; while in *rating* mode, the simulation provides performance data (*i.e.*, flowrates and compositions of product streams) for a column of specified geometry. The modes of operation create a natural break for two lectures.

The design project(s) for the course are designed to compel the students to demonstrate a more advanced level of understanding of these features than the laboratory homework. Whenever possible, it is recommended that previously built examples be used to demonstrate new concepts.

Begin Week 2 with a one-column, two-component, rating mode, RADFRAC simulation. Use a binary system for which data is plentiful (methanol/water) and avoid systems that form an azeotrope (ethanol/water). In rating mode, *Design Specifications* and *Vary* statements are unnecessary since one only seeks to understand the performance of a given column for a specified feedstock. In the absence of these complications, demonstration of Murphree efficiencies and the inclusion of a pressure profile are simplified. Time should be dedicated during this week to considering the wealth of results provided by RADFRAC, as well as to demonstrating the use of the Plot Wizard to visualize results graphically.

Begin the discussion of the design mode in Week 3 by demonstrating use of the DSTWU block (Winn-Underwood-Gilliland method) to estimate the reflux ratio and number of physical stages that are necessary to meet the design specifications of the product stream. Continue working with the same chemical system that was used in demonstrating the rating mode in Week 2. Reinforce to the student that DSTWU results are starting points, based on non-rigorous calculations.

Demonstrate replacing the DSTWU column with a RADFRAC column once the needed design information has been estimated with DSTWU, reconnecting the source and destination streams to the new column. This simulation with RADFRAC will employ the *Design Specification* and *Vary* folders to complete the design calculation, which will also be the first exposure to *Object Managers* in ASPEN Plus. Upon completion of the basic material and energy balance calculations, the simulation can be enhanced with little additional effort to perform tray-sizing calculations, another object manager-based block.

Upon completing these two lectures, students will have been introduced to the basic functions of the RADFRAC block. In addition, the concept of an *object manager* will no longer be foreign, allowing students to confidently explore similar folders.

❒ *Weeks 4 and 5:Stoichiometric and Kinetic Reactor Models*

The primary reactor models with which the student should become familiar can be categorized into three classes: balance-based (RStoich and RYield), equilibrium-based (REquil and RGibbs), and kinetics-based (RBatch, RCSTR, and RPLUG). The first class are the non-rigorous blocks that simply complete a material balance based on specified conversion and yields. The equilibrium-based and kinetics-based blocks use the rigor of equilibrium constants and kinetic rate equations, respectively. As such, this natural distinction should be used to divide the discussion of reactors into two parts.

In Week 4, the reactor blocks are introduced using the balance-based reactors. The object manager into which stoichiometric information is assembled can be demonstrated without the need for a rate equation at this point. In addition, the effect of using this non-rigorous method on the energy balance can be pointed out by performing the simulation by ignoring, specifying, and allowing the simulator to calculate the heat of reaction based on heats of formation, then observing the effect on the duty of the reactor.

In the fifth week, the reactor block capabilities are extended to include the equilibrium-based and kinetics-based blocks, which share kinetic data from the *Chemistry* and *Reactions* subfolders. Students are already familiar with the methods for entering stoichiometry for each reaction at this point. Emphasis can thus be afforded to assuring students understand the reaction types (equilibrium, salt, dissociation, reaction) and the power laws kinetic model (power law, Langmuir-Hinshelwood-Hougen-Watson, reactive distillation, and user-defined models based on FORTRAN code) at their disposal.

❒ *Week 6: Physical Property Methods*

The selection of a property model package tends to be an arduous task for students. To this point in the course, property packages have been specified in demos and on homework assignments without justification, but there have undoubtedly been questions from the more inquisitive students concerning how to select appropriate models.

To address this question, two tasks must be accomplished first. A series of terms relevant to ASPEN Plus physical properties must be defined: property *method*, *model*, *parameter*, and *set*. Secondly, management of Henry's Law components

must be discussed. Point out that Henry's Law can only be used with the Ideal & Activity Coefficient models.

Deliberating justifications for specifying a particular method is usually a necessary aside at this point in the course. It is helpful to summarize this discussion with a graphic decision tree as that provided in Figure 1, providing a quick mechanism for dividing the lengthy list of property methods into two classes. Yet, this interchange does little to further the students' knowledge of the simulator. The educational endeavors associated with Week 6 should include: selecting an appropriate method for a simulation based on the components present; identifying and changing the model used for a physical property calculation when a given method is applied; performing a stand-alone properties analysis; and preparing an object manager containing a user-defined property set for tabulation.

❒ *Week 7: Property Constant Estimation System*

While the ASPEN Plus Database of constituent chemicals is quite large, there is often the need to work with a chemical that is not in the database. The Property Constant Estimation System (PCES) is used to estimate parameters required by physical property models. It is used to estimate (i) pure component physical property constants, (ii) temperature-dependent property constants, (iii) binary interaction parameters, and (iv) group parameters for UNIQUAC. Estimations are based on "group contribution methods" and "corresponding state correlations." Experimental data can be incorporated into the estimation to improve accuracy of results.

The capabilities of the PCES are best demonstrated sequentially. The connectivity of a component is first built in the molecular structure folder, and its properties are generated based strictly on atomic connectivity and molecular weight. The results are improved by then adding some laboratory data for this pure component. Including vapor pressure data demonstrates the input of temperature-dependent data into the data subfolder for a pure component. The estimations are then further improved by including one or more of the functional group contribution methods.

Recommended exercises include

- *Estimate pure component parameters using the general structure method*
- *Define molecular structure using functional group methods and approximate a structure when ASPEN Plus is unable to completely determine all functional groups from the general structure*
- *Incorporate experimental data into a parameter estimation simulation*
- *Compare estimated property results versus experimental values*
- *Apply the PCES Compare function to identify appropriate estimation methods when generating parameters and properties for a component that is similar to a component contained in the ASPEN Plus database.*

❒ *Week 8: Accessing Variables: Sensitivity Analysis*

The ability to access and manipulate the value of a variable in ASPEN Plus represents a knowledge level at which the student becomes capable of preparing simulations of a higher degree of sophistication. The need to modify/record a variable value occurs often in generating a process simulation, particularly when one is attempting to define operating conditions to meet a design specification. The concept of *accessing a variable* refers to references made to flowsheet quantities. It is important to stress that the values of user-entered variables may be manipulated directly; while ASPEN Plus-calculated variables should not be overwritten, but should be varied indirectly.

Emphasis on the introduction to this topic must be on the process of *accessing* variables, and thus the first application should be the least complicated. Introduction of the *Sensitivity Analysis* function provides a tool for applying the accessing variables technique, while providing a user-friendly process evaluation tool that the students can begin using immediately with their design projects, allowing students to study the effect of changes in input variables on process outputs and thus perform rudimentary optimizations. It should also be noted that this method allows one to study the effect of time varying variables using a quasi-steady-state approach. The instructor should demonstrate displaying the results

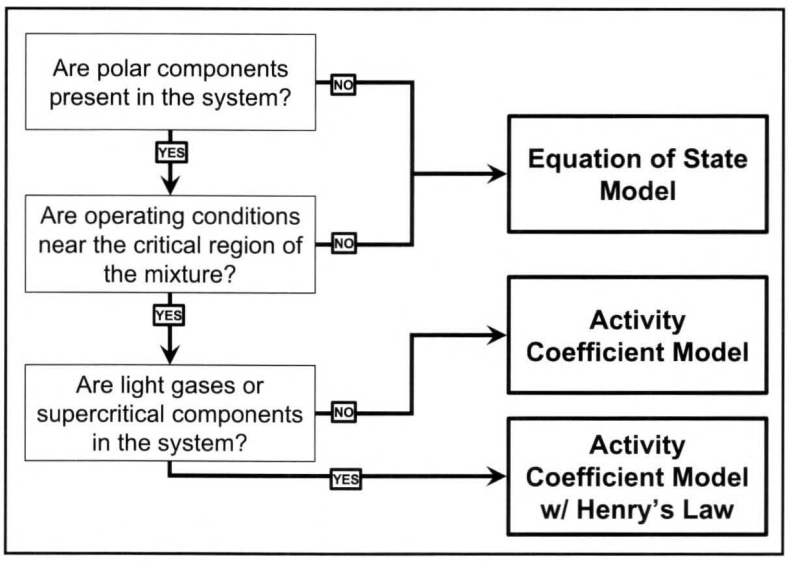

Figure 1. *Decision tree used in selecting an appropriate physical property method in ASPEN Plus.*

graphically based on data in the *Results* form of the sensitivity block object manager, and should point out that changes to flowsheet inputs made by the sensitivity analysis do not affect the simulation as the base-case is run independently.

Homework developed to assess knowledge of the sensitivity analysis should be based on a simulation from a previous homework assignment. A flowsheet with a recycle stream can lead to some interesting results and can lead into a discussion of manual selection and convergence of a tear stream (*i.e.*, a process in which effective convergence of the recycle loop requires user intervention). Emphasis on this material is thus dedicated to the application and interpretation of the accessing variables and sensitivity analysis tools, and expectations of the workload related to these concepts can be increased.

❒ *Week 9: Accessing Variables: Design Specifications*

The *Design Specification* tool in the *Flowsheeting Options* folder provides a type of feedback controller for setting the value of a calculated flowsheet quantity to a particular value. This objective is achieved by manipulating a specified input variable. The *specification* portion of this tool provides a second exercise with *accessing variables*.

It is important to note during this section that design spec calculations are iterative; thus, providing a good estimate for a manipulated variable will help convergence in fewer iterations. This can be best learned by demonstrating a problem that does not seem to work the first time the simulation is run, allowing the students to contemplate the apparent difficulties. During the brainstorming to identify the convergence problem, a checklist of things to investigate can be generated:

- *See if manipulated variable is at one of the bounds*
- *Verify that solution exists over range (hide the design spec and perform a sensitivity analysis)*
- *Confirm the manipulated variable affects the sampled variables*
- *Attempt to provide an improved initial guess*
- *Change the convergence block characteristics (step-size, number of iterations, algorithm, etc.)*

❒ *Week 10: Accessing Variables: In-Line FORTRAN*

The last session covering accessing variables involves manipulating variables within ASPEN Plus through the use of FORTRAN code executed during a simulation run. ASPEN Plus can translate simple FORTRAN statements, with the simulation engine; but complex code requires a FORTRAN compiler. Many engineering degree programs no longer teach FORTRAN, but this does not preclude teaching this tool as the simple FORTRAN is understood by anyone with a structured language background.

When building the simulation that demonstrates the use of inline FORTRAN code, indicate that one must provide access to all flowsheet variables that are to be used within FORTRAN statements, and that all read or written variables must be declared. The execution sequence must also be specified. Further remind students that, as with other accessing variable techniques, only input to the flowsheet should be overwritten by the FORTRAN. When reviewing the simulation output, show that the results of the execution of the FORTRAN block must be viewed by directly examining the values of the variables modified by the FORTRAN block.

❒ *Week 11: Electrolytes*

As noted earlier, the first feature covered in the non-standard materials section is electrolytes. The "Electrolyte Wizard" walks the user through the process of including electrolytes in a simulation. While the wizard makes specifying an electrolyte system simple, there is some information and definitions that need to be provided during this demonstration.

Use of the Electrolyte Wizard

- *Generates new components (ions & solid salts)*
- *Revises pure component databank search order so that first databank searched is ASPENPCD*
- *Generates reactions among components*
- *Sets the property method to ELECNRTL*
- *Creates a Henry's Component List*
- *Retrieves parameters for reaction equilibrium constant values, salt solubility parameters, ELECNRTL interaction parameters, and Henry's constant correlation parameters.*

The student must ensure the simulated chemistry represents the actual system, modifying the wizard-based process as needed. Typical modifications may include

- *Adding to the list of Henry's components*
- *Eliminating irrelevant salt precipitation reactions*
- *Eliminating irrelevant species*
- *Adding species and/or reactions that are not in the electrolyte expert system database*
- *Eliminating irrelevant equilibrium reactions.*

The difference between the True Component Approach (results reported in terms of ions, salts, and molecular species present after considering solution chemistry) and the Apparent Component Approach (results reported in terms of base components present before considering solution chemistry) must be explained.

The limitations of the two approaches should be pointed out. In particular, in the true component approach, liquid/liquid equilibrium cannot be calculated and a number of models cannot be used (Equilibrium reactors: RGibbs, REquil; Kinetic reactors: RPlug, RCSTR, RBatch; Shortcut distillation: Distl, DSTWU, SCFrac; Rigorous distillation:

MultiFrac, PetroFrac). For the apparent component approach, the chemistry may not contain any volatile species on the right side of the reactions, the chemistry for liquid/liquid equilibrium may not contain dissociation reactions, and the input specification cannot be in terms of ions or solid salts.

❑ *Week 12: Conventional-Inert solids, Non-conventional solids & substreams*

ASPEN Plus uses the concepts of *component types, component attributes, substreams,* and *stream classes* to segregate components that require separate equilibria calculations. Conventional components are likely the only component type used to this point in the course. Conventional components participate in vapor/liquid, salt, and chemical equilibria, have a defined molecular weight, and are located in the MIXED substream. Demonstrations and homework to this point should have used only the CONVEN stream class, the default for simulations containing only a MIXED substream.

Understanding the need for multiple substreams, and thus the other *stream classes,* requires an understanding of the two other component types: *Conventional Inert Solids* (CI Solids) and *Nonconventional Solids* (NC Solids). At minimum, it should be pointed out that CI Solids are solids that

- *Are inert to phase equilibrium and salt precipitation/ solubility*
- *May undergo chemical equilibria and reaction with conventional components*
- *Have a molecular weight*
- *Are located in a substream called CISOLID*

while NC Solids are heterogeneous substances that

- *Are inert to phase, salt, and chemical equilibria*
- *Are heterogeneous substances that do not have a molecular weight (e.g., coal, ash, wood pulp, deposited catalytic materials)*
- *May react with conventional or CI Solid components*
- *Are located in the NC substream*

Although these materials are common to commercial chemical processes, they are not necessarily trivial to represent in ASPEN Plus.

Component attributes are typically defined to represent the composition of a component in terms of some set of identifiable constituents as illustrated in Table 2 for the major attribute types. Students must be aware that component attributes are assigned by the user, initialized in streams, and can be modified by unit operation models. An example of a fluidized bed reactor with catalyst regeneration unit is useful to show all three of these concepts.

The number and types of substreams, together with their attributes, define a *stream class*. A stream class can have any number of substreams, but the first substream for each stream class must be of type MIXED. Stream classes include CONVEN, MIXNC, MIXCISLD, MIXNCPSD, MIXCIPSD, MIXCINC, MCINCPSD; where the acronym contains some combination of the substream acronyms MIXED, CISOLID, and NC, and may end with PSD to specify that a particle size distribution has been defined.

Solid properties calculated for conventional components and conventional solids include enthalpy, entropy, free energy, and molar volume using property models in the property method on the *Properties/Specification/Global* form. Enthalpy and mass density are computed by property models specified in the *Properties/Advanced/NC-Props* form.

❑ *Week 13: Optimization Function and Constraints / PFD Customization*

The last couple of sessions of the computation laboratory are used to present subject matter beyond that of the casual user. In the first of the final two sessions, the *Optimization* function is demonstrated as a means to find extrema of an objective function. The objective function is expressed in terms of flowsheet variables and in-line FORTRAN using variable accessing techniques. *Constraints* may be equalities or inequalities. Equality constraints in an optimization are similar to design specifications.

A simple demonstration simulation using both features should be built by following the following steps, identifying each step of the process as it is performed in the simulator:

- *Identify the measured (sampled) variables*
- *Specify the objective function*
- *Specify maximization or minimization of the objective*

TABLE 2
Details of Component Attributes

Attribute Type	*Elements*	*Description*
PROXANAL	Moisture, fixed carbon, volatile matter, ash	Proximate analysis, weight % dry basis
ULTANAL	Ash, C, H, N, Cl, S, O	Ultimate analysis, weight % dry basis
SULFANAL	Pyritic, sulfate, organic	Forms of sulfur analysis, weight % of original coal, dry basis
GENANAL	Up to 20 constituents	General constituent analysis, weight or volume %

function

- *Specify constraints (optional)*
- *Specify the manipulated variables*
- *Specify the bounds for the manipulated variables*

Like design specifications, the convergence of an optimization can be sensitive to the initial values of the manipulated variables. It is best if the objective, constraints, and manipulated variables are in the range of 1 to 100 (accomplished by normalizing the function). Furthermore, it should be stressed that the optimization algorithm only finds local minima and maxima in the objective function. With some objective functions, it is possible to obtain different extrema by starting at a different point in the solution space. A visual demonstration to emphasize this effect will have a lasting impact.

Presentation of the *Optimization* function tends to be completed quickly because the students have already been drilled in the art of accessing variables. Consequently, this discussion can be augmented with a demonstration of the numerous *PFD customizations* that can be applied to the graphical look of the flow diagram, including annotations and OLE Objects. Use the PFD mode to change flowsheet connectivity by adding or deleting unit operation icons to the flowsheet for graphical purposes only. Since the PFD-style drawing is completely separate from the graphical simulation flowsheet, students can improve the visual aesthetics of their flow diagram for use in reports and presentations. One must return to simulation mode to change the simulation flowsheet.

❑ *Week 14: Windows Interoperability*

ASPEN Plus has been designed to achieve a high degree of Windows interoperability. This includes the ability to copy and paste simulation data into spreadsheets or reports, copy/paste flowsheet graphics and plots into reports, create active links between ASPEN Plus and other Windows applications, embed OLE, and automate with ActiveX.

Students value the ability to perform Paste Links (live data links that update applications as the process model is changed automatically propagate results of changes). Most students learn to perform a net present worth analysis in a spreadsheet as a means of comparing project cash flows. Link an ASPEN Plus sensitivity analysis to a spreadsheet that performs a complete net present worth analysis by sizing equipment and estimating capital cost based on key simulation parameters, as well as calculating direct costs based on material and energy balance data. A worksheet based on each run of the sensitivity analysis can be used to graphically build a cost vs. operating parameter figure. If the appropriate operating parameter is used in the sensitivity analysis, a minimum in total cost will be observed in the figure. The direct and indirect costs can be shown as separate additive functions, giving rise to the minimum. Such a demonstration thus represents a strong reinforcement of basic engineering economy concepts.

SUMMARY

ASPEN Plus is the most powerful chemical process simulation tool available, but is not a typical Windows-based program that can be learned by trial-and-error. The most efficient manner to learn the software is through a thought-out curriculum in which examples are introduced in an order that builds on previously learned concepts, and all concepts are reinforced with hands-on demonstrations. Students can complete an undergraduate degree and enter the workforce of the chemical industry with more than a working knowledge of the ASPEN Plus. This can be accomplished without requiring an overly demanding academic workload if the instructor assembles an appropriate curriculum.

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