PROCESS ANALYSIS

An Electronic Version

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Here at Stevens we adhere to the widespread proposition that using the Internet and the Intranet can be substantially beneficial to undergraduate chemical engineering education, both administratively and pedagogically.[1,2] There is also evidence that using software such as spreadsheets and equation solvers[3-5] not only develops the skills and flexibility necessary for ready adoption of different software packages[6] for professional activities in industry, but also substantially supports learning. We believe that effective use of these tools requires a "cultural" change, or enhancement, on the part of both faculty and students. Full course integration is desirable[6] and requires broad faculty participation, which comes slowly in many cases.[7] The skill level and motivation of the students, however, can significantly stimulate the faculty culture.

At Stevens, our initial focus has been on the students. We have attempted to forge a paradigm for a departmental electronic culture in our first chemical engineering course, Process Analysis, that comes in the second term of the sophomore year. Our efforts to do this are summarized in this article.

COURSE SUMMARY

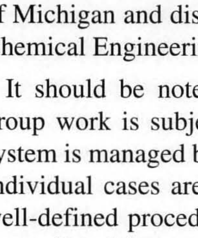
The objectives of the course are to introduce students to chemical engineering, to chemical processing equipment and chemical processes, and to apply material balances and basic phase equilibria to processing systems and the design of equipment from the equilibrium-stage point of view. At the same time, the course is being developed in an electronic environment in order to prepare students for this emerging characteristic of the workplace, to enhance their learning, and to establish a basis for distance learning and asynchronous delivery. By "electronic environment" we mean the ubiquitous use of software for problem solving and transmission, communication between constituencies, presentations, introduction to process simulators, graphics, and computer-aided instruction and learning.

The course, which uses the Luyben and Wenzel text,[8] is summarized in Table 1. Throughout the course the physical and chemical bases of the process or equipment being discussed are emphasized and class discussions are often based on the problem assignments and examples in the text. The students are required to complete a project involving construction or enhancement of a website devoted to a chemical process or to a class of chemical processing equipment, and each group presents its project later in the semester. Throughout the semester, students are encouraged to use the computer-aided instruction modules developed at the University of Michigan and distributed by CACHE (Computer Aids in Chemical Engineering).

It should be noted that the integrity of individual and group work is subject to the Stevens Honor System. This system is managed by the students through an Honor Board. Individual cases are investigated and tried on the basis of well-defined procedures approved by both faculty and students. Penalties range from warnings through grade loss to expulsion from the Institute. All homework and examinations in the course are signed by the students and attest to the fact that they have adhered to the Honor Code.

SOFTWARE

Students are required to purchase computers when entering Stevens. The software suite that comes with the computers includes MS Office Pro 97, Mathcad, Scientific Notebook, X-win32, WinQVT, Netscape, Java, and Matlab. Software used in the course that is not included in this package is available for purchase on campus. An exten-



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sive application of Ethernet supports communications from the academic buildings, computational facilities, and residence halls, and a gateway from the Ethernet is provided for access to the Internet.

WebCT, described at (http://homebrew.cs.ubc.ca/webct) is used to organize the sites summarized in Figure 1, to make grades, examples, and solutions available to the students, to provide E-mail and Bulletin Board communication tools as well as a Calendar. The underlying html files were created with Microsoft Word, except possibly for the student project pages.

TABLE 1
Course Summary

Subject	*Weeks*
Overview of Chemical Industry and Processes Process Equipment: Construction and Operation Process Analyses: Flow Sheets and Process Conditions	3
Mass Balances, Degrees of Freedom, and Chemical Reaction	4
Equilibrium Separations: McCabe-Thiele Analyses	4
Multi-Component Phase Equilibrium: Isothermal Flash	2
Class Presentations	1

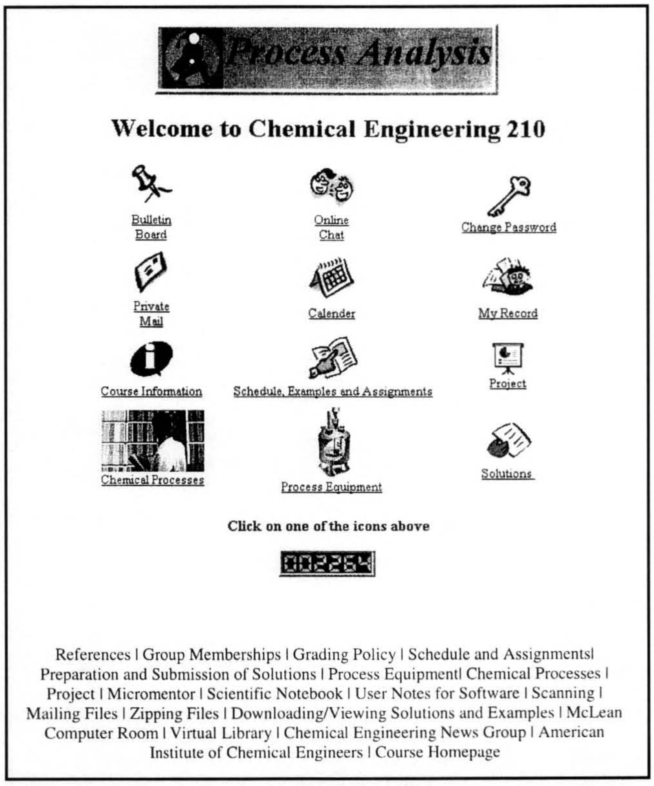


Figure 1. *Course homepage and information hyperlinks.*

The Calendar is used on a class basis to post important events such as examination and assignment due-dates, class activities, vacations, etc. The Calendar can also be used on a personal basis by individual students or the instructor without others being able to view their entries.

Examinations are posted on the Bulletin Board and the students can download/view the examination file. All questions concerning the examination contents are posted on the Bulletin Board along with the responses of the instructor. Postings from both parties may take place at any convenient time and from any convenient location and may be viewed by the entire class. This function is very useful, especially when the exams are not due for several days or over a weekend. Questions involving problem assignments are handled in a similar fashion except that viewing may be limited to the group in question, and the grader for the class may respond as well. The Bulletin Board is also used on a group basis to manage group discussions on project and problem assignments and to transfer files associated with these activities within the group.

E-mail serves the common communication needs as well as being the vehicle for transferring homework, examinations, and project files between two parties. The subject entry on the e-mail message is important for quick overviews of previous messages and for the search function supplied by WebCT.

Scientific Notebook (SNB), found at

http://scinotebook.tcisoft.com

is used primarily for solving systems of nonlinear equations arising from material balances and in phase-equilibrium calculations. SNB has a user-friendly front end with a Maple kernel and supports a word processing format. No special code is required, and SNB can interface with the web and serve as a browser for Tex files. Users can quickly perform symbolic computations, integration, differentiation, matrix and vector operations, and many other more complex computations involved in calculus, linear algebra, differential equations, and statistics. For these reasons, we chose to adopt SNB rather than Mathcad[5,7] or Mathematica.[3] The solution to simultaneous nonlinear equations associated with material balances is illustrated in Example 1, while Example 2 illustrates how SNB is used to solve equilibrium flash calculations.

Microsoft Excel is used for graphical (McCabe-Thiele) solutions of equilibrium-stage problems: stripper with a reboiler, gas absorption and stripping, distillation, and liquid-liquid extraction. We have elected to preserve the graphical construction modality available in Excel for this introductory course rather than the spreadsheet solutions to the material balance equations used at some other institutions.[4] The stage steps are constructed with the drawing tool in Excel.

Distillation is illustrated in Example 3 and extraction in Example 4. Calculations can be done on the spreadsheet or SNB may be used, saved with a screen capturing software (*e.g.,* Snagit) and pasted into Excel. Equilibrium data may be generated from a function (Example 3) or plotted directly as an input data series (Example 4). Stream points are entered as a new data series for convenience when zooming in for stage stepping (Example 3) or zooming out for the operating point in extraction (Example 4).

The course also makes use of the MicroMENTOR system for delivery of the educational software modules developed at the University of Michigan and distributed by CACHE. The modules suggested for use during the class are: UM-Units, UM-Beer, MATBAL, UM-Hawaii, UM-POP, and UM-McCabe. The modules have been required in some cases and left to the discretion of the students in others.

Distill is a program, available from CACHE, that does multicomponent flash and distillation calculations. It considers both the liquid and gas to be nonideal and it includes a database of 98 compounds. The vapor-phase fugacity is calculated with the Redlich-Kwong equation of state. The liquid-phase activity coefficients are based on the Hildebrand solubility parameter. This program is used in several assignments to illustrate the effect of assuming ideal conditions in flash and bubble/dew point calculations for hydrocarbons.

ChemWindows is made available to the students for drawing schematics, flow sheets (see the figure in Example 1, for example) and chemical formulae. They have not yet been required to use this software and may use others if they wish.

EXAMPLE 1

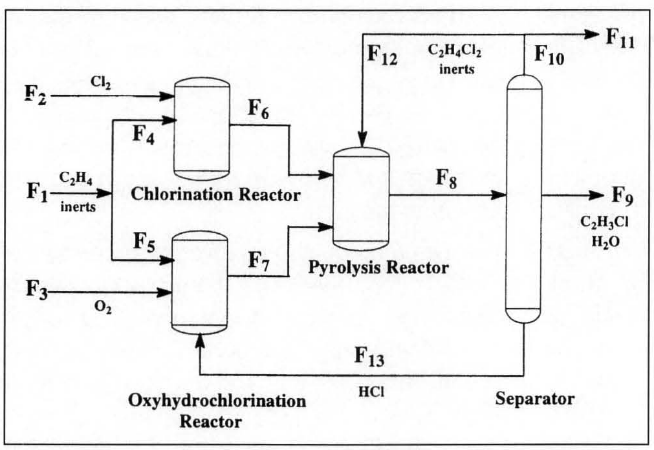


Figure 1

The flow diagram in Figure 1 illustrates a simplified version of the main steps in the production of vinyl chloride (C_2H_3Cl) from ethylene (C_2H_4). The reactions, which occur separately in the different reactors, are:

Chlorination: $C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2$

Oxyhydrochlorination: $C_2H_4 + 2\ HCl + 1/2\ O_2 \rightarrow C_2H_4Cl_2 + H_2O$

Pyrolysis: $C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl$

The ethylene feed, F_1, is 90 mole % ethylene and the remainder is inerts. The chlorine and oxygen feeds, F_2 and F_3, respectively, are pure. All of the ethylene, oxygen, and chlorine react and all of the hydrochloric acid (HCl) fed to the oxyhydrochlorination unit reacts.

Only 50% of the total dichloroethane ($C_2H_4Cl_2$) fed to the pyrolysis reactor is converted, with the remainder being separated and recycled with inerts in stream F_{12}. The inert concentration in the recycle stream is 50 mole %. Pure hydrochloric acid (HCl) is recycled in stream F_{13}. The final product stream, F_9, consists only of vinyl chloride and water.

Determine all of the unknown flow rates, F_j, and mole fractions, $x_{i,j}$ (mole fraction i in stream j). Set F_1=1 mole/hr as a basis. The species are labeled as shown in the following Table 1.

TABLE 1
Labeling of Components

Species	*Index*	*Species*	*Index*
C_2H_4	1	$C_2H_4Cl_2$	5
Cl_2	2	C_2H_3Cl	6
HCl	3	H_2O	7
O_2	4	Inerts	8

SNB solves the material balance equations given in Figure 2 in SNB format (single column) in less than one minute. The solution is shown in Figure 3 after some reordering for convenience.

$F_2=0.90F_4$	$0.50(x_{5,6}F_6+x_{5,7}F_7+0.50F_{12})=x_{6,8}F_8$
$F_3=(0.90/2)F_5$	$0.50(x_{5,6}F_6+x_{5,7}F_7+0.50F_{12})=x_{3,8}F_8$
$F_4+F_5=F_1$	$x_{7,7}F_7=x_{7,8}F_8$
$x_{5,6}F_6=0.90F_4$	$x_{8,6}F_6+x_{8,7}F_7+0.50F_{12}=x_{8,8}F_8$
$x_{8,6}F_6=0.10F_4$	$x_{3,8}+x_{5,8}+x_{6,8}+x_{7,8}+x_{8,8}=1$
$x_{5,6}+x_{8,6}=1$	$x_{3,8}F_8=F_{13}$
$x_{7,7}F_7=0.90F_5$	$x_{5,8}F_8=0.50F_{10}$
$x_{5,7}F_7=0.90F_5$	$x_{6,8}F_8=x_{6,9}F_9$
$F_{13}=2(0.90F_5)$	$x_{7,8}F_8=x_{7,9}F_9$
$x_{8,7}F_7=0.10F_5$	$x_{8,8}F_8=0.50F_{10}$
$x_{5,7}+x_{7,7}+x_{8,7}=1$	$x_{6,9}+x_{7,9}=1$
$0.50(x_{5,6}F_6+x_{5,7}F_7+0.50F_{12})=x_{5,8}F_8$	$F_{10}=F_{11}+F_{12}$

Figure 2. Material Balances

$F_2 = .5, F_3 = .2, F_4 = .55556, F_5 = .44444,$
$F_6 = .55556, F_7 = .84444, F_8 = 3.6, F_9 = 1.2,$
$F_{10} = 1.6, F_{11} = .2, F_{12} = 1.4, F_{13} = .8,$
$x_{3,8} = .22222, x_{5,8} = .22222, x_{6,8} = .22222, x_{7,8} = .11111, x_{8,8} = .22222,$
$x_{5,6} = .9, x_{8,6} = .1,$
$x_{5,7} = .47368, x_{7,7} = .47368, x_{8,7} = 5.2632 \times 10^{-2}$
$x_{6,9} = .66667, x_{7,9} = .33333. F_1 = 1.0$

Figure 3. Solutions

EXAMPLE 2

A petrochemical stream consisting of 30 mole % propane, 10 mole % n-butane, 15 mole % n-pentane, and 45 mole % n-hexane is to be flashed to 200 kPa. **(a)** Determine strict bounds on the operating temperature. **(b)** Find the vapor flow rate per unit of feed and the product compositions for a temperature mid-way between these limits. The equilibrium data are given in Table 1.

TABLE 1
Phase Equilibrium Data

Equilibrium data: $y = Kx$, $T = °R$, and p = psia:

$$\ln K(T,p) = (a_1/T^2) + a_3 + b_1 \ln p + (b_3/p)$$

Species	a_1	a_3	b_1	b_3
C_3H_8	-970,688.5625	7.15059	-0.76984	6.90224
n-C_4H_{10}	-1,280,557	7.94986	-0.96455	0
n-C_5H_{12}	-1,524,891	7.33129	-0.89143	0
n-C_6H_{14}	-1,778,901	6.96783	-0.84634	0

The solution procedure in SNB is as follows:

The functions in Figure 1 are defined in SNB format. Bounds for the bubble and dew points of the feed are at unity K values for propane (j=1) and n-hexane (j=4). These values are obtained from the roots of the K function at the prevailing values of p (200 kPa) and j. The solutions are shown in SNB format in Figure 2. The bubble and dew points of the feed are roots of the associated functions at the prevailing p. The results in SNB format are shown in Figure 3. The vapor flow at the midpoint temperature, 561.4°R, is obtained similarly and is shown in Figure 4.

Equilibrium: $$K(i,T,p)=\exp\left(\frac{a_{i,1}}{T^2}+a_{i,3}+b_{i,1}\ell n\,p+\frac{b_{i,3}}{p}\right)$$

Bubble point: $$f(T,p)=1-\sum_{i=1}^{4}K(i,T,p)z_{i,1}$$

Dew point: $$g(T,p)=1-\sum_{i=1}^{4}\frac{z_{i,1}}{K(i,T,p)}$$

Isothermal flash: $$h(\vartheta,T,p)=\sum_{i=1}^{4}\frac{z_{i,1}[K(i,T,p)-1]}{1+\vartheta[K(i,T,p)-1]}$$

Figure 1

$$\frac{a_{j,1}}{T^2}+a_{j,3}+b_{j,1}\ell n p+\frac{b_{j,3}}{p}=0,\quad T\in(0,\infty)$$, Solution is $\{T=657.27\},\{T=449.88\}$

Figure 2

$f(T,p)=0$, $T\in(449,658)$ Solution is $\{T=509.27\}$ $g(T,p)=0$, $T\in(449,658)$ Solution is $\{T=613.54\}$

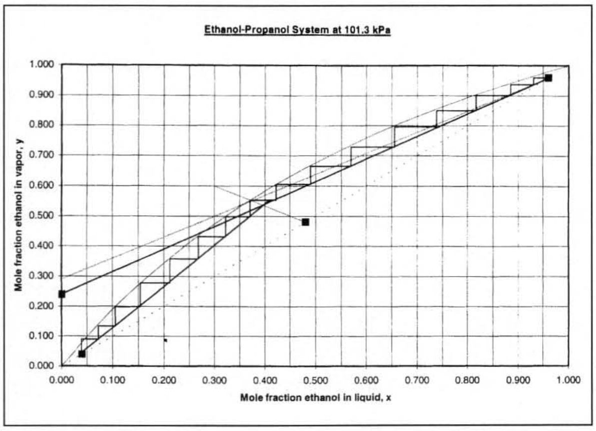
Figure 3

$h(\vartheta,T,p)=0$, $\vartheta\in(0,1)$ Solution is $\{\vartheta=.37704\}$

Figure 4

EXAMPLE 3

Find the number of stages, the best feed location, and the minimum reflux ratio for a distillation column that separates ethanol and propanol at 101.3 kPa. The ratio of the vapor pressure of ethanol to the vapor pressure of propanol is approximately constant at 2.10. The feed is 48 mole % ethanol and 40 mole % liquid. The distillate and bottoms compositions are to be 96 mole % and 4 mole % ethanol respectively. There is to be a total condenser overhead with no sub-cooling. The reflux ratio is 3.0. The graphical construction is shown in the figure in Excel format.



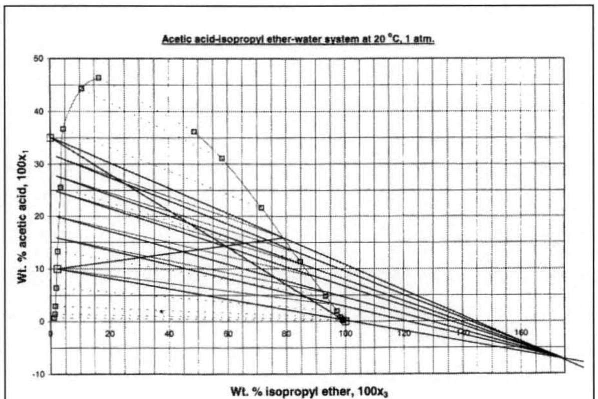
EXAMPLE 4

Acetic acid (species 1) is to be extracted from water (species 2) using isopropyl ether (species 3) as the solvent at 20°C and 1.0 atm. The feed rate is 1000 kg/hr and contains 35 wt % acid in water. The solvent flow rate is 1475 kg/hr and is essentially pure ether. The raffinate is to contain no more than 10 wt % acid. Find **(a)** the minimum solvent flow rate, **(b)** the number of equilibrium stages required for the separation, and **(c)** the outlet concentrations and flow rates. Equilibrium data at the operating conditions are given in the Table and the graphical construction in Excel is shown in the figure.

Water Layer		Ether Layer	
x_3	x_1	x_3	x_1
1.2	0.69	99.3	0.18
1.5	1.41	98.9	0.37
1.6	2.89	98.4	0.79
1.9	6.42	97.1	1.93
2.3	13.3	93.3	4.82
3.4	25.5	84.7	11.4
4.4	36.7	71.5	21.6
10.6	44.3	58.1	31.1
16.5	46.4	48.7	36.2

◄ ***TABLE Phase Equilibrium Data***

▼ ***FIGURE Excel Constuction for Example 4***



FILE HANDLING

An extraordinary amount of time is required to open files to learn the source and/or the contents. This is especially true if more than one course is underway. Consequently, labeling of files is very important. Points are deducted from assignments and examinations (which may not even be accepted in some cases) if the established procedures are not followed. No files are accepted unless adherence to the Honor Code is pledged by the students at the end of the file.

Homework files are prepared weekly by students working in groups. The assignments are numbered and are generally specific problems in specific chapters of the text. Solutions to individual problems are labeled as gxpy-zc210.(tex, rap, doc, xls,...) where x is the group number, y is the chapter, and z is the problem number. The individual solution files are then assembled in a single archive, with WinZip for example. The archive is labeled gxayc210.zip where x is the group number and y is the assignment number. The archive is attached to an e-mail message with an informative subject entry and mailed to the instructor. The archives are placed in a directory named with the group numbers. Solution files for each problem are posted for downloading after the due date for the assignment.

Examination files include a reference to the individual student: exmc210qnabz.(tex, rap, doc, xls,...), where m is the examination number, n is the question number, ab are the student initials, and z is the group number. We have not encountered students with the same initials in the same group yet, but many modifications are possible to handle such an event. The examination files are then grouped in an archive labeled exmc210abz.zip and attached to a relevantly labeled e-mail message to the instructor. The archives are then placed in a directory named with the examination number.

Copies of files received by the instructor are forwarded by e-mail to the grader. The grader is not permitted to accept files directly from the students. The grader has a set of directories similar to those used by the instructor, described above. The grader uses several additional subdirectories associated with the grading process. One directory is for graded files, one for ungraded files, and one for the archive in process of being graded. After the files are graded and the comments and points included, the files are returned directly to the students, the grader retains a copy, and a copy of the file is sent to the instructor. The same file name is retained so that the instructor can replace the previously ungraded file with the graded one in his directory. It has always been possible to track down "missing" files with this procedure.

The grader is responsible for posting grades in WebCT, but a separate grade file is maintained by the instructor and updated with each new assignment or examination. The grade file maintained by the instructor is the official one so that grades, once recorded, cannot be changed without the instructor updating this file. Grade access is limited to the student, the grader, and the instructor, but statistical information is generally available.

PROJECT

The objectives of the project are for the student to gain a special familiarity with a specific chemical process or a category of chemical process equipment and a significant experience with web-based presentation of technical materials. The students are also required to present their projects to the class, electronically if desired.

The bases on which the sites are initiated or enhanced are summarized below.

A) Process equipment (nine sites at present covering major equipment categories):

1) Purpose and operating principle(s)
2) Historical background
3) Construction—schematic/illustrations
4) Pictures of actual equipment
5) Range of duties—sizes
6) Maintenance required
7) Utilities required
8) (Some) design equations
9) References

B) Chemical Processes (nine sites at present spanning range of top 50 chemicals):

1) Chemical formula and form/state of product
2) Uses and market price
3) Historical industry development
4) Common methods of production with raw material sources and side products
5) Major companies, production methods, and production levels
6) Details for a common production method: process chemistry with implications for most favorable process conditions; flow sheet(s); operating conditions and problems; environmental considerations; production costs; utility requirements; hazards; handling of waste and side products
7) References

C) Grading (Engineers from EXXON Research and Engineering and experienced faculty outside the department contribute to site assessment):

1) Content (see above)
2) Layout/format
3) User friendliness
4) Use of colors and graphics
5) Use of relevant hyperlinks and other resources

Html files are prepared or edited with software that is generally available to the students, such as Microsoft Word, or that is the individual preference of the students. Scanning hardware is used for some picture files, which can be edited with Photopaint. The completed project files, including images (gif, jpeg,...) are collected in an archive and mailed to the instructor as described above.

DISCUSSION

The students very quickly become accustomed to the electronic communication features of the course and the file-handling procedures. It is, however, helpful to deduct points for improper file labeling as well as to not answer exam questions online unless posted for viewing by the entire class. Off-campus students find the electronic version helpful and students generally like the option of transferring files and posing questions at their convenience. Such items appear at all hours of the day. For the solutions to assignments, the availability of examples for downloading by the students is crucial for each new application.

The use of SNB for material balances has greatly improved the sophistication and ability of the students to write an independent set of material-balance equations and to be acutely aware of the degrees of freedom. They are also able to spot-check their solutions with quick calculations using time components, inerts, etc. Most students begin with doing the solution on paper and transferring it to SNB. They soon progress, some to doing the solution completely online. A series of user sessions would be helpful at the beginning for learning the software. Some students have prior experience in mathematics classes, which is beneficial. Students have voiced a preference for SNB to similar software packages, but these alternatives have not been explored in a formal way.

The use of Excel for graphical multistage constructions has been very successful and well accepted by students. Errors can be quickly corrected. The students cannot imagine doing liquid-liquid extraction constructions by hand.

When not required, the computer-aided instruction modules in MicroMENTOR are not extensively used. Use of the modules is greatly increased if the students are held accountable, for example, in class discussions on the Bulletin Board of WebCT. The modules, once used, are considered helpful.

Distill is viewed as inconvenient by the students, although the results are very elucidating for comparison purposes. For this reason and for broader objectives, it may be worthwhile to introduce Aspen in a limited way at this stage.

ChemWindows is viewed primarily as a cosmetic add-on for problem assignments when not required. It is used for all examination drawings and for some project work. As it significantly enhances the quality of the presentation, we are introducing some limited requirements for its use.

The class projects have been most successful and well received by the students. The project and equipment sites they have developed are being made an integral part of the course. The students are extremely creative and enthusiastic about finding relevant materials on the Web and using other resources to develop or enhance their site. The technical content of the class presentations attests to the learning component that is present in the projects. The students very easily adopt a full range of software to suit their personal needs for developing the required html files and exploit the extensive range of picture files available on the Web.

The electronic approach used in Process Analysis has been repeated with much less effort by the author in Transport Phenomena, a course offered in the following semester. The approach has not yet been extended further across the chemical engineering curriculum. Software is, however, used in all of the courses to some extent and coding is required in several classes. The students have been observed using the specific skills (especially the graphical solution to multistage equilibrium separations) and exhibiting the electronic dexterity they gained in Process Analysis in subsequent courses.

The time commitment and the background that must be acquired on the part of faculty in order to develop an electronic version of a course as defined here are important related issues and tied very much to the available support and the electronic environment. It must be generally recognized, however, that significant effort is required which must be explicitly recognized and supported within the local educational context and the electronic capabilities of its constituencies. The benefits include presentation of a course in an environment that anticipates the workplace, that is more adaptable to the different life styles of the students, and that can be conveniently modified and maintained with no more effort than a conventional course. The electronic version is more supportive of the learning process and allows more spontaneity and interaction, especially when the students are networked with their own computers. A greater focus on problem structure and formulation can be realized as well as a pronounced increase in the specific and general electronic skills of the students.

REFERENCES

1. Bungay, H., and W. Kuchinski, "The World Wide Web for Teaching Chemical Engineering," *Chem. Eng. Ed.,* **29**(3), 162 (1995)
2. Marr, D.W.M., and J.D. Way, "Using the Intranet in ChE Instruction," *Chem. Eng. Ed.,* **31**(2), 110 (1997)
3. Al-Dahhan, M.H., "Computing in the Undergraduate ChE Curriculum," *Chem. Eng. Ed.,* **29**(3), 198 (1995)
4. Burns, MA., and J.C. Sung, "Design of Separation Units Using Spreadsheets," *Chem. Eng. Ed.,* **30**(1), 62 (1996)
5. Sandler, S.I., "Spreadsheets for Thermodynamics Instruction: Another Point of View," *Chem. Eng. Ed.,* **31**(1), 18 (1997)
6. Davis, J.F., G.E. Blau, and G.V. Reklaitis, "Computers in Undergraduate Chemical Engineering Education," *Chem. Eng. Ed.,* **29**(1), 50 (1995)
7. Harb, J.N., A. Jones, R.L. Rowley, and W.W. Wilding, "Use of Computational Tools in Engineering Education," *Chem. Eng. Ed.,* **31**(3), 180 (1997)
8. Luyben, W.L., and L.A. Wenzel, *Chemical Process Analysis: Mass and Energy Balances,* Prentice Hall, Englewood Cliffs, NJ (1988) ❒