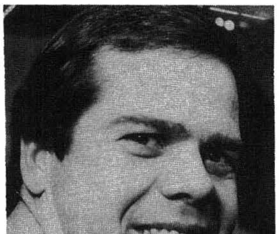
USING SPREADSHEETS FOR TEACHING DESIGN

ERIC A. GRULKE
Michigan State University
East Lansing, MI 48824-1226

THE RAPID INTRODUCTION of microcomputers into the workplace over the past five years has changed the standard "toolkit" for the practicing engineer. We can now expect that our graduating engineers will have microcomputers available either near or on their desks. The software on these computers will probably include a word processor, a graphics package, a spreadsheet, BASIC, FORTRAN, or PASCAL compilers, and a set of statistical and mathematical subroutines. We want our Michigan State students to use similar facilities and software during their time on campus. We recognize that some job assignments will require the use of computer-aided design with graphics, process design packages, dynamic simulators and on-line process control and are trying to provide some exposure to these techniques.

Of the items in the standard toolkit, a spreadsheet program is particularly well-suited to performing the repetitive calculations needed to solve many chemical engineering problems. Students in our department have used spreadsheets for assignments such as numerical integration of absorber design equations and two-dimensional heat transfer problems. Once the equations for a problem have been set up in a spreadsheet format, calculations for new conditions or assumptions can be done rapidly. When the basic problem has been correctly solved, the student can study the response of the system to other inputs without long hours of additional computation. This fast computation for new conditions allows the instructor to deal with some problems in greater depth without excessive demands on student time.



Eric A. Grulke has BChE, MS, and PhD degrees in chemical engineering from the Ohio State University. He worked as a research engineer for the BFGoodrich Chemical Group from 1975 to 1978. In 1978, he joined the chemical engineering department at Michigan State University. His research projects are centered around mass transfer and separations, including polymer devolatilization and phase equilibria, and separations in biochemical processes.

We have been experimenting with spreadsheets in our process design course, where recomputation is a fact of life. Spreadsheets permit computations using formulas to be executed in the form of a table [1,2,3,4,5]. We find that spreadsheets help our students solve design problems more efficiently. The organization of the design problems for a spreadsheet solution gives the student a methodology for finding a design answer.

INTEGRATING MICROCOMPUTERS INTO COURSES

Our college of engineering is now providing a standard "toolkit" of word processing, graphics, spreadsheet and scientific language packages on IBM XT microcomputers. In the Case Center for Computer Aided Design (Prime computer), we have the CHEMSHARE process design package which was recently installed by Dr. Jayaraman of our department. We have been working hard to integrate problems using this hardware and software into our undergraduate and graduate courses. We would like our undergraduate students to be able to use all these tools by the time they reach the process selection and optimization course in the middle of the senior year.

To accomplish this goal, we have been developing problems to be done on the microcomputer for a number of our undergraduate courses. Don Anderson has written software for energy and material balances with graphics and has used it in our energy and material balances course. Dr. Jayaraman has included a CHEMSHARE problem in the process optimization methods course. Dennis Miller has used a CHEMSHARE problem on multicomponent distillation in our course on stagewise separations. Daina Briedis has a two-dimensional heat transfer problem implemented on a spreadsheet in a transport phenomena class. Students in our two laboratory courses are encouraged to use the word processors for writing their final laboratory reports. In 1984, we introduced spreadsheeting in our process design course for both balances and economics. In 1985, Martin Hawley and Dr. Jayaraman used CHEMSHARE for three of the five design problems. We plan to include CHEMSHARE and microcomputer problems in the transport phenomena and separations sequence taught in the junior year as well as in the phase and chemical equilibria course. We hope that the continual use of these computer tools will prepare out undergraduates for the new work environment.

SPREADSHEETS FOR BALANCES AND ECONOMICS

Spreadsheets provide an easy way for students to perform material and energy balances without a process design package. They are adequate for performing the balances needed for moderate size processes except for problems with many recycle streams. Some can even handle modest models for equipment performance. While a process design package such as CHEMSHARE may be easier to use, the spreadsheet does have one advantage. The student is responsible for all spreadsheet input and knows which thermodynamic equations, reactor models, and heat transfer correlations have been used. Spreadsheets relieve the drudgery of recalculating cash flow tables when economic assumptions are changed.

CHOOSING A SPREADSHEET

There are a number of factors to consider when choosing a spreadsheet for process design calculations. The physical location and administration of microcomputers on your campus may place some constraints on the software you select. At Michigan State, we like to provide students 24-hour access to the computing facilities. While our microcomputer labs are almost always open, the rooms are not attended. Therefore, we prefer software which can be installed on the hard disk (legally) and accessed at any time.

Microcomputers are clustered in several rooms in the engineering building at Michigan State. These sites are run by the Engineering Computer Facility, which maintains the software, provides aid to the students, and retains documentation at its central office. We would like to provide 24-hour access to software documentation at each site, but have not found an easy method for doing so. Documentation is available for check-out at the engineering library located in the building. We have also used the microcomputer lab located in the main library. We have not installed software at sites remote from the engineering building because of the lack of convenient ways to retain documentation.

. . . we like to provide 24-hour access to the computing facilities. While our microcomputer labs are almost always open, the rooms are not attended. Therefore, we prefer software which can be installed on the hard disk and accessed at any time.

In order for our students to trouble-shoot their own problems and teach themselves some commands, the software documentation must be well-written, well-organized and well-indexed. We provide them with a "primer" for the spreadsheet which includes information on starting the program, file transfers, editing commands, formulas and functions, and examples of typical screen displays. Tutorials supplied with the software also help. Our most efficient method for getting students acquainted with a spreadsheet is an example problem, which will be discussed in a later section.

The characteristics of the software are also important. A fairly complete set of mathematical functions is preferred. These should include logarithms, exponentials and trigonometric functions. Logic functions and conditional expressions, such as maxima, minima and sums, are also useful. Many of the business spreadsheets have these functions. Some also have graphing capabilities, which can assist the students in preparing reports and presenting homework problems. We prefer software graphics in which the material appearing on the screen is the same as that appearing on the printed page.

It is important to try the software you intend to purchase on the hardware you intend to buy. You'll want to be sure that the printer supports the character fonts supplied with the spreadsheet and that the microcomputer has sufficient memory. On IBM-compatible hardware, an 8087 math coprocessor chip speeds program execution and is recommended.

The key elements in our choice of spreadsheet were not the technical features of how large the program was, how formulas and text were entered, or the details of editing. We were most concerned with software which could reside permanently on the hard disk, which had clearly written documentation with a good index, and which had easy-to-use on-line help.

Supercalc III® provided the best balance of characteristics at the time we made a choice and has functioned well in the MSU environment.

TEACHING THE SPREADSHEET

I try to do as little teaching of the spreadsheet in class as possible. Table 1 contains a portion of a cash-flow table for a methanol process used to illustrate the use of a spreadsheet. Sections of the table are easy to show by making overhead transparencies. The formulas entered into the cells can be displayed while the commands needed to enter them are described. Copies of these example problem files are kept on the hard disk so that students can refer to them as they do their assignment. The example files help the students learn how to organize and construct a spreadsheet. They also provide motivation to use the microcomputers.

I usually end the example problem discussion by suggesting some changes in the problem which require new computations. The advantages of rapid data changing and recalculation quickly become obvious.

USES FOR PROCESS DESIGN

I have used spreadsheets to perform material, enthalpy, and entropy balances for modest size processes (20-40 streams) and for generating equipment cost, capital investment cost, manufacturing costs, and cash flow tables. I can solve the base case design faster using a spreadsheet and can quickly identify high-cost portions of the process for further analysis. This gives me more time to consider design alternatives and decide how to help the students think about the problem.

The spreadsheets provide a convenient format for discussing problem solutions with graders and teaching assistants. They can sit down at the micro and see for themselves the effects of changing assumptions or process conditions. The spreadsheet makes it easy to check solutions of students who may have used different correlations or assumptions. It is particularly helpful in checking the work of students who had a design idea which the instructor did not consider!

CASH FLOW ANALYSIS

Table 1 illustrates a cash flow analysis for a methanol process. In this particular example, the plant is two years in construction and the desired cash flow rate of return is 30%. Students are able to follow example problems such as this and can easily construct similar tables for their design problems. The items in the data block below the title (rows 6-13) are all inputs to the cash flow analysis. Changing the entries in this table will allow recalculation of the spreadsheet. In this problem, the students were to find the selling price needed for discounted cash flow rate-of-return of 30%. This can be done by iterating the selling price until the sum of the present values of the cash flow is zero.

TABLE 1
Methanol Economics: Selling Price for 30% DCF Rate of Return

Cash Flow Analysis: Costs in K $

Capacity, M gpy	100000	
Depr. Cap, M$	70831	str. line
Plant Life	10	years
DCF Rate	.3	
Tax Rate	.5	
Selling Price	.853	$/gallon
Annual Revenue	85300	K $
Manuf. Costs	31450	K $
Working Capital	2151	K $

Item			**Year Start-up**			
	85	**86**	**87**	**88**	**89**	**90**
Cap. Outlay	–70831	0	0	0	0	0
Working Cap.	0	–2151	0	0	0	0
Revenue	0	0	85300	85300	85300	85300
Manuf. Costs	0	0	31450	31450	31450	31450
Depreciation	0	0	7083	7083	7083	7083
Expenses	0	0	38533	38533	38533	38533
Taxes	0	0	23383	23383	23383	23383
Net Profit	0	0	23383	23383	23383	23383
Cash Flow	–70831	–2151	30467	30467	30467	30467
Total Cash Flow	–70831	–72982	–42515	–12049	18418	48884
Present Value, Cash flow	–70831	–1655	18028	13867	10667	7206
Sum of Present Value of Cash Flow		27				
Payout Period	2.32 years					

MATERIAL AND ENERGY BALANCES

Spreadsheets provide a method for structuring material and energy balances when a process design package is not available. Students can discover how to organize their problem and detect balance errors as the subsections of the design are solved.

Table 2 shows a portion of a spreadsheet for solving material, enthalpy, and entropy balances for a distillation column using vapor recompression. The stream numbers are related to a process flow diagram. Each column represents the properties for one stream and includes the flow, the enthalpy and the entropy of the individual components. The liquid-vapor index in the third row ($L = 1$, $V = 2$) is used to include the latent heat in the enthalpy calculations for vapor streams. The enthalpies and entropies are calculated from heat capacity models generated from data around the expected operating conditions. Rather than use a complete model for the heat capacity, we suggest linearizing the data to generate a two constant model applicable in the temperature range of interest. This reduces computation time without much loss in accuracy.

We suggest that the students use "built-in" checks of their energy and material balances. It is easy to set up the overall balances of material and enthalpy around specific process sections at cells outside of the main set of equations on the spreadsheet. This technique allows the student to find balance errors quickly and easily. The last two rows of Table 2 show calculations of compressor work (the difference between the total enthalpy flow of streams 2 and 3) and heat of condensation from the compressed vapor available for boiling bottoms liquid in the reboiler (the difference between the total enthalpy flow of streams 3 and 4). The enthalpy change across the compressor will be used to check its efficiency. The enthalpy change of the condensing stream will be compared to the enthalpy change of reboiled liquid to ensure that the energy flows around the reboiler balance.

One common error of students is formulating a spreadsheet to calculate the material and energy balances for the complete process with very few manual data inputs. The students may try to write the complete spreadsheet file without checking interim calculations. It is usually wiser and more efficient to perform many checks on interim calculations as the balances are being entered, just as a computer programmer would check code for errors as it is being written. For example, I routinely show the energy inputs and outputs around distillation columns to make sure that I have not neglected condenser cooling water or reboiler steam. It is particularly important to resist the temptation to make the spreadsheet iterate on processes with many recycle streams. The spreadsheet is not a sophisticated equation-solver. Some recycle calculations do not converge uniformly and, unless they have done the calculations by hand prior to programming, students may waste a lot of time discovering this. It does not seem convenient to use equipment design algorithms as a part of the energy and material balance spreadsheet (such as would be included in a process design package like CHEMSHARE).

TABLE 2
Section of Material and Energy Balance Table for Vapor Recompression Process

MATERIAL AND ENERGY BALANCES
Vapor Recompression—EtOH Distillation

Stream No.	**1**	**2**	**3**	**4**
Stream ID	Column Feed	Ovrhd. Vapor	Cmprsr. Outlet	Condsr. Outlet
Property				
T, F	198	172.8	254	254
P, psia	14.7	14.7	68.13	68.13
L = 1, V = 2	1	2	2	1
W, lbmol/hr	22898	3857	3857	3857
EtOH, x	.0416	.86	.86	.86
H, Btu/lbmol	5201	21328	22997	6955
S, Btu/lbmol-F	9.11	34.62	37.1	11.67
H_20, x	.9584	.14	.14	.14
H, Btu/lbmol	2988	20437	20851	3641
S, Btu/lbmol-F	5.23	32.83	33.01	6.2
H, Btu/lbmol	3080	21203	22696	6491
S, Btu/lbmol-F	5.39	34.37	36.25	10.9
H flw, K Btu/hr	70520	81781	87540	25037
S flw, KBtu/hr-F	123.5	132.6	139.8	42
Compressor Work				5759 K Btu/hr
Reboiler Heat				62503 K Btu/hr

TABLE 3.
Fermentor Section of an Equipment Cost Table for a Novobiocin Process

Fermentor Section

Item	**Number**	**Size**	**Units**	**Cost, K$**	**Ref.***
R-1 Fermentor	8	10625	gallons	615391	p.790
T-1 Innoculum Tank	1	850	gallons	19356	p.791
A-1 Agitator for T-1	1	1.8	HP	4014	p.572
P-1 Pump for T-1	1	85	gpm	1188	p.556
T-2 Acid Tank	1	850	gallons	12820	p.572
P-2 Pump for T-2	1	30	gpm	1026	p.556
T-3 Base Tank	1	850	gallons	12820	p.572
P-3 Pump for T-3	1	30	gpm	1026	p.556
T-4 Make-Up Tank	1	8500	gallons	68096	p.791
P-4 Pump for T-4	1	800	gpm	3276	p.556
Fermentor Section Subtotal Cost				739013	

---

*Peters and Timmerhaus

EQUIPMENT COSTS

Table 3 is a section of an equipment sizing table for a Novobiocin® process. Each item is process equipment on an associated process flow diagram. The number of items and their size are inputs on the spreadsheet. The cost equation contains exponential equations fitted to cost curves in Peters and Timmerhaus [6]. The cost equation includes the item size, and number of units as inputs. The sizes of some of the items are related to others. In this example, the sizes of the inoculum, acid and base tanks were taken to be one-tenth the size of the make-up tank. The make-up tank size is related to the fermentor size. There are similar relationships between the pump sizes and the tank capacities. Since most equipment

Continued on page 153.

SPREADSHEETS

Continued from page 131.

sizes are linked to the fermentor size, it has been placed first in the list. The rest of the equipment specifications can be changed by entering the new specifications for the fermentor.

This type of table permits rapid computation of equipment costs for different plant capacities or for different fermentor sizes. For example, part of a design problem might be to find the optimum reactor size for a given capacity. The solution could include calculating equipment costs for several different reactor sizes, scheduling the reactors to plan the downtime, and determining overall process costs for each scenario. The student could then plot discrete solutions of cost versus reactor size to graphically determine a minimum cost reactor size.

MANUFACTURING COSTS

Table 4 shows the manufacturing costs for a phthalic anhydride process. Key process design factors (capacity, stream factor, and fixed capital) needed for computing fixed and variable costs are listed at the top. These factors are inputs to cost formulas throughout the table. This format allows the student to change the design basis rapidly.

TABLE 4
Manufacturing Cost Table for a Phthalic Anhydride Process

Economic Example
Manufacturing Costs: Phthalic Anhydride

Capacity	7500 K lb/yr
Stream Factor	.95
Fixed Capital	12100 K $
Depreciable Cap	14900 K $

Variable Costs	**cts/Unit**	**Quantity/ Year**	**Cost, $/Yr**	**Cost, cts/lb**
Raw Materials				
O-Xylene, lbs	15.50	71250000	11043750	14.73
SO_2, lbs	6.50	375000	24375	.03
Sbtl			11068125	14.76
Catalyst, Chem.				
V_2O_5, lbs	720.00	18500	133200	.18
Ht. Trans. Salt, lbs	40.00	12500	5000	.01
N_2, M SCF	75.00	12000	9000	.01
Sbtl			147200	.20
Utilities				
Steam Credit, M lbs	110.00	−214000	−235400	−.31
H_2O, M Gals	20.00	33250	6650	.01
BFW Chem.	1.50	225000	3375	.00
Electricity, KWH	8.00	33750000	2700000	3.60
Sbtl			2474625	3.30
Subtotal, Variable Costs			13689950	18.25

The last column shows the contribution of each item to the manufacturing cost in cents per pound. This breakout is helpful for identifying high cost portions of the process and relating them to the selling price of the product. Listing the cost per unit as well as the quantity needed per year keeps the format flexible. It is simple to assess the sensitivity of the manufacturing costs to changes in raw material costs, labor costs, worker productivity and changes in process conversion.

We have found spreadsheet computations to be helpful to both students and instructors in the design courses. Spreadsheets require organization of the problem material and generate report-quality tables and figures. They help accomplish a rapid solution of the base case and speed analysis of process alternatives.

REFERENCES

1. W. P. Schmidt and R. S. Upadhye, *Chem. Eng.*, **91** (26), 67-70 (1984).
2. S. Selk, *Chem. Eng.*, **20**(13), 51-53 (1983).
3. E. H. Rasmussen, *Chem. Eng.*, **90**(20), 5 (1983).
4. S. M. Goldfarb, *Chem. Eng.*, **92**(8), 91-93 (1985).
5. R. Hirschel, *Chem. Eng.*, **92**(8), 93-95 (1985).
6. M. S. Peters and K. D. Timmerhaus, *Plant Design and Economics for Chemical Engineers*, 3rd Edition, McGraw-Hill, New York, 1980. ☐

REVIEW: Numerical Methods

Continued from page 151.

triangle. This is a terrible mesh and is not allowed in most codes. There is no discussion of natural boundary conditions which is a very important advantage of the finite element method for handling derivative boundary conditions, especially in semi-infinite domains since it reduces the computational costs significantly. Given this presentation of the finite element method, the reader will ask why. The book gives no answer other than that there are codes that are increasingly popular.

Despite these limitations, this is a reasonable treatment and is an improvement in the correct direction. However, the reader will find it necessary to consult other books to solve any problems that are significantly harder than those given in the examples. ☐