# USING MATHEMATICA TO TEACH PROCESS UNITS

## *A Distillation Case Study*

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Today it is well accepted that courses on process units should incorporate some kind of computational and/or simulation tools in order to perform the intensive calculations often required in the analysis and design of process equipment. A common approach in the past, also followed at the University of Coimbra, was to propose a design project where the students had to construct their own programs in a structured language such as Fortran. Nowadays, process simulators, such as Aspen Plus or HYSYS,[1-4] or general-purpose computational platforms, such as Mathematica, MATLAB, or spreadsheet programs,[5-8] are widely accepted tools throughout the chemical engineering curriculum, particularly in the teaching of process units. When compared with Fortran programming, these higher-level computational tools have the obvious advantage of allowing complex calculations with less programming effort. In addition, their graphical interface can be used as a teaching/learning platform, allowing exploratory simulations and quick visualization of the corresponding results.

Process simulators, however, have a potential pedagogical drawback—students may eventually use them as black boxes, without really understanding the physico-chemical model embedded in the simulator. Wankat and Dahm recognize this limitation and propose a cautious use of process simulators, leading students to physically interpret simulation results.[3,4] On the other hand, if a general-purpose platform is used, students have to write down the process model equations and program their basic solution strategy. Therefore, it is the opinion of the authors that this kind of tool is more adequate to support a basic process units course. Process simulators can also be used, but mainly for inductive presentation of concepts[2,4] and to compare solutions and methods.[8] A more intensive use of simulators should be left for later instruction in a senior design course.

In the case study presented in this paper, we have chosen Mathematica, a very powerful general-purpose platform, to support the teaching of distillation in a process units course. Similar experiences have been reported using spreadsheet programs,[7,8] which have the advantage of being easier to learn. Mathematica is much more powerful, however, and has a comprehensible working environment that makes it possible to introduce its key capabilities using engineering problems as a starting point, as will be explained later. In a previous evaluation, made from the viewpoint of an undergraduate student seeking to solve four simple chemical engineering problems, Mathematica received the highest rating, ahead of MATLAB, Maple, and Excel.[6]

Mathematica has been used in our process units course for the last two academic years (2001/2002 and 2002/2003), and in particular, it was used to teach distillation operations. Two initial computer classes introduce students to some key Mathematica capabilities, using vapor-liquid equilibrium cal-

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culations as a starting problem. Later, the interactive user interface of Mathematica (known as *notebook*) is used to illustrate several design methods and modes of operation, making it possible for students to perform complex calculations followed by more perceptible graphical representations. Additionally, a simulation project is given to student teams, with two computer classes supporting it. At the end of this distillation course, students should be able to use Mathematica as a tool in designing other process units in addition to distillation.

In order to evaluate this methodology, a class survey was conducted to judge both the benefits and the difficulties experienced by students, with a resulting general appraisal that was quite positive. In comparison with our previous approach, students now achieve a wider understanding of distillation processes and simultaneously learn a powerful computational tool that they will actually use later in other courses, namely in the senior design course.

The remaining parts of this paper are organized as follows: First, we give a brief introduction to the computational tool we selected (Mathematica) and outline its capabilities; then, the teaching strategy we adopted will be explained in the context of our distillation case study and will be illustrated by two examples (design of a binary continuous distillation column and simulation of a batch distillation operation); finally, the results of the class survey will be discussed and some final conclusions will be drawn.

> ***When compared with Fortran programming, these higher-level computational tools have the obvious advantage of allowing complex calculations with less programming effort. In addition, their graphical interface can be used as a teaching/learning platform, allowing exploratory simulations and quick visualization of the corresponding results.***

## THE COMPUTATIONAL PLATFORM - MATHEMATICA

Mathematica is a general-purpose computational platform that performs numerical and symbolic mathematical calculations. It can be used as a simple calculator, as a high-level programming language, or as a software platform to run previously built packages for specific purposes. An extensive list of internal functions is available that covers a wide variety of mathematical fields, such as numerical solution of algebraic and differential equations, linear algebra, and statistics. All tasks can be performed through an interactive document, known as the *notebook*, in which the user can mix simple calculations or complex function calls with text and graphics, creating an autonomous technical document that can be visualized in class and used as a tool for study. A very good manual is available[9] that describes the Mathematica platform and covers a wide range of mathematical topics; the whole book with extra documentation is also available in the on-line program help, where it is possible to look quickly for information and find clear examples.

In our case study, focused on the distillation process, we have used the standard Mathematica system (Version 4, 1999), applying its capabilities at the levels of numerical solution of algebraic equations, numerical integration, linear algebra and graphics.

## TEACHING STRATEGY: DISTILLATION CASE STUDY

The Process Units II course in the chemical engineering curriculum at the University of Coimbra is dedicated to equilibrium-staged separation operations, based on a mass transfer mechanism—namely distillation and liquid-liquid extraction.[10,11] The organization of the distillation lectures, taking a total of 18 hours, is described below.

Before enrolling in this course, students have already had a course on thermodynamics, so we begin by revisiting the fundamentals of vapor/liquid equilibrium, and we introduce Mathematica in computer classes at this early stage. We then move to the design and analysis of distillation processes, based mainly on both mass and energy balances to each equilibrium stage or to the distillation system as a whole.

The balances can be either in a differential or algebraic form, depending on whether we are dealing with batch or continuous processes. Equations are often organized in an algorithmic form, and we stress the analysis of their degrees of freedom[10] in order to guide their subsequent computational solution using Mathematica. In parallel to this analytical approach, we present graphical methods—namely the McCabe-Thiele method for binary distillation. Although rigorous analytical solutions are preferred, we emphasize that graphical methods are important tools for quickly visualizing interactions between process variables, which are not so perceptible when looking only at model equations.[4,11]

As far as the continuous processes are concerned, we first give students binary problems (feeds with just two components) and then move to multicomponent problems, which are usually solved by putting the balance equations in a matrix form.[10] Simpler problems, with just one feed and two product streams, as well as more complex problems involving multiple feeds and products are approached. Regarding batch operation, we only consider binary feeds and simple models, neglecting column holdup. The differential balances are integrated considering both constant and variable reflux ratios.

The primary goal of the proposed design exercises is to compute the number of ideal stages required for a specified degree of separation. Additionally, we must obtain information on the variation of temperature, composition, and flow rates (vapor and liquid phases) along the column, on the heat needed in the reboiler, and also on the heat withdrawn in the condenser. In the case of a continuous column, we also consider the problem of optimum stages for feeds and purges.

In addition to the aforementioned theory lectures, the practical application of distillation fundamentals is set for students over three different projects:

- (P1) A case study illustrating different distillation operations and calculations involved in their design, using Mathematica notebooks
- (P2) A list of proposed simple problems, most of them solvable by hand calculations and/or graphical methods
- (P3) A simulation project where students are asked to design a multicomponent continuous distillation column

Students are guided through the above projects with three types of practical classes:

- (A) *Full classes* (3 x 2 hours, with 30-40 students) introducing a case study (P1), with the main goal of teaching applied distillation using Mathematica
- (B) *Tutorial classes* (4 x 2 hours, maximum of 25 students), mainly supporting project (P2), where autonomy in problem solving and critical thinking are encouraged
- (C) *Computer classes* (4 x 2 hours, maximum of 15 students, with 2-3 students per computer) with the main goal of leading students to learn the basics of Mathematica and providing support to project (P3)

Table 1 shows the complete program of practical classes for the school year 2002/2003. Comparing it to the 2001/2002 schedule shows that we introduced some minor changes based on the results of the class survey as well as on our own experiences.

## *Introductory Computer Classes*

Students have not previously gone through any formal classes introducing them to Mathematica, although they have had introductory courses on Fortran programming and numerical methods. Therefore, our teaching strategy includes two initial computer classes programmed to informally introduce them to Mathematica fundamentals, motivated by the difficulties that arise even in one-stage distillation calculations.

Our first class, for instance, starts with the question

> *As you know, distillation design calculations are usually based on the concept of equilibrium stage. So, the prediction of vapor/liquid equilibrium conditions in multicomponent systems is an essential tool in the design of distillation equipment. Let us then consider a liquid quaternary mixture of i-butane, n-butane, n-pentane and n-hexane, with molar fractions of 0.10, 0.35, 0.45 and 0.10, respectively. How can we predict the boiling temperature of such a liquid for a pressure of 3 bar (bubble-T calculation)?*

**TABLE 1**

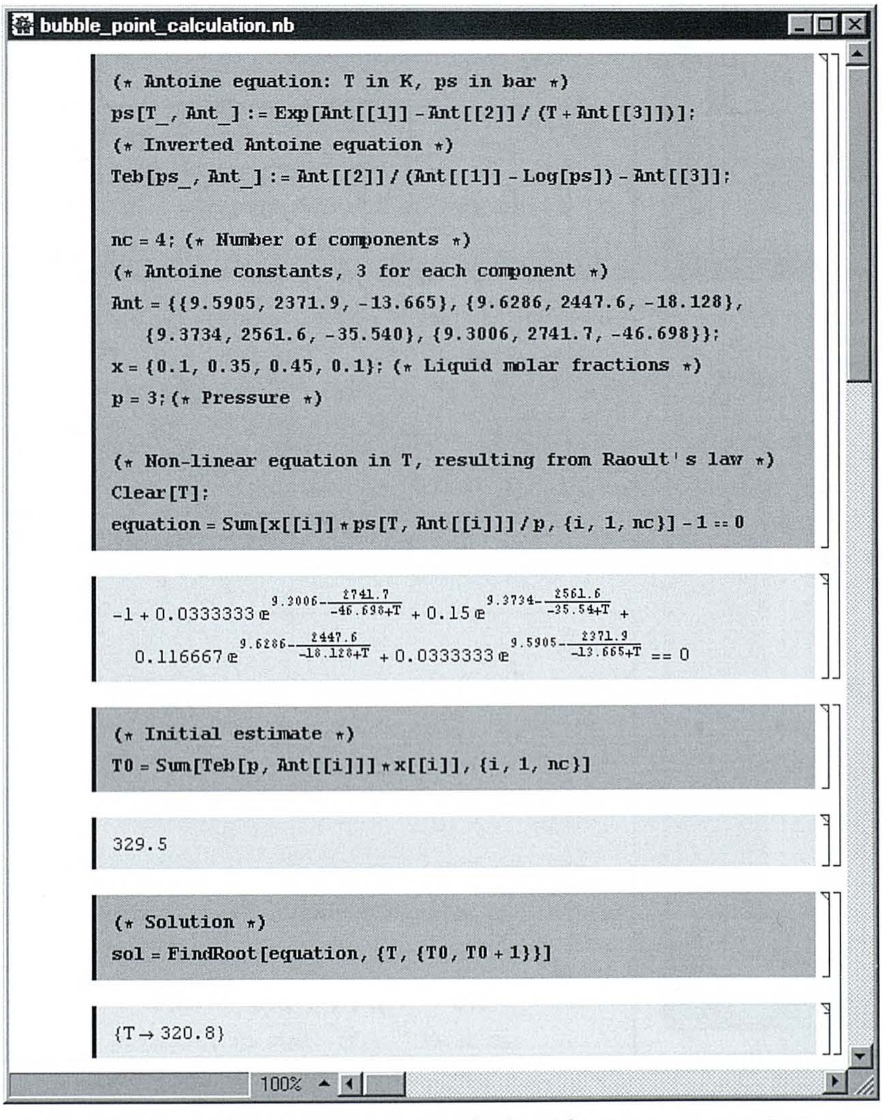
**Program of Distillation Practical Classes (2002/2003)**

| *Class* | *Summary* |
|---|---|
| C1 (2 hrs) | Introduction to Mathematica using vapor-liquid equilibrium (VLE) calculations as a starting point. |
| A1 (2 hrs) | Drawing VLE diagrams in Mathematica. Effect of pressure on relative volatility. One-stage batch distillation; integration of mass balances. |
| C2 (2 hrs) | *Flash* calculations using Mathematica. Partial condensation of vapor coming from the top of a distillation column. |
| B1, B2, B3 (3 x 2 hrs) | Design of a continuous binary distillation column: VLE model based on constant volatility; number of ideal stages computed by Lewis-Sorel method; minimum number of ideal stages; minimum reflux ratio; approximate column sizing; qualitative discussion of the effect of pressure and reflux ratio on column dimensions. |
| A2 (2 hrs) | Design of a continuous binary distillation column using Mathematica; effect of feed location, pressure, and reflux ratio on design results. Simulation of a batch binary distillation column; constant and variable reflux ratio. |
| B4 (2 hrs) | Shortcut design method of Fenske-Underwood-Gilliland for continuous multicomponent distillation. Selection of operating pressure and estimation of the number of stages required. |
| A3 (2 hrs) | Design of a continuous multicomponent distillation column. Shortcut methods and rigorous stage-by-stage calculations by Lewis-Matheson method. Synthesis of distillation column sequences; heuristics to select the most promising alternatives. |
| C3, C4 (2 x 2 hrs) | Programming Wang-Henke rigorous design method in Mathematica. Simulation of a continuous distillation column with multiple feeds and product streams; graphical representation of compositions, temperature, and flow rates along the column. |

The problem formulation, assuming ideal vapor behavior, UNIFAC model to quantify interactions in liquid phase,[12] and the Antoine equation to predict pure components vapor pressures, results in a single nonlinear algebraic equation to be solved for temperature.

Starting from a Mathematica notebook, with the Antoine equation and UNIFAC method already programmed, students are asked to: 1) construct the nonlinear equation in temperature and solve it using the internal function `FindRoot` (Figure 1 shows the notebook for this case, considering the liquid phase ideal), and 2) explicitly program in Mathematica language a numerical method to solve this equation.

While performing these tasks, students learn some fundamentals of Mathematica, such as lists (vectors and matrixes), functions, `For` cycles and modules (subroutines), and how to seek information from the online help. At the end of this class, students are told how to use the modules in the notebook *vle.nb*, which has been pre-programmed by us so as to easily perform the bubble-T calculation they have just programmed as well as other bubble and dew point calculations.



```
(* Antoine equation: T in K, ps in bar *)
ps[T_, Ant_] := Exp[Ant[[1]] - Ant[[2]] / (T + Ant[[3]])];
(* Inverted Antoine equation *)
Teb[ps_, Ant_] := Ant[[2]] / (Ant[[1]] - Log[ps]) - Ant[[3]];

nc = 4; (* Number of components *)
(* Antoine constants, 3 for each component *)
Ant = {{9.5905, 2371.9, -13.665}, {9.6286, 2447.6, -18.128},
   {9.3734, 2561.6, -35.540}, {9.3006, 2741.7, -46.698}};
x = {0.1, 0.35, 0.45, 0.1}; (* Liquid molar fractions *)
p = 3; (* Pressure *)

(* Non-linear equation in T, resulting from Raoult's law *)
Clear[T];
equation = Sum[x[[i]] * ps[T, Ant[[i]]] / p, {i, 1, nc}] - 1 == 0
```

$$-1 + 0.0333333\, e^{9.3006 - \frac{2741.7}{-46.698+T}} + 0.15\, e^{9.3734 - \frac{2561.6}{-35.54+T}} + 0.116667\, e^{9.6286 - \frac{2447.6}{-18.128+T}} + 0.0333333\, e^{9.5905 - \frac{2371.9}{-13.665+T}} == 0$$

```
(* Initial estimate *)
T0 = Sum[Teb[p, Ant[[i]]] * x[[i]], {i, 1, nc}]
```

```
329.5
```

```
(* Solution *)
sol = FindRoot[equation, {T, {T0, T0 + 1}}]
```

```
{T → 320.8}
```

**Figure 1.** *Boiling temperature of a liquid mixture, assuming Raoult's law is valid.*

## *Illustrative Type-A Classes*

The case study (P1) consists of the separation by distillation of a hydrocarbon mixture into two or more streams with specified compositions. A set of problems is formulated and solved in Mathematica notebooks, covering most of the fundamental topics in distillation, from vapor/liquid equilibrium calculations to equipment sizing, including binary and multicomponent feeds and continuous and batch operation. Type-A classes are dedicated to this collection of problems, with Mathematica notebooks being visualized and evaluated throughout the classes. In this way, it is possible to quickly illustrate the influence of several parameters on the performance of distillation processes (reflux ratio, operating pressure, feed location) and also different design methods (short-cut or rigorous stage-by-stage calculations) and their results. Students are provided with Mathematica notebooks so they can explore other situations not covered during class and, at the same time, become more familiar with Mathematica capabilities. Two examples will be described in more detail below.

### ► *Design of a Continuous Distillation Column*

The design of a n-butane/n-pentane continuous distillation column (Figure 2) is set for students using the Lewis-Sorel method (constant liquid and vapor molar flows in each column section). The desired degree of separation is 98% recovery of butane in the distillate and 95% recovery of pentane in the bottom product. We begin by computing the number of ideal stages required assuming certain conditions (approximately constant pressure of 5 bar,

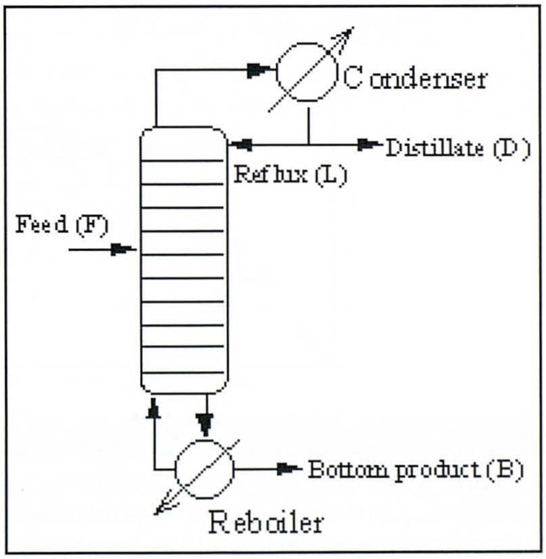
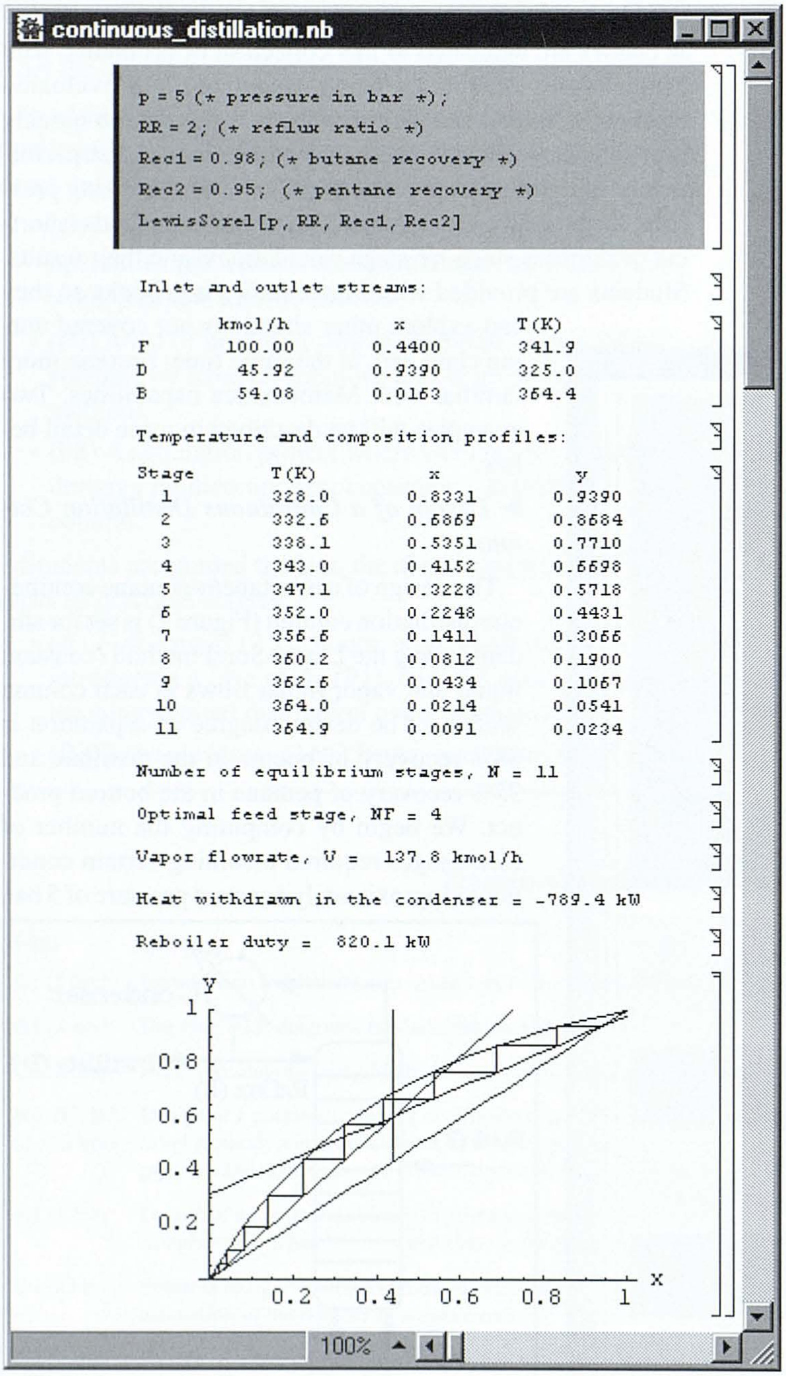


**Figure 2.** *Continuous distillation column.*

saturated liquid feed, total condenser and saturated reflux, reflux ratio of 2), with some of them being discussed further later on. The approximated column dimensioning is left to a subsequent class.

After formulating the solution to the problem on the blackboard, we begin to use the Mathematica platform as a simple calculator, alternating between linear mass balances and dew point calculations (note that at this point students are already familiar with VLE calculations using Mathematica). Then, we show how the Lewis-Sorel procedure can be easily programmed within a module (named as `LewisSorel`), with adequate criteria for optimal feed location being adopted; the module output includes stage-by-stage temperature and composition information and also the respective McCabe-Thiele diagram



```
p = 5 (* pressure in bar *);
RR = 2; (* reflux ratio *)
Rec1 = 0.98; (* butane recovery *)
Rec2 = 0.95; (* pentane recovery *)
LewisSorel[p, RR, Rec1, Rec2]
```

```
Inlet and outlet streams:

        kmol/h        x          T(K)
F       100.00      0.4400      341.9
D        45.92      0.9390      325.0
B        54.08      0.0163      364.4

Temperature and composition profiles:

Stage        T(K)          x            y
  1          328.0       0.8331       0.9390
  2          332.6       0.6869       0.8684
  3          338.1       0.5351       0.7710
  4          343.0       0.4152       0.6698
  5          347.1       0.3228       0.5718
  6          352.0       0.2248       0.4431
  7          356.6       0.1411       0.3066
  8          360.2       0.0812       0.1900
  9          362.6       0.0434       0.1067
 10          364.0       0.0214       0.0541
 11          364.9       0.0091       0.0234

Number of equilibrium stages, N = 11

Optimal feed stage, NF = 4

Vapor flowrate, V =  137.8 kmol/h

Heat withdrawn in the condenser = -789.4 kW

Reboiler duty =  820.1 kW
```

**Figure 3.** *Results from Lewis-Sorel design method (continuous distillation column for butane/pentane separation, with optimal feed location; T is temperature, x and y are molar fractions of butane in liquid and vapor phases, respectively).*

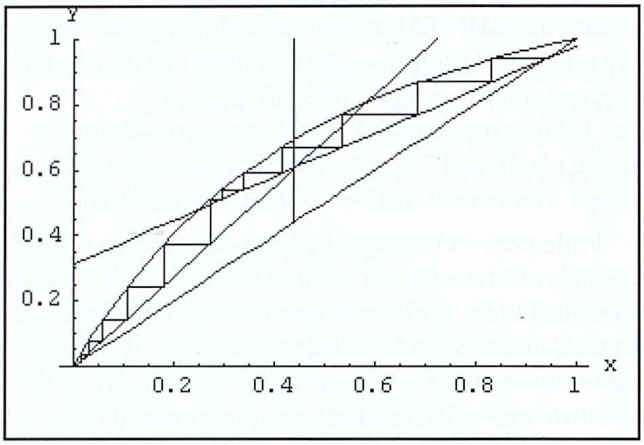


**Figure 4.** *Effect of a non-optimal feed location (7th instead of 4th stage): number of stages required increases from 11 to 12.*

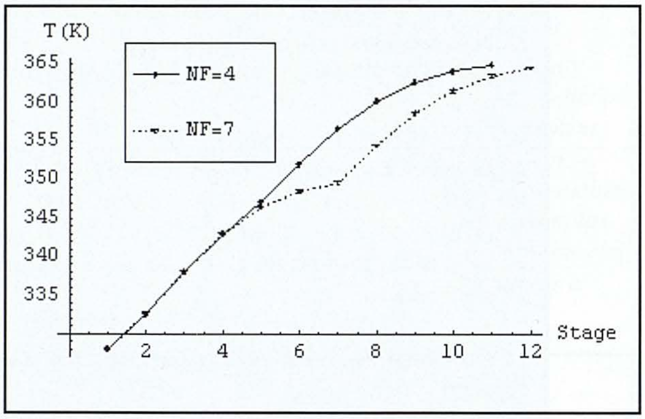


**Figure 5.** *Temperature profiles for optimal (NF=4) and non-optimal feed locations (NF=7).*

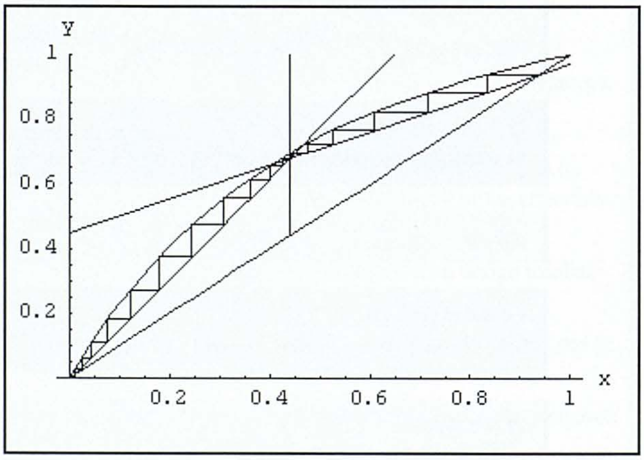


**Figure 6.** *Effect of decreasing the reflux ratio from 2 to 1.1: number of stages required increases from 11 to 17 (minimum reflux ratio = 0.97),*

(Figure 3). This module can now be used to illustrate a non-optimal feed location (Figures 4 and 5) or the effect of decreasing the reflux ratio and, consequently, the concept of minimum reflux ratio (Figure 6), among other relevant points of discussion (effects of operating pressure, optimal reflux ratio, etc.).

### ▶ *Operation of a Batch Distillation Column*

Having applied the Lewis-Sorel method to design a continuous distillation column, students are then confronted with the problem of simulating a batch distillation operation conducted in a boiler + rectifying column (Figure 7). The goal is to separate the same binary mixture of n-butane/n-pentane as before, studying both constant and variable reflux ratio operations. The main simplifying assumptions considered here are constant vapor boilup rate, negligible column holdup, and constant liquid and vapor molar flows along the column.

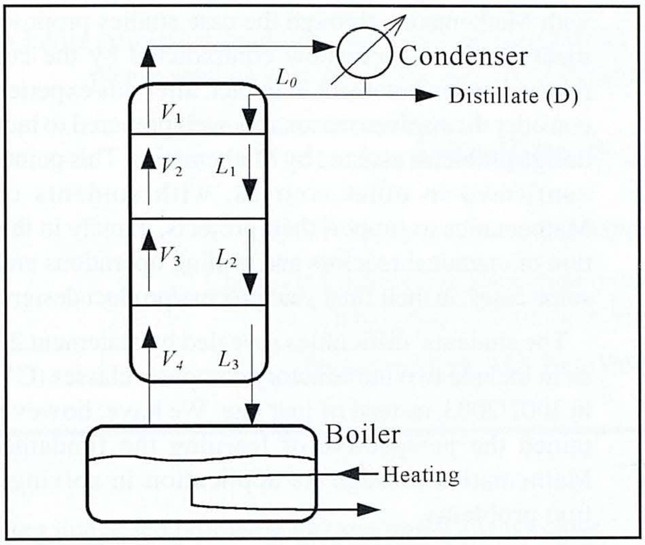
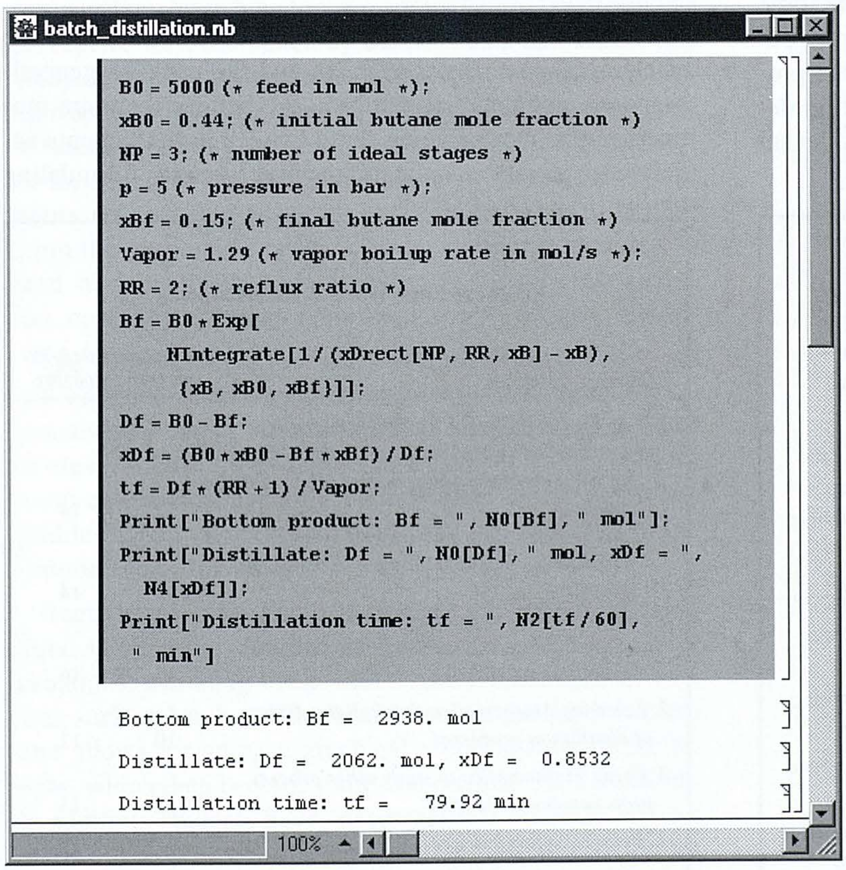


***Figure 7.*** *Batch distillation column.*



```
B0 = 5000 (* feed in mol *);
xB0 = 0.44; (* initial butane mole fraction *)
NP = 3; (* number of ideal stages *)
p = 5 (* pressure in bar *);
xBf = 0.15; (* final butane mole fraction *)
Vapor = 1.29 (* vapor boilup rate in mol/s *);
RR = 2; (* reflux ratio *)
Bf = B0 * Exp[
    NIntegrate[1 / (xDrect[NP, RR, xB] - xB),
     {xB, xB0, xBf}]];
Df = B0 - Bf;
xDf = (B0 * xB0 - Bf * xBf) / Df;
tf = Df * (RR + 1) / Vapor;
Print["Bottom product: Bf = ", N0[Bf], " mol"];
Print["Distillate: Df = ", N0[Df], " mol, xDf = ",
  N4[xDf]];
Print["Distillation time: tf = ", N2[tf / 60],
 " min"]
```

```
Bottom product: Bf =  2938. mol

Distillate: Df =  2062. mol, xDf =  0.8532

Distillation time: tf =   79.92 min
```

**Figure 8**. *Results for a batch distillation simulation with constant reflux ratio.*

For a bottom liquid composition `xB` (molar fraction of butane), a Mathematica module (named `xDrect`) is constructed to predict the distillate composition obtained in the top of a column with `NP` ideal stages and operating with reflux ratio `RR`. For a constant reflux ratio, this module is used in conjunction with Rayleigh equation (differential mass balances) to compute the final bottom product quantity (`Bf`) with a specified composition (`xBf`). After this, the accumulated distillate quantity (`Df`), its average composition (`xDf`) and the distillation time (`tf`) are easily computed through simple mass balances (Figure 8). For a variable reflux ratio operation, the reflux ratio profile (Figure 9) required to obtain a distillate with a constant composition of 90% in butane, using the same column, is computed integrating the mass balances together with the non-linear equation `xDrect[NP,RR,xB] = 0.9`, solved for `RR` (a 4th order Runge-Kutta method is selected and programmed in Mathematica).

<u>*Simulation Project (P3)*</u>

The aim of project (P3) is to confront students with an open engineering problem: design a multicomponent continuous distillation column, with a given feed and certain restrictions on operating conditions, that provides a specified degree of separation. Similar problems are set for teams of 3 elements each, with the final evaluation being based on a technical report (about 20 pages), which is

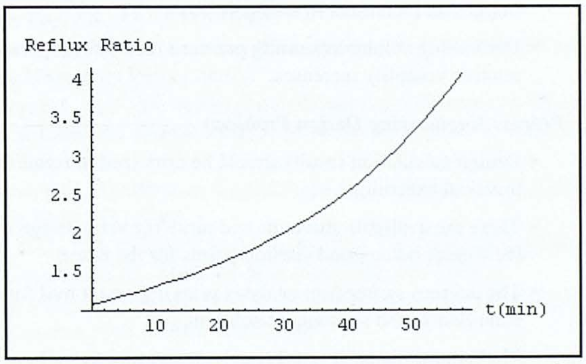


***Figure 9.*** *Results for a batch distillation simulation with constant distillate composition and variable reflux ratio.*

orally discussed. There is also an individual task for each team member.

In order to guide students faced with such an open problem, project (P3) is scheduled in 6 steps: (1) VLE prediction; (2) calculation of stream enthalpies; (3) flash calculations (individual task); (4) preliminary evaluation of operating conditions; (5) shortcut method for column design; (6) rigorous stage-by-stage column design by the Wang-Henke method.[13,14] Teams are advised to use case study (P1) as a starting point to proceed along the various steps and their work is closely followed with short oral discussions. Step (6) is the one requiring most programming skills, and thus two computer classes (C3 and C4) are dedicated to mentor students through it, introducing them, simultaneously, to matrix manipulation and efficient linear algebra calculations with Mathematica. Having completed a base case simulation, students are then encouraged to study and discuss the influence of several operating conditions on column performance and design.

## ASSESSMENT OF STUDENTS' PERCEPTIONS

Students' perceptions of the advantages and disadvantages of the teaching strategy adopted were evaluated through both an oral discussion and a written survey.

In the oral discussion, students were asked to outline some conclusions based on the set of problems studied during type-A classes, and at two different levels: (i) the particular process unit studied (distillation); (ii) process engineering design problems in general. Table 2 presents the most relevant collected opinions.

**TABLE 2**

**Students' Conclusions Regarding Project (P1)**

***Distillation Level***

- Flash distillation promotes a coarse separation appropriate to pretreatment of mixtures with highly volatile components.
- In a continuous column, an increase in the operating reflux ratio implies an increment in energetic costs.
- Decreasing column operating pressure facilitates separation since relative volatility increases.

***Process Engineering Design Problems***

- Design calculation results should be criticized in terms of their practical execution.
- There are available shortcuts and more rigorous design methods, the former being good starting points for the latter.
- The degrees of freedom analysis is an important tool for problem formulation and subsequent solution.
- Mathematica is an accessible calculation tool that allows one to perform parametric studies, but is not very efficient in terms of computational time.

The written survey aimed at evaluating the impact of our teaching strategy under four domains—the main results are given in Table 3.

The overall evaluation is positive, with a relevant improvement in the second school year. The strongest point mentioned by students was related to the advantages of learning distillation with the assistance of Mathematica, especially concerning the software's graphics facilities. Though students mention having experienced some difficulties in getting started with Mathematica through the case studies proposed (statement 2), that is somehow contradicted by the conclusion reached under statement 3. In fact, after this experience, they consider themselves reasonably well prepared to tackle other design problems assisted by Mathematica. This point has been confirmed in other courses, with students choosing Mathematica to support their projects, namely in the simulation of chemical reactors and milling operations and also, in some cases, in their final year process/product design projects.

The students' difficulties revealed by statement 2 have led us to include two introductory computer classes (C1 and C2) in 2002/2003, instead of just one. We have, however, maintained the perspective of learning the fundamentals of Mathematica through its application in solving distillation problems.

## CONCLUSIONS

The strategy presented in this paper combines both the teaching of process units design and the use of a general-purpose computational platform. We believe there are mutual benefits in combining these two subjects. Students acquire a good understanding of the process units, formulating

**TABLE 3**

**Main Results from Written Survey**

| | *Classification (scale 0-20)* | |
|---|---|---|
| *Domains Evaluated* | *2001/02* | *2002/03* |
| ***1. Learning Distillation Using Mathematica*** | | |
| • Mathematica code visualized in type A classes did not perturb the perception of fundamental concepts. | 13 | 14 |
| • Type A classes illustrated a wide range of situations, giving a broad view of distillation processes. | 13 | 14 |
| • The graphical capabilities of Mathematica allowed for quick visualization and several operating aspects. | 17 | 16 |
| ***2. Learning Mathematica through the design of distillation processes*** | 10 | 12 |
| ***3. Using Mathematica to study other process units besides distillation*** | 12 | 13 |
| ***4. Benefit / effort balance*** | 11 | 12 |
| Sample (number of students / students developing project (P3)) | 23/45 | 30/49 |

and solving integrated problems and remaining always close to the underlying physical/chemical phenomena. Simultaneously, they learn how to use a computational platform in a perceptive way, motivated by the problems that arise while studying a given process unit. Altogether, this methodology represents an improvement on the more traditional strategy of teaching process units and computational tools separately. In fact, there is a clear reduction in the total number of hours required for teaching and it is possible to benefit from the graphical facilities of the computational tool to lead students to the understanding of the processes studied, namely the design features.

The computational tool selected (Mathematica) supports our simultaneous teaching strategy in several ways: the interactive document known as notebook can be visualized in class and used by students as a tool of study, the symbolic calculation capabilities help students to formulate problems and check results, and the online help greatly supports the program.

Regarding our distillation case study, Mathematica has offered an adequate environment to illustrate a wide range of situations, including those with a heavy mathematical content, such as batch distillation. Moreover, the notebook feature allows for an easy graphical representation of the results, which then become more comprehensible to students. In addition, students have successfully used Mathematica while developing a proposed simulation project. After this distillation experience, we can confirm that students are reasonably well prepared to tackle other process-design problems using Mathematica.

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