THE PROCESS SIMULATION COURSE – THE CULMINATION OF CORE UNDERGRADUATE COURSEWORK IN CHEMICAL ENGINEERING

Mordechai Shacham, Ben-Gurion University, Beer-Sheva, Israel

Michael B. Cutlip, University of Connecticut, Storrs, CT 06269, USA

Introduction

The status of the incorporation of computational tools in the undergraduate Chemical Engineering curriculum has been recently reviewed by Shacham et al. (2009). This review, as well as some additional references (Dahm et al., 2002, Rockstraw, 2005, Dias et al., 2010), reveal that process simulation is being used to some extent in various courses. Most often commercial simulators (such as HYSIS, AspenPlus and PRO II) are used to model the steady state or dynamic operations of processes. The benefit of such use of a process simulator (as stated by Dahm et al., 2002) is that it "provides a time-efficient and effective way for students to examine cause-effect relationships" among various parameters of the process. A pedagogical drawback to the use of such packages is that "it is possible for students to successfully construct and use models without really understanding the physical phenomena within each unit operation" (Dahm et al., 2002). Furthermore, Streicher et al. (2005) have found that "the majority of students see simulations merely as sophisticated calculators that save time."

In order to promote and emphasize the full educational benefits of process simulation, we have developed a process simulation course where the students need to prepare process models that, in most cases, are ultimately simulated with MATLAB. The course content begins with the steady state operation of simple recycle processes that contain mixers, simple splitters and conversion type reactors. Material balances on such systems can be represented by linear models. For such systems, a direct solution (of a system of linear equations) can be obtained and the performance of various iterative algorithms can be examined. The students learn to establish the computational sequence in the flow-sheet using various partitioning and tearing algorithms. Then, students solve the problems directly and iteratively using the successive substitution, dominant eigenvalue, Wegstein's and Broyden's methods. After understanding the basic principles of the operation of the steady state simulators, models of unit operations with increasing level of complexity (such as isothermal, adiabatic and three-phase flash) are prepared. The models are implemented as MATLAB functions where the input parameters are the vectors of flow-rates and enthalpy of the inlet streams and the design parameters of the process unit. The output parameters are the vectors of flow-rates and enthalpies of the outlet streams. Physical property data and correlations that required for the modeling the unit operation are taken from the DIPPR thermo physical database (Rowley et al., 2006, http://dippr.byu.edu/). Binary equilibrium data, needed for calculations of activity coefficients, are retrieved from the Dortmund Data Bank (http://www.ddbst.com/en/ddbst/index.php) and regressed with the Polymath program. The systems of nonlinear algebraic equations that represent typically the steady state models of the various units operations are solved using the constrained version of the Newton-Raphson method (Shacham, 1986).

In dynamic simulation, the emphasis is on the solution of Multiple-Model, Multiple-Algorithm (MMMA, see Cutlip et al., 2009) problems. An example is a process unit that can operate in different modes (such as a reactor with heating and cooling periods) and requires

different integration algorithms (stiff and non-stiff) in each period. For example, the students can model the operation of a runaway chemical reactor which is described in detail by Eisenberg et al., 2006.

The process simulation course is a challenging course to teach, from the technical standpoint. Derivation of complex equations require the use of a chalkboard, complex diagrams (like flow-sheets) require the use of pre-prepared PowerPoint slides, and demonstrations of computer programs require live interaction with the program in class. In addition to the presentations, note taking by the students is also demanding as they have to add notes to a hardcopies of the PowerPoint slides during the presentations. To assist the students, we have been using a Tablet-PC (which can serve both as chalkboard and computer for PowerPoint presentations and program demonstrations) and can also record the classroom activities and lectures that are later made available from a class site on the internet.

This paper will emphasize in some detail the preparation of complex process models, the use of the DIPPR database as the source of physical and thermodynamic properties, and the use of the "Self-recording with a Tablet-PC" technique.

Non-Isothermal Multi-component Flash Calculation - The Structure of a Unit Operations Module

The general structure of a unit operations module is shown in Figure 1. The purpose of this model is to calculate the flow rate temperature and pressure of the outlet streams using the information on the input streams, design parameters and the physical/thermodynamic properties of the compounds involved.
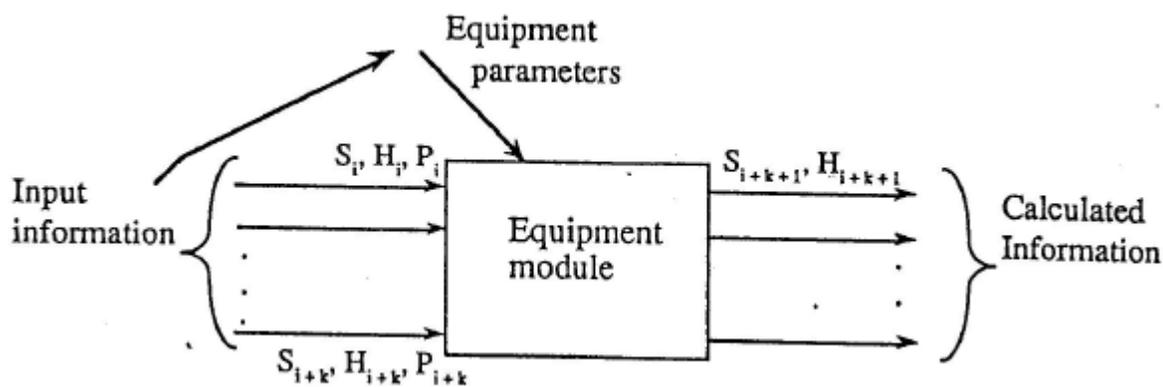

Figure 1. The General Structure of a Unit Operations Module

The notation used in Fig. 1: $\mathbf{S}_i$ is a vector of flow-rates in stream i, H_i is the total enthalpy of stream i, P_i is the pressure of stream i, and i and k – are stream indices.

When process simulators used for modeling a unit operation (or a complete process), the user is responsible for specifying the type of the equipment item, the connections between the various items, input stream flow-rates, compositions, enthalpies and pressure as well as the parameters of the processing units.

Constructing a unit operations module requires much more involvement on the student's behalf. The required knowledge and activities will be demonstrated for the case of a non-isothermal multi-component flash unit. In addition to the information concerning the input

stream(s), there is a need to specify the parameters of the unit which include the heat added or removed from the flash drum (Q) and the pressure. Based on this information, the module has to determine whether under the stated conditions the outlet will be all gas, all liquid, or two streams of different phases. Then the calculations can be carried out accordingly. To determine the state of the outlet stream(s), the bubble point and the dew point temperatures of the feed and the enthalpies at these temperatures need to be calculated. These enthalpies have to be compared with the total enthalpy available (feed stream and heat input) in order to determine the state of the output stream(s). Thus the non-isothermal flash module must contain the model equations for calculating the following: 1. Bubble point temperature of a multi-component mixture, 2. Dew point temperature of a multi-component mixture, 3. Non-isothermal flash of a multi-component mixture, and 4. Mixture enthalpy at a specified temperature.

In addition to the mathematical model, physical property data related to phase equilibrium calculations (vapor pressure as function of temperature, activity coefficients) and to vapor and liquid enthalpy calculations (ideal gas enthalpy and heat of vaporization as function of temperature) are needed.

The calculation of the bubble point and dew point temperatures, and the non-isothermal flash calculations require solution of systems of nonlinear algebraic equations (NLE). The multidimensional Newton-Raphson method can be used for solving the NLE systems. Because of the complex temperature dependence of the vapor pressure (Riedel's equation) and the composition dependence of the activity coefficients, no analytical expression for the partial derivatives can be obtained but they must be estimated by finite differences. The many orders of magnitude differences between the terms of the material balance equations and the enthalpy balance equations require proper scaling of the equations in order to prevent ill-conditioning of the NLE system.

Proper safeguards should be included in the solution algorithm to enable providing sensible output stream flow-rates even in abnormal situations in the early stages of the solution process (zero input to the unit, failure to converge of one of the computations, etc.).

```
File  Edit  Text  Go  Cell  Tools  Debug  Desktop  Window  Help

                                                                      Stack: Base

  1.0    +    ÷  1.1    ×

  1       % function [SV,HV,SL,HL,err]=adbf(SF,HF,P,Q)
  2       % Calculates the composition and the enthalpy of a flash unit with
  3       % specified pressure, feed enthalpy and heat input
  4       % Description of the input parameters
  5       % SF - vector of feed flow rates (kg-mole/hr)
  6       % HF - feeds enthalpy ( J/hr)
  7       % P - pressure (Pa)
  8       % Q - heat input (J/hr)
  9       % Description of the output parameters
 10       % SV - Outlet vapor stream flow rates vector (kg-mole/hr)
 11       % HV -  outlet vapor enthalpy (J/hr)
 12       % SL - outlet liquid stream flow rates vectot (kg-mole/hr)
 13       % HL - outlet liquid enthalpy (J/hr)
 14       % err - Eucledian norm of the final corrections in alpha and TF
 15       % subprograms used bubble.m, dew.m, enthalpy.m, kvalue.m and adbfun.m
```

Figure 2. MATLAB function interface for the non-isothermal flash module

The MATLAB function interface for the non-isothermal flash module is shown in Figure 2. The interface provides details regarding the input and output parameters of the function and the subprograms used by this module (function). The function parameters coincide with the input and output information of the modeled unit operation (Figure 1).

One or more assignments are given to the students which involve non-isothermal flash calculations. In all the assignments the students receive from the instructor some of the MATLAB functions that are needed for these calculations the others they need to prepare on their own. The functions used for physical property calculations (*kvalue.m* and *enthalpy.m*) are always prepared by the students. The use of the Polymath 7.0 interface for the DIPPR database (Rowley et al. 2006) which is used to prepare property-related functions is discussed in the next section.

The use of the Polymath 7.0 interface for the DIPPR database in physical property calculations

Constant physical properties (such as critical properties, normal boiling temperature, etc.) and equations of temperature-dependent properties can be copied from the DIPPR database to Excel spreadsheets, Polymath, and MATLAB using the newly developed Polymath 7.0 interface for the DIPPR database. The process starts with user identification of the compounds and the properties involved. Figure 3 shows the "Temperature-Dependent Properties" communication box where the properties needed for non-isothermal flash calculations (vapor pressure, ideal gas heat capacity and heat of vaporization) are selected for the seven compounds from the database that were identified earlier using the interface.
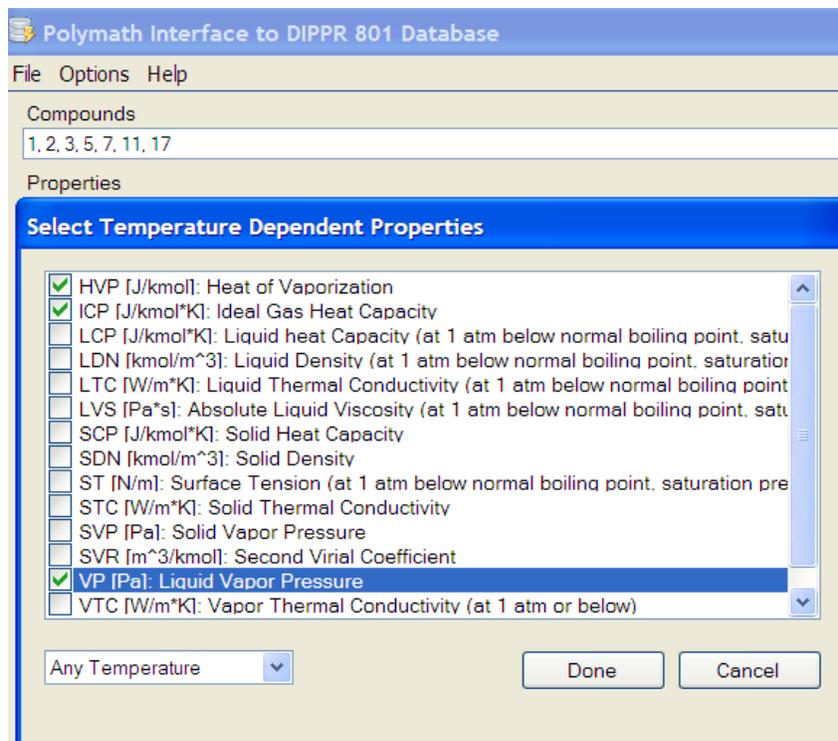

Figure 3. Polymath 7.0 Interface for the DIPPR database showing desired selection from among the available temperature-dependent properties.

After identifying the compounds and desired properties, a report is generated which contains the relevant data, equations and additional information available in the DIPPR database for each property. The data, equations and supporting information can then be copied into an Excel spreadsheet (in tabular form) and into a Polymath or MATLAB program. The relevant property equations for *n*-Pentane, as copied into a MATLAB m-file are shown in Figure 4.

```
File  Edit  Text  Go  Cell  Tools  Debug  Desktop  Window  Help
 1      % Heat of Vaporization of C5H12
 2      % n-PENTANE
 3      % Uncertainty: < 1%; Acceptance: A; Data Type: Experimental; Source Type: Unevaluated;
 4      % Tc=469.7
 5      % Min_T=143.42, Max_T=469.7, Min_Val=33968000, Max_Val=0 [K ; J/kmol]
 6      HVP_C5H12 = 39109000 * (1 - (T / 469.7)) ^ 0.38681; % J/kmol
 7      % Ideal Gas Heat Capacity of C5H12
 8      % n-PENTANE
 9      % Uncertainty: < 1%; Acceptance: A; Data Type: Smoothed; Source Type: Evaluated; Sourc
10      % Min_T=200, Max_T=1500, Min_Val=94039, Max_Val=329270 [K ; J/kmol*K]
11      % HIG_C5H12 = 88050*T+301100*1650.2*coth(1650.2/T)-189200*747.6*tanh(747.6/T)+HCON %
12      ICP_C5H12 = 88050 + 301100 * (1650.2 / T / sinh(1650.2 / T)) ^ 2 + 189200 * (747.6 / 1
13      % Liquid Vapor Pressure of C5H12
14      % n-PENTANE
15      % Uncertainty: < 3%; Acceptance: A; Data Type: Experimental; Source Type: Unevaluated;
16      % Min_T=143.42, Max_T=469.7, Min_Val=0.068642, Max_Val=3364200 [K ; Pa]
17      VP_C5H12 = exp(78.741 - (5420.3 / T) - (8.8253 * log(T)) + 9.6171E-06 * T ^ 2); % Pa
18
```

Figure 4. MATLAB formatted physical property equations and supporting information as generated by the Polymath 7.0 DIPPR interface

The property equations are shown in lines 6, 12 and 17, respectively. The names of the variables which store the numerical values of the properties at a specified temperature are consist of the symbol of the property (HVP-heat of vaporization, ICP-ideal gas heat capacity, VP-vapor pressure) and the chemical formula of the compound involved. The units of the property are shown (as a comment) in the same line as the equation.

The supporting information is provided as "comments". There are three user-selectable levels for this information. The report in Figure 4 was generated using the "basic" (intermediate) level. The first line of supporting information includes: the full name of the property and the formula of the compound, and the 2nd line contains the full name of the compound. In the 3rd line, information concerning the reliability of the property equation, as determined by the DIPPR staff, is shown. This includes the uncertainty in the property value (an upper limit on the experimental or prediction error), information whether the equation is based on experimental data or prediction, and whether the equation was evaluated and accepted by the DIPPR staff. An additional comment line contains the range of validity of the equation in terms of temperature and property limits. In the same line, the units of the temperature and the property are also shown.

The ideal gas heat capacity (line 12 in Figure 4) deserves special discussion. The transcendental equation of Aly and Lee (1981) is used by DIPPR to model this property. The integrated form of this equation for calculation of the ideal gas enthalpy is considerably different than the heat capacity equation. For the benefit of the users, whenever the ideal gas heat capacity is requested, the equation for ideal gas enthalpy is also included as a comment

(see line 11). The enthalpy equation includes an integration constant H_{con}. This constant depends on the standard state selected for the enthalpy calculation. For example, selection of a pure liquid component at 0 ºC (273.15 K) as a standard state yields H_{con} as ideal gas enthalpy at 273.15 K subtracted from the heat of vaporization of the component at the same temperature.

```
File  Edit  Text  Go  Cell  Tools  Debug  Desktop  Window  Help

8        function [HLS,HVS]=enthalpy(XF,YF,T)
9          T0=273.15;
10         %Methane
11         HCON_CH4 = -(33298*T0+79933*2086.9*coth(2086.9/T0)-41602*991.96*tanh(991.96/T0)); %  J/kmol
12         HIG_CH4 = -33298*T+79933*2086.9*coth(2086.9/T)-41602*991.96*tanh(991.96/T)+HCON_CH4; %  J/kmol
13         HV(1,1)=HIG_CH4;
14         if T<190.564
15             HVP_CH4 = 10194000 * (1 - (T / 190.564)) ^ (0 - (0.000771079532335593 * T) + 0.22154 * (T /
16             HL(1,1) =HIG_CH4-HVP_CH4 ;
17         else
18             HL(1,1) =HIG_CH4;
19         end
20         %Ethane
21         HVP_C2H6_0 = 21091000 * (1 - (T0 / 305.32)) ^ (0 - (0.00181750294772697 * T0) + 0.32799 * (T0 /
22         HCON_C2H6 = HVP_C2H6_0-(40326*T0+134220*1655.5*coth(1655.5/T0)-73223*752.87*tanh(752.87/T0)); %
23         HIG_C2H6 = 40326*T+134220*1655.5*coth(1655.5/T)-73223*752.87*tanh(752.87/T)+HCON_C2H6; %  J/kmol
24         HV(2,1)=HIG_C2H6;
25         if T<305.32
26             HVP_C2H6 = 21091000 * (1 - (T / 305.32)) ^ (0 - (0.00181750294772697 * T) + 0.32799 * (T / 3
27             HL(2,1) =HIG_C2H6-HVP_C2H6 ;
28         else
29             HL(2,1) =HIG_C2H6;
30         end
31         %Propane
```

Figure 5. Partial display of the MATLAB *enthalpy.m* function

Part of the MATLAB function: *enthalpy.m* for calculating the molar enthalpy of liquid with composition of $\mathbf{x}_F$ and molar enthalpy of vapor with composition of $\mathbf{y}_F$ at temperature T, is shown in Figure 5. For brevity, most supporting information is not shown. The ideal gas enthalpy (HIG) and heat of vaporization (HVP) equations are used. The integration constants H_{con} are calculated for all the compounds using the standard state of liquid at 273.15 K. Additional programming is required to separate cases where a compound above or below the critical temperature, and the enthalpies must be introduced into arrays.

Thus the Polymath 7.0 DIPPR interface enables very rapid program development for calculating properties of mixtures using state-of-the-art industrial standard correlation equations.

Self-Recording of the Lectures Using a Tablet-PC and a Camtasia Recorder

This new technology allows the lectures to still be delivered face-to-face; however, instead of writing on the chalkboard the instructor writes on the computer screen. At the same time, the instructor uses the computer to record voice and the visual material that is displayed on the PC screen (and also projected to a large screen in the classroom). The Camtasia recorder (a software package loaded on the instructor's computer, http://www.softwarecasa.com) is used for recording.

The visual material of the lecture can be presented with the Tablet PC either using the Windows Journal or Power Point slides. When Windows Journal is used, the computer screen essentially serves as a chalkboard. When power point slides are used, it is preferable to put on them only part of the lecture material, while the rest is added by writing during the presentation. The students are encouraged to bring hard copies of the incomplete slides to the class and to add missing parts during the class presentations. The instructor writes on the Tablet PC screen while explaining the material, and the students complete the missing information on the hard copies. This method gives students sufficient time to absorb the more difficult material and to ask questions of the instructor.

Figure 6. Introduction of the MESH equation for multistage distillation calculations

Consider, for example, the derivation of the MESH equations for multistage distillation calculation, as shown in Figure 6. The sketch of an equilibrium stage and the text characterizing the equations needed are placed in advance on the PowerPoint slide. The equations are derived in class with considerable student involvement.

Figure 7 demonstrates another option in the effective use of the Tablet PC. In this figure, a part of a computer program for solving a recycle problem using Broydens' method is shown. The students bring a hard copy of the program. The connection between the mathematical formulas used, the solution algorithm, and the coding of the method is explained in class by putting markings on the Tablet PC screen while the students write on the hard copy.

The instructor starts the recording at the beginning of the lecture and stops it toward the end. The recorded lecture becomes available on-line within a few hours after some modest editing is done. The main purpose of the editing is to add subtitles that enable accessing separate sections of the lecture rapidly. The students can watch the recorded lectures wherever they have access to the Internet.

Figure 7. Use of Broyden's Quasi-Newton method for recycle convergence

Conclusions

The process simulation course is given as an elective course for fourth year undergraduate students and new graduate students. Success in this course requires that students must review, enhance, update and make practical use of their knowledge of programming, material and energy balances, thermodynamics, numerical methods and reaction engineering. With the integration of such broad content, the course can be considered as a culmination of core chemical engineering coursework.

Use of the Polymath 7.0 – DIPPR database interface enables the students to use state of the art, industrial-standard physical and thermodynamic properties as well as property correlation expressions. They become aware of the uncertainty associated with the property data as well as with the need to respect the range of validity of the correlation equations.

Student evaluation of the new instructional technique, enabled by the Table PC, yielded very positive results. In particular, the students pointed out the following advantages: 1. The lectures are better structured and more interesting than the traditional methods of teaching (PowerPoint or chalkboard) 2. The records kept in their notes are clear and understandable 3. The recorded lectures are beneficial when someone misses a lecture or wishes to review the lecture material when completing homework assignments or preparing for an exam.

References

1. Aly, F. A. and L. L. Lee, "Self-Consistent Equations for Calculating the Ideal Gas Heat Capacity Enthalpy, and Entropy". *Fluid Phase Equilib.* 6, 169(1981)
2. Cutlip, M. B., N. Brauner and M. Shacham, "Biokinetic Modeling of Imperfect Mixing in a Chemostat – an Example of Multiscale Modeling", Chem. Eng. Ed., 43, 243 (2009)
3. Dahm, K. D., R. P. Hesketh and M. J. Savelski, "Is process simulation used effectively in ChE courses?" *Chem. Eng. Ed.*, 36, 192 (2002)
4. Dias, R. S., L. C. Silva, L and A. J. De Assis, Plant wide simulation using the free chemical process simulator Sim42: Natural gas separation and reforming, Published online in Wiley InterScience; DOI 10.1002/cae.20200
5. Eisenberg, S., M. Shacham and N. Brauner, "Combining HAZOP with Dynamic Simulation - Applications for Safety Education", Journal of Loss Prevention in the Process Industries 19, 754–761 (2006)
6. Rockstraw, D. A., "ASPEN Plus in the ChE curriculum. Suitable course content and teaching methodology," *Chem. Eng. Ed.*, 39, 68 (2005)
7. Rowley R. L., W. V. Wilding, J. L. Oscarson, Y. Yang and N. A. Zundel. DIPPR Data Compilation of Pure Chemical Properties Design Institute for Physical Properties. http//dippr.byu.edu, Brigham Young University Provo Utah (2006)
8. Shacham, M., "Numerical Solution of Constrained Non-Linear Algebraic Equations", *International Journal of Numerical Methods in Engineering*, 23, 1455-1481 (1986).
9. Shacham, M., M. B. Cutlip and N. Brauner, "From Numerical Problem Solving to Model Based Experimentation – Incorporating Computer Based Tools of Various Scales into the ChE Curriculum", *Chem. Eng. Ed.*, 43, 299 (2009)
10. Streicher, S. J., K. West, D. M. Fraser, J. M. Case and C. Linder, "Learning through simulation, student engagement," *Chem. Eng. Ed.*, 39, 288 (2005)