

Spreadsheet use in Conceptual Design of Chemical Processes*

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The main purpose of the following work is to present an elemental simulator of chemical processes developed on an Excel® spreadsheet. The simulator consists basically of three main modules: Property Prediction Block: different physicochemical and thermodynamic properties for pure compounds and mixtures can be calculated; Equipment Block: the main dimensions and output streams of typical process equipment are calculated by means of approximate methods; Cost Calculation Block: the investment required by the different equipments is estimated through generic correlations. Several application examples are introduced, as well as the general structure of the program.

INTRODUCTION

DURING THE TEACHING of elemental principles of process design in chemical engineering, a special emphasis should be made on what Douglas calls *Conceptual Design of Processes* [1]. This basic concept implies a systematic search, through succeeding refinements hierarchically ordered, which starts from the simplest solutions and goes on up to the concretion of an entire process diagram.

Douglas proposes the following hierarchy of decisions:

1. Batch vs. continuous processing.
2. Input-Output structure of the flowsheet.
3. Recycle structure of the flowsheet.
4. General structure of the separation system:
 - vapor recovery system,
 - liquid recovery system.

To fulfill these steps, it is necessary to make use of both calculation and economic estimation methods in accordance with the increasing complexity levels implied by the procedure.

In the early stages, it is possible to eliminate design alternatives that are clearly disadvantageous by means of very simple assumptions, a few economic data and unsophisticated computation schemes. Farther on, the search will require a greater volume of information and calculation schemes of higher complexity.

Of course, the final purpose is the simulation of the process, using a program that establishes exactly the stream properties and performance conditions of the different units. This program is clearly oriented to the professional practice, and its

use requires a specific training, whose extent depends on the particular characteristics of the commercial product.

Before running process simulators, the engineer possesses powerful calculation tools that make the analysis easier, using approximate values of the compound and mixture properties as well as simplified methods for equipment calculation.

Among those software tools, it is worth mentioning:

- ASCEND, from Carnegie Mellon University, <http://www-2.cs.cmu.edu/-ascend/>
- GAMS, from GAMS Development Corporation, Washington DC, <http://www.gams.com>
- spreadsheet.

ASCEND and GAMS are modeling systems which are appropriate for engineering problems, in particular, for chemical engineering ones. They have several developments and facilities (prebuilt units, organization routines, etc) that help the user to model the analyzed systems.

The spreadsheet is the most used computation tool in the engineering field, not only in professional practice but also during undergraduate study. Because of this, all the developments for engineering teaching based on spreadsheets imply an environment and techniques well-known to the student, as well as a reinforcement of the required skills for the future professional performance.

Thereby, at the Faculty of Engineering of the Universidad Nacional de La Plata (UNLP), in the Process Engineering course, we have decided to develop a simplified process simulator, SimPro, in Excel® and its associated VBA programming language. Technical and economic analysis of typical systems of the chemical industry is feasible with SimPro, as well as eventual mass and energy recycling and the search for optimal design and

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performance conditions. The basic structure of data entry and property calculation has been taken from Partin [2], the most direct antecedent for the present work.

BASIC REQUIREMENTS FOR A PROCESS SIMULATOR IN SPREADSHEETS

The development of a simulator requires:

- routines for thermodynamic and physicochemical properties of pure compounds and mixtures;
- routines for the design of typical process equipment, with the corresponding calculation procedures;
- routines for the estimation of equipment costs.

To achieve bigger pedagogic effectiveness, the type of simulation problem considered with SimPro will be of reduced complexity: four to ten process units, two to six decision variables and one or two recycle material streams, as it is shown in Fig. 1 [3].

To find the optimal values for the decision variables, Excel® has a specific add-in called Solver that turns out to be sufficient for the magnitude of the analyzable cases. Besides, though it is possible to solve an iteration problem directly with the spreadsheet ('circular reference',

using the Excel® jargon), it is recommended [4] to make that calculation explicit and also to solve it with Solver.

Due to the preliminary approach in which the simulator will be used, the design of the equipment will be made through simplified (shortcut) methods. Nevertheless, it requires a multiplicity of arguments as data and its result will be a set of values. It includes not only composition, pressure, temperature, etc, of each equipment's output stream, but also the main dimensions of the equipment. In this case, matrix functions, which are not familiar to the student, must be used. Thereby, it was decided to implement their handling through a specific menu.

Property prediction and cost estimation routines are of scalar nature, with multiple input arguments and a single output value. In the case of these routines, even though it is possible to use the classical function structure and to handle them through Function Wizard, it was decided to access them from SimPro menu in order to unify the handling of the add-in.

The obtained product, SimPro.xla, is faultlessly adapted to the demands of the final stages of a course on Conceptual Design, in order to make a preliminary analysis of the behavior of a particular equipment structure or the characteristics of some compound mixtures. Also, SimPro can be

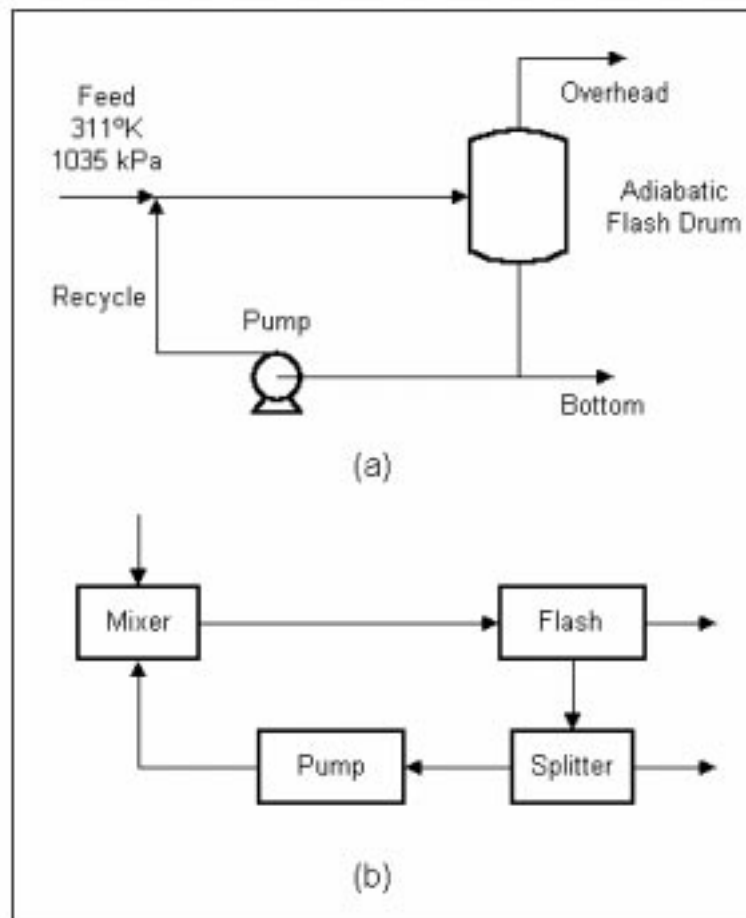


Fig. 1. Typical problem to be solved with SimPro.

extremely useful for other academic activities such as elementary material and energy balances, single process calculations, among others.

MAIN CHARACTERISTICS OF THE SIMPRO ADD-IN

SimPro is an add-in (SimPro.xla) for Excel® 97 and subsequent programs. When it is incorporated, a modification in the menu bar takes place, where the SimPro option appears. Also, two sheets are created, 'DatosProp' and 'Datos-Serv', both destined for data entry of compounds and auxiliary services that will be present during the simulation. In these sheets, several properties and parameters for each compound in the system (name, formula, molecular weight, fusion and boiling temperatures, critical properties, etc.) can be entered using SimPro menu. Those data are necessary to estimate different properties (enthalpies, VLE constants, etc.) of the pure compounds and their mixtures. SimPro has a database with information on 168 typical compounds of chemical and petrochemical process plants. In addition, the user can enter this kind of information for compounds that are not found in the database from the data available in classical bibliographical sources [5, 6]. Figure 2 shows part of the 'Datos-Prop' sheet.

The add-in assigns a number to each compound at the top of the corresponding column. During the simulation, this number will work as the identification code of that compound. The prediction of

properties requires the compound identification code or the mixture composition (it depends on the case) to be entered as arguments, as well as the pressure values and temperature to which the property is to be calculated.

As we have said, the SimPro add-in has several scalar functions in order to predict properties of pure compounds and mixtures. Also, from the SimPro menu it is possible to access several matrix functions that perform the calculation of process equipment and the auxiliary units available in the simulator. These functions are listed in Tables 1, 2 and 3.

Figure 3 shows the sequence of alternatives of the corresponding entry in the SimPro menu. For matrix functions, Excel® requires the user to select a priori the range of results. In the case of equipment, this is troublesome since the dimensions of that range change according to the chosen one. The function cannot perform the selection because this is a forbidden operation to functions, but procedures are allowed to do it.

In this way, the solution to the problem begins with the use of procedures, but only if it is possible to keep the automatic updating of results in order to carry out eventual iterative calculations or optimum searches. Then, the procedure must select the range and fill it with the corresponding function.

The Cost of Equipment block includes the following functions: Absorption and Distillation Tower, Heat Exchanger, Compressor and Pump, Reactor Vessel and Flash Tank.

The cost estimations for the installment equipment are made using the correlations given by

Properties	Comp. 1	Comp. 2	Comp. 3	Comp. 4
Name	Iso Pentane	2-Methylpent	n-Heptane	Toluene
Formula	C ₅ H ₁₂	C ₆ H ₁₄	C ₇ H ₁₆	C ₇ H ₈
MolWt	72.151	86.178	100.205	92.141
Tfp	113.3	119.5	182.6	178
Tb	301	333.4	371.6	383.8
Tc	460.4	497.5	540.2	591.7
Pc	30.4	29.7	27	40.6
Vc	306	367	432	316
ω	0.227	0.279	0.351	0.257
<i>Antoine Vapor Pressure Equation Data</i>				
A	15.6338	15.7478	15.8737	16.0137
B	2348.67	2614.38	2911.32	3096.52
C	-40.05	-46.58	-56.51	-53.67
<i>Ideal Gas Heat Capacity Data</i>				
a	-2.275	-2.524	-1.23E+00	-5.817
b	0.121	0.1477	1.62E-01	0.1224
c	-0.00006519	-0.00008533	-8.72E-05	-0.00006605
d	1.367E-08	1.931E-08	1.83E-08	1.173E-08
<i>Liquid Heat Capacity Data</i>				
a	10.83	142220	6.13E+01	140140
b	0.0146	-47.83	3.14E+05	-152.3
c	-0.0000292	0.739	1.82E+03	0.695
d	0.000000151	0	-2.55E+03	0
e	0	0	0	0
Eq. Type	1	1	2	1
Comp.	71	93	117	105

Fig. 2. 'DatosProp' sheet.

Table 1. Pure compounds properties functions

Liquid heat capacity
Gas heat capacity
Liquid density
Gas density
Liquid enthalpy
Gas enthalpy
Vapor pressure
Viscosity

Table 2. Mixtures properties functions

Heat capacity
Vle constant
Liquid density
Gas density
Liquid enthalpy
Gas enthalpy
Molecular weight
Bubble point pressure
Critical pressure
Dew point pressure
Bubble point temperature
Critical temperature
Dew point temperature

Table 3. Units functions

Absorption column
Distillation column
Compressor
Condenser
Adiabatic flash
Isothermal flash
Heat exchanger
Mixer
Pump
Conversion reactor
Continuous stirred tank reactor
Plug flow reactor
Reboiler
Splitter



Fig. 3. SimPro menu.

Guthrie [7], updated by Marshall Swift's index (M&S) [7].

In addition to the three mentioned modules, there are some edition tools that allow, for instance, extracting the bottom or top conditions of a column from the corresponding range that contains the results of the unit. These functions, as the equipment calculation ones, are of matrix nature and they are accessed from the SimPro menu.

APPLICATION EXAMPLES

SimPro system has been used in several problems of Conceptual Design, complementing the activities of design and cost calculation in complex systems.

Figure 4 partially shows the sheet with the results of one of the five possible schemes for the separation train of a 4-hydrocarbon mixture, which were obtained in the analysis made with SimPro. For clarity's sake, the corresponding process diagram has been added to the sheet. In this case, SimPro is being used as a tool for the analysis of the separation sector of liquid streams. Before using SimPro system, students have already performed a selection of the most promising schemes, taking into account the total annual cost that is associated to each scheme.

To carry out this previous selection, evaluation rates are used, such as Porter and Momoh's ROTÉ equation [9] or Jobson's boiling capacity variable [10]. In this example, the previous study has reduced the analysis to two schemes: the direct sequence (the lightest compound entering the feed is isolated in each column), and the one that is shown in Fig. 4. For both of them, the student has to carry out a series of activities which, in the commercial simulators, are made by the executive program in a transparent way to the user.

The simulation of every process scheme using SimPro requires:

- The preparation of a flow diagram which shows the data that come in and out from each simulation unit. This diagram must consider the interrelations among units. For instance, the variables that are calculated in one unit and which are data in another unit, represent information flowing from the first unit to the second one. It is also necessary to detect the iteration cycles produced by the typical structural stiffness of the modular simulators, usually when there are variables that appear as results in more than one block.
- About the flow diagram: if there are recycle structures, tearing sets allowing sequential calculation must be selected. Also, it is necessary to add control equations that allow performing the adjustment of the guessed values.
- If the previous analysis indicates the existence of independent variables, iteration schemes with guessed variables, or mixed situations with both

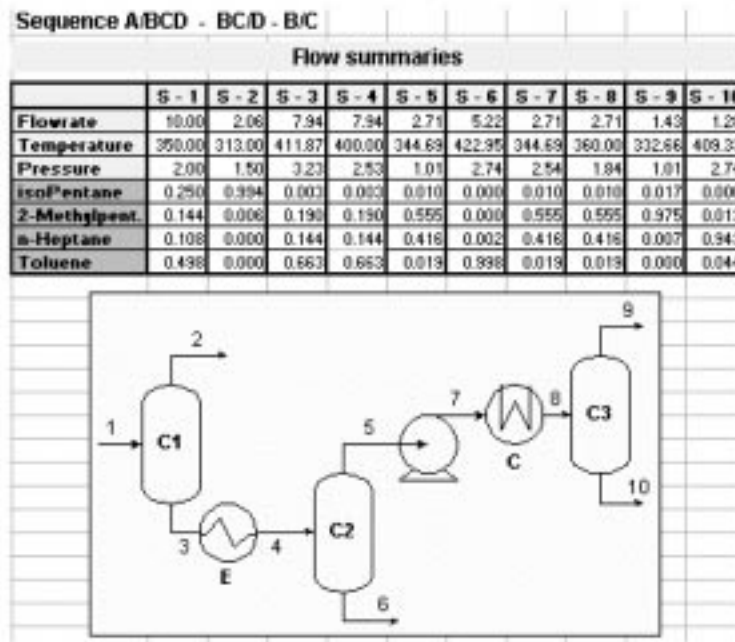


Fig. 4. Flow summaries for a train distillation simulated with SimPro.

types, the Solver add-in has to be used to solve the simulation problem.

Concerning the separation train analysis, there are no iterative schemes in the problem, though there are independent variables such as reflux ratio and top refrigerant temperatures. Figure 5 shows another part of the sheet in which the simulation is carried out. The results of the third tower of the scheme can be observed as well as the total annual cost calculation table. Besides identification labels, the results show the values of the process variables and those ones related to the equipment size.

The user should enter the data for the different units by following the information flow that cor-

responds to the flowsheet. In this way, the information used for the third column is taken from the row corresponding to the distillate of the second one. In turn, the second column is calculated from the bottom of the first one, until the feed is reached.

The results obtained in the example are in accordance with the estimations carried out by the evaluation functions, following Jobson's criteria, being the direct sequence the one that has the lowest total annual cost.

This example allows us to value the possibilities of SimPro, including the analysis of different process alternatives and the selection of the most appropriate one from a technical and economic point of view.

	Iso Pentane	2-Methylpentane	n-Heptane	Toluene	Flowrate [kg/s]	Temp. [°K]	Press. [bar]
Top (Vap)	0.0000	0.0000	0.0000	0.0000	0.00	0.00	0.00
Top (Liq)	0.0173	0.9753	0.0074	0.0000	1.43	332.66	1.01
Bottom	0.0000	0.0127	0.9429	0.0444	1.28	409.33	2.74
Plates	Reflux	Diameter [m]	Height [m]	Water Flowrate [kg/s]	Condenser Area [m ²]	Steam Flowrate [kg/s]	Reboiler Area [m ²]
50	0.80	0.27	35.05	2.57	79.43	0.51	30.28

ANUAL COSTS				
Item	Investment	Water	Steam	Total
M&S Index	1093.3	Cost (\$)	Cost (\$)	Cost (\$)
COLUM C1	675814	532	1769	69882
COLUM C2	598974	379	1791	62668
COLUM C3	229036	205	408	23517
COOLER	27237	304		3028
HEATER	11439		51	1195
PUMP	100			10
Total	1.54E+06	2020	4019	1.60E+05

Fig. 5. SimPro results for a distillation column and cost estimations for the train.

The availability of a cost expression for each process unit allows us to use SimPro in order to carry out the variable significance analysis according to the methodology proposed by Douglas *et al.* [11], detecting the process units and variables that have a bigger influence on the production cost.

In this case, the use of Solver has to be carried out in several steps:

- First, suitable values for the decision variables must be set.
- Second, values for the guessed variables in the iterative schemes will be found. Of course, this step is not necessary if there are no iteration schemes.
- Then, the decision variables will be disturbed one by one, and the entire calculation process will be repeated.
- After that, estimation of the partial derivatives of the total annual cost function components will be carried out.

Finally, the significance of each independent

variable is determined and the optimization problem is reformulated taking into account only those variables that are relevant due to their influence on the objective function.

It is really easy to perform the whole process once the problem has been posed on the spreadsheet, using the SimPro add-in.

CONCLUSIONS

The developed SimPro add-in allows us to carry out approximate calculations (mass and energy balances, equipment dimensions and cost estimation) for chemical processes of medium complexity. The use of this add-in is not different from the usual uses in the handling of functions and procedures in spreadsheet. With SimPro, we can efficiently deal with basic questions of Conceptual Design of Processes such as alternative analysis, specific modifications to a scheme and design variable significance analysis, among others.

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