

A Stochastic Simulator of a Multi-Component Distillation Tower Built as an Excel Macro

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ABSTRACT

Dynamic process simulation is widely used in teaching controller design, as it allows foreseeing the performance of different control configurations and controller tunings. Currently, most college-level controller design exercises that are based on simulation consider deterministic perturbations (i.e. steps or ramps). In real life however, processes are more likely to face fluctuating, random disturbances, so the use of stochastic simulation in controller tuning exercises would provide students with an experience closer to their future professional practice than that provided by deterministic simulation. However, public institutions attempting to use dynamic, stochastic simulators in teaching, are hindered by the need of buying licenses of simulation packages or specialized programming languages (such as Matlab), as there aren't any dynamic, stochastic simulators available as downloadable freeware. This paper shows a dynamic, stochastic simulator with a friendly interface of a distillation tower, developed as an Excel macro. This simulator has the advantage that it can be used at no cost to educational institutions since Excel is almost universally known and used by college faculties.

Keywords-simulation; stochastic; distillation

I. INTRODUCTION

Dynamic simulators are very useful in the teaching of process control in college engineering, as they can be used to compare the performance of different control configurations (i.e. the linking of controlled and manipulated variables) and to optimize the tuning of controllers. However, almost all simulation-based learning experiences of control design use deterministic disturbances (e.g. ramp or step changes) to dynamically assess the candidate controller configurations or tunings [1]. In practice, however, process units are subjected to disturbances that are better described as stochastic, varying continuously and in an unpredictable manner. Therefore, the engineering trainee would benefit from performing process control practices including stochastic disturbances. To carry out the said activities however, dynamic process simulators able to incorporate random elements (i.e. stochastic dynamic simulators) are needed. On the other hand, public institutions of higher education in developing countries are facing severe shortages of economic resources. This hinders their ability to

use process simulators in their teaching activities, due to the need of purchasing user licenses. In the case of steady-state simulators, there are a few free software alternatives that have been sufficiently validated (e.g. the COCO simulator [2]), however, this is not the case of dynamic simulators and certainly not of the subset of these able to handle random disturbances. This paper presents the development of a dynamic three-component distillation tower simulator with stochastic elements and a user-friendly interface (allowing user interaction via buttons and dialog boxes) created using Microsoft Excel macro functionalities. This allows the simulator to be run in said software, that is already being used by most developing countries college engineering faculties.

A. Literature Review

Reviews of dynamic simulation applications for optimizing energy and chemical systems are shown in [3, 4], while applications of discrete event simulation to the optimization of industrial systems can be found in [4-6]. Usage of simulation in

specific situations are presented in [7] for sustainable plant design, in [8] for gasifier pressure modeling, and in [9] for analyzing a petrochemical process wastewater plant. Additional applications include treating a desalination plant [10], optimizing the drying of phosphates [11], analyzing the benzene-toluene-xylene separation train from a sustainable point of view [12].

Regarding the software used for the dynamic simulations, Aspen Dynamics and Matlab have been used for studying separation tower trains [13], ChemCAD for modeling polymerization reactors [14], Aspen HYSIS for treating energy-integrated reactors [15], and Matlab and COSMOL Multiphysics for studying catalysts [16]. Additionally, authors in [17] present a proposal for controlling combustion cycles using Aspen Dynamics, authors in [18] simulated a wastewater system using INSEL (Integrated Simulation Environment Language), and authors in [19] modeled a set of CO₂ absorbers for implementing a predictive control scheme, employing ASPEN and Matlab.

Experiences on the didactic use of chemical process simulators are included in [20], where Aspen HYSIS was used for training engineers in the handling of distillation trains and in [21] where Honeywell Unisim Design was used in training operators of an isopropanol plant. Regarding the reports on the development of home-grown process simulators in educational institutions for pedagogical purposes, authors in [22] describe the steady state simulator Lazarus, run in UML and developed as a freeware with the option of incorporating modules from third parties, authors in [23, 24] developed programs to study the dynamics of heat exchanger networks, authors in [25] provided a web-based natural gas distribution system simulator, authors in [26] described the LABVIRTUAL learning platform which includes steady-state simulators, and authors in [27] presented a dynamic reactor simulator programmed in Matlab.

It can be noted that there is a growing preference for using commercial simulation software (e.g. ASPEN) and programming languages with pre-built routines for model construction (e.g. Matlab) in reported research and pedagogical simulation applications. Since both types of software require paid licenses, the reported applications are of little relevance to the teaching in public institutions which strive to optimize the spending of their limited budgets. In contrast, the simulator presented in this paper is programmed in Microsoft Excel. This program, even though not being freeware, is widely available to college staff as it comes with the MS Office packages purchased by institutions for word processing and administrative tasks. Additionally, none of the reported dynamic simulators built for teaching applications incorporates random disturbances. As in practice, process plant operation is affected by random disturbances, using stochastic dynamic simulators in teaching activities related to controller design and tuning, can better prepare the future engineer for operating real plants.

II. CASE STUDY DESCRIPTION

A ten-plate distillation tower fed with a mixture of benzene, toluene and p-xylene is taken as a case study (Figure 1).

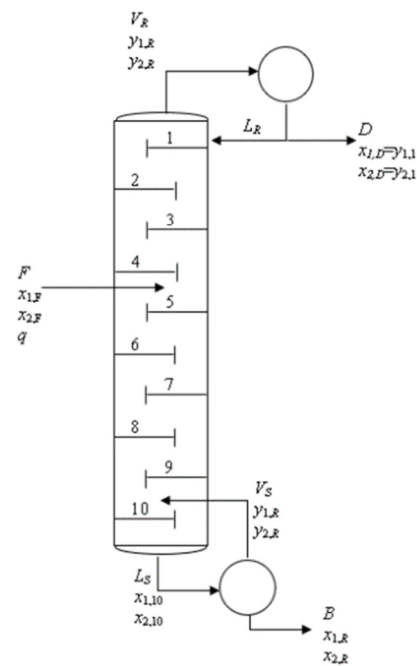


Fig. 1. Distillation tower case study.

V_R and V_S are, respectively, the molar vapor flow in the rectifying and stripping tower sections, with L_R and L_S being the corresponding liquid molar flows. F , D and B are, respectively, the molar flow of feed, distillate, and bottom product, and q is the feed vapor fraction. The feed mole fraction of component i is $x_{i,F}$ ($i=1,\dots,3$). $x_{i,j}$ and $y_{i,j}$ denote, respectively, the mole fraction of component i in the liquid and vapor leaving the plates and the reboiler ($j=1,\dots,10,R$). The dynamic model used the following assumptions:

- The molar flows of vapor and liquid in the stripping and rectifying sections are constant.
- The plate (m) and the reboiler (m_R) holdups are constant.
- The mole fractions of the liquid and vapor in equilibrium follow Raoult's law (1):

$$P y_{i,j} = P_i^0(T_j) x_{i,j} \quad i=1,\dots,3, \quad j=1,\dots,10,R \quad (1)$$

where P is the tower pressure and $P_i^0(T_j)$ the vapor pressure of component i at the temperature T_j of stage j ($j=1,\dots,10,R$). Vapor pressures follow Antoine's relation (2) with A_i , B_i and C_i being component specific constants:

$$P_i^0 = \exp\left(A_i - \frac{B_i}{T_j + C_i}\right) \quad (2)$$

- The tower hydraulics are very fast, with the internal and external flows adjusting to changes in F , q , V_S and r , which is the reflux ratio (L_R/D), according to:

$$V_R = V_S + qF \quad (3)$$

$$D = \frac{V_R}{(1+r)} \quad (4)$$

$$B = F - D \quad (5)$$

$$L_S = V_S + B \quad (6)$$

$$L_R = D r \quad (7)$$

- The mole fractions of the components in the feed $x_{i,F}$ ($i=1, \dots, 3$), may fluctuate randomly.

Mole fractions add to one, so the dynamic model consists of two molar balances for each stage, resulting in 22 ordinary differential equations, i.e. (8)-(13), for $i=1, 2$.

Plate 1:

$$\frac{dx_{i,1}}{dt} = \frac{L_R(y_{i,1} - x_{i,1}) + V_R(y_{i,2} - y_{i,1})}{m} \quad (8)$$

Plate in the rectifying section $j=2, 3, 4$:

$$\frac{dx_{i,j}}{dt} = \frac{L_R(x_{i,j-1} - x_{i,j}) + V_R(y_{i,j+1} - y_{i,j})}{m} \quad (9)$$

Feed plate:

$$\frac{dx_{i,5}}{dt} = \frac{F x_{i,F} + V_S y_{i,6} + L_R x_{i,4} - V_R y_{i,5} - L_S x_{i,5}}{m} \quad (10)$$

Plate in the stripping section $j=6, \dots, 9$:

$$\frac{dx_{i,j}}{dt} = \frac{L_S(x_{i,j-1} - x_{i,j}) + V_S(y_{i,j+1} - y_{i,j})}{m} \quad (11)$$

Plate 10:

$$\frac{dx_{i,10}}{dt} = \frac{L_S(x_{i,9} - x_{i,10}) + V_S(y_{i,R} - y_{i,10})}{m} \quad (12)$$

Reboiler:

$$\frac{dx_{i,R}}{dt} = \frac{L_S x_{i,10} - B x_{i,R} - V_S y_{i,R}}{m_R} \quad (13)$$

Equations (8)-(13) are integrated using an implicit Euler method: Defining a state vector $\mathbf{X} = [x_{1,1}, x_{2,1}, \dots, x_{1,R}, x_{2,R}]^T$, a disturbance vector $\mathbf{D} = [F, q, x_{1,F}, x_{2,F}]^T$, and a manipulated variables vector $\mathbf{U} = [r, V_S]^T$, the value of \mathbf{X} at time $t+h$, is obtained from its value at time t by solving the system of nonlinear equations (14), h being is the step size.

$$\mathbf{X}(t+h) = \mathbf{X}(t) + \frac{d\mathbf{X}}{dt} \Big|_{(\mathbf{X}(t+h), \mathbf{D}(t), \mathbf{U}(t))} \quad (14)$$

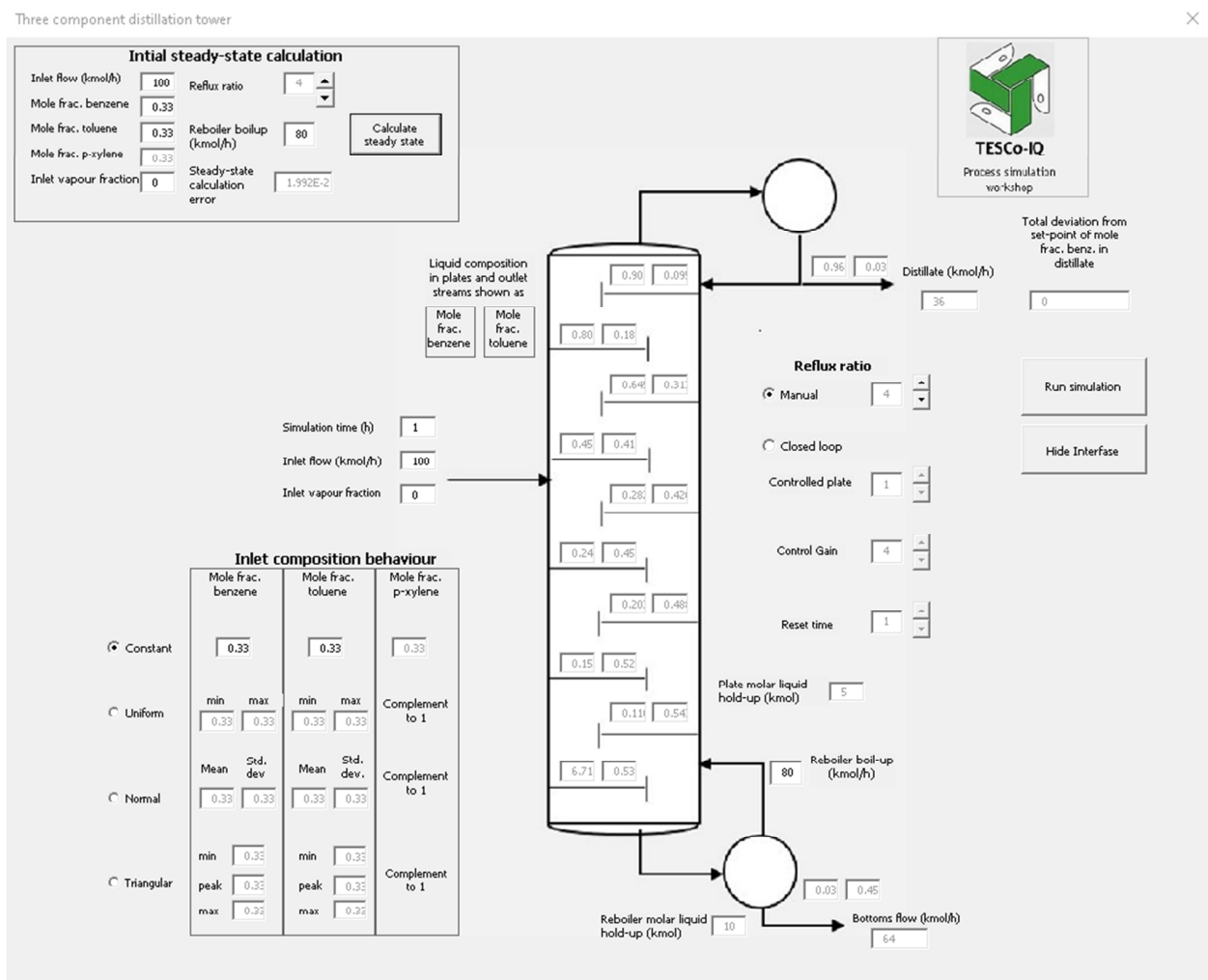


Fig. 2. Main simulator interface.

For simulating a tower with stochastic feed mole fractions, $x_{1,f}(t)$ and $x_{2,f}(t)$ are sampled from their probability distributions (using the methods described in [28]) and are substituted in (14) before solving these equations to calculate $\mathbf{X}(t+h)$. When running a controlled tower, an integral proportional logic (15) changes the reflux ratio r to control the temperature of a given plate in the rectifying section:

$$r = r_0 + K_C \left(e + \frac{1}{\tau} \int_0^t e dt \right) \quad (15)$$

where e is the deviation of the controlled plate temperature from its set-point, K_C is the gain of the controller, τ is its reset time, and r_0 the initial value of the reflux ratio.

III. SIMULATOR DESCRIPTION

The simulator is given to the user as a macro-enabled Microsoft Excel file. By clicking the "Begin Simulation/Show Interface" button (Figure 3) the main simulator interface is displayed (Figure 4). The program works in desktop Excel versions supporting visual-basic macros, i.e. those in MS Office versions from 2010 onwards.

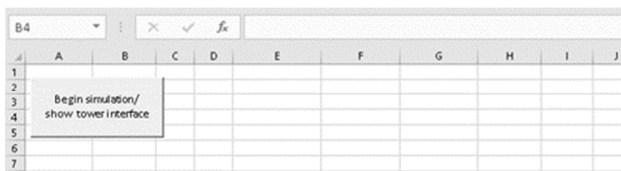


Fig. 3. Initial screen when the Excel file is opened.

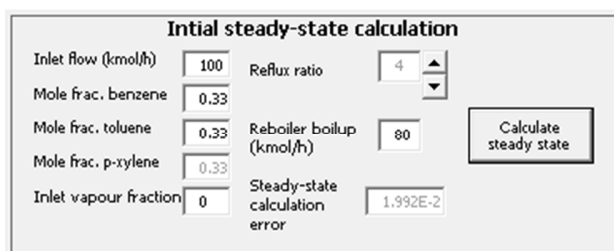


Fig. 4. Detail of the controls in the steady state interface section.

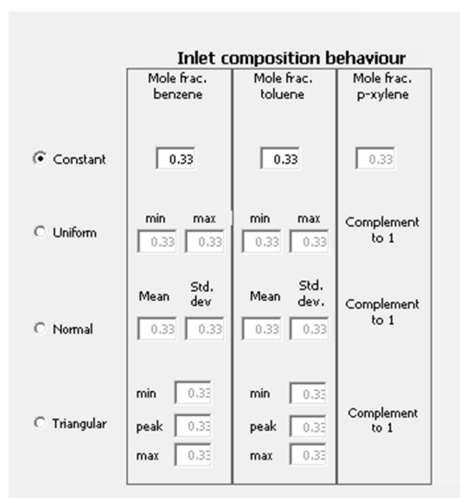


Fig. 5. Controls for specifying the inlet composition behavior.

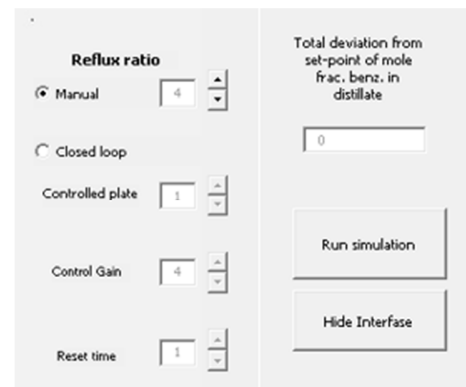


Fig. 6. Controls for defining the reflux ratio policy

Initially, only the controls in the "Initial steady state calculation" zone appear active (Figure 4). Through these controls, the user specifies the steady-state condition the tower is in before the dynamic simulation starts. Once the qualities of the feed, reflux ratio, and reboiler boil-up (V_3) have been entered, by clicking the "Calculate steady state" button the initial steady state of the system is calculated. The total error achieved in solving the steady state problem (that is formed by making the derivatives in (8)-(13) equal to zero) appears in the corresponding dialog box. The steady-state composition of the liquid in the plates and the flowrate and compositions of the outlet streams appear in the boxes placed on the plates and close to the outlets of the sketched tower (Figure 2). Once the steady-state solution has been achieved, the buttons associated with the dynamic simulation become active.

The feed flowrate and vaporization and total simulation time are entered in the dialog boxes located to the left of the tower in Figure 2. The probability distributions of the feed mole fractions, which are to be varying randomly, are defined through the controls in the section "Inlet composition behavior" of the interface (Figure 5).

The control ratio to the left in Figure 5 allows selecting how the behavior of the feed mole fractions of benzene and toluene is going to be. These mole fractions can remain constant or follow a probability distribution: uniform (specifying minimum and maximum values), normal (specifying mean and standard deviation), or triangular (specifying minimum, most likely and maximum values). The sampled feed mole fractions are standardized in case their sum exceeds unity and, as can happen when sampling from a normal distribution, if the simulated value is either negative or greater than 1, new values are produced until they lie in the required (0,1) range.

Figure 6 shows the interface section in which the reflux ratio management is defined. It can be set constant (by choosing "manual" and selecting its value) or used to keep the temperature of a rectifying plate close to its temperature at the initial steady state. The controller specifications are also entered here. The total absolute deviation (i.e. the absolute value of the deviation integrated along the simulated time) of the fraction mole of benzene in the distillate, with respect to its steady state value, is displayed in the relevant text box.

Once the simulation is complete, a dialog box asks the user if graphs of the simulation results are to be produced. If "yes" is answered, graphs of the controlled plate temperature and the mole fraction of benzene in distillate against time are displayed. These graphs are produced using the Excel spreadsheet functionalities, as shown in Figure 7.

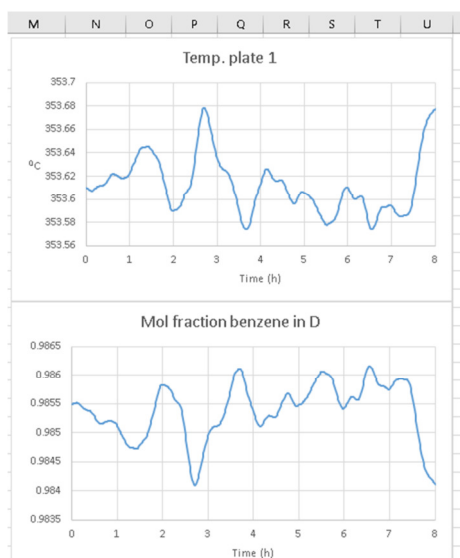


Fig. 7. Example of charts produced by the simulator.

To illustrate the simulator results, the top chart of Figure 8 shows the behavior of plate one temperature when the feed mole fractions of benzene and toluene are uniformly distributed between 0.1667 and 0.5.

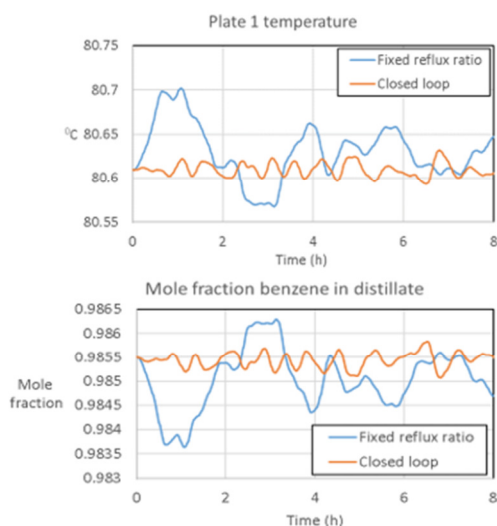


Fig. 8. Closed loop vs. manual operation contrast

Responses for a constant reflux ratio set to its steady state value, and for a manipulated reflux ratio controlling plate one temperature, with controller gain of 20 and reset time of 0.1h, are included. The bottom chart of Figure 8 shows the

corresponding behavior of the distillate mole fraction of benzene. The total absolute deviation of the distillate benzene mole fraction for the closed loop case is 0.0672, while that for the fixed reflux ratio case is 0.21.

It is easy to visualize the usage of this simulator for training students in controller design under stochastic conditions, through exercises in which they need to tune the controller and select controlled plates so to minimize the benzene distillate composition deviation, and asking them to discuss the effect of the feed composition behavior on the results.

IV. CONCLUSIONS

As there is a lack of freeware dynamic simulators, educational institutions seeking to use them in teaching must purchase licenses. This situation is exacerbated for dynamic simulators capable of including stochastic disturbances, as these are more specialized and have more expensive licenses than deterministic simulators. As in practice engineers need to control plants facing unpredictable, continuously varying disturbances, implementing process control exercises for engineering students using simulated stochastic disturbances can be a valuable preparation for their future practice.

In this paper, a stochastic simulator intended for this purpose is presented. As the simulator runs in Microsoft Excel, that is already used in most engineering colleges, no specific license software is needed for its pedagogical use. A limitation of the simulator, however, is that it only runs in desktop Excel versions. It wouldn't run in Libre or OpenOffice, GoogleSheets, or web-based Excel, as these do not support visual basic macros. It is expected that the work presented here encourages engineering faculties to develop their own simulators.

The interested reader can download the simulator at [29]. The users are encouraged to report any bugs to the corresponding author email address.

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