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Aspen Dynamics simulation of a middle-vessel batch distillation process

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ABSTRACT

Aspen Dynamics is a powerful dynamic simulator that is widely used to explore the dynamics and control of continuous processes around some steady-state design operating point. This paper explores its use to study the dynamics of a batch process. The example studied is a middle-vessel batch distillation system for separating a ternary mixture. The batch system is operated by adjusting the two reflux flowrates (one from the reflux drum to the top of the upper column and the second from the middle vessel to the top of the lower column). The liquid inventories in the three drums vary with time. This paper shows how this batch operation can be conveniently simulated by first using the steady-state simulator Aspen Plus to correctly size the equipment. Then the file is exported into Aspen Dynamics where a rigorous dynamic simulation can explore alternative control strategies by using the large library of control functions.

1. Introduction

Control studies of both batch and continuous chemical processes have been widely used for many decades. Dynamic models of all the units and accurate physical property relationships are required as well as numerical methods for solving the large set of nonlinear algebraic and dynamic differential equations. Early studies required the engineer to develop the required dynamic equations from fundamental models (energy and component balances with appropriate phase equilibrium and reaction kinetics relationships). Then numerical integration methods were used to obtain dynamic responses.

In recent years, commercial steady-state and dynamic simulators have been developed that provide built-in quite rigorous models of many unit operations. They also provide a large library of physical property data and a reliable selection of numerical integration algorithms. They have an extensive array of realistic control models (controllers, multipliers, selectors, deadtimes, etc.), which permit dynamic simulations capable of accurately predicting the dynamics of quite sophisticated control structures.

The vast majority of studies have considered the dynamics and control of continuous processes. The process operates around a design steady-state condition. Alternative process designs and control structures can be quickly and easily evaluated.

Most studies of batch processes have used user-developed models and solution methods. The pioneering middle-vessel control paper by Skogestad et al. [1] is a good example. The model for a hypothetical chemical system was developed and implemented using SPEEDUP. A more recent study of the middle-vessel batch process by Rao and Barik [2] used a first-principles model for the ethanol/propanol/butanol separation.

Gruetzmann and Fieg [3] presented both simulation and experimental results for a middle-vessel batch distillation column for the hexanol/octanol/decanol separation. Aspen Custom Modeler was used for the simulations. They considered the detailed startup procedure from a cold start (column filled with nitrogen). It took 41 min for the vapor coming from the reboiler to reach the top of the column and begin building liquid in the reflux drum. When an adequate level was obtained, reflux to the top of the column was initiated (at 79 min). When the liquid reached the middle vessel and its level rose to an adequate level, reflux to the lower section of the column was begun. It took 180 min for the counter-current flow of vapor and liquid to be established so that fractionation could develop composition and temperature profiles under total reflux operation. Then various control strategies were explored for manipulating the two reflux flowrates to achieve the desired purities in the three vessels.

It is important to note that developing dynamic simulations in SPEEDUP or in Aspen Custom Modeler is a daunting task. The programming is complex and non-intuitive (at least to this author). A level of expertise is required that is well above that of the normal control engineer. This paper demonstrates that the more common

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and much more easily used (than user-developed models) software of Aspen Plus and Aspen Dynamics can be effectively used for the task of studying batch processes.

A number of simulators have been developed over the years for handling batch processes: BATCHFRAC, Aspen Batch Modeler, Aspen BatchSep, etc. All these require learning a different simulation language. Some studies [4] of batch processes have used hybrid systems combining Aspen Plus and Matlab. A study [5] using Aspen Plus and Aspen Dynamics developed a very complex simulation involving multiple steps and "Scripts" in a very lengthy design and analysis procedure. The method presented in this paper is much more straightforward and easy to implement.

Chien et al. [6,7] combined the steady-state simulator Aspen Plus with the dynamic simulator Aspen Dynamics for the simulation of two batch processes: batch extractive distillation and batch heterogeneous distillation. No details are provided in these papers of the required procedure in setting up the initial steady-state simulation in Aspen Plus and then converting it into a batch dynamic simulation in Aspen Dynamics.

There are a number of significant advantages in being able use the many capabilities of a rigorous but simple-to-use simulator to study batch processes. These advantages include extensive physical property libraries, built-in models of many process units, rigorous numerical integration algorithms and rigorous models of control elements (valves, controllers, deadtime, selectors, etc.). The Aspen *Radfrac* distillation column model is quite rigorous and gives realistic predictions of column hydraulics during dynamic changes (tray holdup and pressure drop). These are often ignored in simple simulations but can be significant in dynamic batch distillation.

The purpose of this paper is to provide the important step-by-step details ("the devil is in the details") of starting with steady-state Aspen Plus to size equipment and then performing the dynamic batch simulation in Aspen Dynamics. The important batch middle-vessel process is used as a realistic example to demonstrate how the widely used and user-friendly Aspen software can be conveniently applied for studying a batch process.

The middle-vessel configuration has some distinct advantages over more conventional batch processes. The major advantage is that there are no "slop cuts" (material that is off specification) that have to be managed (determine when to produce) and have to be further processed (e.g. recycle back to the next batch). See Ref. [8].

2. Process studied and design procedure

The numerical example studied has a ternary feed of benzene, toluene and o-xylene. The NRTL physical properties are used in the Aspen Plus and Aspen Dynamics simulations. The number of stages in each column section (upper and lower) is set at 16 since the separation is fairly easy with the minimum number of trays well below 16. A *Radfrac* rectifier model (condenser but no reboiler) is used for the upper column. A *Radfrac* stripper model (reboiler but no condenser) is used for the lower column. Operating pressure in the reflux drum is 1.1 bar since operation at about atmospheric pressure eliminates issue with vacuum columns.

2.1. Setup of continuous process in steady-state Aspen Plus

The first step is to set up a simulation in Aspen Plus that has the required pieces of equipment and to size the columns and vessels for the desired capacity (vapor boilup) and batch size (volume of initial charge to the sump of the lower column). Remember that in Aspen Plus the flowsheet must be a continuous process with feed and product streams. These will be eliminated (valves shut) in the dynamic simulation.

The most critical design parameter is to set the vapor and liquid load in the column to be approximately equal to what is desired for the batch operation. This is necessary so that the column diameter is appropriately sized. For example, in the numerical example we assume that a vapor boilup rate of 100 kmol/h is going to be used in the batch process. To achieve this objective, the vapor stream from the lower section into the upper section is "torn" as shown in Fig. 1. The stream "VUPPER" is specified to be 100 kmol/h with an

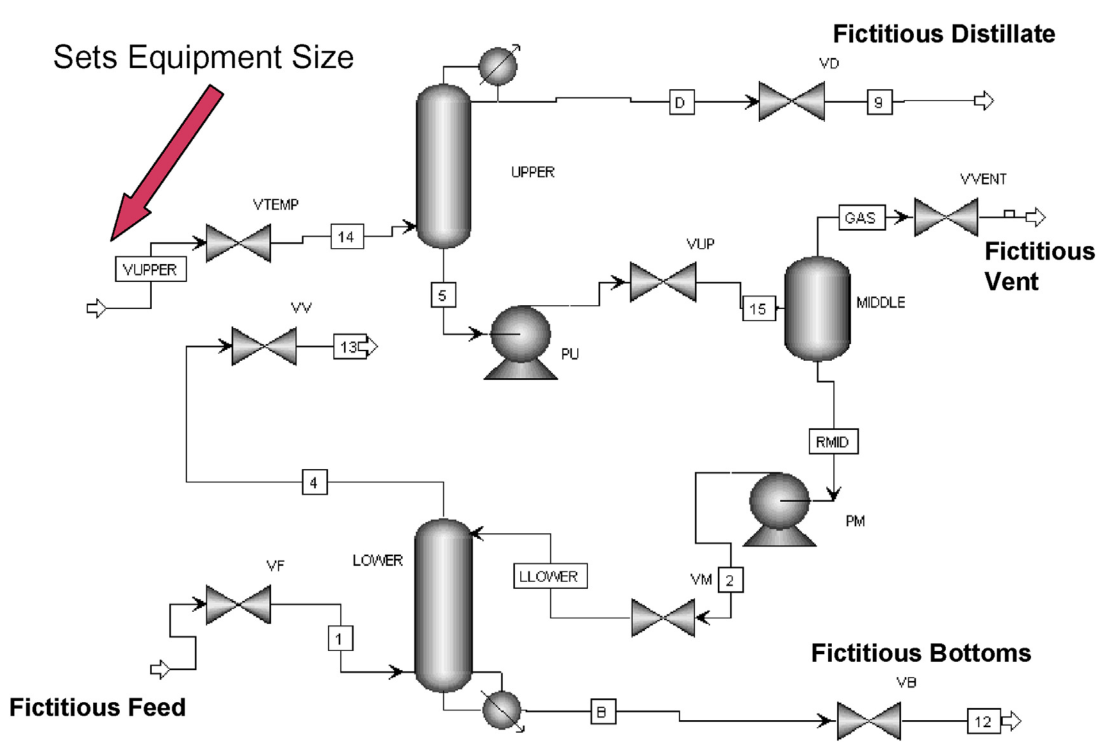

Fig. 1. Aspen Plus PDF showing fictitious streams.