OPTIMAL BATCH DISTILLATION SEQUENCES USING ASPEN PLUS®

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Abstract

After the original design is completed, optimum batch distillation sequencing and operation in a chemical plant is usually a matter of trial and error that evolves as operators gain experience with the system. Predictive tools, such as Batchfrac™ in Aspen Plus®, have been used with success in designing new batch separation systems and in analyzing existing systems. However, these tools require the user to define all the operation steps for each cut. The number of case studies required to approach an optimum scenario is very large, and the time required to perform each case study makes a comprehensive analysis commercially impractical. Optimal design and operation, however, is the ultimate goal. In this paper we propose how to quickly optimize batch separation sequences. Combining Batchfrac™ and SQP with other flowsheeting and modeling features in Aspen Plus® provides an advantageous way to analyze and optimize operating scenarios for optimum batch separation sequencing. This approach is demonstrated with the optimization and debottlenecking of several batch distillation scenarios to separate and recover a heavy product, a partially water-miscible solvent, and water from a batch reactor effluent. Simulations identified a >25% increase in capacity with a minimum capital investment.

Keywords

Batch distillation, batch distillation sequencing, optimization, debottlenecking, Aspen Plus®, Batchfrac™

Introduction

Process engineers are often tasked to find more capacity in existing plants. In batch plants, the engineer traditionally starts with a cycle time analysis. The engineer evaluates a particular unit operation to determine the time required for each step. For example, in a batch distillation unit operation, the steps can be charging the still, heating the still, reaching total reflux, taking Cut 1, taking Cut 2, etc., and finally, discharging the pot.

Based on the results of the cycle time analysis, the engineer then focuses on the step or steps that take the longest because these steps intuitively have the most impact on rates. The engineer then generates ideas and options for improvement, quantifies the benefits and validates the feasibility for each option, selects the best option, and implements the solution.

The major disadvantages of this approach are

- The approach is manually iterative to obtain a feasible solution.
- The identified step(s) may not be the critical path step(s).
- The approach may produce a local optimum, not a global optimum.
- The approach is labor intensive – fewer options can be evaluated.

A methodology and technique that eliminates these shortcomings is a worthwhile goal. This paper focuses on the engineering quantification and validation of ideas for debottlenecking a batch distillation sequence using commercially available CAPD tools, specifically Batchfrac™ [1] within the Aspen Plus® framework. Batchfrac™ is a rigorous batch distillation model in Aspen Plus®. Combined with flowsheeting features within Aspen Plus®, Batchfrac™ can be used to systematically evaluate and optimize generated batch distillation scenarios, while manipulating all potential process variables to meet all process constraints. The proposed approach saves engineering time, allows the engineer to evaluate more ideas, and increases accuracy and confidence in the quantification of benefits.

Debottlenecking Methodology

A business premise usually sets the objectives or goals the process engineer must deliver. The business premise for higher rates in a batch plant may be to meet customer demand or to better utilize the assets with more products. Often the business premise defines the boundaries or constraints of the ideas, for example project execution time or capital spending.

With the goals defined, the process engineer must generate ideas and options to debottleneck the plant. The ideas come from process understanding, cycle time analysis, operator feedback, and simulation analysis. These ideas could include a larger reboiler, larger condenser, larger reflux pump, etc. The process engineer then quantifies and validates the benefits of each idea to debottleneck the plant.

The production rate from each idea must be quantified. These quantified benefits must also be validated to determine if it they are truly achievable. Validation often requires the process engineer to look at constraints outside of the particular unit operation in question.

After the ideas are validated and the benefits quantified, the ideas must be sorted to determine if the business goals will be met within the defined constraints. If the idea will debottleneck the plant to the extent needed, a rough capital estimate is generated. With the capital estimate, the process engineer determines if the idea will meet the business constraints. The ideas are then sorted by a cost and benefits analysis to select the best option. The final step is to execute the selected option.

Process Description

The current bottleneck in the process is the crude product and solvent recovery system. The system consists of a single batch distillation column, including condenser and reboiler; five storage tanks; a reflux pump; a pot bottoms pump; and three charge pumps. The system contains three major components: water, a partially miscible solvent, and the heavy product.

As shown in Figure 1, the single batch distillation column performs three different distillations: Crude Product, Wet Solvent, and Very Wet Solvent. The purpose of the distillations is threefold: to remove the partially miscible solvent and water from the crude product, to recover dry solvent for recycle into the reactor system, and to minimize organics in the wastewater.

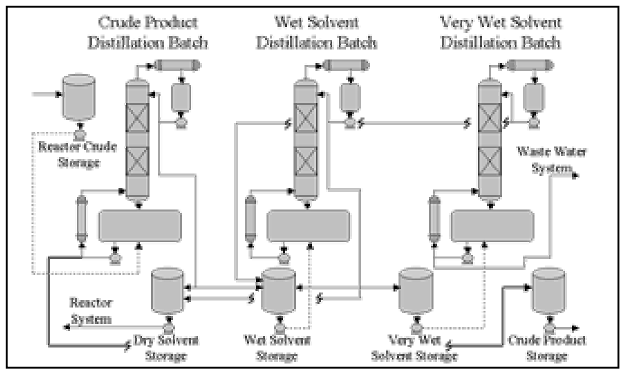


Figure 1. One Column, Three Distillations.

The crude product has a maximum specification for solvent and water content. The dry solvent has a maximum specification for the water that can be recycled to the reactor. The wastewater has a maximum specification for organics. Each distillation has its own cycle time, and each distillation must be sequenced to make full use of the single batch distillation column. Since the solvent and water are partially miscible, intermediate storage and recycle within the recovery system are required.

As seen in Figure 1, the reactor effluent is stored in the reactor crude storage tank. The Crude Product Distillation requires a wet solvent cut, a dry solvent cut, and a pot discharge. The pot discharge is the crude product that is further refined in other equipment. The dry solvent is recycled to the reactor.

When several Crude Product Distillations have been completed and the wet solvent storage tank is full, a Wet Solvent Distillation is performed. The Wet Solvent Distillation requires a very wet solvent cut, a wet solvent cut, and a dry solvent cut. Similarly, when several Wet Solvent Distillations have been completed and the very wet solvent storage tank is full, a Very Wet Solvent

[1] BatchSep™ will supersede Batchfrac™ in 2004. BatchSep™ is currently under development by AspenTech.

Distillation is performed. The Very Wet Solvent Distillation requires a wet cut, and the pot discharge is wastewater.

The sequencing of the three distillations is determined by wet and very wet solvent storage tank capacities. If one of the very wet or wet solvent storage tanks is nearly full, the contents of that particular tank must be distilled to lower the tank level to allow room for the cuts from a Crude Product Distillation.

Baseline Simulation

The first step in the quantification and validation process is to develop a baseline model that adequately simulates the existing process. The development of a model for this process is complicated by the fact that batch distillation is a dynamic operation, and the framework for the SQP model is a steady-state simulator. Batchfrac™ is incorporated within Aspen Plus® using time-averaging. The amount charged to the batch column is specified using a charge time within the Batchfrac™ input. The steady-state flow rate of the charge stream is divided by this charge time to get the batch amount charged to the column. The batch distillation products are converted to steady-state rates using this same specified time.

Also complicating the simulation is the fact that the same column is used for three separate distillations; the frequency of each distillation is dictated by the storage tank capacities. To relate the three distillations on the same basis within a steady-state simulator, interacting streams must be scaled to reflect the frequency of each distillation. For example, if the process executes four Crude Product Distillations for every Wet Solvent Distillation, the flow into the wet solvent storage tank from the Wet Solvent Distillation needs to be scaled by ¼ to keep the flows into the tank on the same basis as the Crude Product Distillation. It is necessary to keep the flows to the cut tanks on the same basis so that the distillations are properly sequenced, for example, eight Crude Product Distillations to two Wet Solvent Distillations to one Very Wet Solvent Distillation, or a distillation frequency of 8:2:1.

In Aspen Plus® the three distillations can be related on the same basis by using factors to relate all continuous streams on the basis of one Crude Product Distillation. Aspen Plus® has a Multiplier Unit Operations Model that allows us to manipulate stream flows.

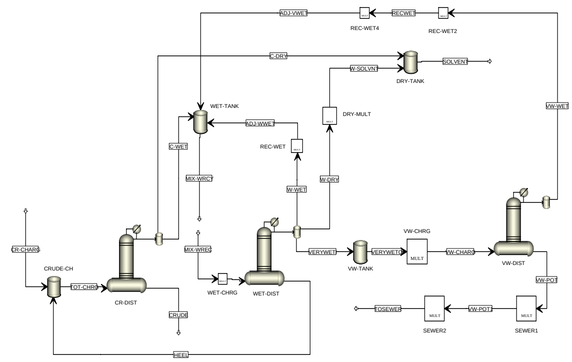


Figure 2. Aspen Plus® Flowsheet-Baseline Model

Figure 2 depicts the Aspen Plus® schematic used for the baseline model. Notes on the flowsheet:

- The heel of the Wet Distillation (Stream *Heel*) is recycled back to the Crude Product Distillation in case any heavies are taken overhead in the Crude Product Distillation.
- The wet solvent tank feed to the Wet Solvent Distillation is a tear stream.
- Stream *Crude* is the crude product to be sent downstream for further purification.
- Stream *Solvent* is the dry solvent to be recycled to the reactor.
- Stream *ToSewer* is the wastewater stream.
- All of the units represented by squares are Multiplier Blocks to represent flows on the same basis.

The Crude Product Distillation consists of the following steps: flushing, pot charge, heat up, total reflux, a Wet Solvent Cut, a Dry Solvent Cut, and pot discharge. The Wet Distillation consists of the following steps: pot charge, heat up, total reflux, a Very Wet Cut, a Wet Solvent Cut, a Dry Solvent Cut, and heel discharge. The Very Wet Distillation consists of the following steps: pot charge, heat up, total reflux, a Wet Solvent Cut, and pot discharge. The only steps that are rigorously modeled in Batchfrac™ are the Cuts. All other step times are fixed, based upon plant values. The baseline distillation frequency (Crude : Wet : Very Wet) is 5:2:1.

Each of the rigorously modeled Cuts is segmented into Operation Steps. An Operation Step within Batchfrac is defined as a period of time where operating conditions (e.g., pressure, reflux ratio, pot duty) are constant, or optionally ramped (pressure).

Validation of the baseline simulation requires plant data, and may require refinement of the physical property model. Once the model is validated, it can be modified to perform what-if scenario simulations.

Scenario Modeling Using SQP

Demand for the product of the plant is expected to exceed 5% CAGR (compound annual growth rate).

However, the existing assets are already in full use. This means that a 5% expansion is required for next year, and the capacity needs to be 22% greater in four years to meet demand. The product has a high value, so it is desired to capture as much of the demand as possible. At the same time, it is necessary to minimize capital spending, as a major capital expenditure cannot maintain the plant's high return on investment.

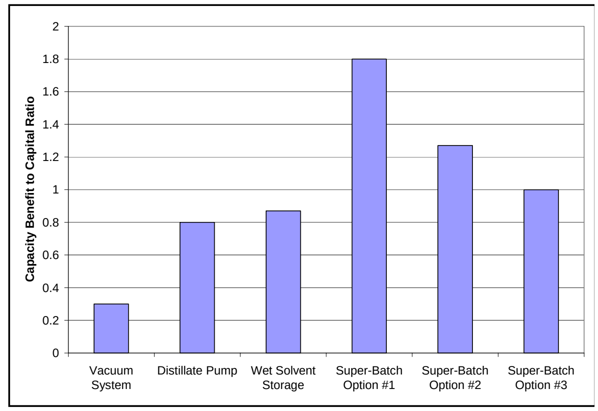
Several ideas were generated to debottleneck the crude product and solvent recovery system:

- Install vacuum capability on the distillation column to exploit the pressure swing separation.
- Increase distillate pump capacity to decrease the Crude Product Distillation cycle time
- Increase wet solvent storage capacity for more flexibility in distillation sequencing
- Implement a SuperBatch (semi-batch) feed scheme to make full use of pot capacity during the Crude Product Distillation
- Upgrade the reboiler to make full use of column hydraulic capacity
- Increase very wet solvent storage capacity for more flexibility in distillation sequencing

Some were combined as additional options, and the benefits of all the options were quantified and validated. Starting with the baseline model, the SQP (Successive Quadratic Programming) feature in Aspen Plus® is overlaid on the model, and the model is modified to represent the desired scenario. Input to SQP includes the optimizer objective function, the constraints, and the variables to be manipulated. The objective function is to maximize crude product rate. The following constraints must be satisfied:

- Crude product, dry solvent, and wastewater purity specifications
- Column hydraulic limitations
- All storage tank capacities
- All pump capacities
- Reboiler heat transfer capacity
- Condenser heat transfer capacity
- Vessel maximum allowable working pressure

The manipulated variables include operating pressure, reflux ratio, and cut time for all cuts in each distillation. Reboiler duty is assumed to operate at maximum capacity for all cuts. Other manipulated variables include two multiplication factors to relate the three distillations on the same basis; the reactor effluent charge rate and the tear stream flows; and, in the case of the super batch scenarios, the continuous feed rate to the Crude Product Distillation.



Scenario Modeling Results

The results of the SQP optimization define the optimum operating conditions and stop criterion for each modeled operation step, the optimum continuous feed rate for superbatching, and the optimum distillation frequency. The model also quantifies the effect of relaxing constraints. This is valuable information in identifying bottlenecks.

The multiplication factors, which are the modeling equivalent of the distillation frequency, are treated as continuous variables in the model. This results in an optimum solution that may not have discrete distillation frequencies. A second SQP optimization may be required where the optimum distillation frequency consists of whole numbers; that is, the multiplication factors are rounded from the first SQP optimization and fixed (not manipulated).

Figure 3 shows the percentage increase over base capacity for the following options:

- Install vacuum capability on the distillation column to exploit the pressure swing separation
- Increase distillate pump capacity to decrease Crude Product Distillation cycle time
- Increase wet solvent storage capacity for more flexibility in distillation sequencing
- SuperBatch Option 1: Combine a SuperBatch feed scheme to make full use of pot capacity during Crude Product Distillation, plus increased wet solvent storage capacity, increased distillate pump capacity, and elimination of the Dry Solvent Cut in the Crude Product Distillation.
- SuperBatch Option 2: Option 1 plus increased very wet solvent storage capacity
- SuperBatch Option 3: Option 2 plus upgrade reboiler to make full use of column hydraulic capacity

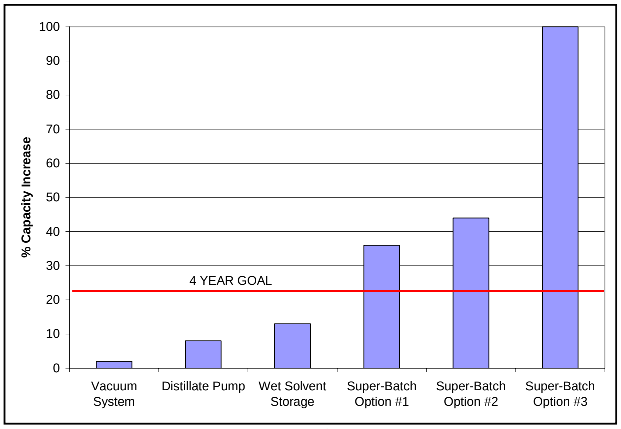


Figure 3. Benefits Compared.

As shown in Figure 3, the vacuum system would not even meet the 5% capacity increase needed for the first year. Only SuperBatch Options 1-3 would meet the capacity needs in four years.

Figure 4. Cost-adjusted Benefits Compared.

After the benefits of each option are quantified and validated, they are sorted to determine if the business goals are met within the defined constraints (Figure 4). Even though SuperBatch Option 3 has the highest capacity increase, SuperBatch Option 1 has the highest ratio of benefit/cost due to the implementation cost of Option 3. SuperBatch Option 1 best meets the business goal of achieving 22% capacity increase.

The SuperBatch Option 1 optimization results suggest a distillation frequency of 3:3:1 (Crude Product : Wet Solvent : Very Wet Solvent). It also suggests the continuous feed rate during the Crude Product Distillation and the operating conditions for all the modeled cuts to satisfy all the process constraints.

The schematic for the Aspen Plus® flowsheet that represents the SuperBatch Option 1 is shown in Figure 5. The only differences between this schematic and the baseline schematic is the addition of a continuous feed to the Crude Product Distillation (stream Feed) and the elimination of the Dry Solvent Cut in the Crude Product Distillation.

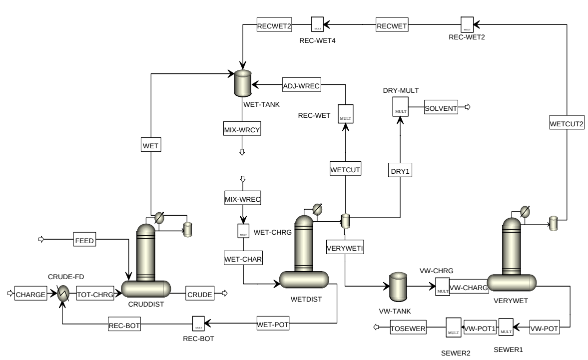


Figure 5. Aspen Plus® Flowsheet-SuperBatch Option 1

Conclusions

A rigorous batch distillation model within a continuous process simulator with SQP capability provides a powerful tool to evaluate and validate scenarios to debottleneck and optimize batch distillation systems. Complicated systems that include recycles and intermediate storage tanks are easily handled in this environment.

It has been shown that such a tool will allow the engineer to quickly evaluate more scenarios, while increasing the accuracy and confidence in the quantification of benefits. In the process demonstrated, the team identified a potential increase of >25% in capacity using SuperBatch Option 1.