gPROMS Application brief

# Azeotropic distillation

## Optimal process and control system design

Based on the report "*Simultaneous Design and Control of the Shell Azeotropic Distillation System using Mixed-Integer Dynamic Optimization"* by Vikrant Bansal and Roderick Ross, Centre for Process Systems Engineering and PSE (2001). *Please note that for confidentiality reasons, exact details of the process and the control and design alternatives mentioned are not provided.*

## Summary

Mixed-integer and dynamic optimisation were used to select the best of several proposed control schemes for an existing two-column coupled distillation unit operating under low and high-frequency disturbances. This led to a significant improvement in the controllability of the unit. Mixed integer Optimisation (MIO) was then used to improve the design of future units by selecting optimal feed and draw tray locations, while simultaneously optimising the column diameters. This identified significant improvements in capital and annual operating cost.

The project was performed on a Shell alcohol separation unit at Pernis in the Netherlands.

## Process

The two-column distillation system forms part of the Shell alcohol separation train at Pernis in the Netherlands. Figure 1 shows the separations taking place. There is a ternary azeotrope at the top of Column 1. The unit is subject to regular low frequency disturbances resulting from changes in feed rate and high-frequency disturbances resulting from fluctuation in the feed composition.

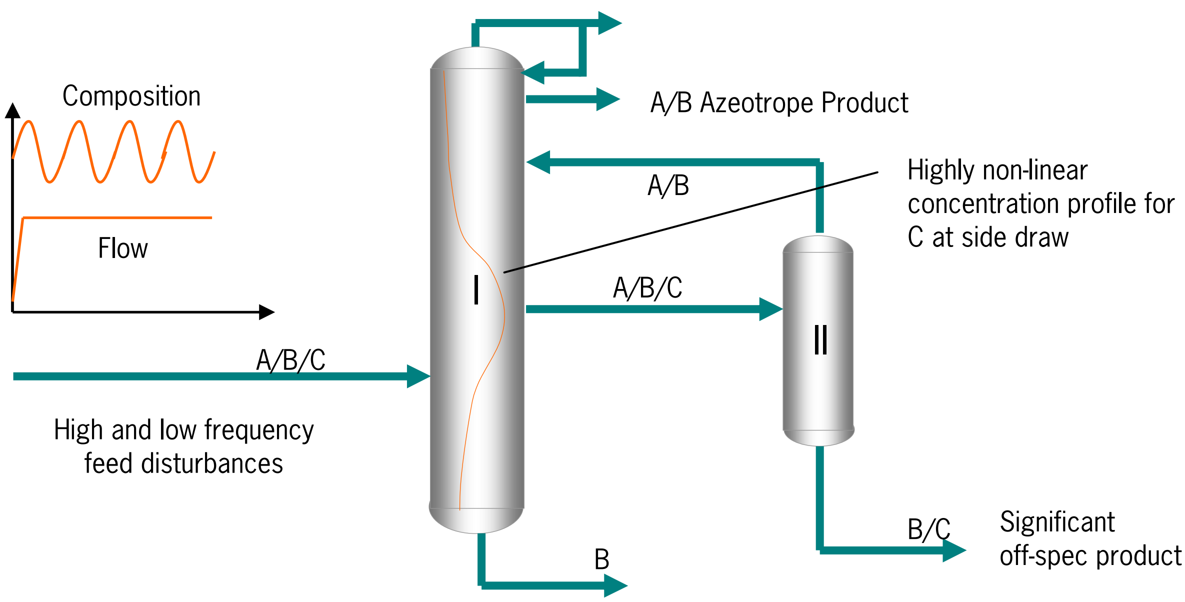



*Figure 1. The two-column azeotropic distillation process*

For many years the system had been very difficult to control. Good operation depends critically on the composition around the side draw tray in Column I being within a certain range. If the composition goes outside that range, Column II cannot operate correctly and the system enters into a sustained period of unsteady behaviour.

## Study 1 – operational improvement on an existing unit

Several control schemes were proposed in order to improve the process behaviour under disturbance. These are shown in approximate form in Figure 2.

### Modelling approach

The system was modelled in PSE's gPROMS package, using a detailed dynamic tray-by-tray model for the distillation columns. The model was tuned to existing plant operational data, using gPROMS' parameter estimation capabilities, in order accurately to quantify parameters such as tray efficiency and heat transfer coefficients.

Once a suitably accurate model of the process had been built, the existing control scheme was added and the model tested for response against various disturbances. Having established that the existing control scheme and tunings were not capable of restoring stability under these disturbances, a dynamic optimisation was performed (using the same input disturbances) in order to establish the optimal control tunings. This showed some improvements over the existing settings.

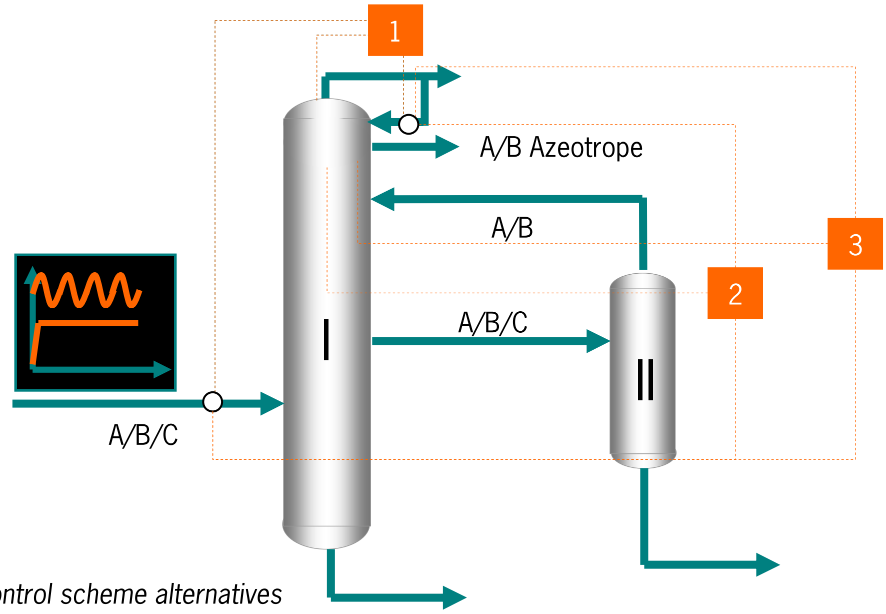



*Figure 2. Control scheme alternatives*

### Control scheme alternatives

Having proven that there was scope for improvement in the control system, several alterative proposed control schemes were added to the model. A dynamic optimisation was set up which included integer (discrete) selection between the alternative control schemes. This was configured to allow the dynamic optimisation to select the best control scheme to handle the disturbances, and to ensure that only one scheme was selected rather than a combination of the schemes.

### Result

The results of the dynamic optimisation not only identified a better control scheme than the existing one, but provided optimal tunings (gain and integral action) for each of the controllers. The improved control scheme meant that for the first time it was possible to control the system properly during normal operation.

By including alternative optimisation variables in subsequent runs – for example, column diameter – it was shown that significant improvements could be made in the design of such plants that would lead to improved inherent controllability.

In addition to the results obtained here it would also be possible to use the dynamic model to, for example, optimise start-up procedure, or investigate optimal transition policy between different modes of operation.

## Project 2 – process and control improvements for new design

Having built a detailed predictive model of the system, it was possible to use it to design more economic units for the future, with better controllability characteristics.

A particular feature of the project described here was the use of integer optimisation to determine the optimal locations of the Column I feed and side draw locations, while simultaneously optimising the values of other “continuous” variables such as the column diameters.

### Objectives

The objective was to design the distillation system and its control system at minimum total annualised cost. It was necessary that:

- the unit was capable of feasible operation over the whole of a given time horizon in the face of disturbances in the feed flow rate and composition
- the solution satisfied composition specifications on the various column product streams
- the column diameters calculated would be sufficient to avoid flooding in either column, and ensure that entrainment limits were observed.

This required the simultaneous determination of the optimal process design and the optimal control design, by calculating optimal values for the following integer (discrete) and continuous variables:

- locations of the feed and draw-off trays in Column I (discrete decisions)
- the column diameters, reboiler heat duties and flow rates of the draw-off stream to Column I and the return stream back to Column II (continuous decisions)
- tuning parameters – gain and reset – of all control loops (continuous decisions).

In principle, other discrete decisions could also have been considered, such as the optimal return tray location in Column I and the numbers of trays in the two columns. However the client asked for these to be excluded.

### Modelling approach

The modelling approach was essentially the same as that used before, with the optimised control scheme from the previous project (above) implemented. However it was necessary to providing a number of potential locations for feed tray and side draw locations for Column I, shown in Figure 3, from which the optimiser could choose the optimal combination.

The optimisation used an economic objective function that includes both capital and operating cost, to find the lowest *annualised* cost for the system.

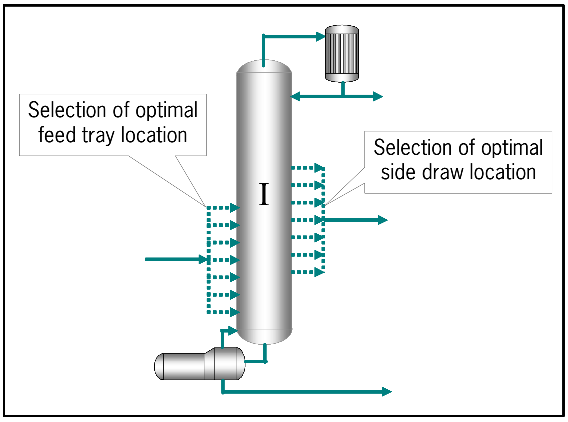



*Figure 3. Possible feed and side draw locations*

## Results

A summary of the results is shown in Table 1. It can be seen that the optimiser has changed the feed and draw tray location significantly, and has altered the relative sizes of Column I and II.

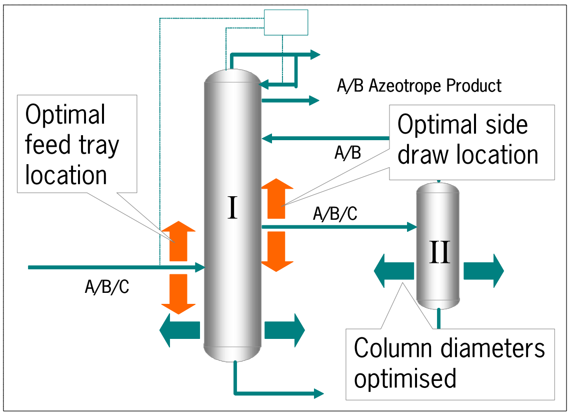
The total annualised cost of the re-designed unit is 18% lower than the existing Shell design. These savings are achieved by drawing more product B from Column I, resulting in a smaller Column I, with the size of Column II increased correspondingly. The reduced capital cost and reboiler duty for Column I easily outweighs the increases in these quantities for Column II.

The resulting optimal solution is about 18% cheaper than the existing design, indicating both the benefits of considering process design and process control simultaneously and the viability of using this MIO technology for solving complex, industrial problems.

The optimal solution was found on the fourth iteration of the integer optimisation loop. In fact the MIO algorithm was able to find three structures (second, fourth and eighth solutions) that are cheaper than the original structure. If optimisation had not been used, it would have been necessary to evaluate 68 alternative combinations in order to achieve this result.

*Table 1 – existing vs. optimal design*

| | **Existing design** | **Design using MIO** |
|---|---|---|
| Feed location | 14 | 8 |
| Draw location | 22 | 18 |
| Q column I (MW) | 19.5 | 14.7 |
| Q column II (MW) | 0.87 | 2.45 |
| Capital cost M$/year | 0.63 | 0.56 |
| Operating cost M$/year | 4.37 | 3.56 |
| **Total cost M$/year** | **5.00** | **4.12** |




The study showed that if such a simultaneous optimisation approach had been used when the distillation system was originally designed, not only would the total annualised cost of operation been substantially lower, but the operability difficulties experienced during its operation would have been avoided.