Simultaneous Optimal Configuration, Design and Operation of Batch Distillation

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A methodology for simultaneous determination of optimal batch distillation configuration, design and operation is presented. The configuration design methodology utilizes a mixed integer dynamic optimization (MIDO) formulation approach, where the optimal batch distillation system is obtained automatically, based on its maximum overall profitability for a given separation duty. Using rigorous models, the MIDO problem is solved using a practical stochastic solution approach of genetic algorithm and penalty function. The feasibility of this methodology is demonstrated for both binary and multicomponent separation scenarios. In the binary separation case study, the effect of feed composition for different binary mixtures on the optimal configurations, that is, regular vs. inverted columns, is investigated and discussed. The regular column was found to be more profitable for feeds with a high fraction of the light component, whereas the inverted column is optimal for heavier feeds. The optimality of a particular configuration over another is, however, case study specific, depending on, for example, how easy the mixture is to separate. In the multicomponent separation case study, the results obtained highlight the superiority of the multivessel configuration over the regular and inverted configurations. *AIChE J,* 51: 1700–1713, 2005
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Introduction

Batch distillation is widely used in the fine and speciality chemical and pharmaceutical industries for the purification or recovery of high value liquid mixtures. Traditionally, the batch distillation configuration design problem is seldom posed because the design engineer typically starts off the batch distillation design process with a batch rectifier, that is, with a regular column configuration, in mind. However, in recent years, motivated by the drive for greater process performance and efficiency, the fundamental configuration of the batch distillation process itself is being exploited, resulting in the emergence of new unconventional columns, such as the inverted, middle vessel and multivessel columns. As a result, the design engineer is faced with the challenging task of determining the best configuration, design and operation for a given distillation duty.

The performance of alternative batch distillation configurations has been actively researched through many comparative studies, where the process operation in different configurations are compared either through parametric simulation or optimal control studies, based on various performance indexes (see Chiotti and Iribarren,[1] Mujtaba and Macchietto,[2] Davidyan et al.,[3] Meski and Morari,[4] Hasebe et al.,[5] Sørensen and Skogestad,[6] Noda et al.,[7] Furlonge et al.,[8] Ruiz Ahón and de Medeiros[9] and Low and Sørensen[10]). Recently, Warter et al.[11] compared the practicality of the competing configurations by conducting a pilot plant scale experimental study on the operations of the middle vessel and regular columns. However, the performance indexes compared are often based on a specific aspect of the operation, that is, batch processing time, production rate and energy consumption. In a previous article (Low and Sø-

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rensen[12]), the simultaneous optimal design and operation of the different column configurations were compared for the first time, based on an overall profitability performance index, which provided a fairer and more conclusive comparison for batch distillation column configuration selection.

In an effort to aid batch distillation column configuration screening by means of providing insights into the behavior of different column configurations, Kim and Diwekar[13] performed the most comprehensive comparative studies to date where the performance of the column configurations, that is, the regular, inverted and middle vessel columns, based on various performance indexes, were obtained via parametric simulations using statistical sampling of design and operation variables within specified ranges. Due to the high number of simulations conducted in the study, a simplified model that assumes zero holdup in the column section, constant molal overflow and constant relative volatility was used. The work demonstrated how the screening of column configurations could be elicited through a sort of heuristic analysis of the trade-off among the performances indexes of the competing column configurations.

In short, although the numerous works mentioned above may provide some general insights on the comparative performances of the various batch distillation systems, which may be used as a basis for heuristic screening, ultimately a more general and deterministic approach for the determination of the best batch distillation system is needed. Oldenburg et al.[14] formulated a mixed-logic dynamic optimization approach to batch distillation design. The method consisted of a disjunctive model with a given set of equipment modules and logical relationships provided by the design context.

As the number of possible batch distillation column configurations proposed in the literature continues to increase, it becomes important to be able to choose the best one among them in an automatic manner without the need for manually considering each one of them separately. To the best of our knowledge, work on simultaneous optimal configuration and design has not been reported in the open literature. The aim of this article is to propose a configuration design methodology based on a discrete-continuous dynamic optimization formulation that can automatically and simultaneously generate the optimal configuration, design and operation of batch distillation for a given separation duty. The use of a rigorous model and an overall profitability index are also key characteristics of this study. In the next section, the batch distillation configuration design problem is presented, that is, the degrees of freedom considered and their general trade-offs as well as the performance index for optimality. Next, the formulation of the optimization problem is presented followed by the optimisation solution technique based on a genetic algorithm framework. The feasibility of the approach is demonstrated for a number of case studies which include several binary separation scenarios and a multicomponent separation scenario. In the binary separation case studies, the effect of feed composition on the optimal configuration is also investigated.

Batch Distillation Problem Definition

Degrees of freedom and trade-offs

Typically, the general objective in batch distillation design is the specification of the most cost effective batch distillation system for the separation of a mixture(s) into its components to a specified, or minimum, degree of purity. This involves the optimal determination of its configurational, design and operation decision variables.

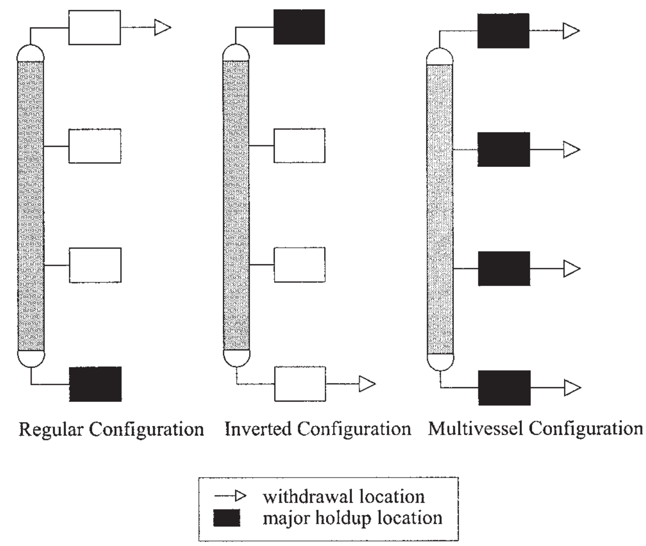


Figure 1. Different batch distillation column configurations.

In batch distillation, the configurational decision of the system is primarily characterized by the location of the initial feed charge and the location of product withdrawal, thus, giving rise to alternative column configurations, such as the regular, inverted and multivessel columns as shown in Figure 1. There is also the choice of the number of column sections and holdup vessels in the case of multicomponent distillation where the multivessel column is chosen. This configurational degree of freedom is proportional to the number of components N_C, that is, N_C needing $N_C - 1$ column sections to allow for the separation of all the components simultaneously. Driven by stricter need for a more efficient and economical process, the choice of utilizing these alternative batch distillation configurations instead of the traditional rectification system, has been an active area of research over the past decade. Many of these works presented comparative studies on the different configurations based on particular performance indexes, such as process time and energy rate. A few works are available which provide insights into the trade-offs among the various configurations. Notably, Kim and Diwekar[13] discussed considering trade-offs of the product purity and yield, design feasibility and flexibility, as well as thermodynamic efficiency for a given separation duty in heuristically arriving at a most suitable configuration. In another work, Low and Sørensen[15] contrasted the individual economics components of capital cost, production revenue and operating cost of the regular and multivessel columns for different separation duties.

In terms of design and operation, works on operational optimization of batch distillation have demonstrated the interdependent nature of these decision variables, thus, the need to consider these simultaneously. This interdependency is fundamental as the operation of batch distillation is linked to the reflux ratio profile and reboiler duty—operational parameters which needs to be set as a basis for a particular design. For continuous distillation, the opposing design limits are based on these parameters being fixed *a priori* at the minimum and infinite values, resulting in the highest and lowest investment costs, respectively. However, in the batch mode, even with constant operational parameters, the batch system is nonsteady state. Furthermore, the lowest capital cost design does not necessarily make for the most economical solution due to the low performance and high operating costs associated with a high reflux column. The optimal condition is achieved by balancing the additional performance obtainable against investment in a bigger column. For example, it is possible for a given set of separation requirements to be met using a column with the minimum number of trays for a particular reflux ratio profile, or alternatively, using a column with more trays operated over a shorter period of time at a lower reflux ratio profile. Operating at high boil-up rate would reduce batch time but would conversely incur an increase in reboiler and column investment costs, as well as utility cost. Thus, the design problem involves several complicated economical trade-offs between capital investment and operating costs, subject to the separation requirements.

Theoretically, a batch distillation system capable of handling large batch sizes is more cost effective due to economy of scale and reduction in total setup time over a production period. However, the nominal batch size is normally dependent on the short or medium term inventory requirement of a particular plant. The batch size can be determined *a priori* via optimal capacity and product portfolio planning, or even as a result of a wider supply chain optimisation study, and, hence, is not considered within the configuration design framework described in this article.

In conclusion, the development of a configuration design methodology for batch-distillation systems is a challenging task due to the dynamic behavior of the process and the concurrent consideration of the system configurational, design and operation degrees of freedom. The objective of this work is to present for the first time a methodology to simultaneously determine the optimal configuration, column size and operating policy of batch distillation using a mixed discrete optimization approach.

Economics performance index

Here, the general design objective is to simultaneously obtain the most economical batch distillation column configuration, design and operating policy that will satisfy the specified separation requirements. Ideally, this implies that the targeted batch distillation system should be the result of an optimal trade-off in initial investment, energy consumption, product yield and batch processing time. This can be translated into an economics model of sales margin, capital cost and operating cost using monetary units base on a production time scale, for example, hourly or annually. The optimal batch distillation system will be a trade-off between lower capital and operating costs against higher production revenue, thus, the performance index should be formulated to encapsulate all of these costs. In this study, the performance index economics models for operating cost and capital cost based on Guthrie's correlation (Douglas[16]) is used. The same profitability index has also been used in the works by Logsdon et al.,[17] Mujtaba and Macchietto[18] and Low and Sørensen[12,15] (where details of the derivation can be found) and is given by

$$P = \frac{\sum_{i=1}^{Nc} C_i H_i(t_f) - C_{feed} H_{feed}}{t_f + t_s} - K_3 V - (K_1 N^{0.802} V^{0.533} + K_2 V^{0.65}) \quad (1)$$

where C_i and C_{feed} represent the unit costs of product i and feed, respectively, H_i and H_{feed} the quantity of on-specification product i collected and feed, respectively, N the number of stages for tray columns, V the column vapour loading, and K_1, K_2 and K_3 the economics correlation coefficients for the shell, exchangers and utilities costs, respectively, given by

$$K_1 = \frac{C_{shell,BC}}{N_{BC}^{0.802} V_{BC}^{0.533}} \quad (2)$$

$$K_2 = \frac{C_{exchangers,BC}}{V_{BC}^{0.65}} \quad (3)$$

$$K_3 = \frac{C_{utilities,BC}}{V_{BC}} \quad (4)$$

where the costs are correlated using the Guthrie's correlation from values in a base case (BC) distillation column, for example, from the predetermined costs associated with installing a carbon steel column of a certain size with hydrocarbon feedstock. Note that, alternative correlation models to those in this work can also be used, and industrial design engineers may wish to utilize their own in-house costing models. The methodology proposed in this study is open to any form of performance index as the solution approach used are insensitive to this, as described in the following sections.

Formulation as a Discrete-Continuous Optimization Problem

The aim of batch distillation design is to maximize the profit performance index P, described above, subject to the set of system model equations and all the separation constraints, namely the product purities. Thus, batch distillation design can be based on the solution of a dynamic optimization problem.

The batch distillation configuration design problem is complicated because, in addition to determining the set of design and operation variables which gives the optimal trade-off in capital and operational costs, the problem here is expanded to also explore configurational variables in an effort to further increase the profitability of a particular batch distillation process.

The configurational decision of the system is mainly characterized by the location of the feed and product withdrawal locations (Figure 1) which correspond to different column configurations, such as the regular, inverted and multivessel columns. Conceptually, the determination of the optimal configuration for a particular separation duty can be tackled by optimization in the continuous domain, that is, by optimizing the initial feed holdup distribution $M_j(t_0)$, and the reflux ratio profiles, $R_j(t_i)$, for all control intervals, Δt_i, at all potential output locations j, on a dynamic superstructure model. The maximum and minimum bounds of these continuous variables $M_j(t_0) \in [0, H_{feed}]$ and $R_j(t_i) \in [0, 1]$, correspond to the distinct column configurations known as the regular, inverted and multivessel columns as illustrated in Figure 1. However, the final solution would in all probability lie within the continuous range in between the bounds, and, thus, despite offering the highest possible degrees of freedom, result in none of the straightforward distinct column configurations as those shown in Figure 1, but in less practical configurations with complicated implementation.

To obtain distinct structures, the configurational degrees of freedom must be treated in a discrete manner. For example, discrete decisions may be incorporated into the mathematical model as a set of time-invariant binary variables $y \in \{0, 1\}$, each representing the existence or nonexistence of a particular connecting stream or a process unit (for example, side vessels), or part thereof (for example, accumulators at a particular task interval). Optimal streams between process units can easily be incorporated into the superstructure model by algebraic equations (see Sharif et al.[19]). The development of the dynamic superstructure model is by no means a trivial task, because it needs to encompass all the different options available. Furthermore, the mathematical superstructure model formulation may have a significant impact on the robustness and efficiency of the numerical integration and optimisation solution techniques. For these reasons, considerable effort may be spent in defining ways to build superstructure models that are generic to the extent possible, and provide favourable properties in conjunction with specially designed numerical solution algorithms (Oldenburg et al.[14]). In this work, the need for a superstructure model is avoided.

In this work, the discrete decisions is characterized by disjunctions, where a disjunction represents the discrete decision as to whether the batch distillation process is to be operated in the regular, inverted or multivessel mode. For example, this could be achieved by using the boolean type variable, $Y \in \{Regular, Inverted, Multivessel\}$, where a direct relationship is preestablished between the discrete boolean variable, Y, and the grouped configurational variables and conditions, for example, top and bottom streams and initial holdups conditions

$$\begin{bmatrix} Y = \{Regular\} \\ M_{bottom}(t_0) = H_{feed} \\ R_{LB} \leq R_{top}(t_i) \leq R_{UB} \\ R_{bottom} = 1 \end{bmatrix} \vee \begin{bmatrix} Y = \{Inverted\} \\ M_{top}(t_0) = H_{feed} \\ R_{top} = 1 \\ R_{LB} \leq R_{bottom}(t_i) \leq R_{UB} \end{bmatrix} \vee \begin{bmatrix} Y = \{Multivessel\} \\ M_i(t_0) = H_{feed}/N_C \\ R_j = 1 \\ \forall\, j \in \{top,\ sides,\ bottom\} \end{bmatrix} \quad (5)$$

Note that for the multivessel configuration, only the simplest operating policy of total reflux constant holdup $R_j = 1$, is considered here (refer Low and Sørensen[15]).

In summary, the approach to batch distillation configuration design presented in this work is based on a discrete-continuous dynamic optimization problem, where the discrete aspect of the problem formulation includes the integer variable associated with the number of trays N, and the logical boolean variable Y, for the selection of distinct column configurations, in addition to continuous variables, such as the time invariant boilup rate V, and the reflux ratio profile, $R_j(t_i)$. Hence, given the minimum product purity specifications $x_i^{\min}$, the price structure of the feed and products C_i and C_{feed}, as well as the economics correlation coefficients K_1, K_2 and K_3, the aim is to determine the optimal system configuration Y, optimal set of design variables u_d, and optimal operating control variables u_o, so as to maximise the objective function P. In mathematical terms, the optimization problem is posed as follow

$$\max_{Y,u_d,u_o} P \quad (6)$$

subject to

$$f(\dot{x}, x, t, u) = 0 \quad (7)$$

$$x_i(t_f) \geq x_i^{\min} \quad \forall\, i = 1, \ldots, N_C \quad (8)$$

$$Y \in \{Regular, Inverted, Multivessel\} \quad (9)$$

$$u_d^{\min} \leq u_d \leq u_d^{\max} \quad (10)$$

$$u_o^{\min} \leq u_o \leq u_o^{\max} \quad (11)$$

Equation 7 represents the batch distillation model (see below), where x is the vector of state variables, u the vector of control variables, u_d is the set of design variables (that is, $u_d = \{N\}$), u_o the set of operating control variables (that is, $u_o = \{V, R_j(t_i)\}$), and t is the process time.

Mathematical model

The mathematical model of the dynamic batch distillation system is a set of differential-algebraic equations (DAE). The stochastic optimization solution framework proposed in this study (see below) can be utilized in conjunction with any level of model abstraction and the choice is dependent on the level of detail or accuracy required vs. the computational cost. Although many previous batch distillation studies commonly utilised simple and semi-rigorous models, the batch distillation configuration design work here has been successfully conducted using a rigorous model which includes the following features:

- Fast energy dynamics instead of relying on the usual assumption of constant molal overflow.
- Constant liquid holdup in trays and reflux drum, hence, not requiring details associated with tray hydraulics which is not available nor required during the preliminary design stage.
- Negligible vapour holdup, hence, eliminating the need to specify detailed flow characteristics during the preliminary design stage.
- Rigorous thermodynamic models which replace the quite common constant relative volatility assumption through the use of liquid and vapor fugacities as functions of temperature, pressure and composition.
- Total condenser, phase equilibrium, perfect mixing and adiabatic trays.

The models were constructed using the *gPROMS*® modeling tool (Process Systems Enterprise Ltd.[20]). Thermophysical properties (including density, enthalpy and fugacity) required in the rigorous model were calculated using the *Multiflash* (Infochem Computer Services Ltd.[21]) physical properties package interfaced to *gPROMS*. The Soave Redlich Kwong (SRK) equation of state was used for both the vapor and liquid phases for the case studies.

Stochastic Optimization Solution Approach

In this work, the optimization problem consists of continuous (for example, boil-up rate and reflux ratio profile), integer (for example, the number of stages) and logical (for example, column configuration) variables. In addition, the batch distillation DAE model, and the profitability performance index are nonlinear with a nonconvex solution space. The coupling of these aspects translate into a complex discrete-continuous dynamic optimization problem. The solution of this type of optimisation problem is nontrivial, especially the determination of its global optimum, and there is much ongoing research on developing practical and global solution algorithms (for example, Liberti and Pantelides[22] and Bjork et al.[23]).

Conventional deterministic mathematical programming approaches, such as outer approximation (OA), and generalized Bender's decomposition (GBD), require gradient information for the nonlinear programming (NLP) solver, and are, therefore, not robust for solving problems with highly nonlinear functions, stiff models and complex search spaces like those exhibited by the batch distillation column design. The batch distillation design problem is nonconvex, thus, convexity conditions required by many of these gradient-based approaches to locate the global optimum are not satisfied. Recently, Oldenburg et al.[14] proposed a deterministic gradient-based solution method to solve a mixed logic dynamic optimization (MLDO) problem for batch distillation design. The tailored logic-based solution approach proposed in their study was based on the decomposition strategy, which consists of a primal subproblem and a master subproblem.

Genetic algorithm

In this article, the configuration design optimization problem is solved for the first time by a stochastic method of steady-state genetic algorithm and penalty function framework. Genetic algorithm is an optimization technique inspired by the theory of biological evolution which attempts to imitate the process of natural selection. In this process, fitter individuals (such as designs) characterized by their genomes (that is, dezign and operation variables) are favored over weaker individuals and, therefore, are more likely to survive longer and produce stronger offsprings for the next generation. The fitness of the general population thereby increases from generation to generation. The optimization framework proceeds according to the following algorithm:

(1) Initialization—An initial population is created consisting of random points in the search space.

(2) Fitness function evaluation—The fitness of each genome in the population is evaluated through the objective function and penalty function.

(3) Reproduction genetic operators—The search is performed by creating a new population generation from the previous one through the application of genetic operators.

(4) Convergence criteria—Steps 2 and 3 are repeated until the population converges according to a prespecified optimality criterion.

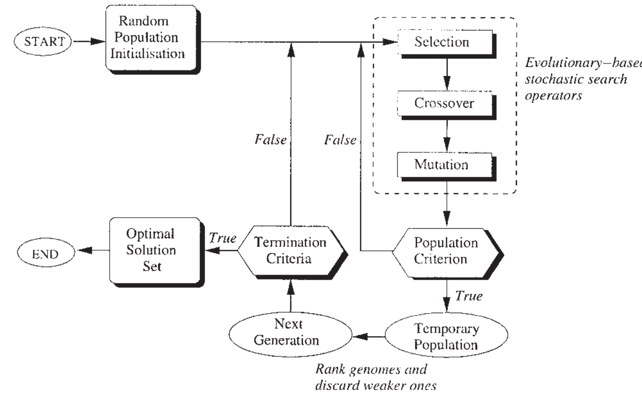


Figure 2. General structure of the genetic algorithm.

A steady-state genetic algorithm that uses overlapping populations is used in this study, the basic structure of which is shown in Figure 2. First, an initial population of a specified size N_{pop} number of genomes, is randomly generated. This is N_{pop} different combinations of column design and operation variables. Then, in each generation, the fitness of each genome is evaluated, that is, the profitability performance index of Eq. 1 (adjusted by the penalty function described later). Based on the fitness function of each genome, the algorithm creates a new set of temporary genomes via the three operators, that is, selection, crossover and mutation, and adds these to the previous population, and at the same time removes the weaker genomes in order to return the population to its original size. The number of new genomes created in each generation depends on the percentage of population overlap P_{ss}, specified. In this algorithm, the new genomes may or may not make it into the next population, depending on whether they are better or weaker than the rest in the temporary population. This allows the retention of fitter genomes for use in the next generation, as well as provides the opportunity to discard new genomes that are weaker than those of the parents' generation. Further details of the genetic algorithm operators used are discussed in our article, Low and Sørensen.[12]

Penalty function

A mechanism is needed to check the constraints of the returned simulation results represented by the genome and to map the objective function to an appropriate fitness function, if necessary. In the batch distillation design problem, the purity constraints of the products are checked for each returned results and the objective function is manipulated using a penalty function to obtain the corrected fitness functions for each genome. The purpose of the penalty function is to penalize designs that violate the required purity constraints by imposing a penalty on the objective function. The penalty imposed is proportionally related to the magnitude of the violation, and can be adjusted using a power coefficient

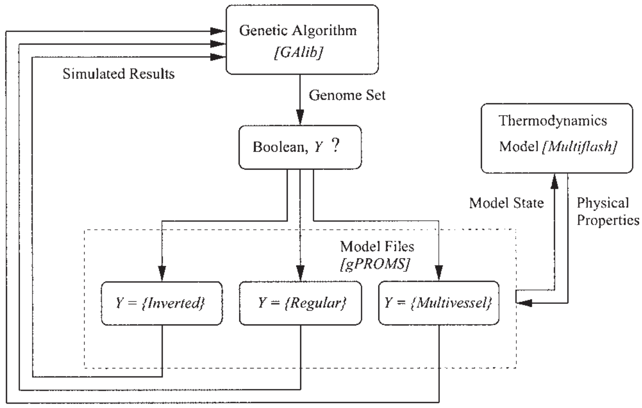


Figure 3. Batch distillation configuration design optimization implementation.

$$\kappa_i = \begin{cases} \left[1 - \dfrac{x_i^{\min} - x_i(t_f)}{x_i^{\min}}\right]^{p_i} & \text{if } x_i(t_f) < x_i^{\min} \quad \forall\, i = 1, \ldots, n_c \\ 1 & \text{otherwise} \end{cases} \tag{12}$$

$$f = \begin{cases} \Omega \prod_{i=1}^{n_c} \kappa_i & \text{when } \Omega \geq 0 \quad \text{(profit)} \\ \Omega\left(2 - \prod_{i=1}^{n_c} \kappa_i\right) & \text{when } \Omega < 0 \quad \text{(loss)} \end{cases} \tag{13}$$

where κ_i denotes the penalty function for each n_c constraint, p_i the penalty power coefficient, Ω the original objection function value, and f the corrected fitness value.

Disjunction handling

One of the key advantage of this approach is that the framework can easily accommodate the continuous, integer and logical variables within its genome set without any modification to the adaptive search procedure. In terms of implementation, the framework can also be applied to handle the logical disjunctions in a simple manner, whereby the genetic algorithm program performs a directed call to the specific model file that contains the relevant conditions and constraints (Eq. 5) that correspond to a particular genome's boolean variable Y, that is, regular, inverted or multivessel models (Figure 3). Hence, the need to develop a superstructure model is avoided.

Advantages and drawbacks of the stochastic approach

In this work, a nondeterministic algorithm, that is, genetic algorithm-penalty function, is used to arrive at the optimal batch distillation configuration and design results. For such optimization problems, where discrete variables are introduced in addition to continuous variables, only a handful of deterministic works have been reported in the literature—they ranged from various NLP methods where the discrete variable is treated as continuous, to MINLP method that requires superstructure modeling. Compared to these approaches, the genetic algorithm approach provides some inherent advantages as follow:

(1) It offers greater robustness as it can handle nonlinear objective functions with complex search space topography in a single continuous optimization run without the algorithm terminating due to instability. This is because genetic algorithm is a black box or gradient-free search algorithm which means it only requires scalar values of the objective function, that is, it does not require derivative information or a smooth, continuous and differentiable search space.

(2) It has global optimization capability and eliminates the difficult task of deciding the initial starting point. Rather than starting from a single arbitrary point within the search space, the genetic algorithm is initialized with a population of points which is spread randomly throughout the search space. Furthermore, the mutation operator subsequently ensures the diversity of the population by allowing the algorithm to jump to a new solution and sample the entire search space.

(3) The fitness of the solution set improves over each generation. Since the algorithm operates on a population of solutions, and the average population fitness of each generation improves in line with the best genome fitness, the final population may supply some viable alternative designs and operations which are near the optimum solution.

(4) Genetic algorithm offers the opportunity for parallel processing to reduce computational time.

(5) The approach is practical, flexible and easily implemented. Since only the optimized variables and value of the objective function are passed between the algorithm and the model, the approach can be applied to different types and complexity of model with minimal implementation effort, and different modeling packages can be connected to the algorithm. The nature of the approach also means that it can treat continuous variables, as well as discrete variables like integer and logical variables easily within its genome set.

The main drawbacks of the genetic algorithm approach are:

(1) Unlike methods which direct the optimization search based on the sensitivity of an individual solution, the inherent need for a population of solutions in the genetic algorithm approach may translate to a relatively higher computational cost (in the order of 48 h to seven days in this work). Note that a possible alternative is to have a population size of one. Since there is only one individual or solution, there would be no crossover, but only mutation. This stochastic method is recognisable as *simulated annealing* where the so-called *mutation* is conventionally called *random move,* and the solution typically moves to the next one with a probability function.

Table 1. Specifications and Operating Conditions for the Binary Separation Case Study

Available annual production time, T_A (h/year)	8760
Batch setup time, t_s (s)	1800
Operating pressure, P (Pa)	101325
Major holdup (batch size), H_{feed} (mol)	3000
Minor holdup, M_{rd} or M_{reb} (mol)	45
Tray holdup, H_{tray} (mol)	4.5
Feed composition, $x_{1,feed}$, $x_{2,feed}$ (mol fraction)	
Cyclohexane, toluene	varied
Product purity specifications, (mol fraction)	
First product, $x_1(t_f)$	0.99 of cyclohexane
Second product, $x_2(t_f)$	0.99 of toluene
Cost, C_i (\$/mol)	
Cyclohexane, C_1	0.034
Toluene, C_2	0.034
Feed, C_{feed}	0.002

Table 2. Decision Variables Bounds for the Binary Separation Case Study

Decision Variables	Bounds
Y	{Regular, Inverted}
N	[4, 30]
V (kmol/hr)	[0.6, 6.0]
$R(t_{2,3})$	[0.4, 1.0]
Δt_1 (s)	[0, 2000]
Δt_2 (s)	[0, 10000]
Δt_3 (s)	until purity achieved

(2) The *optimality* (or *accuracy*) of the final solution is, since genetic algorithm is stochastic in nature, dependent on the convergence setting. This is a drawback of genetic algorithm—the trade-off between the accuracy and computational time, especially at the latter part of the optimization where the growth in fitness is slower than in the initial stages. Furthermore, the algorithm itself requires careful tuning of a number of parameters (Low and Sørensen[12]) in order to obtain an acceptable performance in terms of its efficacy and computational efficiency.

Case studies

In the following sections, several batch distillation design case studies involving binary and multicomponent separation processes are presented.

Optimal Configuration for Binary Separation

In this section, the design of optimal batch distillation processes is investigated for the case of binary mixture separation. Previous works by, for example, by Sørensen and Skogestad,[6] have indicated that the optimal configuration, that is, either rectification or stripping mode, is dependent on the separation duty, for example, the composition of the feed. In this study, the optimal batch distillation configuration, column size and operating conditions, that is, constant boil-up rate and reflux ratio profiles, for a given feed composition and product purity requirement will be automatically found using the approach outlined earlier.

Separation of a binary mixture of cyclohexane and toluene is considered in this case study, and the effect of different feed compositions on the optimal solution is investigated. A summary of the column specifications and operating conditions is given in Table 1. The 3000 mol major holdup corresponds to the batch size, and the decision on its initial location, that is, either in the reflux drum or reboiler pot, is optimized through the boolean variable Y. Accordingly, the minor holdup occupies the vessel at the opposite end of the column. The batch distillation operation is separated into three task intervals, starting with a total reflux period followed by a first product withdrawal period, and finally, an offcut period to purify the other product. Again, whether cyclohexane or toluene is withdrawn first, from the top or bottom of the column, respectively, depends on the disjunction represented by Y. The minimum product purity specifications are set at 99.0 mol% for both cyclohexane and toluene. The cost coefficients K_1, K_2 and K_3 of the objective function were set to the values of 1500, 9500 and 180, respectively (taken from Logsdon et al.[17]).

The optimized decision variables are the column configuration Y, number of trays N, column constant boil-up rate V, and reflux ratio profile, that is, the values of the normalized reflux ratio, $R(t_i)$ (except in the first task interval where $R(t_1)$ is set to 1 for total reflux), and the durations of each of the first two task intervals Δt_1 and Δt_2. In the final task interval, the duration, Δt_3, is set corresponding to the minimum time needed to purify the remaining component (in either the reboiler pot or the reflux drum) to its required purity of 99.0 mol% (that is, set as a termination condition during simulation). The bounds for each variable are given in Table 2.

Case I: Effect of Different Feed Compositions

The optimal results for the cases of different feed compositions are summarised in Table 3 for both fixed and optimal column size. The results are illustrated in Figure 4 which highlights the optimal configurations and their associated objective function values for a range of feed compositions. The shape of the optimal profitability curve indicates that feeds with a relatively higher fraction of either component, that is, towards both ends of the feed composition, achieved higher profitability. The figure clearly suggests that it is economically beneficial to consider alternative column configurations. In this case study, for example, the optimal column configuration varies, depending on the feed compositions. For a mixture with a higher fraction of the heavy component, the inverted column gave a higher profitability than the regular column, but the opposite is true for a mixture with a higher fraction of the light component.

The results are in agreement with the findings of Sørensen and Skogestad[6] who proposed that the reason why the inverted column configuration is better than the regular column with small amounts of light component is that, when this light component is to be removed from the column at high purity, a very high reflux ratio must be used in order to meet the product specification in the conventional rectification mode. For the inverted configuration, however, a large amount of heavy component is withdrawn very quickly from the bottom using a low reboil ratio, thus, resulting in a relatively lower operating time and higher profit value.

Figure 4 also displays the results for the cases where the column size, that is, number of trays, is fixed (N = 10), and

Table 3. Summary of Optimal Results for the Separation of the Cyclohexane-Toluene Binary Mixture

	Fixed Column Size (N = 10)		Optimal Column Size		
Feed Composition (mol fraction)	Optimal Configuration	Profit ($/yr)	Optimal Configuration	Optimal Size, N	Profit ($/yr)
0.90, 0.10	Regular	330 063	Regular	22	342 989
0.75, 0.25	Regular	185 963	Regular	21	203 953
0.50, 0.50	Inverted	163 602	Inverted	16	183 078
0.25, 0.75	Inverted	215 719	Inverted	20	224 953
0.10, 0.90	Inverted	343 999	Inverted	23	372 788

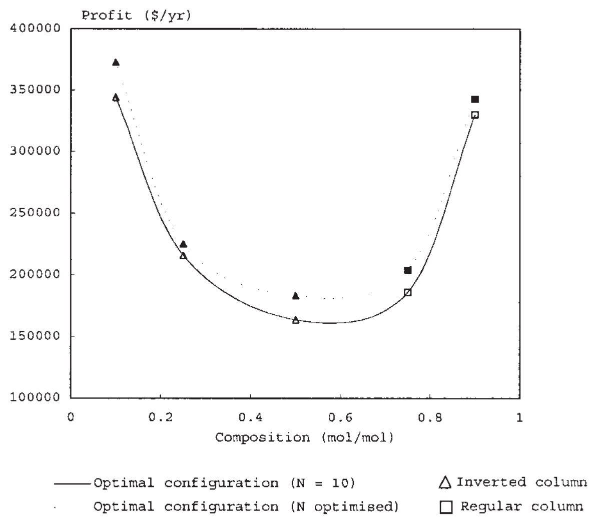


Figure 4. Optimal profits and configurations for different feed compositions (cyclohexane-toluene mixture).

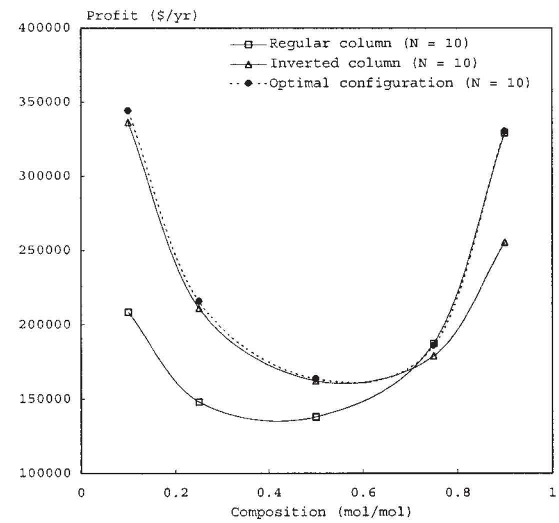


Figure 5. Optimal profits for different column configurations and feed compositions (cyclohexane-toluene mixture).

where it is optimized. As expected, the profits were increased in all cases when the number of trays is optimized. The trend of the curve for the case where N is optimized matches the one obtained for fixed number of tray in terms of shape, as well as the optimal configuration obtained for a particular feed composition. In Table 3, it can be observed that the optimal number of trays for all the cases are above the previously fixed 10 trays, indicating that a favorable economics trade-off has been made, whereby the performance gained from a bigger column, that is, lower batch processing time, is worth the higher capital cost incurred. However, the magnitude of increase in the number of trays is not uniform across the cases, but appeared to establish some sort of pattern. The optimal number of trays were 22 and 23 for feeds with 0.90 mol fraction of either components, and slightly lower at 20 and 21 trays for feeds with a 0.75 mol fraction. The lowest increment in the optimal number of trays occurred for the equimolar feed. This observation can be explained by the fact that the opportunity to increase performance through minimizing reboil or reflux ratios, that is, higher production per unit time or lower batch time per fixed product volume, is greater for the separation of a mixture with a more asymmetrical molar ratio than for an equimolar mixture.

To investigate the accuracy of the batch distillation design optimization, the optimal results for fixed column configuration and column size ($N = 10$) were obtained for a regular and an inverted configuration for the same set of feed compositions (Table 4). The results are plotted in Figure 5, with the optimal configuration curve (dashed line) of Figure 4 (for $N = 10$) superimposed on it. For both the fixed regular and inverted column cases, it is demonstrated that the profitability curves were influenced to a unique extent by the different feed compositions, and that there exists a point where the two curves intersect. This intersection at approximately 0.69 mol fraction of the light component for this study, is the location where the advantage of one configuration over the other is flipped. It can be seen in Figure 5 that the optimal configuration profitability curve was able to trace accurately the optimal path, that is, it matches the profitability curve of the inverted column to the left of the flip point where the inverted column is superior, and then followed accordingly the profitability curve of the regular column to the right of the flip point to take advantage of the rectification configuration.

Table 4. Summary of Optimal Results for Fixed Column Configurations and Sizes

Feed Composition (mol fraction)	Fixed Column Size ($N = 10$)	
	Fixed Configuration	Profit ($/yr)
0.90, 0.10	Regular	**329 113**
	Inverted	255 162
0.75, 0.25	Regular	**187 550**
	Inverted	178 902
0.50, 0.50	Regular	137 982
	Inverted	**162 164**
0.25, 0.75	Regular	148 111
	Inverted	**211 092**
0.10, 0.90	Regular	208 556
	Inverted	**336 176**

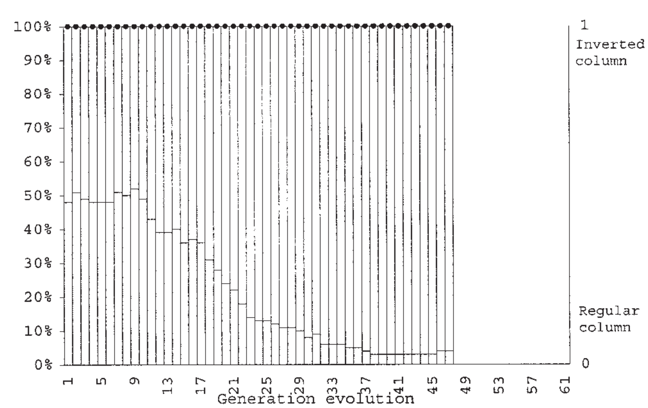


Figure 6. Percentage of column configurations in each generation of the genetic algorithm (feed 69.0 mol% cyclohexane).

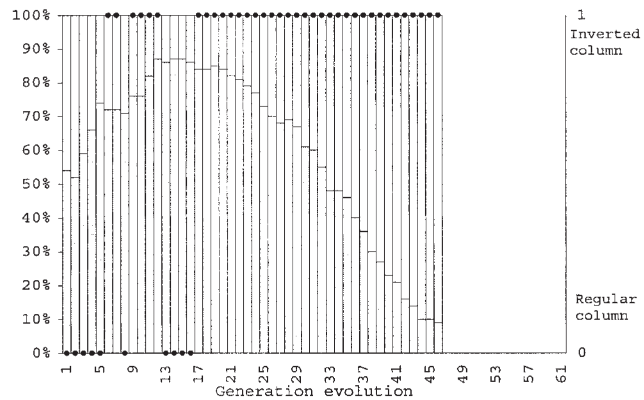


Figure 7. Percentage of column configurations in each generation of the genetic algorithm (feed 69.1 mol% cyclohexane).

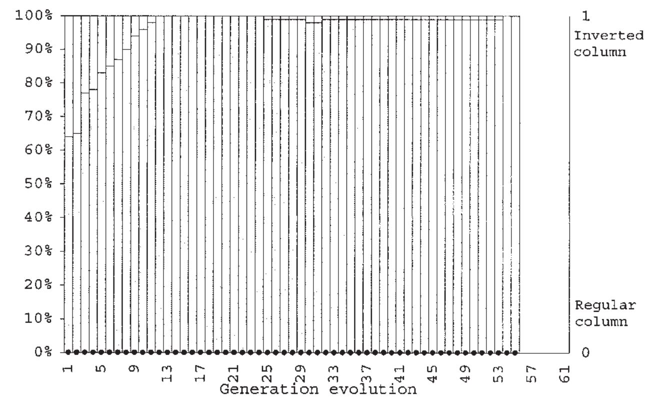


Figure 9. Percentage of column configurations in each generation of the genetic algorithm (feed 70.0 mol% cyclohexane).

Location of the flip point

It is interesting to note that in Figure 5, the location of the flip point is not at the symmetrical separation ($x_{i,feed} = 0.50$). This phenomenon has also been observed by Sørensen and Skogestad[6] who put forward the explanation that the inverted column is not the true inverse of the regular column since the feed and product are in liquid, and not vapor, phase. However, the optimal configuration for a particular separation is also determined by other factors depending on the feed mixture (see the following section) and product purity specification.

The exact location of the flip point can be estimated from the intersection of the profitability curves in Figure 5. Figures 6, 7, 8 and 9 show the percentage of the number of regular columns (white area) and inverted columns (shaded area) represented by all the genomes in each generation of the genetic algorithm for the cases of feed composition $x_{1,feed}$ = 69.0 mol%, 69.1 mol%, 69.2 mol% and 70.0 mol%, respectively. For the case of feed composition 69.0 mol% of cyclohexane, the population of the first generation (that is, the one after the initial random population) consisted of an equal percentage of genomes representing the regular and inverted configurations. However, over the subsequent generations, the genomes representing the inverted configuration began to steadily dominate the population of best solutions (Figure 6). In contrast, Figure 9 shows that for the case of feed composition 70.0 mol% of cyclohexane, genomes representing the regular configuration dominates the population quickly, and by the 13th generation it is already clear that the regular column would emerge as the optimal configuration. Therefore, it can be surmised that the flip point is located between the feed composition 69.0 mol% and 70.0 mol% of cyclohexane, which confirms the approximation obtained from the intersection of the curves in Figure 5. Figures 7 and 8 demonstrate the characteristic of the genetic algorithm's search in the vicinity of this flip point. Note that, in the case of feed composition 69.2 mol% of cyclohexane, the best 100 solutions in every generation over the course of the evolution consisted of both configurations. The best solution in each generation also switched between the regular and the inverted configuration. In the final generation, the evolved population contained solutions for both configurations. Table 5 indicates that at the flip point, of 69.2 mol% cyclohexane, the regular and inverted column configurations give equal performance (difference of 0.1%) in terms of economics, that is, 146 091 and 146 299 \$/yr, respectively.

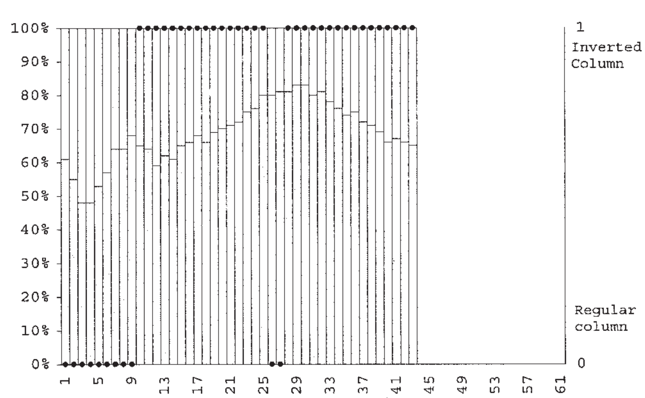


Figure 8. Percentage of column configurations in each generation of the genetic algorithm (feed 69.2 mol% cyclohexane).

Case II: Different Scenario

In this case study, the optimal configuration design is performed for another separation scenario, that is, a different

Table 5. Optimization Solution Vectors for Feed 69.2 mol% Cyclohexane (top 10 genomes)

Optimum Profit (\$/yr)	Optimal Genome Y, N, V, $R(t_1)$,[†] $R(t_2)$, $R(t_3)$, t_1, t_2, t_3[‡]
146 299	Inverted, 10, 1.667, 1, 0.91, 0.95, 250, 4100, —
146 091	Regular, 10, 1.667, 1, 0.81, 0.92, 150, 5200, —
145 814	Inverted, 10, 1.667, 1, 0.91, 0.95, 200, 4050, —
145 064	Inverted, 10, 1.667, 1, 0.91, 0.94, 200, 4100, —
144 413	Regular, 10, 1.667, 1, 0.81, 0.92, 250, 5200, —
144 192	Inverted, 10, 1.667, 1, 0.91, 0.94, 250, 4100, —
143 499	Regular, 10, 1.667, 1, 0.81, 0.93, 300, 5200, —
142 844	Inverted, 10, 1.667, 1, 0.91, 0.95, 150, 4300, —
141 369	Regular, 10, 1.667, 1, 0.84, 0.94, 0, 6350, —
141 154	Regular, 10, 1.667, 1, 0.83, 0.95, 200, 6100, —

[†]Set as total reflux.
[‡]Minimum duration to achieve the required purity of the remaining component.

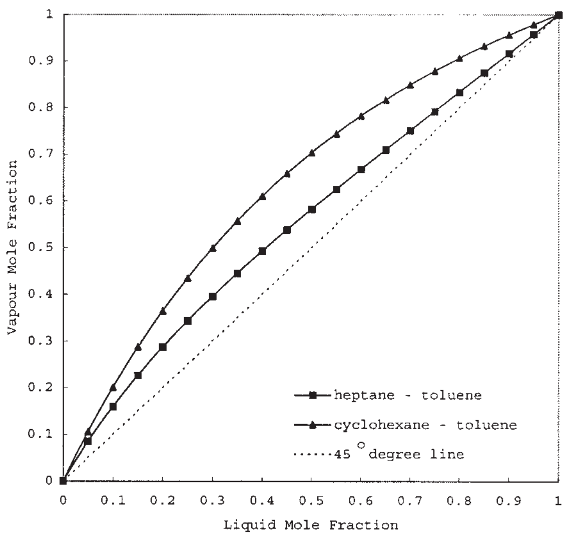


Figure 10. Equilibrium diagram for binary systems (SRK method at 101.32 kPa).

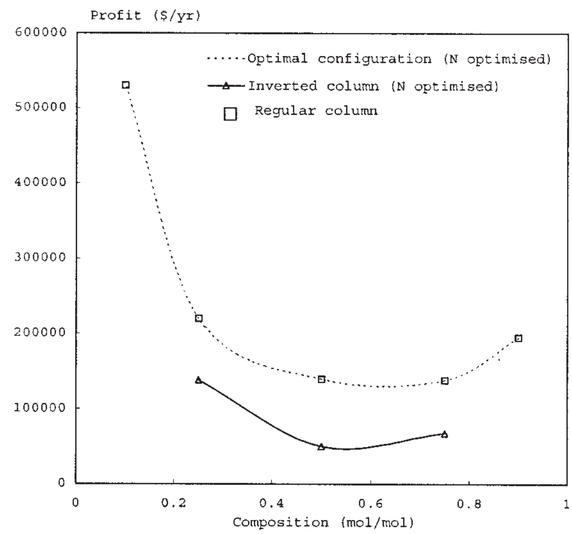


Figure 11. Optimal profits and configurations for different feed compositions (heptane-toluene mixture).

binary mixture of heptane and toluene, in order to investigate whether the mixture to be separated has any influence on the trend of results shown in case study I earlier. The vapor-liquid phase equilibrium relationships in Figure 10 suggest that the distillation of heptane-toluene is more difficult compared to the previous case of cyclohexane-toluene separation. The specifications and decision variable bounds are similar to those of the previous case (given in Tables 1 and 2, respectively) except for the product purities requirement, which was set at 95 mol% of cyclohexane and toluene. In addition, the upper bound for the number of trays variable N, was raised to 40.

The optimal results for different feed compositions of heptane-toluene are presented in Table 6. For the range of feed compositions considered, the regular column configuration was found to be optimal in all cases. This is contrary to the previous case study where the optimal column configuration changes at a flip point location. In this case study, there appeared to be no flip point. This is confirmed in Figure 11 where the results of the optimally designed fixed inverted configuration show lower profit values than those of the regular column configuration obtained from the optimization. The results obtained in this investigation highlight the complex dependence of the optimal economics and performance trade-offs on various factors, such as feed composition, mixture type and product specification.

It is also interesting to note the contrast between how the optimal design and operation variables are affected by different separation scenarios. In the previous case study with cyclohexane-toluene mixture, greater optimal column sizes were needed for feed mixtures with a higher deviation from equimolar composition. For this case study of heptane-toluene, the optimal number of trays for the symmetrical feed (50:50 mol%) and for compositions with a higher disproportion (10:90, 90:10 mol%) were similar ($N = 31$), while for the intermediate compositions (25:75, 75:25 mol%), the optimal column sizes are greater at 37 and 38 trays (Table 7). This observation implies a shift in the weighting of the economics trade-off, for examples, between capital costs and batch time—that is, the justification of higher capital cost by lowering batch time might have been altered moving towards the composition edges for the case of a more difficult separation such as in the case of the heptane-toluene mixture.

A more detailed analysis of the configuration design outcome can be elicited by contrasting it with the results for the optimal inverted column configuration, that is, fixed $Y = \{Inverted\}$, as given in Table 7. For the equimolar composition (50:50 mol%), the more profitable configuration, that is, regular column, had 1452 mol of heptane-rich product withdrawn with 1520 mol of toluene-rich product remaining in the reboiler pot, while for the inverted configuration, the toluene-rich product withdrawn and the heptane-rich product in the reflux drum were 1170 mol and 1368 mol, respectively. This comparison revisits previous similar observations, for example, obtained in the previous case study (case I) as well as by Sørensen and Skogestad,[6] that the regular configuration and its inverted form performed differently even at symmetrical feed composition, and goes on further to highlight that, for more difficult separations, such as the heptane-toluene separation investigated here, the difference in performance could become more prominent (note the significant difference in total batch

Table 6. Summary of Optimal Results for the Separation of the Heptane-Toluene Binary Mixture

Feed Composition (mol fraction)	Optimal Configuration	Optimal Size, N	Profit ($/yr)
0.90, 0.10	regular	31	195 041
0.75, 0.25	regular	38	138 306
0.50, 0.50	regular	31	139 673
0.25, 0.75	regular	37	220 218
0.10, 0.90	regular	31	530 457

Table 7. Details of Optimal Results for the Separation of the Heptane-Toluene Binary Mixture

Feed Composition (mol fraction)	Optimal Size	Reflux Ratio		Task Duration (s)		Batch Time (s)	Separated Products (mol)		
	N	$R(t_2)$	$R(t_3)$	Δt_1	Δt_2	$\Delta t_1 + \Delta t_2 + \Delta t_3$	Heptane	Toluene	Offcut
0.90, 0.10	31	0.80	0.93	0	8750	8818	2935	57	8
0.75, 0.25	38	0.85	1.00	600	9450	10932	2403	597	0
	26	*0.97*	*0.98*	*300*	*10000*	*17008*	*2276*	*500*	*224*
0.50, 0.50	31	0.91	0.99	300	9400	11295	1452	1520	28
	28	*0.91*	*0.97*	*150*	*7800*	*17192*	*1368*	*1170*	*462*
0.25, 0.75	37	0.93	0.96	450	3750	7048	454	2349	197
	18	*0.80*	*0.70*	*50*	*5850*	*8022*	*1*	*1942*	*1057*
0.10, 0.90	31	0.98	0.96	1300	1550	3060	54	2931	15

Italicized: results for the inverted column, i.e. fixed $Y = \{Inverted\}$.
Note: all product cuts were at the minimum purity of 95.0 mol%.

time, 17 192 s for inverted compared to 11 295 s for regular) and unrecovered product (462 mol for inverted against 28 mol for regular). In the heavier feed scenario (for example, 0.25: 0.75 mol%) whereby the inverted configuration has generally been shown to be more favorable, a significantly smaller column (about half the size of the regular column), and lower reflux ratios resulted in lower capital cost and batch time (17 192 s to 8022 s). Despite a much lower capital cost and bigger percentage of reduction in batch time compared to the regular configuration (53% against 38%), the inverted configuration still performed worse in terms of the overall profitability objective function, with lower yield (1057 mol of offcut) being the main cause. Thus, this work serves as an indication that, although the general guideline of "regular column for light feeds and inverted column for heavier feeds" is true for some cases (as shown in case I), the exact location of the flip point is case specific and has to be determined. It is dependent on factors like the mixture to be separated, as demonstrated here. It also highlights the need for a configuration design methodology, such as the one proposed in this study to analyze each case separately.

Optimal Configuration for Multicomponent Separation

In this section, the optimal configuration design of a multicomponent batch distillation system is investigated. The distillation involves the separation of a quaternary mixture of pentane, hexane, heptane and octane. There is a choice to set-up the process in either the rectification, stripping or multivessel configurations. The latter option would consist of a system with three column sections and four major holdup vessels including the reflux drum, two side vessels and the reboiler pot.

The case study specifications and operating conditions are listed in Table 8. The batch size or major holdup (600 mol) is charged wholly to either the reboiler pot or reflux drum in the cases of the regular and inverted configurations, respectively, or in the case of the multivessel configuration, the major holdup is equally distributed across the four vessels (150 mol in each) depending on the uptake of the optimized boolean decision variable Y. For the multivessel column, it is also possible to optimise the initial feed distribution on the vessels (Low and Sørensen[15]). Variable holdup and product withdrawal during the operation can also be considered. In this study, however, the simplest *total reflux constant holdup* policy is considered, $R_j = 1$.

The minimum product purity specifications were set at 90.0 mol% for all four (pentane, hexane, heptane and octane-rich) cuts. The cost coefficients, K_1, K_2 and K_3, of the objective function were set to similar values of the previous case study, that is, 1500, 9500 and 180, respectively.

The optimized decision variables include the column configuration Y, the number of trays in each column section N_1, N_2 and N_3, the constant boil-up rate V, and the reflux ratio profile, that is, the values of the normalized reflux ratio $R(t_i)$ (except in the first task intervals where $R(t_1)$ is set to 1 for total reflux), and the durations of each of the first six task intervals, $\Delta t_{1,2,3,4,5,6}$. Task intervals Δt_2, Δt_4 and Δt_6 represent the withdrawal period of the three lightest or heaviest product cuts, respectively, with Δt_3 and Δt_5 representing the intermediate off-cuts. In the final task interval, the duration Δt_7 is set corresponding to the minimum time needed to purify the remaining component (in either the reboiler pot or reflux drum) to its required purity of 99.0 mol%. The bounds for each variable are given in Table 9. The size of the single column in the regular and inverted configurations is taken as the sum of N_1, N_2 and N_3. For the multivessel configuration, the simple *total*

Table 8. Specifications and Operating Conditions for the Multicomponent Separation Case Study

Available annual production time, T_A (h/year)	8760
Batch set-up time, t_s (s)	1800
Operating pressure, P (Pa)	101325
Major holdup (batch size), H_{feed} (mol)	600
Minor holdup, M_{rd} or M_{reb} (mol)	3.5
Tray holdup, H_{tray} (mol)	3.5
Feed composition, $x_{i,feed}$ (mol fraction)	
Pentane, $x_{1,feed}$	0.25
Hexane, $x_{2,feed}$	0.25
Heptane, $x_{3,feed}$	0.25
Octane, $x_{4,feed}$	0.25
Product purity specifications, (mol fraction)	
First product, $x_1(t_f)$	0.90 of pentane
Second product, $x_2(t_f)$	0.90 of hexane
Third product, $x_3(t_f)$	0.90 of heptane
Fourth product, $x_4(t_f)$	0.90 of octane
Cost, C_i (\$/mol)	
Pentane, C_1	0.035
Hexane, C_2	0.035
Heptane, C_3	0.035
Octane, C_4	0.035
Feed, C_{feed}	0.001

Table 9. Decision Variables Bounds for the Multicomponent Separation Case Study

Decision Variables	Bounds
Y	{Regular, Inverted, Multivessel}
N_1, N_2, N_3	[2, 20]
V (kmol/hr)	[0.6, 6.0]
$R(t_{2,3,4,5,6,7})$	[0.4, 1.0]
Δt_i (s)	[0, 2000]

reflux constant holdup policy is considered here, hence, when the boolean variable $Y = \{\text{multivessel}\}$, the reflux ratios $R(t_i)$, for the seven task intervals are ignored and set to total reflux $R(t_i) = 1$.

Optimal Result

The result of the optimization is presented in Table 10. In this case study, the optimal configuration was found to be the multivessel system with an optimal design structure of 7, 11 and 12 trays in the top, middle and bottom column sections, respectively. For comparison, optimisation were performed with fixed $Y = \{\text{Regular}\}$ and $Y = \{\text{Inverted}\}$, and it is evident from the results that the optimal profits of these two configurations, 45 339 and 50 489 $/yr, respectively, are significantly lower than that of the multivessel configuration (169 588 $/yr). The result obtained from the optimization is in agreement to our earlier findings by Low and Sørensen[15] which demonstrated the superiority of the multivessel system compared to the regular column. The intermediate components of hexane and heptane are at and near their minimum specifications of 90 mol%, respectively, which suggest that they are the limiting components in this particular case study example.

The composition profiles of the four components in the regular, inverted and multivessel configurations are presented in Figure 12. Compared to the separation of the regular and inverted columns where each product is purified and withdrawn in sequence, the multivessel arrangement performs the separation tasks simultaneously (in parallel), resulting in a significant reduction in processing time.

The progress of the genetic algorithm search indicates that genomes bearing the gene, $Y = \{\text{multivessel}\}$, dominated the population from the first generation (Figure 13). In contrast, the total number of genomes representing the regular and inverted configurations were only 18, 25 and 3 out of the top 100 genomes in the first, second and third generations, respectively. By the fourth generation, the multivessel configuration occupied all the best 100 solutions in the population. The termination criteria was fulfilled in 37 generations.

Note that in this quaternary mixture separation case study, the multivessel configuration has two additional side vessels. Although the capital cost of these vessels is relatively smaller compared to the cost of the column, this fixed cost can be easily accounted for within the optimization methodology. Since the genetic algorithm is a black box search algorithm, that is, not dependent on the derivative information of the objective function, the inclusion of the vessel cost C_{vessel}, can simply be achieved as part of the logical disjunction statement within the program, that is, $Y = \{Multivessel\} \rightarrow P = P + C_{vessel}$.

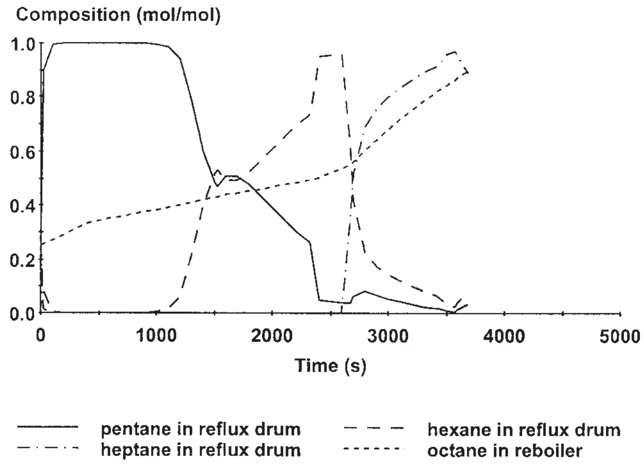
Conclusion

In this article, the optimal batch distillation configuration, design and operation have been determined simultaneously

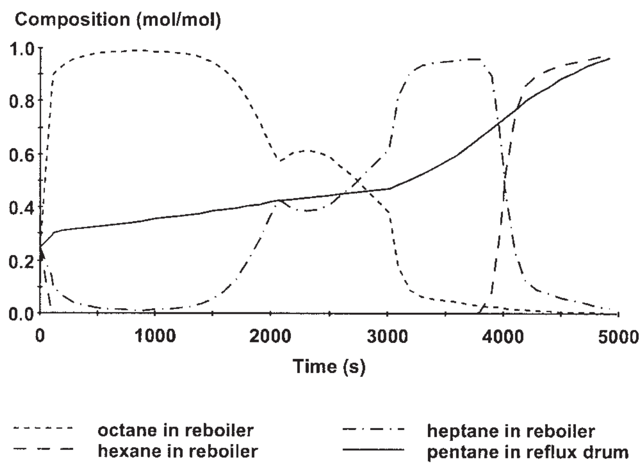
Table 10. Summary of Optimal Results for the Multicomponent Separation Case Study

Optimum Profit ($/yr)	Optimal Configuration	Optimal Design	Optimal Operation
169 588	$Y = \{\text{multivessel}\}$	$N_1 = 7$ $N_2 = 11$ $N_3 = 12$ $N_T = 30$	$V = 6.0$ kmol/hr $R_i = 1.0^‡$ $t_f = 701$ s§ Product purities: (0.99, 0.90,* 0.91,† 0.96)
Optimum Profit ($/yr)	**Configuration**	**Optimal Design**	**Optimal Operation**
45 339	$Y = \{\text{regular}\}$ (fixed)	N=20	$V = 2.4$ kmol/hr $R_1 = 1.0,^‡$ $\Delta t_1 = 24$ s $R_2 = 0.87$, $\Delta t_2 = 1501$ s $R_3 = 0.91$, $\Delta t_3 = 800$ s $R_4 = 0.53$, $\Delta t_4 = 350$ s $R_5 = 0.83$, $\Delta t_5 = 748$ s $R_6 = 0.71$, $\Delta t_6 = 150$ s $R_7 = 1.0$, $\Delta t_7 = 117$ s $t_f = 3690$ s§ Product purities: (0.93, 0.94, 0.96, 0.90*)
50 489	$Y = \{\text{inverted}\}$ (fixed)	N=18	$V = 2.0$ kmol/hr $R_1 = 1.0,^‡$ $\Delta t_1 = 929$ s $R_2 = 0.85$, $\Delta t_2 = 1950$ s $R_3 = 0.92$, $\Delta t_3 = 944$ s $R_4 = 0.72$, $\Delta t_4 = 952$ s $R_5 = 0.74$, $\Delta t_5 = 50$ s $R_6 = 0.73$, $\Delta t_6 = 94$ s $R_7 = 0.98$, $\Delta t_7 = 0$ s $t_f = 4919$ s§ Product purities: (0.96, 0.90,* 0.91,† 0.92)

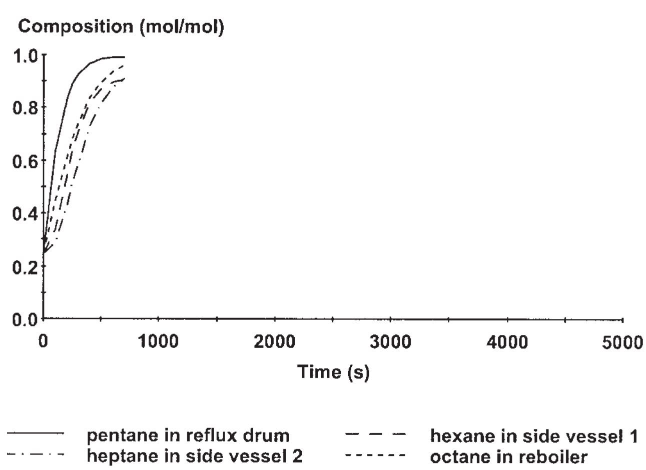
*On or †near the lower bounds.
‡Pre-set in disjunction.
§$t_f = \sum_{i=1}^{7} \Delta t_i$.



(a) Regular column



(b) Inverted column



(c) Multivessel column

Figure 12. Optimal composition profiles for different batch distillation configurations.

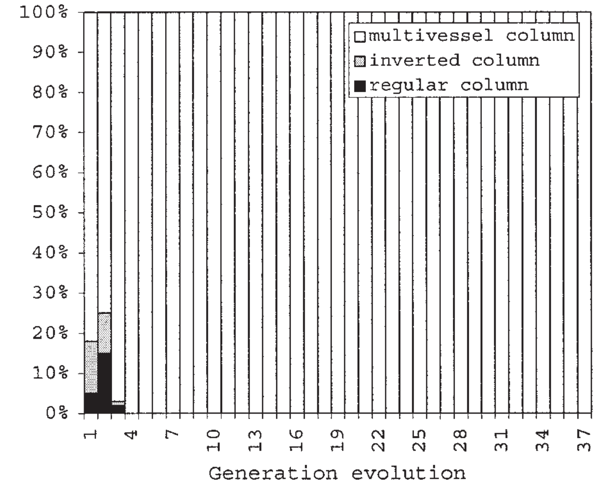


Figure 13. Percentage of column configurations in each generation of the genetic algorithm.

based on the solution of a mixed discrete dynamic optimization problem using a genetic algorithm and penalty function framework. The optimization was based on a rigorous column model and a comprehensive economics performance index that takes into account production revenue, capital and operational costs was utilized as the basis of the configuration design.

The separation of binary and multicomponent mixtures were considered. In the binary separation case study, the optimal configuration, that is, regular vs. inverted configurations, was found to be dependent on feed composition. The inverted column was found to be more profitable for feeds with high fraction of the light component while the regular column is optimal for heavier feeds. For some separations, such as that investigated for the cyclohexane-toluene mixture, there exist a flip point where a switch in the most profitable configuration occurs. The optimization results were verified by pin-pointing the location of the flip point where the switch in the optimal configuration occurs. Through another case study, of a heptane-toluene mixture, it was shown that optimal column configuration is also dependent on conditions such as the difficulty of separation as no flip point existed for this mixture.

In conclusion, the choice of optimal column configuration is dependent on different separation scenarios, thus, the configuration design approach presented in this article serves as a useful tool in the determination of the most economical configuration, design and operation for specific separation cases.

The optimization procedure was also found to be feasible in the multicomponent separation scenario, whereby the number of configurational, design and operational decision variables are greater than that in the binary case. The optimization result obtained provided a further demonstration of the superiority of the multivessel configuration over the regular and inverted configurations as highlighted in our previous work (Low and Sørensen[15]).

Notation

$C_{exchangers}$ = installed heat exchangers cost, \$
C_{feed} = unit cost of feed, \$/mol
C_i = selling price of product i, \$/mol
C_{shell} = installed column shell cost, \$

$C_{utilities}$ = utilities cost, \$
f = corrected fitness of genome
H_i = amount of accumulated product i, mol
H_{feed} = amount of feed, mol
K_1 = Guthrie's correlation coefficient for shell cost
K_2 = Guthrie's correlation coefficient for exchangers cost
K_3 = Guthrie's correlation coefficient for utilities cost
M = liquid holdup, mol
n_c = number of constraints
N_C = number of components
N_{pop} = number of genomes in one population
p = penalty function power coefficient
P = profit, \$/s
P_{ss} = percentage of population overlap, %
$Q(t)$ = instantaneous rate of reboiler heat transfer, W
R = internal reflux ratio
t = time, s
t_f = final batch processing time, s
t_i = time duration for interval i, s
t_s = batch setup time, s
u = vector of control variables
u_d = vector of design variables
u_o = vector of operation variables
V = column vapor loading, mol/s
x = vector of state variables
$x_i^{\min}$ = minimum purity of product i, mol/mol
$x_i(t_f)$ = final purity of product i, mol/mol
y = vector of discrete variables
Y = configurational boolean variable

Greek letters

κ = penalty function
Ω = objective function

Subscripts and superscripts

BC = base case
C = total number of component
f = final
i = component/control interval/constraint
j = location
LB = lower bound
UB = upper bound

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