SIMULTANEOUS OPTIMAL DESIGN AND OPERATION OF MULTIPURPOSE BATCH DISTILLATION COLUMNS

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ABSTRACT

This work presents a robust method for the integrated design and operation of batch distillation whereby optimal column sizing, process flexibility and operating policies are obtained simultaneously based on the complex economic trade-offs between capital investment, production revenue and utility costs. The proposed stochastic framework, which utilises a genetic algorithm and a penalty function strategy is found to be successful in obtaining profitable and feasible column designs for many design scenarios including binary and multicomponent mixtures, single duty and multipurpose columns as well as for regular and complex column configurations. The method can also be used with models of different complexity. Given a set of design specifications and separation requirements, the optimal number of stages, reboiler duty, reflux profiles, product recoveries, time interval of each distillation tasks, process allocation and number of batches can be obtained. Several design case studies are presented and a comparison of optimal designs for various design scenarios such as different production time, capital costs, process allocation and mixture characteristics, are discussed.

Keywords : batch distillation, optimal design, optimal operation, stochastic optimisation, genetic algorithm

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INTRODUCTION

Although batch distillation is widely used in high-value and low to medium scale production, such as those found in the fine and speciality chemical and pharmaceutical industries, the development of design methods for batch distillation columns remains a challenging task. The main reasons being the dynamic behaviour of the process and the concurrent consideration of the column design variables and its operating conditions. The task is also further complicated when the batch column flexibility as a multipurpose separations unit has to be taken into consideration at the design stage.

Design of batch distillation columns is still being carried out using the heuristic approach which relies on intuition, engineering knowledge and experience starting with an order of magnitude calculation followed by repeated calculations either by hand or aided by a computer. Al-Tuwaim and Luyben [1] performed a large number of parametric simulations and condensed them into graphs for correlation whilst Salomone *et al.* [2] presented design correlation based on the simple Fenske-Underwood-Gilliland approach developed initially for continuous columns. However, the design correlation data presented were limited, *i.e.* specific range, control profile and mixtures, and it might be too computationally expensive and tedious for the designer to conduct the same analysis.

With the emergence of greater computational power and better solution algorithms, computer-aided optimisation approaches using mathematical programming techniques is beginning to be used to tackle the design of batch distillation columns. However, to the best of our knowledge, only works by Diwekar *et al.* [3], Logsdon *et al.* [4], Diwekar [5], Mujtaba and Macchietto [6], Sharif *et al.* [7] and Kim [8] are available in the open literature.

Most of these works involved the use of short-cut methods and decomposition of the mixed integer dynamic optimisation (MIDO) problem into a nonlinear programming problem (NLP) [3,4,5]. Mujtaba and Macchietto [6] presented a two-loop algorithm where the number of trays is treated as a continuous variable in the outer loop and rounded off in the NLP subproblem which is solved by sequential quadratic programming. Sharif *et al.* [7] solved the design problem as a finite dimensional mixed integer nonlinear problem (MINLP) using the outer approximation/augmented penalty technique. Kim [8] optimised the operational variables for columns of different sizes, solved using NLP techniques, and from the multiple objective functions, the net profits were deduced after subtracting the capital costs. The column with the highest net profit was then taken as the optimum design.

In summary, the problem of finding the simultaneous optimal design and operation of batch distillation columns has been tackled using various NLP and MINLP techniques. However, the nonconvexity of the search space can cause these gradient-based sequential search methods to converge into arbitrary local optimal designs, this has been the case for many optimal control studies using standard NLP techniques. The design of a multipurpose column, a single column used to separate more than one mixture, has not been tackled properly other than considering short-cut models and subsets of the available degrees of freedom. Furthermore, the design of columns with complex configuration, such as the multivessel column, has so far not been attempted.

The objective of this work is to propose a robust optimisation method, namely Genetic Algorithm, for the integrated design of batch distillation columns which is applicable to different scenarios including multicomponent mixtures, multiple separation duties and complex column configurations. This work also aims to highlight the effects of different design scenarios, *i.e.* production time, capital costs, mixture characteristics and process allocation, on the final design and operating policies of batch distillation.

In the next section, the batch distillation design problem is presented including the formulation of the objective function and definition of the optimisation problem. Next, the mathematical modelling of batch distillation used in this study is presented. A general overview of the stochastic evolutionary-based solution technique is presented, followed by a full description of the Genetic Algorithm framework developed for the batch distillation design problem. The implementation of the method is then outlined. Finally, the design problem and its solution algorithm are applied to several case studies, in particular the design of a regular column for a ternary system, the design of multipurpose regular columns involving multiple mixtures with different separation duties and finally, the design of a multivessel column for a quaternary system.

THE BATCH DISTILLATION DESIGN PROBLEM

Problem Definition

The objective in batch distillation design is to determine the most economical column specification capable of fulfilling all separation requirements intended for the unit. Works on operational optimisation of batch distillation have demonstrated the interdependent nature of design and operation issues and thus, the need to consider these simultaneously (Figure 1). This interdependency is fundamental as the operation of batch distillation is linked to the reflux ratio profile, an operational parameter which needs to be set as a basis for a particular design. For continuous distillation, the opposing design limits are based on the reflux ratio being fixed *a priori* at the minimum and infinite values, resulting in the highest and lowest investment costs, respectively. However, in the batch mode, for a constant reflux ratio, the batch system is non-steady state.

Furthermore, the lowest capital costs 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 boilup 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.

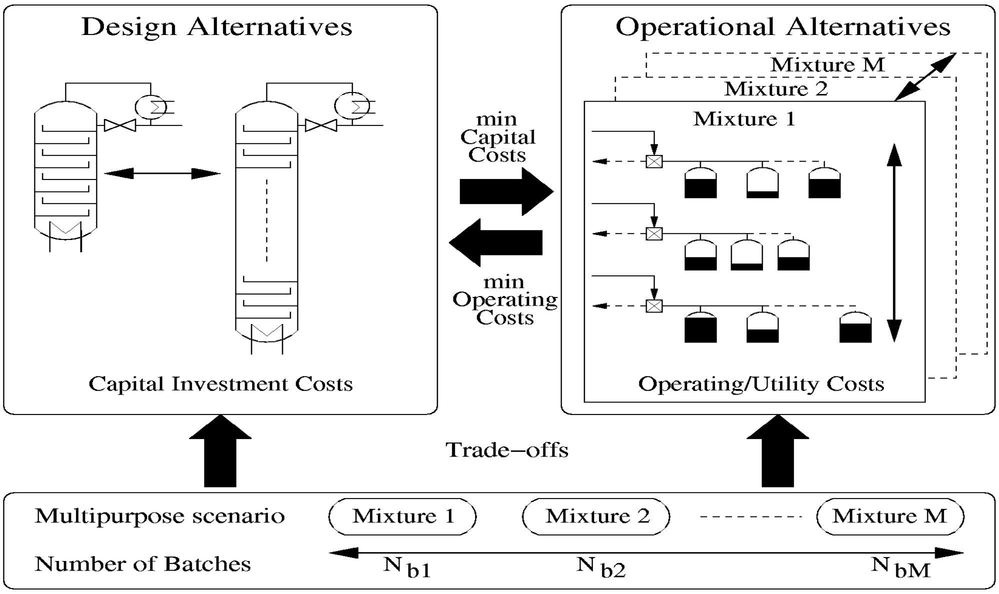

Figure 1: Batch distillation design problem

The trade-off problem is further complicated when the batch distillation column is designed for separation of multiple mixtures. In industry, batch distillation is commonly used as a flexible multipurpose unit and there may be a need for the same column to be used for a wide range of feed mixtures or at different stages in a single process. In this multipurpose scenario, the optimal number of stages and optimal control of each duties is different and therefore a third dimension is added whereby the design has to take into account the balance of trade-offs among the various duties. Production time allocation, *i.e.* the *importance* of a particular mixture with regard to the others, would also influence the final design solution. For example, if a particular separation is performed much more frequently than the others, the ultimate design tend to be bias toward this weighting. It also depends on the characteristics of the mixtures including the ease of separation and the price structure of the separated products. In this paper, the process time allocation of the mixtures is treated as an extra degree of freedom and incorporated into the optimum design problem. Thus, the optimal design variables, the different optimal operating policies of each mixtures as well as the optimal allocation of process time among the mixtures will be solved simultaneously.

Objective Function

The general design objective of a batch distillation system is to obtain the most economical column and operating policies that will satisfy all specified separation requirements. The economical design will be a trade-off between lower capital and operating costs against higher production revenue, thus the objective function must be formulated to encapsulate all of these costs. The objective function for the design of a multipurpose column as used in this paper is given by:

$$P_A = \left(\frac{\sum_{i=1}^{N_C} C_i H_i \left(t_f\right) - C_{feed} H_{feed}}{t_f + t_s} \right)_m \phi_m T_A - \left(K_1 N^{0.802} V^{0.533} + K_2 V^{0.65} + K_3 V \right) \quad (1)$$

The derivation and notation for the objective function is given in Appendix I.

Optimisation Problem Formulation

The aim of the batch distillation design problem is to maximise the objective function or profitability defined above, subject to the column model equations and all the separation constraints. In this paper, it is assumed that the purity of main products are driven by customer demand and distillation is undertaken to achieve these specifications. The optimisation is then:

Given N_M number of mixtures to be separated, each with $N_{C,M}$ components, the minimum products purity specification $x_{i,m}^{\min}$ (where $x_{i,m}$ refer to the recovered i product of mixture m), the price structure of the feed and products, C_i and C_{feed}, as well as the total production time available per year, T_A, determine the optimum set of design variables, u_d, optimum operating control variables, u_o, and production schedule among the mixtures, $\phi_m \subseteq [0,1]$, so as to maximise the objective function P_A (Equation 1). In mathematical terms, the optimisation problem is posed as follow:

$$\max_{u_d, u_o, \phi_m} P_A$$

subject to

$$f(\dot{x}, x, t, u) = 0 \quad (2)$$

$$x_{i,m}(t_f) \geq x_{i,m}^{\min} \quad \forall i = 1,\ldots,N_C; m = 1,\ldots,N_M \quad (3)$$

$$u_d^{\min} \leq u_d \leq u_d^{\max} \quad (4)$$

$$u_o^{\min} \leq u_o \leq u_o^{\max} \quad (5)$$

where Equation 2 represents the basic mathematical model for the description of a batch distillation process; x is the vector of state variables (*i.e.* holdups, concentrations, temperatures, pressures *etc.*), u denotes the vector of control variables (*i.e.* reflux ratio profile) and t is the process time. Equation 3 represents the product purity constraints on all main cuts subintervals which must be satisfied for all the mixtures. Equations 4 and 5 represents the physical and optimisation bounds of the design and operating control variables, respectively.

The set of design variables includes the optimal number of trays, batch size and vapour flowrate through the column, *i.e.* u_d = { N, H_{feed}, V }, respectively. The optimal vapour boilup rate, V, can subsequently be used to design the diameter of the column (*e.g.* using Guthrie's correlation $D \propto \sqrt{V}$) as well as the heat exchanger loading. The operating control variables includes the interval durations of each main and offcut periods for each mixtures, $t_{i,m}$, and the corresponding reflux ratio profiles, *i.e.* u_o = $R(t_{i,m})$. Thus, indirectly, the total batch time for each mixture, $t_{f,m}$, the recovery of each product and offcuts and the withdrawal rate profiles can be obtained in an optimal manner.

If the design scenario is based on a given total production time, T_A, and process distribution, ϕ_m, then a larger batch size, H_{feed}, will be favoured since a greater quantity per batch can be processed resulting in fewer number of batches and greater reduction in setup time. The trade-off caused by higher capital costs becomes insignificant as the capital costs typically increase with capacity by an exponent of less than 1 due to economy of scale. Hence, the batch or reboiler pot size has to be specified *a priori*. From a practical point of view, this is an acceptable design scenario as the designer would normally have a desired batch capacity suited to a particular plant inventory and short-term scheduling.

In a multiple separation duties scenario, if the optimal process allocation, ϕ_m, is treated as a degree of freedom, the optimisation would supply decision support on the ranking of the duties, *i.e.* duration of time allocated for each particular duty, for maximum profitability in addition to the optimum column size and all the operating policies.

In mathematical terms, the need to consider design and operation simultaneously translates into both discrete (*e.g.* the number of trays) and continuous variables (*e.g.* reflux ratio profile). The optimisation objective function (Equation 1) is nonlinear with a potential non-convex search space. Coupled with a dynamic and nonlinear model of the batch distillation column, this translate into a complex mixed integer dynamic optimisation (MIDO) problem. This type of problem is difficult to solve and there is much ongoing research on developing practical solution algorithms (Sakizlis *et al.* [9]). In this paper, the use of a stochastic algorithmic method to solve the batch distillation design MIDO problem, is proposed.

Batch Distillation Model

The mathematical model of the dynamic batch distillation system is a set of differential-algebraic equations (DAE). The optimisation framework proposed in this study, can be utilised in conjunction with any level of model abstraction and the choice is dependant on the level of detail or accuracy required at a particular design stage as well as the computational cost available. In the case studies presented in this work, three batch distillation models of different complexity are used for different purposes (Table 1).

Table 1: Different models used in case studies

Model Characteristics	Detailed Model	Simple Model	Rigorous Model
Component balance	dynamic	dynamic	dynamic
Energy balance	fast	X	dynamic
Liquid holdup in trays	constant	constant	variable
Vapour holdup	negligible	negligible	variable
Flow characteristics	mass and energy balance	constant molal overflow	hydraulics and pressure flow relationships
Total condenser	√	√	√
Perfect mixing	√	√	√
Adiabatic trays	√	√	√
Phase equilibrium	√	√	√
Thermodynamics	ideal or nonideal	constant relative volatility	ideal or nonideal
Model Usage	suitable for column design	for quick optimisation such as sensitivity studies	advanced design stage or retrofit of existing column

STOCHASTIC OPTIMISATION STRATEGY: GENERAL CHARACTERISTICS AND ADVANTAGES

Genetic Algorithm is an optimisation technique inspired by the theory of biological evolution which attempts to imitate the process of natural selection. In this process, fitter individuals characterised by *genome* are favoured 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 increases from generation to generation.

To translate this strategy into a search technique for the batch distillation optimisation problem, firstly, the design and operational decision variables of the problem have to be represented as *genes* in the genome. Then, a measurement of fitness has to be assigned to every genome depending on the quality of its genes. The fitness measurement correspond to the optimisation objective function and the aim is to maximise its value over time. The Genetic Algorithm starts by an automatic initialisation of a random population. It then employs three operators, *i.e.* selection, crossover and mutation, to evolve the initial solution set and drive it towards convergence at the global optimum.

Conventional deterministic mathematical programming approaches such as gradient-based search methods, are not robust for solving problems with highly nonlinear functions, stiff models and complex search spaces like that exhibited by the batch distillation column design. Hence, the probabilistic method proposed here has the potential to be a more attractive solution technique.

There are several advantages to the use of Genetic Algorithm:

(1) It offers greater stability and robustness as it can handle nonlinear objective functions with complex search space topography. This is due to the fact that Genetic Algorithm is a black box or zeroth order search algorithm which means it only requires scalar values of the objective function, *i.e.* do not require derivative information and a smooth, continuous and derivable search space. In addition, the solutions are manipulated in parallel rather than the sequential adjustment of a single solution performed in many traditional methods. This reduces dependability on search path history, *e.g.* derivative information, and thus the likelihood of the algorithm failing due to a previous infeasible solution. This is important for the batch distillation model which often experience initialisation or integration difficulties due to either stiff models, sharp operational switches, or more likely, infeasible solutions.

(2) It has global optimisation capability and eliminates the difficult task of selecting initial conditions. The solution obtained by many deterministic methods such as random search and gradient-based search, depends on manual setting of the initial starting point or the quality of the initial guess. Rather than starting from a single point within the search space, the Genetic Algorithm is initialised with a population of guesses which is spread 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. Due to the fact that the algorithm operates on a population of solutions and the average fitness of each generation improves in line with the best genome, the final population may supply some viable alternative designs and operations which are near the optimum solution. This is not generally available from deterministic mathematical programming approaches.

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

A GENETIC ALGORITHM FRAMEWORK FOR THE BATCH DISTILLATION PROBLEM

The optimisation framework proceeds according to the following algorithm:

1. Initialisation - 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 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 pre-specified criterion.

The Genetic Algorithm strategy employed in the work is described in the following sections.

Genome Coding

The batch distillation design problem consists of both design and operational variables and are represented in the genome as direct real values instead of binary bits and mapping which has been found to be less efficient (Coley [10]). The design parameters include the number of trays, N, which is an integer variable, and vapour boilup rate, V, whilst the operational variables include reflux ratio profiles, $R(t_{i,m})$, and the interval times, $t_{i,m}$ which are continuous variables. For a multiple separation scenario without a pre-specified production schedule, the decision variable, ϕ_m, can also be included into the genome. The reflux ratio profile is assumed to be a constant piecewise profile and thus is represented in the genome as a series of constant reflux ratio values, $R(t_{i,m})$, applied for the duration of their corresponding time intervals, $t_{i,m}$ for each task i of mixture m as shown in Figure 2. Each parameter in the genome including the time intervals can have different bounds depending on the design problem.

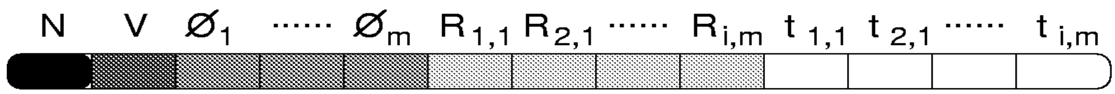

Figure 2: Genome coding

Steady-State Algorithm

A steady-state Genetic Algorithm that uses overlapping populations is used in this study, the basic structure of which is shown in Figure 3. Firstly, an initial population of a specified size, N_{pop} number of genomes, is generated randomly. This is N_{pop} different column design and operating variable combinations. Then, in each generation, the fitness of each genomes are evaluated. Based on the fitness function of each genome, the algorithm creates a new set of temporary genomes via the three operators, *i.e.* selection, crossover and mutation, and adds these to the previous population, and at the same time removing the weaker genomes in order to return the population to its original size. The amount of new genomes created in each generation depends on the percentage of population overlap, P_{ss}, specified. In this algorithm, the new offsprings 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. It allows the retention of the 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 parent generation.

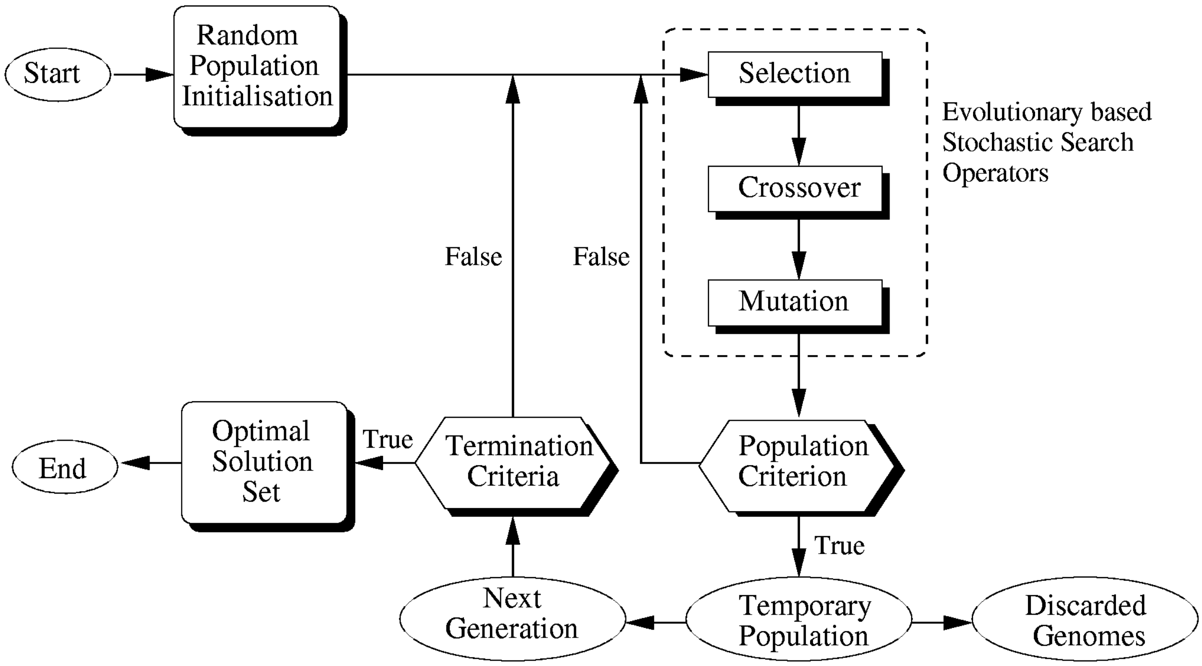

Figure 3: General structure of the Genetic Algorithm module

Solution Infeasibility and Constraints Checking

In many constrained problems such as the batch distillation design, the majority of possible solutions represented by the genomes will prove to fall short of the requirement of the constraints. 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:

$$\kappa_i = \begin{cases} \left[1 - \dfrac{x_i^{\min} - x_i\left(t_f\right)}{x_i^{\min}}\right]^{p_i} & if \quad x_i\left(t_f\right) < x_i^{\min} \quad \forall i = 1,\ldots,n_c \\ 1 & otherwise \end{cases} \tag{6}$$

$$f = \begin{cases} \Omega \prod_{i=1}^{n_c} \kappa_i & when \quad \Omega \geq 0 \quad (profit) \\ \Omega\left(2 - \prod_{i=1}^{n_c} \kappa_i\right) & when \quad \Omega < 0 \quad (loss) \end{cases} \tag{7}$$

where κ_i denotes the penalty function for each n_c purity constraints, p_i the penalty power coefficient, Ω the returned objective function and f the corrected fitness function.

It is also possible for many genomes to represent unrealistic or impractical solutions especially when the bounds set for the design and operational variables are generous. For example, when the maximum bounds or high values are chosen for boilup rate, product withdrawal rate and task duration, the reboiler pot may run dry during the task causing the simulation to crash due to infeasibility. In this case, a poor fitness function is assigned to the genome so that the probability of it being promoted to the next generation is reduced.

Selection Operator

In order to obtain good offsprings, genomes with higher fitness values should have a greater probability of being selected to undergo reproduction, *i.e.* crossover and mutation. A stochastic sampling method called *fitness-proportional* or *roulette wheel* is used here as the selection operator. In this approach, the probability of selection is proportional to the fitness of the genome. The algorithm is summarised as follow (Figure 4):

- Sum the fitness of all the population members, f_{sum}.
- Generate a random number R_s where $R_s \in [0\ , f_{sum}]$.
- Add, one at a time, the fitness of the population members stopping immediately when $f_{sum} \geq R_s$. The last member added is the selected genome.
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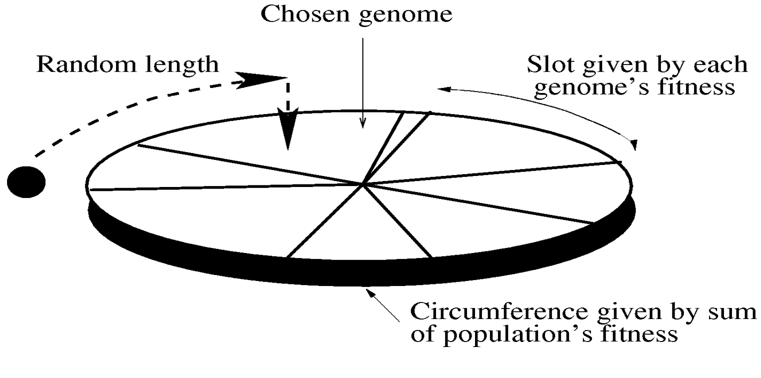

Figure 4: Fitness-proportional selection

The selection operation is applied twice in order to select a pair of genomes to undergo crossover. Selection is continued until enough genomes have been created according to the percentage of population overlap specified, P_{ss}.

Fitness Scaling

If during an early generation, one particularly fit genome is created, the fitness-proportional selection algorithm can allow a large number of its copies to rapidly dominate the subsequent generations and cause rapid and erroneous convergence towards a local optimum. Once the population has converged, crossover of almost identical genomes produces little that is new and thus the ability of the Genetic Algorithm to search for better solutions is effectively eliminated. Only mutation remains to explore entirely new space and this simply performs a slow and random search. During later stages of the optimisation, after many generations, the population would have largely converged but again there may be little difference between the best and the average genomes. Thus there is insufficient gradient pressure to distinguish between the high fitness genomes and push the population quickly towards the global optimum.

Here, *sigma truncation scaling* is used to overcome both premature convergence and slow finishing. Fitness scaling works by pivoting the fitness of the population members about the average population fitness. The mapping from objective function to fitness score for each individual is given by

$$f^S = f - \left(f_g^{ave} - c f^{\sigma} \right) \tag{8}$$

where f is the corrected fitness of a genome, f^S the scaled fitness, f_g^{ave} the average fitness of the population, c the scaling parameter and f^{σ} the standard deviation of the genome's fitness from the average.

Crossover and Mutation Operators

The crossover operator in the Genetic Algorithm is employed to mate genomes from the population to form new offsprings. Due to the fact that the genomes hold a mix of discrete and continuous variables and that each gene represents a distinct design or operational variable, the crossover method have to respect the structure of the genome, *i.e.* crossover is only allowed between genes at the same location, or allele position, of the parent genomes and the resulting length of the offspring genome must not be altered. This is done via a *uniform crossover* technique as shown in Figure 5. The genes in each genome are only allowed to swap with the gene at the same location in the other genome with a probability, P_c. A random number, $R_c \in [0,1]$, is generated for each pair of genes along the genome and the genes undergo crossover only if $R_c \le P_c$, otherwise the pair proceed without crossover.

After passing through the crossover operator, the offspring genomes undergo *Gaussian type mutation* with a probability of P_m. Again a random number, $R_m \in [\,0,1\,]$, is generated and if $R_m \le P_m$ the gene is mutated using a Gaussian function around the current value. If the mutated value goes out of the gene's allele range, it is reset to the violated boundary.

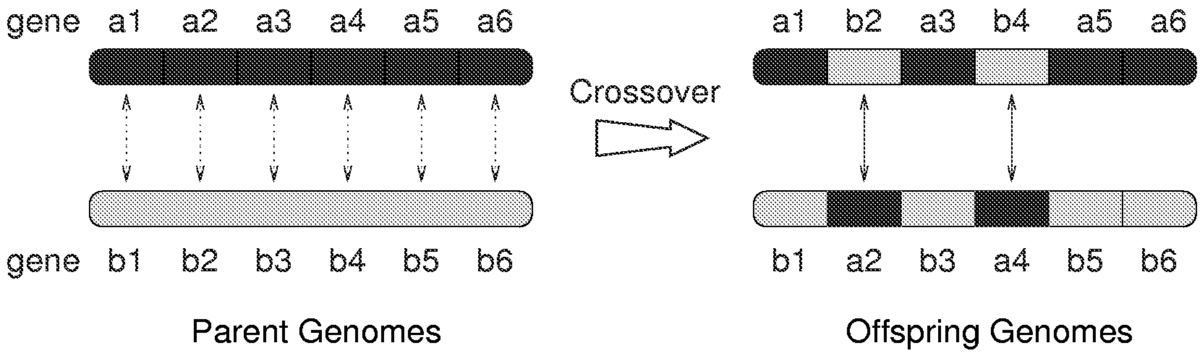

Figure 5: Uniform crossover operator

Termination Criteria

If the Genetic Algorithm is implemented correctly, the population will evolve over sequential generations so that the fitness of the best genome and the average fitness of the population in each generation increases towards the global optimum. There are a number of ways to terminate the algorithm. One of the criteria is termination when a specified number of generations has been generated and tested. However, the required number of generations to obtain a solution is difficult to estimate for a new problem. Here, the termination is based on convergence percentage, *i.e.*, either the current best of generation is compared to the N previous best of generation or current generation average. Termination criteria can also be combined, namely the algorithm stops when the ratio of the current population best to the population average *and* to the population best of the previous N generation is equal or greater than the convergence percentage specified.

IMPLEMENTATION

The dynamic models used in this paper are constructed using the *gPROMS* modelling program [11]. Thermophysical properties including density, enthalpy and fugacity required in the detailed model are calculated using the *Multiflash* physical properties package [12] interfaced to *gPROMS*. The Genetic Algorithm library *GAlib* (Wall [13]) is used in the implementation (Figure 6). The Genetic Algorithm program operates on the genome populations. During the genome evaluation step, the program performs a foreign process call to the *gPROMS* batch distillation model. In the batch distillation model, the column design and operating policy represented by the genome is dynamically simulated using an implicit backward differentiation formulae (BDF) method. The profit objective function together with the values of the constrained parameters are then passed back to the Genetic Algorithm program where a fitness value is obtained based on the penalty function.

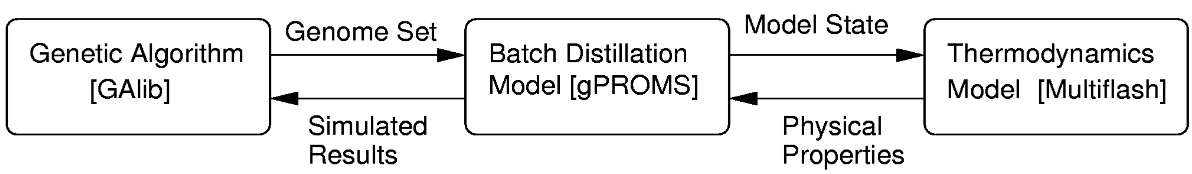

Figure 6: Schematic diagram of the program structure

Figure 7: Best fitness function and number of generation for different population sizes, N_{pop}

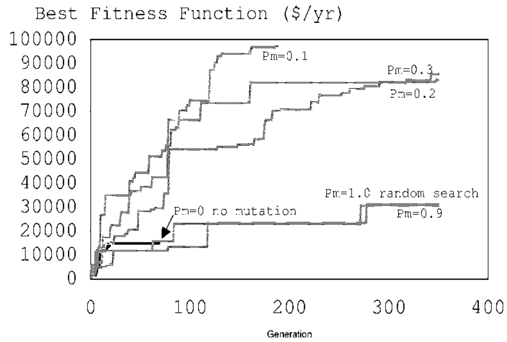

Figure 8: Best fitness function evolution for different mutation rates, P_m

The choice of Genetic Algorithm parameters (*i.e.* N_{pop}, P_{ss}, p_i, P_m and P_c) play a crucial role in the solution quality and speed of convergence of the algorithm. Sensitivity analyses have been performed to obtain the optimal settings for these parameters. Figure 7 indicates that for the batch distillation design problem, a critical population size is required to support the algorithm. A population size less than 100 will result in suboptimal solutions, *e.g.* the solution for a population size of 50 is around 60% lower than the optimal solution. This is despite the fact that about the same number of generations are needed for convergence. Hence it can be concluded that the decision is basically a trade-off between the quality and reliability of the solution and the computer cost, so long that a critical mass of population size is established. Table 2 shows that when the penalty function coefficient, p_i, is set too low, the Genetic Algorithm produces a batch distillation design that does not statisfy the separation duty, *e.g.* constraint violation of 44% when p_i is set to 1. The overall constraints violation is reduced as the penalty function coefficient is set at a higher weighting. On the other hand, if the coefficient is set too high, the genetic algorithm converged prematurely on any feasible solution it can find, *e.g.* when p_i is set at 20, the algorithm converges prematurely at the 124*th* generation, compared to more than 200 generations for p_i set at 8 and lower. Figure 8 clearly illustrates how high mutation rates (*e.g.* P_m = 90% or 100%) can disrupts the power of the algorithm and basically causes it to act like a purely random search. On the other side of the spectrum, a Genetic Algorithm with no exploration capability at all (*e.g.* P_m = 0%) causes it to be trapped in the local area of the best solution found and to converge early to a sub-optimal value.

Table 2: Effect of penalty function coefficient (p_i) on the handling of constraints (constraints specifications: 0.895, 0.863, 0.990)

Penalty Function Coefficient, p_i	Constraints Values (mol fraction)	Constraints Violation (%)	Overall Violation (%)	Generation Converged
1	[0.518] [0.855] [0.979]	[-42.1] [-0.9] [-1.1]	-44.2	279
6	[0.891] [0.857] [0.980]	[-0.4] [-0.7] [-1.0]	-2.2	229
7	[0.895] [0.863] [0.989]	[0] [0] [-0.1]	-0.1	228
8	[0.897] [0.863] [0.988]	[+0.2] [0] [-0.2]	0	219
9	[0.898] [0.858] [0.990]	[+0.3] [-0.6] [0]	-0.2	131
20	[0.894] [0.877] [0.992]	[-0.1] [+1.6] [+0.2]	+1.7	124

CASE STUDIES

In this section, several batch distillation design case studies involving binary and multicomponent mixtures are presented. This includes column design for single separation duty, design of a multipurpose column and design of a column with complex configuration. Three different batch distillation models (described earlier) are employed which showcase the flexibility of the Genetic Algorithm framework; a detailed model for the design stage, a simple model which might be useful during preliminary sensitivity studies, and finally, a rigorous model for a more definitive investigation during the advanced stages of design.

Case Study I : Design of a Column with Single Separation Duty

For this case study, a similar design scenario as that described in Mujtaba *et al.* [6] is considered. The objective is to find the optimal design and operating policy for a batch distillation column with a single separation duty of a multicomponent mixture. A detailed model is utilised with the thermodynamics described by the Soave-Redlich-Kwong equation of state. Table 3 gives a summary of the column specifications and operating conditions.

Table 3: Column specifications and operating conditions for case study I

Feed composition, $x_{i,feed}$ (mol fraction)	
Cyclohexane, $x_{1,feed}$	0.407
n-Heptane, $x_{2,feed}$	0.394
Toluene, $x_{3,feed}$	0.199
Batch size, H_{feed} (mol)	2930
Reflux drum holdup, H_{rd} (mol)	43.95 (1.5% H_{feed})
Tray holdup, H_{tray} (mol)	7.325
Available production time, T_A (hr/yr)	8760
Operating pressure, P (Pa)	101325
Batch setup time, t_s (s)	1800
Cost, C_i ($/mol)	
Cyclohexane, C_1	0.034
n-Heptane, C_2	0.026
Toluene, C_3	0.024
Feed, C_{feed}	0.002
Waste	Negligible
Product purity specifications, (mol fraction)	
First product, $x_1(t_f)$	0.895 of Cyclohexane
Second product, $x_2(t_f)$	0.863 of *n*-Heptane
Final product, $x_3(t_f)$	0.990 of Toluene

Figure 9 shows the schematic of the batch distillation process. The batch distillation operation is separated into five task intervals, starting with a total reflux period followed by a Cyclohexane product withdrawal period, offcut period, *n*-Heptane product withdrawal period and finally another offcut period to purify the Toluene product in the reboiler. The minimum product purity specifications are 89.5, 86.3 and 99.0 mol% of Cyclohexane, *n*-Heptane and Toluene, respectively. Given these specifications, the aim is to find the design and operating policy for the separation duty that would give a maximum annualised profit. The cost coefficients for the total annual cost were based on carbon steel column and hydrocarbon feedstock using cost data as shown in Logsdon *et al.* [4] resulting in the coefficients K_1, K_2 and K_3 having the values of 1500, 9500 and 180, respectively.

The design and control variables are the optimum number of trays, N, the optimum constant boilup vapour rate, V and optimal reflux ratio profile, *i.e.* the value of the normalised reflux ratio, $R(t_i)$ (except for $R(t_1)$ which is set at 1 for total reflux), and the durations, t_i, of each of the five (i = 5) task intervals. The bounds for each variable are given is Table 4.

Based on the sensitivity analysis discussed earlier, the Genetic Algorithm parameters are set as follow - the population size for each generation, N_{pop}, is set at 120, population overlap, P_{ss}, is 70% whilst crossover and mutation probability, P_c and P_m, are set at 0.75 and 0.10, respectively. The penalty function power coefficients, pi, are set at 8 for each purity constraints. The algorithm is terminated with two combined stopping criteria, *i.e.* when a convergence of 95% is obtained over 50 generations as well as over the current population average.

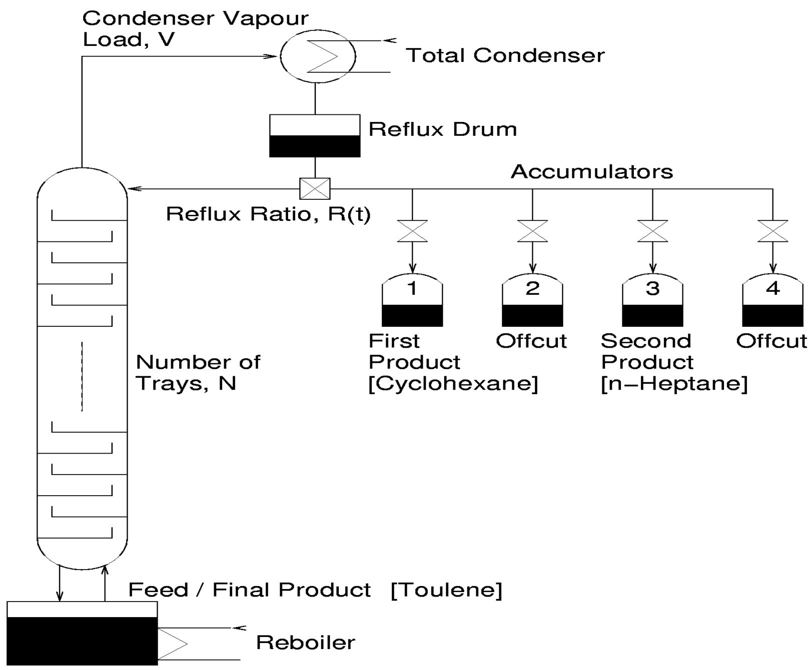

Figure 9: Schematic of batch distillation for case study I

Optimal solution

The optimum solution genome is shown in Table 5. The optimal design variables, number of trays and condenser vapour load, are found to be 29 and 6.0 kmol/h, respectively, whilst the optimal operating policy is shown as the distillate composition profiles in Figure 10. Assuming non-stop year round production (T_A = 8760 hr/yr), a profit of 97942 $/yr is achieved.

A column size of 29 trays, close to the maximum bound, is found to be optimal in this particular case study because the greater performance obtained from a bigger column achieved a revenue of 187502 $/yr which is enough to offset the annual

Table 4: Decision variables bounds for case study I

Decision Variables	Bounds
N	[4, 30]
V (kmol/hr)	[0.6, 6.0]
$R(t_i)$	[0.6,1.0]
$t_{1,2,4}$ (s)	[1000, 15000]
$t_{3,5}$ (s)	[0, 15000]

Table 5: Optimisation solution vector for case study I

Optimum Profit ($/yr)	Optimal Genome [N , V , $R(t_1)$* , $R(t_2)$, $R(t_3)$, $R(t_4)$, $R(t_5)$, t_1 , t_2 , t_3 , t_4 , t_5]
97942.9	[29, 6.00, 1, 0.86, 0.84, 0.84, 0.99, 1100, 5700, 100, 4400, 500]

(set as total reflux)*

capital investment cost of 88480 $/yr for a 29 trays column. This situation is obvious for a production plant whereby the products are of high relative value. If the design is based on a longer return outlook, *e.g.* biennial or longer, the possibility of a bigger column being more profitable in the long run increases. Similar explanation holds for the vapour load, V. For a specified amount of distillate, the batch time is inversely proportional to V and, alternatively, for a given batch time the amount of product is directly proportional to V. Since the utility and capital costs grow with V by an economic factor less than 1, a column with large V will be favourable.

The optimal operation consists of a short total reflux period (1100 s) during which the composition of the distillate rises steeply to well above the required purity of 89.5 mol% of Cyclohexane (Figure 10). Then the Cyclohexane product is withdrawn for a period (5700 s) with a reflux ratio of 0.86 until the purity in the first accumulator falls below specification. Despite the non-sharp product changeover, the offcut period is very brief (100 s). This is followed by the *n*-Heptane withdrawal period (4400 s). Finally, there is a short period of slight offcut or close to total reflux ($R(t_5)$= 0.99) to obtain the final Toluene product remaining in the reboiler. The purities obtained are 90.1, 86.5 and 98.9 mol% of Cyclohexane, *n*-Heptane and Toluene respectively, which satisfy the separation specifications.

Table 6: Genetic Algorithm statistics

Number of generations	188
Number of genome evaluations	15912
Mean fitness in initial population	-61239
Maximum fitness in initial population	3088
Mean fitness in final population	92372
Maximum fitness in final population	97230

Table 6 shows the statistics of the stochastic optimisation, *i.e.* 188 generations with 15912 function evaluations were required to achieve convergence. The mean fitness of the population increased from 61239 ($/yr loss) to 97230 ($/yr profit). Figure 11 shows that the progress of the algorithm is rapid initially with both the best and mean fitnesses of the population climbing steeply. However, the progress became slow towards a steady state. The optimisation duration is about one week on an IBM RISC

System/6000 workstation with 256 Mb of RAM running under the AIX 4.3.2 operating system. The majority of the computation time was spent on function evaluation.

Effect of production time and capital costs

In this case study example, the optimal batch distillation column consist of 29 trays, which is near the maximum bound, giving an annual profit of 97942 $/yr. At this point, it would be interesting to see the effect of another design scenario on the optimal design and operating policy. In the previous scenario, the production was run continually all year round without any stoppages. Here, a more realistic annual production time, T_A, with a 20% downtime (0.8 x 8760 = 7008 hr) is assumed, taking into account labour and maintenance work. Also, a 50% inflation of the capital and utility costs is assumed in order to study the effect of higher costs on column sizing. The new design scenario B is shown in Table 7.

A feasible solution would be to use the same column and operating policy optimised for the previous scenario A. The separation duty purity constraints would be satisfied as previously and the profit can be calculated (Table 8). Due to production

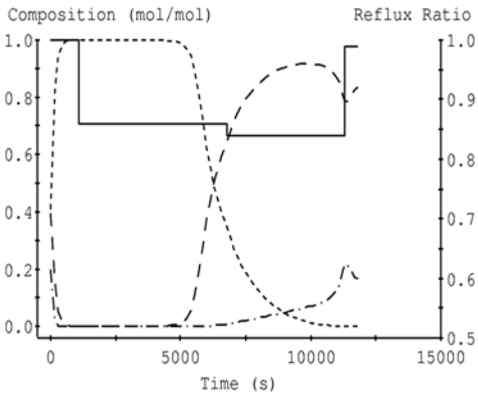

Figure 10: Optimal reflux ratio and distillate composition profiles (— Reflux ratio, - - - Cyclohexane , – – n-Heptane, –.– Toluene)

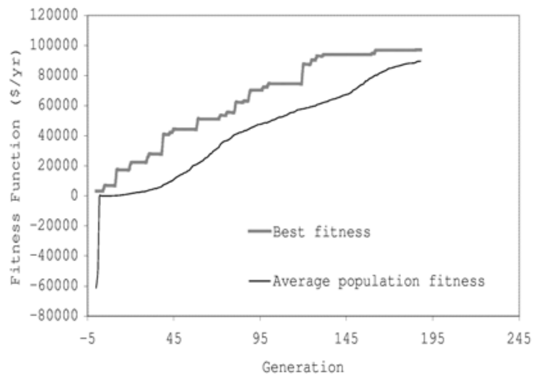

Figure 11: Fitness function evolution

downtime, the number of batches processed per year would be reduced from 2318 to 1855, giving a revenue of 150002 $/yr. The higher capital cost and utility cost are 132720 $/yr and 1620 $/yr, respectively (equations 8 in Appendix I). This gives an annualised profit of 15662 $/yr which is the maximum value achievable for a column with 29 trays, and serve as a base case because any better alternative design and operating policy must be able to provide at least this amount of annualised profit.

The Genetic Algorithm is set to run under the new design scenario to search for possible better solutions. As shown in Table 8, the new column design consists of 17 trays and vapour flowrate of 6.0 kmol/hr whilst the new operating policy is shown in Figure 12. The smaller column has lower efficiency than the base case column, *i.e.* higher reflux ratios across all the task intervals and longer offcut periods to satisfy the purities requirement, causing an overall longer process time (Figure 12) and thus a decrease in number of batches per year (N_b = 1627) compared to the base case. However, the smaller column also reduces the capital investment cost and the overall offset has resulted in a higher profitability than the base case. In other words, the 17% loss in production revenue (from 150002 to 124524 $/yr) is positively offset by a greater reduction (23%) in the cost of installing a smaller and less efficient column. The net profit for the revamped design and its corresponding operating policy is 20514 $/yr, a 30% increase from using the base case 29 tray column.

Table 7: Design scenarios

Design Scenario	A	B
Production time per annum, T_A (hr)	8760	7008
Capital costs coefficients, K_1, K_2	1500 , 9500	2250 , 14250
Utility cost coefficient, K_3	180	270

Table 8: Optimal designs for different scenarios

Design Scenario	A	B	
	Optimised Design	Base Case Design	Revamped Design
Number of trays, N	29	(29)	17
Vapour boilup rate, V (kmol/hr)	6.0	(6.0)	6.0
Batch processing time, t_f (hr)	3.28	(3.28)	3.81
Number of batches, N_b	2318	(1855)	1627
Purity constraints, x_i (mol%)	90.1, 86.5, 98.9	(90.1, 86.5, 98.9)	89.6, 86.4, 99.0
Production revenue ($/yr)	187502	(150002)	124524
Capital costs ($/yr)	88480	(132720)	102390
Utility costs ($/yr)	1080	(1620)	1620
Profit, P_A ($/yr)	97942	(15662)	20514

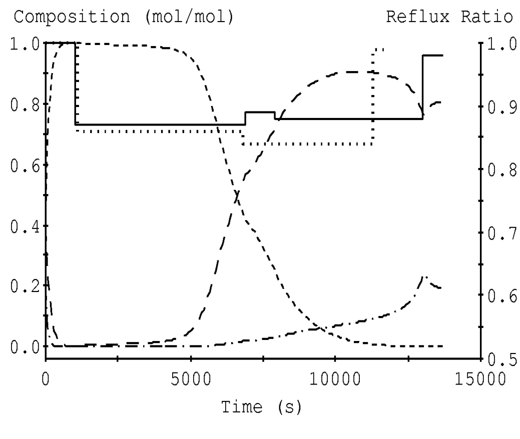

Figure 12: Optimal reflux ratio and distillate composition profiles

(— Reflux ratio of scenario B, …. Reflux ratio of scenario A, - - - Cyclohexane , – – n-Heptane, –.– Toluene)

Case Study II : Design of a Multipurpose Column
In this case study, the design of a column with multiple separation duties (two binary mixtures) is considered. The aim is to obtain the optimal column design, *i.e.* number of trays and vapour boilup rate, as well as optimal operating policies for each of the separation duties in a scenario whereby the column is used to separate mixtures with different thermodynamic characteristics. Here, the ease of separation of one mixture is greater than the other via the specification of relative volatilities.

Table 9 gives the summary of the column specifications and operating conditions. The two binary feeds are of equimolar composition. The separation requirements is to obtain 95 mol% of the lighter components for each mixtures, both having the same selling price of 20 $/kmol, thus the only difference between the mixtures is the ease of separation. A total production time of 8000 hr (9% downtime) is allocated per year to be distributed between the two separation duties (ϕ_m). The column setup time for each batch is 1440 s. Figure 13 shows the schematic of the batch distillation process whereby each operating policy consist of two time intervals. The same values as in the previous case study are used for the coefficients K_1, K_2 and K_3 as well as the Genetic Algorithm parameters. The bounds for each variable are given is Table 10.

Table 9: Column specifications and operating conditions for case study II

Number of mixtures, N_m	2 binaries
Relative volatilities, α_{ij}	
Mixture 1	1.5, 1.0
Mixture 2	2.5, 1.0
Feed composition, $x_{i,feed}$ (mol fraction)	
$x_{1,feed}$, $x_{2,feed}$ Mixture 1	0.5, 0.5
$x_{1,feed}$, $x_{2,feed}$ Mixture 2	0.5, 0.5
Batch size, H_{feed} (mol)	10000
Reflux drum holdup, H_{rd} (mol)	100 (1.0% H_{feed})
Tray holdup, H_{tray} (mol)	3.0% H_{feed}
Available production time for both mixtures, T_A (hr/yr)	8000
Operating pressure, P (Pa)	101325
Batch setup time, t_s (s)	1440
Cost, C_i ($/mol)	
C_1 , C_2 Mixture 1	0.020, 0
C_1 , C_2 Mixture 2	0.020, 0
Product purity specifications, (mol fraction)	
First product mixture 1	0.950
First product mixture 2	0.950

Table 10: Decision variables bounds for case study II

Decision Variables	Bounds
N	[12, 22]
V (kmol/hr)	[5, 15]
ϕ_m	[0, 1]
$R(t_{i,m})$	[0.4, 1.0]
$t_{i,m}$ (s)	[100, 18000]

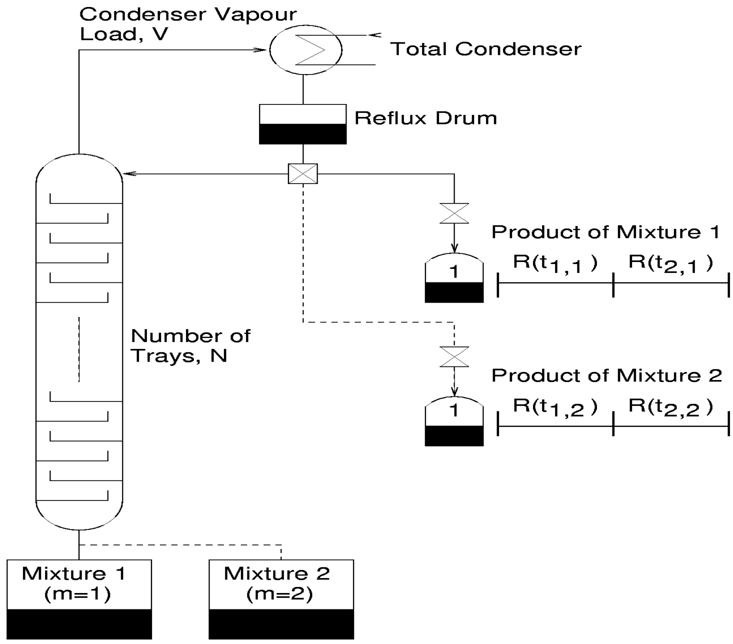

Figure 13: Schematic of batch distillation for case study II

Optimal solutions

Table 11 and Table 12 show the optimal column design and optimal operating policies for different cases of process allocation scenario. Case A and B represent the optimal designs when the column is used exclusively to separate a particular mixture. The optimal number of trays for separating the mixture with a relative volatility of 1.5 is 21 (case A), close to the maximum bound, whilst a column with 12 trays, minimum bound, is found to be optimal for the separation involving the mixture with a relative volatility of 2.5 (case B). The solution is in accord with engineering intuition, *i.e.* a smaller column can be used to satisfy purity specification for a mixture with greater ease of separation. The results also show that it is more profitable to allocate production time on easy to separate mixture (247333 $/yr) rather than for the more difficult separation (55702 $/yr). This is because, in addition to lower capital cost for a smaller column, the operating policy is also economically more advantageous in case B, *i.e.* greater ease of separation allowing for lower reflux ratios and thus lower batch times (1.25 hr compared to 2.47 hr) and greater number of batches processed per year (4848 compared to 2785). In addition to more batches, a greater amount of product is collected per batch in case B (4.364 kmol) than in case A (3.767 kmol).

Case C represent the design scenario whereby a single column is used for different separation duties. When the production time is distributed equally between the two mixtures, a column with 16 trays is found to be optimum with a profit of 144529 $/yr. The batch processing time for the easy separation is 1.19 hr compared to 3 hr for the more difficult separation. An interesting observation can be seen when case C_1 is contrasted to case A and B whereby a column of 16 trays seems to be a compromise between the optimum 21 trays in case A and the optimum 12 trays in case B. This is reflected in the operation where, as a result of compromising a smaller column (16 instead of 21), the batch time has suffered for the more difficult duty (3.00 hr compared to 2.47 hr) whereas on the other hand, the batch time has improved slightly (1.19 hr compared to 1.25 hr) for the easier duty when a larger than necessary column is compromised (16 instead of 12).

Case C_2 highlights the possibility of alternative solution for a particular design scenario. The profit objective function is very close to case C_1 (+1.0%). However, by adding another two trays to make a total of 18, the extra capital investment costs can be more than recouped within a year by a 10% increase in the total number batches processed (3685 to 4061). Thus, it may be worthwhile to use the Genetic Algorithm to search for possible alternative solutions or as a mean of checking for global solution by simply conducting more than a single run.

Table 11: Optimal process allocation and column design for two separation duties (N_M=2)

Case	Process Allocation $[\phi_1, \phi_2]$	Vapour Boilup Rate, V (kmol/h)	Optimal Number of Trays, N	Profit, P_A ($/yr)
A	[1,0]	10.0	21	55702
B	[0,1]	10.0	12∗	247333
C_1	[0.5,0.5]	10.0	16	144529
C_2	[0.5,0.5]	10.0	18	146001
C_3	[0.5,0.5]	14.9 (optimised)	16	204498
D	[0,1] (optimised)	10.0	12∗	245361

(∗ minimum bound)

Table 12: Details of Optimal Operating Policies for two separation duties (N_M=2)

Case	Batch Times (hr) $[t_{1,1}+t_{2,1}]$, $[t_{1,2}+t_{2,2}]$	Amounts of Product (kmol/batch)	Number of Batches $N_{b,1}$, $N_{b,2}$ (total)
A	2.47 , ------	3.767 , -------	2785 , ------- (2785)
B	------ , 1.25	------- , 4.364	------ , 4848 (4848)
C_1	3.00 , 1.19	3.931 , 4.258	1176 , 2509 (3685)
C_2	2.78 , 1.03	3.986 , 3.908	1259 , 2802 (4061)
C_3	2.22 , 0.92	4.090 , 4.641	1525 , 3038 (4563)
D	0.00 , 1.39	0 , 4.625	0 , 4472 (4472)

In case C_3, the vapour boilup rate, V, is optimised along with the other variables. Similar to the observation in case study I, a high vapour boilup rate (14.9 kmol/hr, close to the maximum bound) maximises the objective function. The capital and utility costs associated with high vapour boilup rate is insignificant relative to the greater performance and production gained from the faster separation and more number of batches.

Finally, in case D, the process allocation parameter, ϕ_m, is relaxed as a degree of freedom. In other words, the algorithm is free to make decision on how much *importance* should be placed on each mixtures so as to maximise profit, in addition to determining the column design and its associated operating policies. It can be expected from the previous cases that the highest profit can be obtained when all the available production time is allocated solely on the easier separation (case B), which is duly confirmed in case D. The optimal number of trays, 12, and objective function (-0.9%) is the same as case B. However, interestingly there are alternatives within the operating policy, *i.e.* 4848 batches per year collecting 4364 mols per batch (case B) compared to 4472 batches (376 less) but collecting slightly higher 4625 mols per batch (case D).

The optimisation duration for each run is about one day on the same machine used in case study I. This is due to faster simulation associated with the simpler model as well as faster convergence (< 25 generations) compared to case study I (188 generations).

Case Study III : Design of a Complex Column

The design of a batch distillation column with complex configuration, *i.e.* multivessel column, is considered (Figure 14). Furlonge *et al.* [14] solved the optimal operation problem of this column for a fixed number of stages based on minimum energy consumption. The aim here is to consider both the optimal number of trays and operation simultaneously using the more general objective of maximising profit. Table 13 gives the column specifications and operating conditions. A rigorous model is used and the mixture assumed to be ideal. The column dimensions and flow characteristics are similar to those given in [14]. The values of the coefficients K_1 and K_3 are taken as 0.0663 and 1.5 respectively to obtain the hourly profit (assuming the heat exchangers costs has been set for this example, *i.e.* K_2 = 0).

The feed is distributed equally among the reboiler, two side vessels and reflux drum. All these holdups are kept constant throughout the operation which takes place under total reflux. The operating policy is divided into six control intervals of variable duration bounded between 12 and 3000 s (Table 14). In addition, the optimal number of trays for each column section, $N_{i=1,2,3}$, and reboiler duty profile, $Q_{reb}(t_i)$, are determined.

Table 13: Column specifications and operating conditions for case study III

Feed composition, $x_{i,feed}$ (mol fraction)	
Methanol, Ethanol, *n*-Propanol, *n*-Butanol	0.25, 0.25, 0.25, 0.25
Batch size, H_{feed} (mol)	100
Reboiler, side vessels and reboiler holdups (mol)	25 each
Tray holdup, H_{tray} (mol)	0.12
Column dimensions and flow coefficients	as in reference [14]
Operating pressure, P (Pa)	101325
Batch setup time, t_s (s)	1800
Cost, C_i ($/mol)	
Methanol, C_1	0.035
Ethanol, C_2	0.035
n-Propanol, C_3	0.035
n-Butanol, C_4	0.035
Feed, C_{feed}	0.001
Product purity specifications, (mol fraction)	
Reflux drum, $x_1(t_f)$	0.928 of Methanol
Vessel 1, $x_2(t_f)$	0.854 of Ethanol
Vessel 2, $x_3(t_f)$	0.914 of *n*-Propanol
Reboiler, $x_4(t_f)$	0.970 of *n*-Butanol

Table 14: Decision variables bounds for case study III

Decision Variables	Bounds
N_1, N_2, N_3	[2, 20]
$Q_{reb}(t_i)$ (kW)	[0.75, 5.5]
$T_{i,m}$ (s)	[12, 3000]

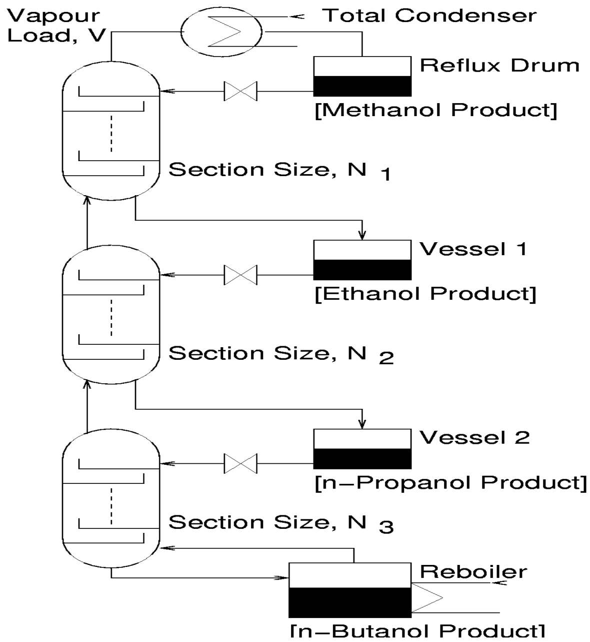

Figure 14: Schematic of batch distillation for case study III

Optimal solutions

Table 15 shows the optimal results for three different scenarios. Firstly, the optimal operation obtained by Furlonge *et al.* [14] is compared to the result in scenario A. Both cases considered fixed number of trays in each column sections, *i.e.* 10 each. The comparison highlights the disadvantage of using an objective function that focus on a particular aspect of the batch distillation process (in this case, energy consumption) instead of an overall economical evaluation like profitability. Scenario A argues that the better alternative to operating a column with the lowest energy consumption rate (1478 W) is to operate the column with a 40% increase in energy consumption (2065 W) with a reduction in operating time by 46% (5115 to 2774 s). Thus for a production plant with unlimited demand, this would result in greater number of batches and more than 2.5 fold increase in profitability (0.40 to 1.07 $/hr).

In scenario B, the optimal design and operation are considered simultaneously, i.e. the optimal number of trays in each sections of the multivessel column is optimised and hence taking into consideration the capital investment cost. The results shows that by investing in just one more tray (31 instead of 30) and by optimally distributing the trays in the column (11,11,9 configuration instead of 10,10,10 configuration), the profitability can be increased by 22% from 1.07 $/hr in scenario A to 1.31 $/hr. This comparison shows how economical insights can be gained by considering both design and operating parameters concurrently during the design stage and the benefits of doing so.

The optimisation duration for each run is about 3 days on the same machine used in case study I and II.

Table 15: Optimal results of the multivessel column for different scenarios

Scenario	Furlonge *et al.* [11]	A	B
Objective function	Minimise E	Maximise P_A	Maximise P_A
Optimisation Method	CVP/SQP[1]	Genetic Algorithm	Genetic Algorithm
Number of trays, N_I			
Section 1, N_1	10	10	11 (optimised)
Section 2, N_2	10	10	11 (optimised)
Section 3, N_3	10	10	9 (optimised)
Energy consumption, E (W)	1478	2065	2148
Profit, P_A ($/hr)	0.40	1.07	1.31
Batch processing time, t_f (s)	5115	2774	2255
Purity constraints, x_i (mol%)	92.8*, 85.4*, 91.4*, 97.0*	92.8*, 87.0, 92.5, 98.6	92.8*, 87.6, 91.4*, 97.3

(minimum bound [1]control vector parameterisation/sequential quadratic programming)*

CONCLUSION

In this work, optimal design and operating policies of the batch distillation system has been solved simultaneously, for single duty columns, multipurpose columns with multiple separation duties as well as for columns with complex configuration. The problem consists of a nonlinear annualised profit objective function that encapsulates the various trade-offs between the design and control decision variables, between the production revenue, capital and utility costs as well as between the different mixtures. The case studies highlighted the importance of considering all the design and operational degrees of freedom available in order to gain a comprehensive economical insight into the batch distillation process. Optimal column design and operating policies depends highly on the design scenario, *i.e.* production time, capital costs, mixture characteristics, process allocation *etc*.

The stochastic optimisation framework, *i.e.* Genetic Algorithm, used in this work was found to be a robust and viable way to solve the batch design problem and can be used with a range of models with different complexity. The proposed algorithm is found to be robust compared to other deterministic approaches as it does not rely heavily on information from previous iterations for the search direction or on the topography of the search space. The Genetic Algorithm is also more robust in absorbing infeasible solutions. However, the Genetic Algorithm parameters have to be selected appropriately in order to fulfil the problem constraints as well as to avoid premature convergence.

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APPENDIX I

The objective function used in this paper is derived here. The production sales revenue for each batch may be given by:

$$\Psi = \sum_{i=1}^{N_C} C_i H_i(t_f) - C_{feed} H_{feed} \tag{1}$$

where C_i and C_{feed} represent the unit costs of product i and feed, respectively, and H_i and H_{feed} the quantity of on-specification product i collected and feed, respectively. The revenue per unit time is obtained by dividing by the batch processing time, t_f, plus the setup time for each batch, t_s, as follows:

$$\Psi_t = \frac{\sum_{i=1}^{N_C} C_i H_i(t_f) - C_{feed} H_{feed}}{t_f + t_s} \tag{2}$$

The total number of batches processed per annum for a particular mixture is calculated as:

$$N_b = \frac{T_A}{t_f + t_s} \tag{3}$$

where T_A is the total time available for processing per year.

The total annual costs associated with a batch distillation column includes installed equipment capital costs and operational utilities cost. Using Guthrie's correlations (Douglas [15]), the installed cost of a distillation column shell can be written as:

$$C_{sh} = C_{sh,BC} \left(\frac{N}{N_{BC}} \right)^{0.862} \left(\frac{D}{D_{BC}} \right)^{1.066} \tag{4}$$

where N is the number of trays, D is the diameter of the column and the subscript BC represents the base case column from which the Guthrie's correlation is obtained. Assuming the column diameter varies as the square root of the column vapour rate [15], $D \propto \sqrt{V}$, so Equation 4 can be written as:

$$C_{sh} = C_{sh,BC} \left(\frac{N}{N_{BC}} \right)^{0.802} \left(\frac{V}{V_{BC}} \right)^{0.533} \tag{5}$$

Apart from the column shell, the column reboiler and condenser would also contribute significantly to the installed equipment cost of batch distillation. The annual installed costs of a heat exchanger can be written as [15]:

$$C_{ex} = C_{ex,BC} \left(\frac{V}{V_{BC}} \right)^{0.65} \tag{6}$$

The main operating cost in batch distillation is utilities cost, *e.g.* steam for the reboiler and cooling water for the condenser. In the simplest case, the following correlation can be used [15]:

$$C_{uty} = C_{uty,BC} \left(\frac{V}{V_{BC}} \right) \tag{7}$$

Equations 5, 6 and 7 can be written respectively as:

$$C_{sh} = K_1 N^{0.802} V^{0.533} \ , \ C_{ex} = K_2 V^{0.65} \ , \ C_{uty} = K_3 V \tag{8}$$

where the value of the correlation coefficients K_1, K_2 and K_3 can be calculated according to a base case column:

$$K_1 = \frac{C_{sh,BC}}{N_{BC}^{0.802} V_{BC}^{0.533}} \;,\; K_2 = \frac{C_{ex,BC}}{V_{BC}^{0.65}} \;,\; K_3 = \frac{C_{uty,BC}}{V_{BC}} \qquad (9)$$

The objective function of the simultaneous batch distillation design and operation problem used in this paper is set up as profit per unit time, *i.e.* annualised profit, given by the total annual sales revenue minus the capital and utility costs. Mathematically, the objective function can be written as:

$$P_A = \Psi_t - C_{sh} - C_{ex} - C_{uty} \qquad (10)$$

Substituting Equations 2 and 8 into 10:

$$P_A = \left(\frac{\sum_{i=1}^{N_C} C_i H_i (t_f) - C_{feed} H_{feed}}{t_f + t_s} \right) T_A - \left(K_1 N^{0.802} V^{0.533} + K_2 V^{0.65} + K_3 V \right) \qquad (11)$$

or from Equation 3,

$$P_A = \left(\sum_{i=1}^{N_C} C_i H_i (t_f) - C_{feed} H_{feed} \right) N_b - \left(K_1 N^{0.802} V^{0.533} + K_2 V^{0.65} + K_3 V \right) \qquad (12)$$

The term Ψ_t (Equation 10) itself is an objective function which combines the maximum distillate production and minimum processing time problems commonly used separately in optimal control optimisation for fixed column size. The addition of the capital costs and utilities cost terms completes the interaction between the design and operating variables.

For a multipurpose batch column, a single unit is used to separate a number of mixtures. Consider each mixture m where a total quantity of M_m is processed in a number of $N_{b,m}$ batches of size H_{feed} requiring a total time of T_m, thus:

$$N_{b,m} = \frac{T_m}{t_{f,m} + t_{s,m}} = \frac{M_m}{H_{feed}} \qquad (13)$$

and the time allocation or *importance* of each mixture m can be defined as:

$$\phi_m = \frac{T_m}{T_A} \qquad (14)$$

where T_A is the total available production time per annum. Substituting Equation 14 into 13:

$$N_{b,m} = \frac{\phi_m T_A}{t_{f,m} + t_{s,m}} \qquad (15)$$

This is then substituted into Equation (12) to give the final objective function equation.