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Self-optimising Control, a Batch Distillation Simulation Study

Taj Alasfia M. M. Barakat

Department of Chemical Engineering, Faculty of Engineering University of Khartoum
P. O. Box 321 Khartoum, Sudan (E-mail: tmbarakat@uofk.edu)

Abstract: A dynamic mathematical model of batch distillation columns is formulated using four basic assumptions: binary separation, negligible vapour holdup, constant pressure and constant molar flows. Simulations performed in the modelling tool MATLAB, proved that the model gives satisfactory description of the process behaviour. Simulations studies were then used to apply the theory of self-optimising control to batch distillation columns, in order to provide a systematic procedure for the selection of controlled variables based on operational economics. It was found that the distillate and boilup flows have good self-optimising properties. The study has also shown the unsuitability of the reflux ratio (R_{in}) and reflux return (LT) to self-optimising control due to their sensitivity to disturbances in batch distillation of the system.

Keywords : *Batch distillation; Dynamic model; MATLAB; Simulation; Self-optimising control.*

1. INTRODUCTION

The use of distillation as a separation and purification process is very old. According to historians, the first recorded description of a batch distillation occurred in Cleopatra's time in Egypt around 50 B.C. In the early sixteenth century, distillation was being applied to separation and recovery of alcohol, water, vinegar, essences, oils and other products.

Recent interest in batch distillation in such industries as fine chemical and pharmaceutical companies is growing fast. In these industries, the separation of multiple components from a product mixture is one of the major difficulties in the production processes. Batch distillation is popular because of its several advantages in many cases. In particular, it is more flexible than continuous distillation making it possible to cope with variation in feed compositions and product specifications. In addition, completely different mixtures can be separated using the same column, the latter is of a great advantage considering today's frequently changing product specification and market's requirement [1]. Furthermore, batch distillation often means simpler operation and lower capital cost than continuous distillation [2]. The most obvious disadvantage of batch distillation is the high cost of energy, as it most often requires more energy than continuous distillation.

The increase of batch distillation use as well as competitiveness in industry during the last years [3] makes it interesting to model the process and to use this model for optimisation, minimising energy requirements (which, in practice, often means minimising production time) and loss of product, always maintaining high purity requirements. Further motivation is provided by the increasingly stringent environmental regulations, which make effective control of processes vital [4].

Batch distillation is an inherently complex dynamic process (the holdup and composition of material change with time during operation). The model size of batch distillation quickly grows with increasing model accuracy, number of components and number of trays, making a successful modelling and optimisation which relies to a great extent on today's fast development in computer hardware and software.

In this work, the dynamics of batch distillation columns is used to apply the concept of self-optimising control by Skogestad [5] to batch distillation systems. The method has been applied successfully for continuous processes by Engelien *et al.* [6] in their investigation of heat integrated distillation columns. The same model in examined in this paper.

Skogestad [5] has developed a procedure to find candidate controlled variables with good self-optimising properties, for which a constant policy results in a small (economic) loss where there is uncertainty (e.g. disturbances, implementation errors and model errors). The controlled variables should normally include active constraints, which may depend strongly on the actual operation, including cost data. The most difficult issue is to select as controlled variables to satisfy the remaining unconstrained degrees of freedom. Even if individual measurements are selected as controlled variables, there may be thousands of possible combinations for a typical process. If a combination of variables is allowed, then the number of possible choices is infinite. There is therefore a need for tools to assist in eliminating and selecting candidates.

The basic idea of self-optimising control was formulated about twenty years ago by Morari *et al.* [13]. They write that "*in attempting to synthesize a feedback optimising control structure, our main objective is to translate the economic objectives into process control objectives*". Skogestad [5] explains this as to "*find a function c of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables, and with it, the optimal operating conditions"*.

Similar to Skogestad work [5] on minimising the losses of a control system implementation, Narrway and Perkins [14] strongly stress the need to base the selection of the control structure on economics. They also discussed the effect of disturbances on the economics but have not formulated any rules or procedure for the selection controlled variables.

Mizoguchi *et al.* [15] and Marlin and Hrymak [16] acknowledged the need to find a good way of implementing the optimal solution in terms of how the control system should respond to disturbances. They suggested that the selection of optimal control systems should yield the highest profit for a range of disturbances. Whereas, Zheng *et al.* [17] presented a procedure for selecting controlled variables based on economic penalties in their application to a reactor-separator-recycle system.

Skogestad [5] has connected the ideas that inspired control scientists for the past twenty years formulating a clear structure for the selection of "Self-optimising control". He included implementation errors in his analysis, and presented case studies for continuous distillation and reactor systems.

2. BATCH DISTILLATION MODELLING

Inspired by Skogestad [9] in his modelling of continuous distillation, and also by simplifying Distefano [7] rigorous multicomponent batch distillation model, a dynamic model has been developed to carry out the necessary simulation studies.

2.1 Assumptions

A binary batch separation case is considered with the following assumptions:

- Constant pressure
- Negligible vapour holdup
- Total condenser with constant liquid holdup
- Constant molar flows
- Equilibrium on all stages
- Constant relative volatility,
- Linearized liquid flow dynamics

These assumptions may seem restrictive, but they are reasonable, except possibly for the assumption of constant pressure. The main objective of this paper is to capture the main effects necessary for dynamics and control.

2.2 The Model

The states are the mole fractions of light component x_j and the liquid holdup M_j : a total of $2(NT + 1)$ states.

All equations quoted here correspond to the model given in **Fig. 1.**

Stage j, Section II;

Total material balance;

$$dM_j/dt = L_{j+1} - L_j + V_{j-1} - V_j \qquad (1)$$

Material balance for light component at stage j, Section II;

$$d(M_j\, x_j)/dt = L_{j+1}\, x_{j+1} - L_j\, x_j + V_{j-1}\, y_{j-1} - V_j\, y_j \qquad (2)$$

which gives the following expression for the derivative of the liquid mole fraction ;

$$d(x_j)/dt = [d(M_j\, x_j)/dt - x_j d(M_j)/dt]/M_j \qquad (3)$$

Algebraic Equations

The vapour composition y_j is related to the liquid composition x_j on the same stage through algebraic vapour-liquid equilibrium:

$$y_j = \alpha x_j/(1+(\alpha-1)x_j) \qquad (4)$$

where α is the relative volatility.

Based on the assumption of constant molar flows and no vapour dynamics the vapour flows has the following expression:

$$V_j = V_{j-1} \qquad (5)$$

The liquid flows depend on liquid holdup (on the stage above) and the vapour flow. This is a linearized relationship that can be used as an alternative to Francis' Weir formula [8].

$$Lj = L_{0,j} + M_j - M_{0,j}/\tau_L + (V_{j-1} - V_{0,j-1})\lambda \qquad (6)$$

where $L_{0,j}$ [kmol/min] and $M_{0,j}$ [kmol] are the nominal values for the liquid flow and holdup on stage j.

This means that it takes some time, about $\theta_L = (NT-1)\,\tau_L = 15 \times 0.063 \approx 1$ [min] for a change in the liquid at the top of the column (L_T) to affect the liquid holdup in the reboiler. This is good for control as it means that the initial ("high-frequency") response is decoupled. That is, there is a delay which could be of an advantage for sufficiently fast control to accommodate the changes in top product flow rate. It will help avoid some of the strong interactions that exist between the control of compositions at the top and bottom of the column. [9]

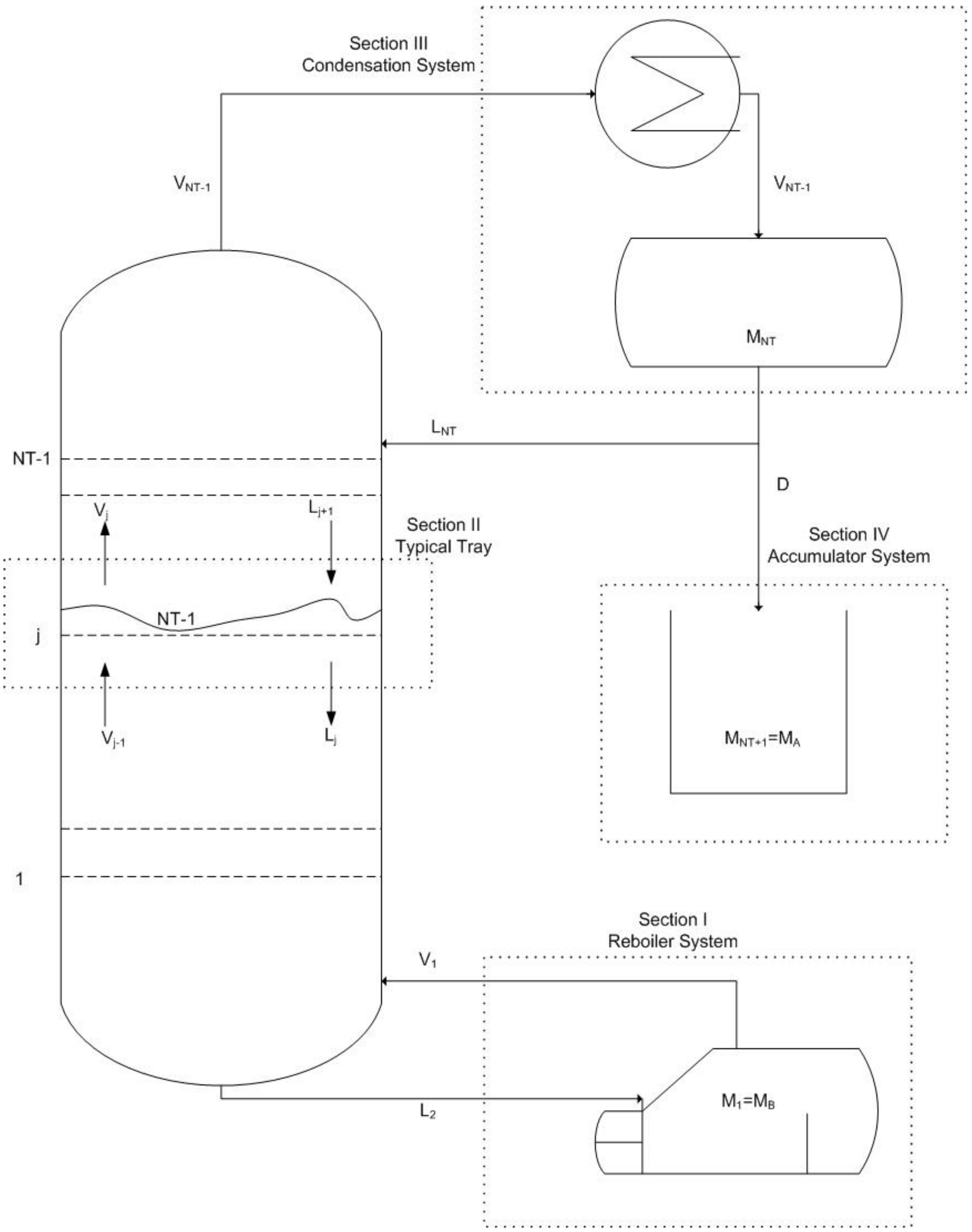

Fig. 1. Batch distillation model sections

The vapour flow into the stage may also affect the liquid holdup as given by the parameter λ (sometimes denoted the K_2-effect). A positive value of λ may result if there increase in vapour flow giving more bubbles and thus pushes the liquid off the stage. For packed columns λ is usually close to zero. In this paper λ is considered to be zero [5].

Reboiler, Section I (Fig. 1.1)**,** j=1

$$M_j = M_B \qquad (7)$$

$$V_j = V_B = V \qquad (8)$$

$$d(M_j)/dt = L_{j+1} - V_j \qquad (9)$$

$d(M_j\,x_j)/dt = L_{j+1}\,x_{j+1} - V_j\,y_j$ (10)

Total Condenser-Drum, Section III (Fig. 1.1)**,** j=NT

$M_{NT} = M_D$ (11)

$L_{NT} = L_T$ (12)

$d(M_j)/dt = 0$ (13)

$V_{j-1} = L_j + D$ (14)

$d(M_j\,x_j)/dt = V_{j-1}y_{j-1} - L_j\,x_j - Dx_j$ (15)

Accumulator Tank, Section IV (Fig. 1.1)**,** j=NT+1

$x_{NT+1} = x_{NT}$ (16)

$d(M_j)/dt = D$ (17)

$d(M_j\,x_j)/dt = Dx_j$ (18)

3. SIMULATION

The model is solved using the ordinary differential equations solver function ODE15s, it was selected according to the recommendations in **Table 1** [10]:

`ode15s` is a variable order solver based on the numerical differentiation formulas (NDFs). It uses the backward differentiation formulas (BDFs, also known as Gear's method) that are usually less efficient. Like ode113, ode15s is a multistep solver [11].

`ode45` was first tried to solve the model but it has appeared to be relatively slow and the problem is suspected to be stiff (it also contains differential-algebraic equations). Instead `ode15s` is used, [12].

3.1 Results

The batch distillation columns model was simulated with the following nominal data as shown in **Table 2.**

Table 1. List of MATLAB solver functions

Solver	**Problem Type**	**Order of Accuracy**	**Usage**
`Ode45`	Nonstiff	Medium	Most of the time. This should be the first solver you try.
`Ode23`	Nonstiff	Low	If using crude error tolerances or solving moderately stiff problems.
`Ode113`	Nonstiff	Low to high	If using stringent error tolerances or solving a computationally intensive ODE file.
`Ode15s`	Stiff	Low to medium	If `ode45` is slow because the problem is stiff.
`Ode23s`	Stiff	Low	If using crude error tolerances to solve stiff systems and the mass matrix is constant.
`Ode23t`	Moderately Stiff	Low	If the problem is only moderately stiff and you need a solution without numerical damping.
`Ode23tb`	Stiff	Low	If using crude error tolerances to solve stiff systems.

Table 2. Column nominal data

Property	**Value**	**Units**
Number of Stages (NT)	15+1	
Initial Reboiler Charge	100	Kmol
Initial Charge Composition z_F	0.50	mole fraction
Reboiler charge liquid fraction q_F	1.00	
Reflux Ratio (Internal 0<R<1)	0.9	
Boilup V	10	kmol/min
Distillate flow D	1.00	kmol/min
Reflux flow LT	9.00	kmol/min
Initial trays liquid holdup is M_j	0.50	Kmol
Initial Condenser-Drum liquid holdup is M_{NT}	10.00	Kmol
Initial Accumulator liquid holdup is M_A	$0.001 \approx 0.0$	Kmol
Time constant for the liquid flow dynamics τ, [9]	0.063	Min
Effect of vapour flow on liquid holdup, λ	0.00	-

The model is capable of producing values for composition and holdup in all stages of simulated column. The main results are the final products composition as well as the holdup in the reboiler and the accumulation tanks (see **Figs 1-4)**. The column is set to operate for 50 minutes. This results in a distillate amount M_A= 50 [kmol] in the accumulator with composition y_D = x_{NT} = 0.96 [mole fraction units], and a bottoms product M_B = 50 [kmol] in the reboiler with composition x_B = x_1 = 0.01 [mole fraction units]. These results are shown graphically in **Figs1-4**

Fig. 1 illustrates a steady increase in the accumulator holdup to 50 kmol. This was obtained because of the steady flow of the distillate *D* into the accumulator at 1.00 kmol/min for the operation time of 50 minutes. It also means that all light components are removed from the reboiler ($M_B = 100$, $z_{F,light} = 0.5$). **Fig. 2** shows the overhead products compositions. As it can be seen the distillation was allowed to continue until its composition falls to 0.82, because the distillate composition had become very pure after the first 10 minutes exceeding our products specification. It was allowed to drop until the final accumulator composition reaches its desired value of 0.960 as shown in the accumulator composition curve. **Fig. 3** shows the reboiler holdup decreases to 44.90 kmol. A sharp decrease was experienced during the first five minutes due to column trays being filled up. This is reflected in the purification of the reboiler inventory (**Fig. 4**) resulting in an increase in the reboiler heavy component composition (0.990).

4. SELF-OPTIMISING CONTROL, APPLICATION TO BATCH DISTILLATION

4.1 Degree of Freedom Analysis

The batch distillation column (see **Fig. 1**) has 5 degrees of freedom for optimisation. The reboiler charge M_B, boilup *V*, distillate flow *D* into accumulator, reflux flow *LT*. The condenser drum level has to be controlled as well. With the initial reboiler charge given, the reflux flow *LT* is automatically adjusted when controlling the distillate *D* and the boilup *V*, leaving 2 degrees of freedom for optimisation, which may be selected as the boilup and the distillate flow (not unique).

4.2 Objective Function and Constraints

Ideally, the optimal operation of the column should follow the overall economics of the plant. To be able to analyze the column separately, however, prices are introduced for all streams/products as well as any energy usage. Consider the following profit function *P* which should be maximized,

$$Profit\ (P) = P_D D + P_B B - P_V V \qquad (19)$$

The objective is to maximise profit ($P = -J$) and thus minimise *J*

The following nominal prices are used (£/kmol)

$p_D = 20, p_B = 15, \ p_V = 0.5$

The price p_V =*0.5 £/kmol* includes the cost for heating and cooling which both increase proportionally with the boilup *V*. The price for reboiler initial charge p_{MB} = 10 £/kmol. Although, this value has no significance for the optimal operation in the case with a given initial charge M_B.

The distillate product is assumed to be the more valuable product with a selling price of 20 £/kmol, and its purity specification is assumed to be

$$x_A \geq 0.960 \qquad (20)$$

Batch operation time of 50 minutes is used for the purpose of this study in order to correctly evaluate the effects of various disturbances. In fact it would be more realistic to work with a minimum amount of products.

4.3 Disturbances

d_1 : An increase in initial reboiler charge composition $(zf)_1$ from 0.50 to 0.65 for the light component.
d_2 : A decrease in initial reboiler charge composition $(zf)_1$ from 0.50 to 0.45 for the light component.
d_{ec} : An increase in the required purity of the distillate product x_A from 0.960 to 0.970

4.4 Optimisation

Extensive simulation studies are performed instead of optimisation. This is mainly due to the fact that the dynamic model and the objective function result in a dynamic optimisation problem. These problems are challenging to solve using conventional optimisation techniques due to the high non-convexity and complex search space topography nature of these problems. However, there is much ongoing research on developing robust and practical solution algorithms [18]. The simulation studies have resulted in what is believed to be approximately the optimal operating points (sufficient for the purpose of this study) for the three disturbances given in the **Table 3**.

Table 3. Optimal operating points

	x_A	$1-x_B$	R_{in}	LT kmol/min	V kmol/min	D kmol/min	Time min	M_A kmol	M_B kmol	- J (£)
Nominal*	0.960	0.990	0.90	9.00	10.00	1.00	50	50.00	44.90	1423.50
$z_{F,light} = 0.65$	0.960	0.996	0.86	6.14	7.14	1.00	50	50.00	48.00	1541.50
$z_{F,light} = 0.45$	0.960	0.990	0.92	8.28	9.00	0.72	50	36.00	61.00	1395.00
$x_A = 0.970$	0.970	0.820	0.95	9.50	10.00	0.50	50	25.00	69.43	1291.45

* Nominal values, $MB_{initial}$ = 100, $z_{F,light}$ = 0.50, p_D = 20, p_B = 15, p_V = 0.50

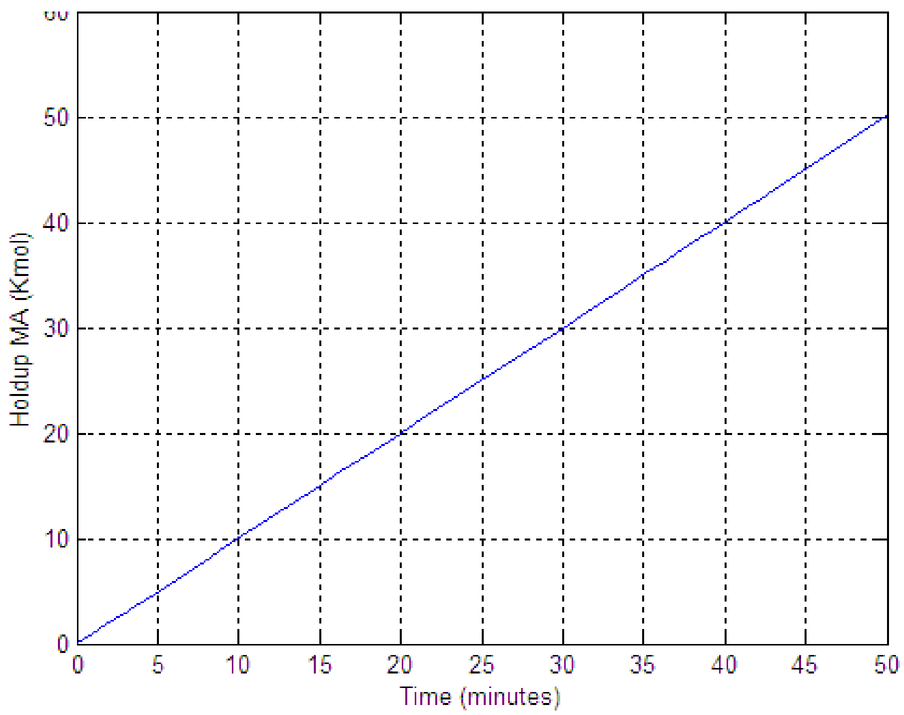

Fig. 1 Accumaltor Holdup (MA [Kmol]) vs Time

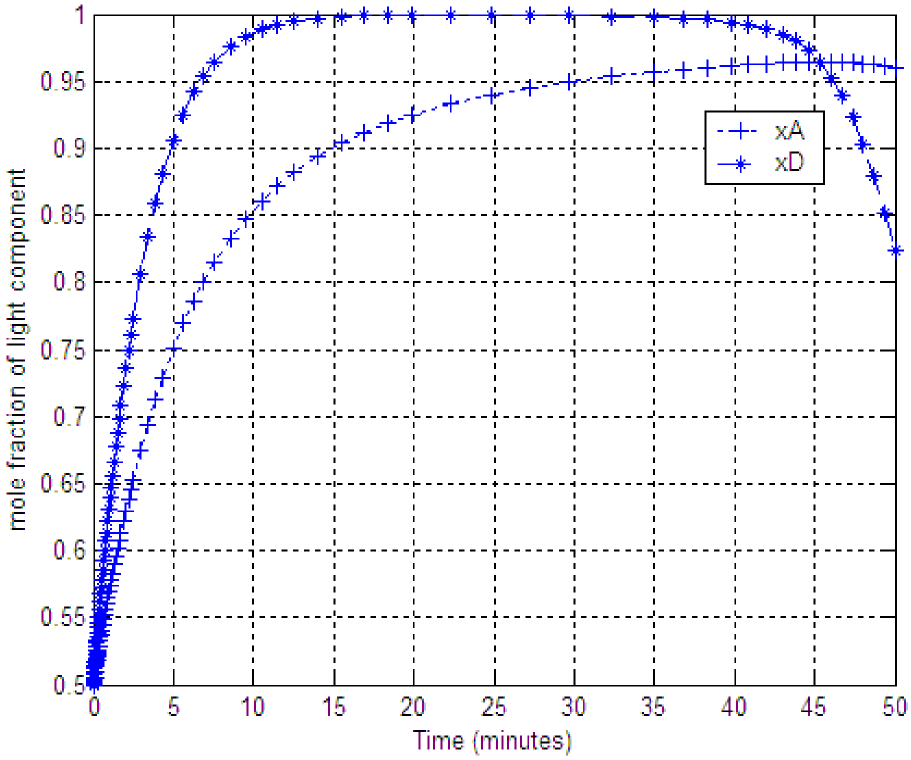

Fig. 2. Overhead product composition (xD, xA) vs Time

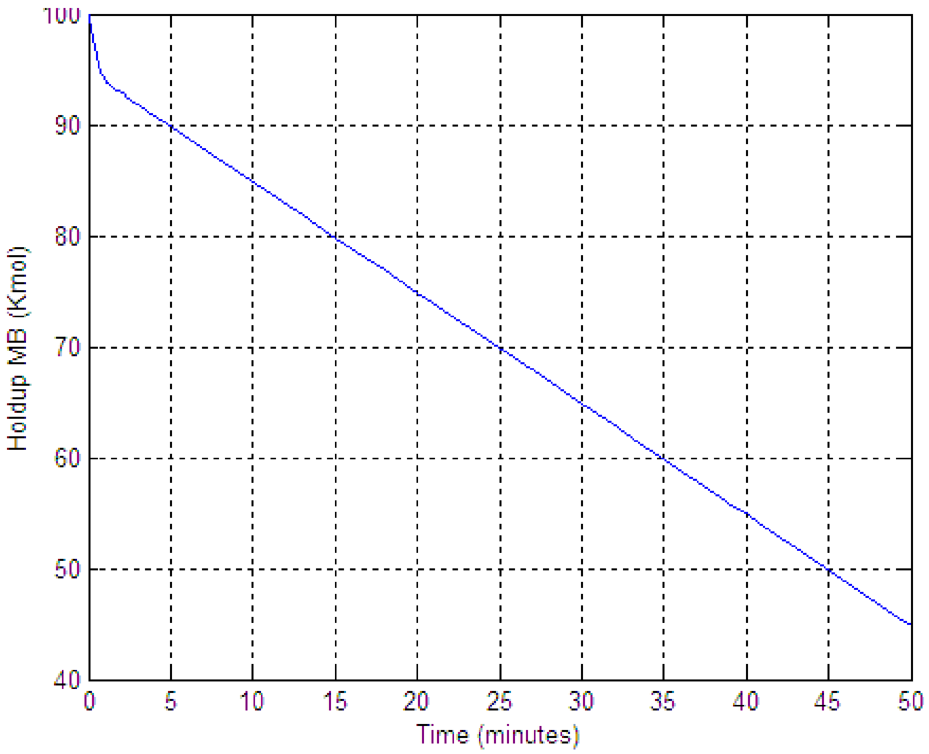

Fig. 3 Reboiler Holdup (MA [Kmol]) vs Time

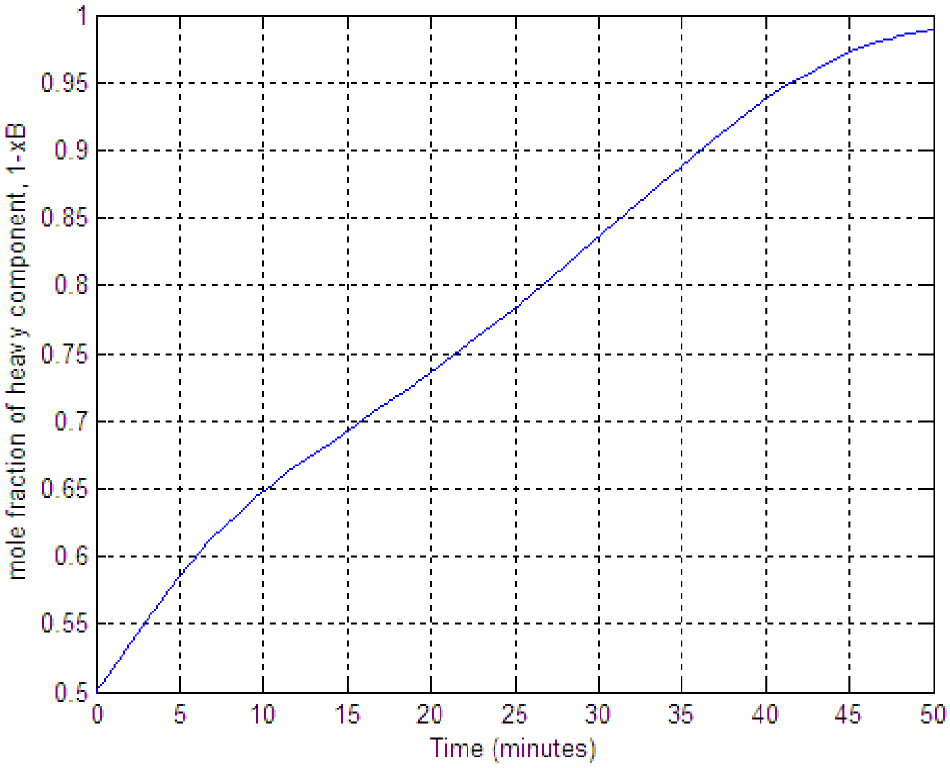

Fig. 4. Reboiler composition (1-xB), vs Time

Table 4. Loss £/min for the batch distillation column

	$x_B = 0.990$	R_{in} =0.9	L = 9.0 kmol/min	V = 10 kmol/min	D = 1.0 kmol/min
Nominal*	0	0	0	0	0
$z_{F,light}$ = 0.65	0.38	**1.76**	**5.5**	0.28	0
$z_{F,light}$ = 0.45	0	Inf.	**5.32**	0.5	0.90
x_A = 0.970	inf.	Inf.	**4.47**	0	**4.88**
+10 % implementation error	0	**4.74**	0.26	0.26	0.26
Rank	**3**	**5**	**4**	**1**	**2**

Table 5. Loss evaluation for constant reflux ratio example

	x_A	**1-x_B**	**R_{in}**	**LT kmol/min**	**V kmol/min**	**D kmol/min**	**Time min**	**Acc kmol**	**Boiler**	**- J (£)**
$z_{F,light}$ = 0.65	0.960	0.999	0.90	6.43	7.14	0.71	50	35.50	61.48	1453.70

4.5 Candidate Control Variables

The distillate composition at the accumulator x_A should be selected as a controlled variable as it is always optimal to have it meeting its constraint.

Only one unconstrained degree of freedom is now available, which we want to specify by keeping the set point of a controlled variable at a constant value. From **Table 4** it could be seen that the optimal purity of the bottom product stays fairly constant except in the last case when the required purity of the top product has changed. This indicates a good strategy for implementation to control x_B. However, there are at least two practical problems associated with this choice. First, on-line composition measurements are often unreliable and expensive. Second, dynamic performance may be poor because it is generally difficult to control both products composition ("dual" control) due to strong interactions. Thus; if possible other variable is preferred to control [5].

The following five controlled variables are considered:
x_B; R; L_T; V; D

4.6 Loss Evaluation

In **Table 4**, calculation of the loss in £/min is calculated for all of the variables to be controlled, an implementation error of 10% is also considered.

Example
Loss = $P_{opt} - P$

For the case of an increase in feed composition to 0.65, fixing the internal reflux ratio (R) at a value of 0.9 rather than its optimal value in this case of 0.86 has resulted in the following data.
Therefore, the loss $= P_{opt} - P$
$= (1541.50-1453.70)/50 = 1.76$ £/min

As expected, the losses are found to be small when x_B is kept constant, except in the case of overpurification of the top product. Keeping the boilup V constant has resulted in the least overall losses. This indicates a good strategy for self-optimising control. Furthermore, keeping the distillate flow D has resulted in the second least overall losses, and hence provides good alternative to the control of the boilup.

Control of the internal reflux ratio or the reflux flow is not suitable for self-optimising control as a relatively large loss will result. The acceptable level of loss is desired not to exceed 1 £/min, equivalent to £50 for this particular simulation. Unacceptable losses are shown in bold in **Table 4**.

For overpurification in x_D where x_D is 0.97 rather than 0.96, all of the alternatives gave an unacceptable loss of about 4-5 £/min except in the case of boilup control. From this it could therefore be concluded that x_D should be controlled close to its specification.

4.7 Selection of Controlled Variables

From **Table 5** the following three candidate sets of controlled variables yield the lowest losses

$$C_1 = \begin{pmatrix} V \\ x_D \end{pmatrix}; \qquad C_2 = \begin{pmatrix} D \\ x_D \end{pmatrix}; \qquad C_3 = \begin{pmatrix} x_B \\ x_D \end{pmatrix}$$

As previously shown "dual" control structure C_3 where both compositions are controlled, result in a difficult control problem. The loss will then be larger than indicated. Therefore it is probably better to keep V or D constant.

Since it is usually simpler to keep a liquid flow D rather than a vapour flow V constant (less implementation error), the following control structure is proposed.

D = 1.0 [kmol/min] is kept constant
V is used to keep $x_A = 0.960$

Alternative control system

V = 10.0 [kmol/min] is kept constant
D is used to keep $x_A = 0.960$

4.8 Summary of Results

This section discussed the concept of self optimising control and its application to batch distillation columns. It was found that the distillate and the boilup flows have good self-optimising properties, whereas the reflux ratio and the reflux flow do not.

5. DISCUSSION

The dynamic process model used to simulate batch distillation columns resulted in the presentation of products purity, the amount accumulated in the reboiler, and the accumulation tank. Stages temperature as well as reboiler and condenser energy requirements may be added for a more rigorous modelling.

In the self-optimisation procedure only the operational effects of the system has been considered. That is, the control structure proposed is based on the operational economics when the column is on normal operation (no shut-down or start-up). In addition, the dynamic effects of the control structure have not been considered in detail.

With the suggested control structure, an increase in reflux flowrate will first give an increase in the concentration of light component. But as the reflux reaches the bottom part of the column, the level increases and thus boilup increases. As a result, there will be more of the heavy component going up the column and the light component concentration will therefore decrease. Hence, the dynamic effects of the selected control structure should be taken into account and considered in future work.

5. CONCLUSIONS

A model to simulate the dynamics of batch distillation columns was created using MATLAB 6.0. Skogestad's [5] method of self-optimising control has been applied to a batch distillation column case. It was found that overhead product purity should be controlled at its constraints. This left one unconstrained degree of freedom for which the choice of a suitable controlled variable was not obvious. It was found that selecting the distillate flow rate D into the accumulator has good self-optimising properties. The selection of the boilup flow V has also presented a good alternative with the possibility of more difficult control of vapour (V) rather than liquid (D). It has also been shown that certain variables were very sensitive to disturbances and might have multiplicities in the objective function. Therefore, they were not suitable for self-optimising control.

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NOMENCLATURE

c	Controlled variables
D	Distillate flow rate [kmol/min]
e_c	Setpoint error
J	Scalar cost function to be minimised
$J_{opt}(d)$	Minimum value for *J* [£]
L	Liquid flow from stage [kmol/min]
LT	Reflux flow [kmol/min]
M	Liquid holdup [kmol]
m	Manipulated variables (degree of freedom for control)
N = NT	Number of trays
n	Noise on measurements for control
N_0	Number of variables with no effect on *J*
N_m	Number of degrees of freedom for control
$N_{opt} = N_u = N_c$	Number of degrees of freedom for optimisation
P	Profit [£]
p	Price [£/kmol]
Q	Heating/Cooling duty [kw]
q	Fraction of liquid in reboiler charge
R	Reflux ratio
t	Time [min]
u	Base set for the N_u optimisation degrees of freedom
V	Vapour flow from stage [kmol/min]
VB	Boilup flow [kmol/min]
x	Vapour composition of light component (light component) [mole fraction]
y	Liquid composition of light component (light component) [mole fraction]
Zf	Initial composition of the boiler charge (light component) [mole fraction]
Greek	
α	Relative volatility
ρ	Density [kg/m^3]
λ	Constant for effect of vapour flow on liquid flow
τ	Time constant for liquid flow dynamics on stages [min]
Subscript	
A	Accumulator
B	Bottom/Reboiler
D	Distillate
i	Component i
in	Internal
j	Stage j
l	Liquid
Light	Light component
s	Set point
V	Vapour, boilup