

NEURAL NETWORK BASED MODELLING AND OPTIMISATION IN BATCH REACTIVE DISTILLATION

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In this work rigorous dynamic model of batch reactive distillation is replaced by a neural network based model which can predict the column dynamics very well in few CPU seconds. Also a neural network based optimisation framework is developed. A simple esterification reaction system is used in the batch reactive distillation column to demonstrate the ideas. The proposed tool can forecast profitability, productivity, batch time, energy cost and can give optimal operating policy in few CPU seconds for changing product specifications, raw material and energy costs and products prices, which is highly needed in this new era of fast changing market environment.

KEYWORDS: neural network, modelling, dynamic optimisation, batch reactive distillation

INTRODUCTION

During the last decade considerable interest has been generated in new hybrid processes carrying out reaction and separation simultaneously in one single operation. These new processes, called reactive separation processes, combine the benefits of traditional unit operations with a substantial progress in reducing capital and operating costs and environmental impact (BP Review, 1997). While Wilson (1987) considered design and operation of batch reactive distillation, Doherty and Buzad looked at similar issues for continuous reactive distillation. Taylor and Krishna (2000) provided a comprehensive review of research in both batch and continuous reactive distillation. Sorensen and Skogestad (1994) developed control strategies for batch reactive distillation.

This work focuses on batch reactive distillation which is inherently a dynamic process. In a competitive environment where the prices of raw materials, products, energy and utility and product specifications (as dictated by the customers) change frequently, the business decision in the area of batch reactive distillation has to be based on a number of key interdependent factors. These are conversion of reactants to main products, amount of unwanted or environmentally damaging side products and associated recovery and disposal cost, raw material and energy cost, product quality and prices, batch size, batch time, productivity, etc. An optimum combination of all these factors will lead to a desired objective of the business which is often the maximisation of

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profit. A *maximum profit* problem can be formulated as follows:

$$\begin{array}{lll}
 \mathbf{PI} & \text{Max} & P \\
 & t_f, C, r(t), D_1 & \\
 \text{subject to:} & \text{product purity constraints} & \\
 & \text{DAE model equations etc.} &
 \end{array}$$

Mujtaba and Macchietto (1997) defined a typical profit function P for batch reactive distillation as:

$$P = \frac{C_{D1}D_1 - C_{B0}B_0 - C_h Q_R}{t} \quad (1)$$

where D_1 is the amount of desired product (kmol), B_0 is the amount of raw material (kmol), Q_R is the total heat input (kJ), t is the batch time (hr), C_{D1} is the product price (\$/kmol), C_{B0} (\$/kmol) is the raw materials cost and C_h (\$/kJ) is the energy cost for heating (operating cost).

Using the above profit function, the solution of problem \mathbf{PI} will automatically determine the optimum batch time (t_f), conversion (C), reflux ratio (r) and the amount of product (D_1). However, as the cost parameters (C_{D1} , C_{B0} , etc.) and product purity can change from time to time, it will require a new solution of the dynamic optimisation problem \mathbf{PI} (as outlined in Kerkhof and Vissers, 1978), to give the optimal amount of product, optimal batch time and optimal reflux ratio. And this is computationally expensive. To overcome this problem Mujtaba and Macchietto (1997) calculated the profit of the operation using the results of a *maximum conversion* problem which were obtained independent of the cost parameters.

In the past, dynamic optimisation framework using rigorous models (Albet et al., 1991; Mujtaba and Macchietto, 1997) have been developed to obtain optimal operating policies that will minimise time, maximise conversion, maximise profit, etc. All these approaches require excessive computation time (in the case of dynamic optimisation). However Mujtaba and Macchietto (1997), after solving a series of cost independent *maximum conversion* problem for different batch times, used polynomial curve fitting techniques to develop time dependent maximum conversion, optimal distillate, reflux ratio and energy usage profiles for two different product purities.

These were:

$$(a) \text{ Maximum Conversion: } C = g_1(t) \quad (2)$$

$$(b) \text{ Optimum Amount of Distillate (kmol): } D_1 = g_2(t) \quad (3)$$

$$(c) \text{ Optimum Reflux Ratio: } r = g_3(t) \quad (4)$$

$$(d) \text{ Total Reboiler Heat Load (KJ): } Q_R = g_4(t) \quad (5)$$

where, $g_1(t)$, $g_2(t)$, etc. are polynomial functions. The profit function (equation 1) now simplifies to:

$$P = \frac{C_{D1}g_2(t) - C_{B0}B_0 - C_h g_4(t)}{t} \quad (6)$$

which is a function of only one variable (t) for a given set of values of (C_{D1} , C_{B0} , C_h). The dynamic optimisation problem would now become a single variable algebraic optimisation and the solution of the problem does no longer require full integration of the dynamic model equations.

FREQUENTLY CHANGING MARKET PRICES

For a fixed product specification but under frequently changing market prices of (C_{D1} , C_{B0} , C_h) the method will solve the *maximum profit* problem very cheaply and will thus determine new optimum batch time for the plant. The functions represented by equations (2–5) can then be used to determine optimal values of C , D_1 , r , Q_R , etc. Note the profit maximisation using the results of *maximum conversion* problem via the polynomial functions does not require solution of the dynamic *maximum profit* optimisation problem, every time the market prices change.

FREQUENTLY CHANGING PRODUCT SPECIFICATIONS

For every product specification, a series of dynamic *maximum conversion* optimisation problem will have to be solved to obtain the functions (2–5).

In recent years neural network techniques have been found to be computationally less expensive in dynamic modelling and optimisation (Greaves et al., 2003). In this work rigorous dynamic model of batch reactive distillation is replaced by a neural network based model which can predict the column dynamics very well in few CPU seconds. Also a neural network based optimisation framework is developed. A simple esterification reaction system is used in the batch reactive distillation column to demonstrate the ideas. The proposed tool can forecast profitability, productivity, batch time, energy cost and can give optimal operating policy in few CPU seconds for changing product specifications, raw material and energy costs and products prices, which is highly needed in this new era of fast changing market environment.

THE BATCH REACTIVE DISTILLATION PROCESS

Let us assume that Ethyl Acetate (lowest boiling component) is to be produced at a specified purity (x_D^*) using the reversible esterification reaction: **Acetic Acid + Ethanol \rightleftharpoons Ethyl Acetate + Water** in a batch distillation column. The problem is defined by the data in Table 1. The kinetic and thermodynamic models are given in Mujtaba and Macchietto (1997).

Table 1. Input data for ethanol esterification using batch distillation column

No. of ideal separation stages = 10,	Total fresh feed, B_0 (kmol) = 5
Feed composition (acetic acid, ethanol, ethyl acetate, water) x_{B0} (mole fraction) = 0.45, 0.45, 0.0, 0.1	
Column holdup (kmol): Condenser = 0.1,	Internal Plates = 0.0125
Condenser vapour load (kmol) = 2.5,	Column pressure (bar) = 1.013

NEURAL NETWORK BASED DYNAMIC MODEL AND OPTIMISATION

For a given set of inputs, Neural Networks (NNs) are able to produce a corresponding set of outputs according to some mapping relationship. This relationship is encoded into the network structure during a period of training (also called learning), and is dependant upon the parameters of the network, i.e. weights and biases. Once the network has been trained (on the basis of known sets of input/output data), the input/output mapping is produced in a time that is orders of magnitude lower than the time needed for rigorous deterministic modelling. Therefore, the resulting NN model is particularly suited for optimisation studies (Greaves et al., 2003).

Most recently Greaves et al. (2003) has developed NN based dynamic process model and optimisation framework for batch distillation column with middle vessel. The model was validated using experimental pilot plant data. The NN based *maximum profit* optimisation was at least 10 times faster compared to rigorous model based optimisation. In this work we use NN based optimisation framework of Greaves et al. in batch reactive distillation producing ethyl acetate by esterification of ethanol and acetic acid. Also here, the profit maximisation is done using the results of *maximum conversion* problem and the NN based functions (2–4) instead of a polynomial based functions. This greatly reduces the computation time compared to that by existing tool (Mujtaba and Macchietto, 1997).

THE MAXIMUM CONVERSION PROBLEM

The *maximum conversion* optimisation problem (**P2**) can be written as:

$$\begin{array}{ll}
 \mathbf{P2} & \begin{array}{ll} \text{Max} & \\ r(t) & \end{array} \\
 & C \\
 \text{subject to} & t = t_f^* \\
 & x_D(t_f) \geq X_D^* \quad (\text{inequality constraint}) \\
 \text{and} & f(t, \dot{x}, x, u, v) = 0 \quad (\text{model equation, equality constraints}) \\
 \text{with} & f(t_0, \dot{x}_0, x_0, u, v) = 0 \quad (\text{initial conditions, equality constraints}) \\
 & \text{Linear bounds on reflux ratio} \quad (\text{inequality constraints})
 \end{array}$$

where $x_D(t_f)$ is the composition of distillate at the end of the operation (t_f). In this work the number of specified purities are extended from two (as used by Mujtaba and Macchietto,

1997) to five using $x_D^* = [0.6, 0.7, 0.75, 0.8, 0.85]$ to cover a wider product range within 5 to 30 hrs of batch time operation. For each product purity the optimal profiles (C , D_1 , R_f and Q_R) are generated by solving the full dynamic optimisation problem (P2). These results are used to develop NN based dynamic models for maximum conversion, maximum distillate, and optimal reflux ratio and energy consumption.

NN BASED MODEL

The input/output specification for the NN based dynamic model is shown in Figure 1a. A multi-layered feed forward network is used which is trained with the back propagation method using a momentum term as well as an adaptive learning rate to speed up the rate of convergence, as found in the Mathworks MATLAB Neural Network toolbox. The error between the actual variable value (obtained from DAE Model) and that predicted by the network is used as the error signal to train the network (Greaves et al, 2003).

As can be seen (Figure 1a) the prediction at any time t is only dependent on Z_0 and not any other value of Z . Three data sets were used to train and validate the neural networks, two for training and one for validation. The data sets were made up from the following data for each network:

Training Set 1 – $x_D^* = [0.6, 0.7, 0.8, 0.85]$ for each NN (C , D_1 , R_f , Q_R)

Training Set 2 – $x_D^* = [0.85, 0.7, 0.6, 0.8]$ for each NN (C , D_1 , R_f , Q_R)

Validation Set – $x_D^* = [0.75]$ for each NN (C , D_1 , R_f , Q_R)

A sample data set for $x_D^* = 0.6$ is shown in Figure 1b for all the NNs. During training and validation only the values corresponding to the NN (C , D_1 , R_f , Q_R) under investigation are used as the set points for the error signal. The final configuration of each of the NNs can be seen in Table 2 as well as the final errors associated with Training and Validation.

(a)		(b)					
		x_D^*	tf (hr)	Neural Networks Setpoints (Z)			
NN Inputs	NN Output	Q_R (kJ/hr)	D_1 (kmol)	R_f	C		
x_D^*, t_1	Z_1	0.6	5.0	4.61	1.180	0.9056	0.540
x_D^*, t_2	Z_2	0.6	7.5	6.93	1.968	0.8950	0.611
	.	0.6	10.0	9.25	2.348	0.9061	0.659
	.	0.6	12.5	11.55	2.562	0.9180	0.693
x_D^*, t_i	Z_i	0.6	15.0	13.86	2.698	0.9280	0.719
	.	0.6	17.5	16.16	2.795	0.9361	0.739
	.	0.6	20.0	18.46	2.866	0.9427	0.755
$Z_1 = \{C, D_1, R_f, Q_R\}_{t=t_1}$		0.6	22.5	20.76	2.920	0.9481	0.768
$Z_i = \{C, D_1, R_f, Q_R\}_{t=t_i}$		0.6	25.0	23.06	2.966	0.9525	0.778
		0.6	27.5	25.36	3.003	0.9563	0.787
		0.6	30.0	27.65	3.034	0.9595	0.794

Figure 1. (a) Input and output specifications for each ANN; (b) A sample data set member for $x_D^* = 0.6$

Table 2. Neural network configurations and final errors

NN	Layer Transfer Functions		No. of Hidden Layer Nodes	Errors	
	Hidden	Output		Training	Validation
C	logsig	tansig	6	5.54E-07	2.24E-06
D ₁	logsig	satlin	4	7.26E-04	2.53E-05
R _f	tansig	purelin	6	1.95E-06	2.12E-04
Q _R	logsig	poslin	6	2.26E-08	1.29E-07

NN BASED OPTIMISATION

Functions g 's in the profit function (equation 6) can now be replaced with the NN based models for C, D₁, R_f and Q_R and the optimisation problem **PI** can be solved for different cost parameters. The only parameter to be optimised reduces to just batch time.

CASE STUDY

For the esterification process described in section 2, comparison between the predictions of C, D₁, R_f and Q_R obtained by using rigorous dynamic model and those obtained using NN based model are shown in Figure 2 (note, Ha = D₁) for two product specifications (one used for training and the other used for validation). The results clearly show that NN based models predict the dynamics of the column very well for both product specifications. From *Chemical Market Reporter, January 2001* the price for 99% (mole fraction) pure ethyl acetate was found to be 2335 \$/kmol and it seemed a fair assumption that for 85% (mole fraction) pure ethyl acetate a price of 500 \$/kmol was reasonable. The prices for ethyl acetate with other purity values assuming an exponential trend are as follows:

x_D^*	0.60	0.70	0.75	0.80	0.85
Price (\$/kmol)	32	96	166	289	500

Table 3 shows the optimum values of batch time (t_f), amount of product (D₁), total heat load (Q_R), maximum conversion (C) and reflux ratio (R_f) for each product purity specification to achieve the maximum attainable profit for the operation. Table 3 shows that for all the purity specifications the operation will make a profit except when the purity $x_D^* = 0.6$. This makes sense, as it is more profitable to make a higher priced product than a lower priced product and it is cheap to dilute a product than it is to concentrate a product in practical terms. It is important to note here that once trained the NN based model can generate optimal C, D₁, R_f, Q_R profiles for any specified purity between $x_D^* = [0.6, 0.85]$ in

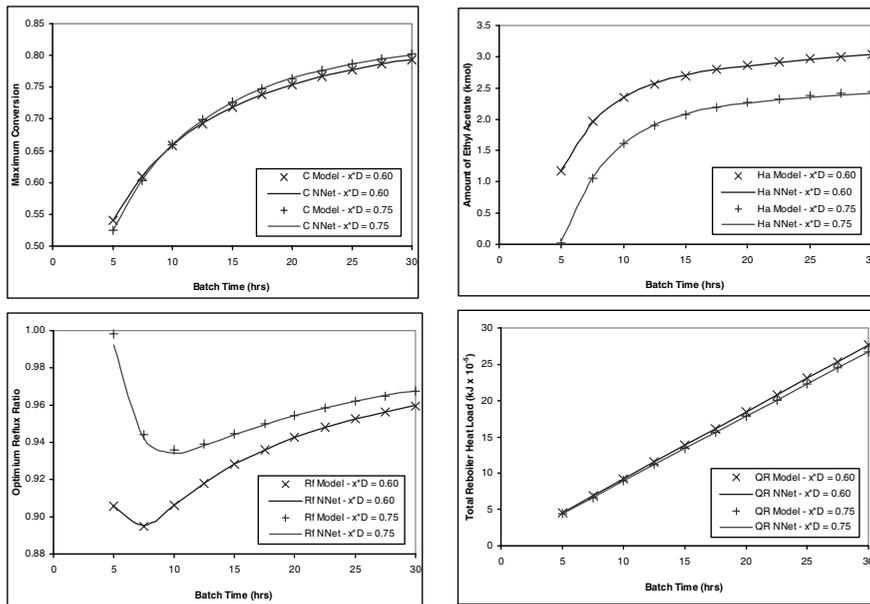


Figure 2. Comparison between the dynamic rigorous model based and the NN based results

under a second. However, the method proposed by Mujtba and Macchietto (1997) would require the solution of full dynamic optimisation problem to generate optimal C , D_1 , R_f , Q_R profiles for any specified purity between $x^*_D = [0.6, 0.85]$ and this would be computationally expensive (as mentioned earlier). This is the major strength of this work. A typical solution of the optimisation problem using rigorous dynamic model approximately required 600 CPU sec in a SPARC-1 Workstation and about 120 CPU sec in a NN Inputs NN Output SPARC-10 Workstation. On the other hand, the solution with NN based model took 10–12 CPU sec using SPARC-10 Workstation.

Table 3. Optimum operation information with single reflux interval

x^*_D	Product Price, \$/kmol	t_f (hr)	Profit (\$/hr)	D_1 (kmol)	Q_R (kJ/hr)	C	R_f
0.6	32	30.00	-0.79	3.043	27.65	0.794	0.960
0.7	96	12.28	7.20	2.127	11.12	0.700	0.931
0.8	166	13.81	26.87	1.686	12.21	0.699	0.951
0.85	500	18.03	35.81	1.526	15.72	0.706	0.966

Table 4. Optimum operation information with two reflux intervals

x_D^*	t_f (hr)	Profit (\$/hr)	D_1 (kmol)	Q_R (kJ/hr)	C	R_f (1)	R_f (2)	%Improvement	
								t_f	Profit
0.6	30.00	-0.78	3.052	27.49	0.795	0.964	0.961	0.00	1.51
0.7	11.58	7.34	2.090	10.46	0.696	0.954	0.904	-5.70	2.01
0.8	9.83	30.03	1.419	8.75	0.658	0.979	0.903	-28.85	11.77
0.85	9.72	46.74	1.139	8.56	0.644	0.993	0.911	-46.07	30.51

MULTIPLE REFLUX RATIO OPERATION

Mujtaba and Macchietto (1997) and the work presented above only presented a study of single interval reflux ratio operation, however it is common practice in industry to use more than one reflux interval to allow higher recovery of the desired product in the shortest period of batch time (Farhat et al., 1990). This strategy also allows production of high purity product. As the distillation progresses the purity of the product decreases with time for a fixed reflux and therefore it is desirable to increase the reflux to maintain the purity. In this work the single reflux interval NN based optimisation framework is extended to a two reflux interval strategy of operation to see if the results obtained could be improved upon.

The dynamic optimisation problem was resolved for all the purity specifications presented above but with two reflux intervals, the first interval was from time $t = [0, t_f/2]$ and the second interval was from $t = [t_f/2, t_f]$. Table 4 shows the optimum values of batch time (t_f), amount of product (D_1), total heat load (Q_R), maximum conversion (C) and reflux ratio (R_f) for each purity specification to achieve the maximum attainable profit for the operation for two reflux ratio intervals.

Table 4 shows that for all the purity specifications the operation will make a profit except when the purity $x_D^* = 0.6$. This observation is the same as for one reflux ratio interval operation showing that it is not profitable to produce such low purity product. Table 4 shows that there is a distinct advantage, in terms of profit and batch time, to run using more than one reflux ratio interval. Apart from purity specification $x_D^* = 0.6$, the optimal batch time was reduced from 5.7% to up to 46%. This has a knock on effect to the profitability of the operation and the profit is improved for all purity specifications from 1.5% to 30.5%.

CONCLUSIONS

The solution of dynamic optimisation problems using a detailed model is computationally expensive, as they require many solutions of the detailed model. In this work a NN based dynamic optimisation framework has been developed for batch reactive distillation using very little computational effort. The method requires the solution of the dynamic optimisation problems (*maximum conversion problems* for example), independent of cost

functions, parametrically for different batch times and purities to generate a region of feasibility to study. The optimal product yield, optimal heat load, optimal maximum conversion and optimal reflux ratio profiles are predicted using NN techniques that are only dependent on purity and batch time inputs. Using these NNs it is possible to formulate the *maximum profit problem* for any cost functions, thus making the solution of the problem very easy and removing the need for full solution of the dynamic optimisation problem as presented by Mujtaba and Macchietto (1997). This reduces the computational time down from minutes to under a second. Also the NNs, once trained and validated, are able to predict other purity specifications within the valid range ($x_D^* = [0.6, 0.85]$, $t_f = [5, 30]$ hrs) instead of one purity specification at a time (Mujtaba and Macchietto, 1997). However it must be stressed that the NNs are unable to accurately predict (with confidence) results outside of the feasible region.

The framework developed can be applied to other batch processes, with or without chemical reaction, as long as the data used to train and validate the neural networks is accurate enough to provide the required degree of confidence.

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