EFFICIENT MODEL IDENTIFICATION THROUGH SENSOR LOCATION IN BATCH DISTILLATION

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Abstract: Prime areas in model based process control are process identification and optimization. This paper presents their linkage for a binary batch distillation pilot plant using minimum experimental data which is necessary in practice if the batch column is to be used as a multiproduct unit. Here, minimum experimental data from plant runs is used to determine the model parameters with minimum error. The main motivation behind this work is the efficient state and parameter estimation for which measurement locations play an important role. Hence optimum measurement locations are first determined and model identification is done based on these measurements.

Keywords: Distillation Column, Sensors, Observability, Condition number, Extended Kalman Filter, State estimation, Error, Optimization, Identification.

1. INTRODUCTION

Efficient model based control demands a sufficiently accurate model. The main areas in model based process control are process identification and optimization. Both these areas could depend on each other as optimization needs a model and model is obtained by identification. This paper presents the linkage of these two areas for a six tray binary batch distillation pilot plant unit in Nottingham's L3 lab. At the same time the focus has been on using minimum experimental data (which is necessary if the batch column is to be used as a multiproduct plant) and also to study the behaviour of the column in minimum runs to set up initial batches to achieve desired product purity. Here, run based optimization addresses this issue and identifies the model structure and its parameters by minimising the process-model mismatch under steady state, total reflux operation of the batch distillation system. More recently, the identification of nonlinear systems, from process measurements was addressed by application of artificial intelligence techniques (Dutta and Rhinehart, 1999; Ruiz-Gomez et al. 2000). Mujtaba and Hussain (1998) presented the optimization framework by using process-model mismatch. Alvarez-Ramirez et al. (2000) have used a modelling error compensation technique to counteract the effects of process-model mismatch, by estimating modelling error using observer. As model plays an important role in prediction of future states, in fact this is the main motivation behind the presented work, the optimum measurement locations are determined first, so as to increase the state estimation accuracy. Here, optimum sensor locations are determined for estimation of states only and compared with optimum locations obtained for state and parameter estimation (Wilson and Guhe, 2005). Also, the minimum number of sensors required has been justified using the Extended Kalman Filter (EKF) algorithm. The temperature sensor probes have been installed on the pilot plant at the optimal tray locations and finally, the model identification has been carried out using the temperature profiles obtained from these optimally placed sensors. The strategy of minimum number of sensors and minimum number of batch runs resulted in capital and operational cost savings respectively.

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2. BATCH DISTILLATION SYSTEM

The system under study is a single product binary batch distillation pilot plant unit with a reboiler and six trays in Nottingham's L3 Laboratory. Sixth tray is the top tray. A binary mixture of Methanol-Water is separated and methanol is recovered as top product. The product composition can be controlled by manipulating the reflux ratio, using tray temperatures as secondary measurements. A PI control algorithm has been developed (Wilson and Zou, 2003) and installed on the pilot plant control architecture. The random disturbances in the system are varying cooling water temperature in the overhead condenser, ambient temperature variations, a slight variation in feed composition due to recycling of bottom product with the fresh batch of feed and the fluctuations in steam line pressure to the reboiler. The system is operated at fixed reboiler duty and atmospheric pressure. The characteristics of the initial model representing the pilot plant are based on simple vapour-liquid equilibrium (VLE) calculations using fixed relative volatility, considering minimum information availability of the pilot plant behaviour. At a later stage Antoine and VanLaar equations are used in the model for rigorous VLE calculations. Both models incorporate simplifying assumptions. The process state in the model is methanol mole fractions in the liquid phase on each tray together with or without relative volatility as a parameter, augmented as a state. The efficiency of all six trays is 60%. The pilot plant has empty slots between the reboiler and the physical tray number one.

3. OPTIMIZATION AND IDENTIFICATION

Steady-state analysis of the batch distillation system i.e. at total reflux has been considered for determination of the optimum sensor location and their number. Next the model identification has been done by the optimization based on experimental data from plant runs. This section is divided in three parts. First part explains the optimum sensor location strategy considering state estimation with or without estimation of parameter as an augmented state. Second part suggests the criterion for deciding the optimum number of sensors and finally the method for model identification based on optimization has been presented.

3.1 Optimum sensor location

More recently the determination of sensors location has been addressed by Wilson and Guhe (2005). Here, the same approach of observability matrix condition number has been extended to compare the sensor locations for state estimation, with or without inclusion of parameter as an augmented state in a process model, provided system is fully observable which is required for implementation of state estimation sequence. The continuous time dynamic model can be represented as a set of nonlinear equations of the form:

$$\dot{\mathbf{x}}(\mathbf{t}) = \xi\,(\mathbf{x}(\mathbf{t}),\mathbf{u}(\mathbf{t}),\mathbf{w}(\mathbf{t})) \qquad (1)$$

where, $\xi(.)$ is a non-linear m valued function, $\mathbf{x}(t)$ is $m \times 1$ vector of state variables, $\mathbf{u}(t)$ is $r \times 1$ vector of input variables, $\mathbf{w}(t)$ is the vector of Gaussian white noise with zero mean and covariance $\mathbf{Q}$. Here, the discrete-time, time invariant linearised model of the system (Eq. (1)) can be written as

$$\mathbf{x}(k+1) = \mathbf{A}\,\mathbf{x}(k) + \mathbf{B}\,\mathbf{u}(k) + \mathbf{C}\,\mathbf{w}(k) \qquad (2)$$

where $\mathbf{x}$ is a state vector of order m with or without augmentation of unknown parameter vector of order p. For the steady state analysis of the system, at total reflux, $\mathbf{B}$ and $\mathbf{C}$ are null. $\mathbf{x}$ relates to measurement $\mathbf{y}$ which is of the order n and it is given by

$$\mathbf{y}(k+1) = \mathbf{H}\,\mathbf{x}(k+1) \qquad (3)$$

Here matrix $\mathbf{A}$ can be written as

$$\mathbf{A} = \begin{bmatrix} \mathbf{A_{m\times m}} & \mathbf{A_{1\times p}} \\ \mathbf{A_{p\times 1}} & \mathbf{A_{p\times p}} \end{bmatrix} \qquad (4)$$

where m is the number of states and p is the number of parameters as an augmented state. The observability matrix is given by (Ray, 1981)

$$\mathbf{O} = \left[\mathbf{H'} \quad \mathbf{A'H'} \quad \mathbf{A'^2\,H'} \quad \ldots\ldots \quad \mathbf{A'^{M-1}\,H'}\right]' \qquad (5)$$

Actually $\mathbf{O}$ relates $\mathbf{x}(0)$ with the number of measurements acquired over M samples. The standard test for system to be observable is that the rank of $\mathbf{O}$ must be equal to order of $\mathbf{x}$. Different sensor location are tested in $\mathbf{H}$ to check the observability of the system. The optimality of selection of sensor location is given by

$$\min_{\boldsymbol{\varphi}} \ \mathrm{J1} = \mathrm{cond}(\mathbf{O}) \qquad (6)$$

where, cond($\mathbf{O}$) represents the condition number of $\mathbf{O}$ and $\boldsymbol{\varphi}$ represents the combination of locations of one or more sensors. cond($\mathbf{O}$) is the ratio of maximum and minimum singular values of $\mathbf{O}$.

It is worth mentioning here that proposed method has been used aiming at efficient estimator design by optimum sensor location and not for controller design e.g. determining actuator location. The approach in this study can easily be extended to jointly improving the state observability and controllability in terms of observer-controller design considering *balanced realization* (Marx et al., 2004) through maximization of respective Gramians. Note, this technique cannot be applied here as the presented approach is at total reflux and autonomous i.e. **B** is null and controllability has no relevance.

3.2 Optimum number of sensors

The number of sensors to be installed on the pilot plant has been proposed by employing a state estimator namely Extended Kalman Filter (EKF). It can be described as: Given a current best estimate of the process state $\mathbf{x}_f(k)$, and its error from $\mathbf{x}(k)$ has an associated covariance $\mathbf{G}(k)$, then the prediction $\mathbf{x}_p(k+1)$ of the state at the time k+1 can be obtained using linearised model as

$$\mathbf{x_p}(k+1) = \mathbf{A}\ \mathbf{x}_f(k) \tag{7}$$

at steady state total reflux (autonomous) and its error about $\mathbf{x}(k+1)$ has an associated covariance $\mathbf{P}(k+1)$ given by

$$\mathbf{P} = \mathbf{A}\ \mathbf{G}(k)\ \mathbf{A}' + \mathbf{CQC}' \tag{8}$$

where, $\mathbf{CQC}'$ represents process noise covariance. As the non-linear model is available, prediction $\mathbf{x}_p(k+1)$ is achieved by numerical integration of $\xi(.)$ across a single sample period with initial conditions $\mathbf{x}_f(k)$, instead of using Eq. (7). The operation is presented symbolically as

$$\mathbf{x_p}(k+1) = \mathbf{\Psi}(\mathbf{x}_f) \tag{9}$$

where $\mathbf{\Psi}(.)$ is in effect a non-linear, discrete time, m-valued function. Eq. (8) then represents only an approximation to the non-linear prediction error covariance associated with $\mathbf{\Psi}(.)$ which is computationally straight forward and adequate. At each sample instant, in addition to having a prediction of the system state $\mathbf{x}_p(k+1)$, added information is available in the form of the n-vector of available process measurements $\mathbf{y}(k+1)$ which is taken to relate to the actual state by the model

$$\mathbf{y}(k+1) = \mathbf{H}\ \mathbf{x}(k+1) + \mathbf{v}(k+1) \tag{10}$$

where $\mathbf{v}(k+1)$ contains stochastic measurement error, having zero mean and error covariance $\mathbf{R}$. The minimum error variance estimate of system state at the current time interval $\mathbf{x}_f(k+1)$ is then given by the filter equation

$$\mathbf{x}_f(k+1) = \mathbf{x}_p + \mathbf{F}\ (\ \mathbf{y} - \mathbf{H}\ \mathbf{x}_p\ ) \tag{11}$$

where values now refer to time interval (k+1) unless stated. The term $(\mathbf{y} - \mathbf{H}\ \mathbf{x}_p)$ is called innovation sequence i.e. if this term is zero the best estimate is the predicted state. **F** is the Kalman Filter gain matrix which is in turn given by

$$\mathbf{F} = \mathbf{PH}'\mathbf{S}^{-1} \tag{12}$$

where **S**, the covariance of the innovation sequence is

$$\mathbf{S} = \mathbf{HPH}' + \mathbf{R} \tag{13}$$

Finally, $\mathbf{G}(k+1)$ the error covariance of the new best estimate $\mathbf{x}_f(k+1)$ is given as

$$\mathbf{G} = \mathbf{P} - \mathbf{FHP} \tag{14}$$

Equations 7 – 14 define the Extended Kalman Filter Algorithm (Wilson and Zorzetto, 1997).

The EKF is used to estimate the states and unknown parameters based on different optimally located number of sensors. Here, a property of error covariance matrix **G** has been used as a measure of optimality. As **G** indicates the accuracy of the estimate and since it is a non-negative matrix, the optimal policy is considered which minimises its *trace* (Kumar and Seinfeld, 1978). The optimality index for a number of measurements is given by

$$\min_{\boldsymbol{\gamma}}\ J2 = \mathrm{trace}(\mathbf{G}) \tag{15}$$

where, $\boldsymbol{\gamma}$ is the number of optimally located sensors. It is noted that here the EKF has been implemented under steady state condition of the plant.

3.3 Model identification

In the context of obtaining an appropriate mechanistic/mathematical model of the system, the process-model mismatch is minimised by proper selection and adjustment of an appropriate model structure and parameters. In this section the steady state measurement profiles from optimum sensor locations are considered to identify the model structure and its parameters to achieve minimum process-model mismatch. The task is to minimise root mean square error (RMSE) between experimental and simulated measurement at steady state operation as a generalised case. Biases in experimental measurements are also taken into consideration during the minimization. The loss function to be minimised at steady state operation is:

$$\arg\min_{\boldsymbol{\theta}} V(\boldsymbol{\theta}, Z, N) = \sqrt{\frac{1}{Z*N}\left(\sum_{i=1}^{N}(\mathbf{T}(t) - \hat{\mathbf{T}}(t))' * (\mathbf{T}(t) - \hat{\mathbf{T}}(t))\right)} \tag{16}$$

where N **-** number of batches over which optimization is carried out, $\boldsymbol{\theta}$ - global parameter vector. Z - number of process outputs $\mathbf{T(t)}$. The prediction of measurement $\mathbf{T(t)}$ is given by $\hat{\mathbf{T}}\mathbf{(t)}$.

4. RESULTS AND DISCUSSION

The basis for model identification of batch distillation pilot plant is to get tray temperature profiles from it.

Here, instead of getting temperature profiles from an arbitrary set of trays, a systematic approach of deducing the optimum sensor location has been adopted using observability matrix condition number for the state and parameter estimation (Wilson and Guhe, 2005) and further extended to notice variations in sensor location from the case of state estimation only to state and parameter estimation. This analysis has been carried out considering the availability of minimum information of the plant at initial stage. Hence a process model representing the pilot plant having reboiler and six trays has been developed using simple VLE calculations based on fixed relative volatility. The relative volatility has been considered as an unknown parameter to be estimated as an augmented state. The observability matrix **O** given by Eq. (5) is evaluated for both cases based on all combinations of temperature sensors at various trays in the column provided the system is fully observable in terms of the rank test. Sensor locations with minimum cond(**O**) are chosen to be optimal because a large condition number is undesirable as it indicates numerical ill-conditioning. Table 1 shows the optimum sensor location and their numbers along with comparison of two cases viz. state estimation only and state and parameter estimation, highlighting fully observable system even with one sensor in former case but unobservable with one sensor in the latter. The effect of 'relative volatility' as a parameter on optimal measurement location was studied and compared with state estimation only. The comparison of results shows that unknown relative volatility influences the observability of the system.

Table 1 Optimum tray locations for various numbers of temperature sensors in a batch distillation pilot plant for 'state estimation' and 'state and parameter estimation' (Wilson and Guhe, 2005)

No. of Sensors	Measurement Locations (Tray Nos)	
	State Estimation	State and Parameter Estimation
1	0 (Reboiler)	0 (Reboiler) *
2	0, 6	0, 4
3	0, 5, 6	0, 2, 4
4	0, 2, 4, 6	0, 2, 3, 6
5	0, 2, 4, 5, 6	0, 1, 2, 3, 6
6	0, 2, 3, 4, 5, 6	0, 1, 2, 3, 4, 6
7	0, 1, 2, 3, 4, 5, 6	0, 1, 2, 3, 4, 5, 6

* Unobservable system with one sensor

The analysis shows that the optimal sensor locations vary by addition of relative volatility as a parameter to be estimated. However, it is observed that in all optimal sensor locations, in both cases, one sensor is always located at the reboiler. This indicates that the reboiler temperature sensor is essential for the system to be observable. It is noted that these results are obtained on the hypothesis of 100% tray efficiency and distillation column operating at total reflux, steady state. As it is always significant to establish a robust estimation sequence and relative volatility plays a vital role in separation, the sensor locations based on state and parameter estimation are preferred over the case of state estimation only. In case of a state and parameter estimation the number of sensors required to make the system observable is more than for state estimation alone (i.e. here, 2 instead of 1).

Secondly, to justify the minimum number of sensors to install on the plant, EKF strategy is employed. The steady state system under total reflux has been considered with measurement and process noise. The methanol compositions on trays are considered as states of the system and relative volatility as a parameter to be estimated. The *trace* property of the error covariance matrix **G** is considered for selection of minimum number of temperature sensors on batch distillation column. To obtain better performance of the estimation sequence, a criterion of minimizing a cost associated with temperature sensor and their quantity has been adopted. Although, here two temperature measurements are competent to satisfy observability criteria, the effects of more measurements on the EKF speed of convergence has been considered. Fig.1 indicates that less error of states and parameter estimate can be obtained using more measurement sensors. Thus capital cost and maintenance cost can be optimized by selecting above the minimum number of sensors through faster or more accurate estimation. Fig. 1 shows simulation

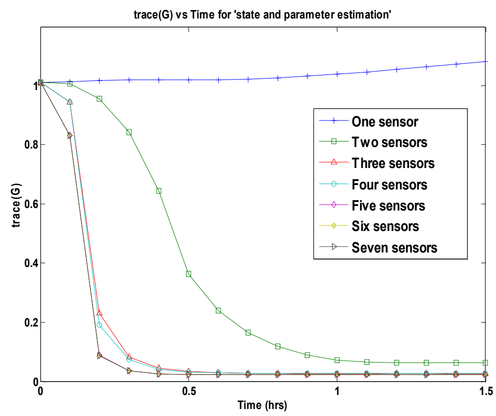

Fig. 1. trace(**G**) for different number of optimally located sensors.

results of *trace* of **G** for different numbers of sensors, clarifying that except the cases of one and two measurements all other cases from three to seven, the values of trace of **G** converge quite closely to each other. But the time taken by five, six and seven measurements to converge is slightly less than three and four measurements. From economic point of view it is always good practice to choose minimum number of measurements which will give comparatively better performance. Here, it is observed that three measurements is the economic choice giving approximately the same performance in comparison with other cases of higher number of measurements. It is noted that only one parameter i.e. relative volatility has been estimated. Moreover, after deciding the sensor location and their number a check on the results has been repeated again by using random scaling of temperature measurements. It has been found that though the value of condition number of observability matrix changes with different scaling constants the optimum sensor location remains the same.

Finally, after deciding the optimum number of sensors and their location (which are at reboiler, Tray 2 and Tray 4) the temperature probes are installed on the respective trays in the pilot plant and temperature profiles have been obtained by using PI control strategy. The initial model representing the pilot plant has been amended with inclusion of rigorous VLE calculations. The temperature profiles of process and model at different trays under steady state operation have been compared. Based on steady state reboiler temperature, Methanol composition in the column has been calculated from reboiler up the column using bubble point calculations. And thus Methanol temperature on trays by model has been generated from respective tray composition using bubble point calculations. The process-model mismatch at steady state on Tray 2 and Tray 4 has been noticed around 6 ^{o}C and 2.34 ^{o}C respectively as a result of empty slots in the pilot plant between the reboiler and actual Tray one, which is equivalent to four physical trays. Here, the task of modeling the pilot plant by taking care of the effect of empty space which is termed as a 'notional tray' has been addressed by optimization and identification of the model, mainly the efficiency of notional tray and the possible bias in experimental Tray 2 and Tray 4 process temperatures due to empty tray space in the column. Objective has been to minimize the process-model mismatch during the dynamic response. First, the notional tray efficiency 'eff01', and temperature bias are manually looked at by drawing a McCabe-Thiele diagram based on steady state temperatures at reboiler, Tray 2 and Tray 4 and back calculating respective Methanol composition profile across the column using rigorous VLE. This approach has given the range of values of 'eff01' and biases as an initial guess, which are used in optimization sequence as constraints. Four different batch runs spanning the random process disturbances in the system has been considered for optimization. The criteria of minimum RMSE of temperatures at Tray 2 and Tray 4 using particular 'eff01' and respective biases over 3-dimensional numerical grid points in a finite space has been adopted to minimize the objective function subject to prescribed constraints for this case. The RMSE has been determined by calculating temperature difference between steady state temperature profile by model and the process for all four pilot plant batch runs at the same time. The grid point at which the model parameter vector $\boldsymbol{\theta}$ i.e. eff01, bias on Tray 2 (bias2), bias on Tray 4 (bias4) gives minimum RMSE has been selected and considered as approximate vector $\boldsymbol{\theta}$ covering four batches. These biases are adjusted on the pilot plant. Thus, the Eq. (16) is interpreted in terms of $\mathbf{T} = (\mathbf{T_2}\ \mathbf{T_4})'$. Where,
T2 = (Experimental temperature on Tray 2 – bias2)
T4 = (Experimental temperature on Tray 4 – bias4)
$\hat{\mathbf{T}}$ – predicted temperatures on Tray 2 and Tray 4 respectively.

Therefore, the approximate $\boldsymbol{\theta}$ has been used as initial guess to find the truly global $\boldsymbol{\theta}$ using Simplex-Marquardt method as a direct search method. This method attempts to minimize a RMSE as a function value based on an approximate $\boldsymbol{\theta}$ as an initial guess. Fig. 2 shows the global minimum model parameter vector $\boldsymbol{\theta}$ found. The optimum values of parameters which are given in the caption to Fig. 2 are therefore implemented into the model.

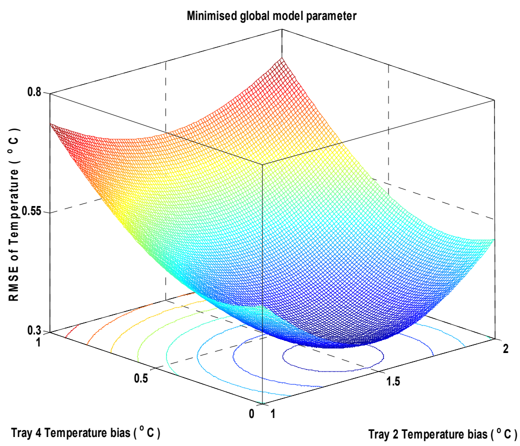

Fig. 2. Optimized global model parameters (eff01 = 149.24%; Overall RMSE = 0.3311 ^{o}C; bias in Tray 2 =1.5094 ^{o}C; bias in Tray 4 =0.2137 ^{o}C)

To demonstrate the effectiveness of the model derived above, its dynamic response has been tested against the experimental one during pilot plant runs taken on partial offtake using PI action to control the Methanol composition by manipulating the reflux ratio using tray temperature as a secondary measurement. The Methanol temperature profile on trays has been generated by the amended model i.e. inclusion of notional tray and its efficiency using rigorous VLE calculations based on tray compositions. The dynamic response by the model has been generated taking the reflux ratio value from the pilot plant. Fig. 3 shows the performance of the new identified model with inclusion of optimum $\boldsymbol{\theta}$ against process under partial offtake condition for Methanol temperature on Trays. As model follows the experimental profile, it clearly shows that the process-model mismatch has been reduced to the minimum. Here, only reflux ratio has been used as a manipulated variable to govern the performance of process and the model.

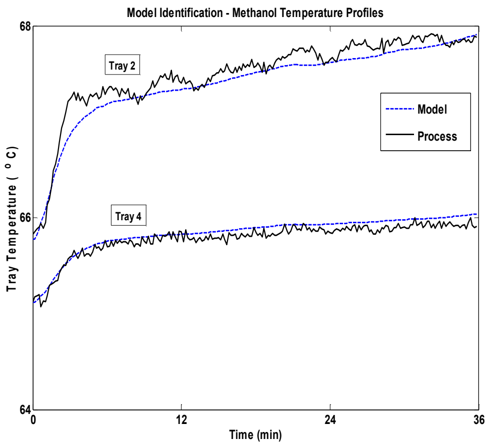

Fig. 3. Performance of the new model in terms of dynamic response under partial offtake.

5. CONCLUSIONS

Based on the results presented it can be concluded that the proposed model identification strategy coupled with optimization method which uses the experimental temperature profile based on optimal sensor location has been successful to identify a model and its parameters which represents the dynamics of the batch distillation pilot plant with minimum process-model mismatch. The effect of inclusion of relative volatility as a parameter to be estimated as an augmented state clearly demonstrated the advantage of optimal sensor location. Also the strategy of inclusion of notional tray and its efficiency has clearly illustrated a vital role in identifying a model which can predict the plant behaviour. Furthermore, the number of sensors has been shown to provide a tradeoff between sensor number and state estimation speed and accuracy. Scaling of temperature measurement had no effect on optimum sensor choice. It is also noted that the model has been identified using a low number of experimental runs, thus reducing the operating cost.

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