BK1064-ch57_R2_250706

© 2006 IChemE

DISTILLATION COLUMN CONTROL USING THE WHOLE TEMPERATURE PROFILE

M Chew, W E Jones & J A Wilson*

School of Chemical, Environmental & Mining Engineering (SChEME) University of Nottingham, University Park, Nottingham, NG7 2RD, UK

Industrial distillation column control typically relies on one (or maybe two) carefully located tray temperature sensors. Here our aim is enhanced control by responding to movements in both the position and shape of the whole measured temperature profile. The control objective is to maintain end product specifications against feed composition disturbances using the measured temperatures and without recourse to composition sensors. While recent approaches to this make use of non-linear wave theory (Han and Park 1993, Roffel et al, 2003) we instead use a mechanistic dynamic state space column model to encapsulate the profile behaviour and an adapted version of the Minimum Error Profile (MEP) strategy to exercise control. Proposed for general profile control by Wahl et al (2002), use of the MEP strategy in controlling fixed-bed catalytic reaction systems has shown advantages (Chew-Hernandez et al, 2004 and Wilson et al, 2005). Here, at each sample period the measured temperature profile allows an Extended Kalman Filter (EKF) to estimate the current feed composition and a Linear Quadratic Regulator (LQR) to set the control moves that will drive the column optimally towards the MEP target steady state, this being the closest match possible to the desired operating condition with the current feed composition. In re-calculating the optimal sequence of future control moves at each measurement sample and taking the first move in the sequence, our approach may be termed a Non-linear Model Predictive Profile Control strategy. Significant performance gains over conventional dual composition control were found in three column case study simulations.

While above the reflux ratio and the reboiler steam valve were manipulated for control, the ease of extending the MEP strategy offers the chance to look in principle at including feed enthalpy as a third manipulated variable. Henry and Mujtaba (1999) looked its use for feedforward control against measured feed composition swings (i.e. using a composition sensor) with success limited by the size of allowable feed enthalpy changes. Here, for the MEP strategy including feed enthalpy for true feedback control we found significant further performance gains and the MEP strategy also provided an explicit way to limit the size of control moves called for in feed enthalpy.

KEYWORDS: temperature profile control, Kalman filtering, feed composition estimation, minimum error profile control, non-linear model predictive profile control, feed enthalpy manipulation

*Corresponding author, Tel: +44(0)115 951 4179, E-mail: j.a.wilson@nottingham.ac.uk

© 2006 IChemE

INTRODUCTION

Industrial distillation column control schemes typically rely on using a small number of carefully located temperature sensors (usually one but sometimes two) in the column. Here we focus on use of the whole measured temperature profile (i.e. sensors on every column tray) as a basis for end product composition control, without recourse to use of on-line composition sensors (i.e. using the temperature profile itself as an inferential measurement). The aim is enhanced control by responding to transient fluctuations in not just the position but also the shape of the profile. While some authors have investigated control schemes involving up to three or four probes in a variety of ways (e.g. temperature differences, averaged temperatures etc.) we view these as only approximate versions of a more complete profile control strategy. A related recent approach treats the profile as the product of a travelling wave and control as a problem of locating and controlling the position of the profile on the basis of non-linear wave theory (Han and Park, 1993; Roffel et al, 2003). However, in applying this non-linear wave theory approach to distillation control, it is assumed that the profile is constant in shape, and so only one point on the profile needs to be controlled. In addition these studies do not consider use of an estimated value of the disturbance to improve the control effectiveness, relying instead on master PI controllers based on measured product composition with long sample periods to provide longer term offset free product composition control.

The control strategy we propose here doesn't need assumptions on the shape of the column temperature profile being based solely on measured temperatures and use of an inferred value of the unmeasured disturbances to get the control actions. In effect we use a detailed mechanistic model-based approach to the problem, employing an adapted version of a general profile control strategy proposed earlier by Wahl et al (2002) based on the idea of a Minimum Error Profile (MEP). Advantages of this strategy have already been shown in control of fixed-bed catalytic reaction systems (Chew-Hernandez et al, 2004 and Wilson et al, 2005). Here the strategy is adapted and applied to distillation column control, the objective being to maintain end product specifications primarily against feed composition disturbances.

Towards the end of the paper, the addition of the feed enthalpy as an extra manipulated variable is explored. This option has not been exercised conventionally, often for the very practical reason that equipment capable of manipulating the feed enthalpy is not always installed (or indeed appropriate) though Henry and Mujtaba (1999) looked at manipulating feed enthalpy via a feed pre-heater as a basis for feedforward control against measured feed composition disturbances (i.e. requiring a composition sensor).

A MINIMUM ERROR PROFILE CONTROL STRATEGY

An EKF is used to estimate the unmeasured column states (compositions) and also the fresh feed composition based on the measured temperature profile. Yu and Luyben (1987), through steady state analysis, and more recently Chew (2006), from a dynamics standpoint, have demonstrated that for an n_c component feed, both the state and the unknown feed composition of a column system are observable via $n_c - 1$ column tempera-

© 2006 IChemE

ture sensors. In the work reported here we assume availability of temperature sensors on all trays and thus complete system observability in our case studies is assured. The control algorithm uses the EKF generated state and feed estimates to decide moves in the reflux ratio (R), the reboiler steam valve position (X_S) and, in the final section of the paper, the feed vapour enthalpy (H_F), to effect control.

For control purposes, the MEP steady state target profile is re-calculated at each measurement sample period from knowledge of the disturbance vector $\mathbf{w}(\mathbf{k})$ (Wahl, 2003) which in our case is the unknown feed composition ($n_c - 1$ mole fractions). The discrete-time linearised model of the column system can be written as

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

where **x** is the state vector, **u** is the vector of manipulated inputs (either $\mathbf{u} = [R X_S]^T$ or $\mathbf{u} = [R X_S H_F]^T$) and **w** is the vector of $n_c - 1$ unknown feed component mole fractions $(\mathbf{w} = [x_{F,1} \dots x_{F,nc-1}]^T)$. The process state **x** is made up largely of $n_c - 1$ component mole fractions in the liquid phase in each column stage (in some cases column tray hydraulic dynamics have also been included) together with corresponding variables defining the reboiler and overhead system conditions. With feed at its normal composition the optimum column steady state (which includes the optimum steady state profile) \mathbf{x}_{OP} is achieved with inputs at \mathbf{u}_{OP} . With a change in feed composition, a different steady state **x** will arise from actions **u**, hence **e** a weighted cost of deviations from the optimum (\mathbf{x}_{OP} , \mathbf{u}_{OP}) becomes

$$\mathbf{e} = (\mathbf{x}_{\text{OP}} - \mathbf{x})^{\mathrm{T}} \mathbf{Q}_{\text{MEP}} (\mathbf{x}_{\text{OP}} - \mathbf{x}) + (\mathbf{u}_{\text{OP}} - \mathbf{u})^{\mathrm{T}} \mathbf{R}_{\text{MEP}} (\mathbf{u}_{\text{OP}} - \mathbf{u})$$
(2)

 \mathbf{Q}_{MEP} and \mathbf{R}_{MEP} are weight matrices that enable different cost penalties to be applied to steady deviations in individual states or manipulated variables. Minimising quadratic cost **e** by choice of **u** at measurement/EKF sample instant k gives

$$\mathbf{x}_{\text{MEP}}(\mathbf{k}) = \mathbf{f}_{\text{I}} \mathbf{u}_{\text{MEP}}(\mathbf{k}) + \mathbf{f}_{\text{B}} \mathbf{w}(\mathbf{k})$$
(3)

with

$$\mathbf{u}_{\text{MEP}}(\mathbf{k}) = -1(\mathbf{f}_{\text{I}}^{\text{T}}\mathbf{Q}_{\text{MEP}}\mathbf{f}_{\text{I}} + \mathbf{R}_{\text{MEP}})^{-1}\mathbf{f}_{\text{I}}^{\text{T}}\mathbf{Q}_{\text{MEP}}(\mathbf{f}_{\text{B}}\mathbf{w}(\mathbf{k}) - \mathbf{x}_{\text{OP}})$$
(4)

where

$$\mathbf{f}_{\mathrm{I}} = [\mathbf{I} - \mathbf{A}]^{-1}\mathbf{B} \text{ and } \mathbf{f}_{\mathrm{B}} = [\mathbf{I} - \mathbf{A}]^{-1}\mathbf{C}.$$
 (5)

The target steady state profile \mathbf{x}_{MEP} is the closest feasible match to \mathbf{x}_{OP} under the prevailing feed conditions.

Transient control perturbations $\mathbf{u}_{C}(k)$ are then superimposed on $\mathbf{u}_{MEP}(k)$ so as to drive the column in an optimal dynamic sense from current state $\mathbf{x}(k)$ to steady state at

© 2006 IChemE

target set point $\mathbf{x}_{MEP}(k)$. A linear quadratic regulator (LQR) is used to determine $\mathbf{u}_{C}(k)$ as perturbations \mathbf{u} minimising the quadratic dynamic cost J where

$$\mathbf{J} = \sum_{i=1}^{\infty} [(\mathbf{x}_{\text{MEP}} - \mathbf{x})^{\mathrm{T}} \mathbf{Q}_{\mathrm{C}} (\mathbf{x}_{\text{MEP}} - \mathbf{x}) + \mathbf{u}^{\mathrm{T}} \mathbf{R}_{\mathrm{C}} \mathbf{u}].$$
(6)

 \mathbf{Q}_{C} and \mathbf{R}_{C} are weight matrices that enable different cost penalties to be applied to dynamic perturbations in individual states or inputs. The full control move $\mathbf{u}(k)$ at the current time instant then follows as

$$\mathbf{u}(\mathbf{k}) = \mathbf{u}_{\mathrm{MEP}}(\mathbf{k}) + \mathbf{u}_{\mathrm{C}}(\mathbf{k}) \tag{7}$$

Thus at any sample instant k, $\mathbf{u}(\mathbf{k})$ represents the first step along the predicted optimal path towards steady state at $\mathbf{x}_{MFP}(\mathbf{k})$ on the infinite-time horizon, the whole procedure being repeated at instant k + 1. On this level our strategy might be viewed as a variant of the Model Predictive Control paradigm. However, the novel MEP component here forces convergence as close as feasibly possible to global optimum operation of the column in the face of the prevailing feed composition disturbances. Within this, control of the whole temperature/composition profile in the column is also implicitly included. Furthermore, local linearisation of the non-linear model at each measurement/estimation sample ensures convergence towards the global optimum steady state. The strategy might thus be more precisely termed 'non-linear model predictive profile control'. Fundamentally, with no process/model mismatch (as we assume here), performance of our approach is contingent on fidelity of the feed composition estimates, which drive the MEP element. As with all optimal control strategies, there are application specific subtleties in setting the weight matrices (Q_{MEP} , R_{MEP} , Q_C and R_C) to deliver desired system performance (an example of this is given later in Case Study 3). Our prime objective here is simply to demonstrate the feasibility and potential of this integrated approach to distillation column control. A more complete exploration of its global stability and robustness properties, including the effect of process/model mismatch on system performance, are topics of on-going research.

THREE CASE STUDY SYSTEMS

We now turn to application of the MEP control strategy to three simulated distillation systems that together exhibit many of the characteristics that feature in column process dynamics.

Case Study1 – is a 10 tray column with a binary nC5/nC6 feed. To improve speed of simulation while retaining a close match to a previous Hysys case study system, the dynamic model (developed by Vais, 2002) uses polynomials fitted across the normal operating region to the rigorous thermodynamic and physical properties embedded in Hysys. With varying phase density, the column hydraulic dynamics are also included, resulting in a high fidelity, non-linear representation of the process.

Case Study 2 – is a 27 tray column again with binary nC5/nC6 feed, this time represented under the usual simplifying assumptions (i.e. equimolal overflow, ideal VLE, fixed tray hold-up etc). With a high purity product spec, this longer column exhibits both strong non-linearity and a sharper temperature profile which flattens significantly towards the ends of the column where an individual temperature probe becomes insensitive and thus useless for inferring end product composition.

Case Study 3 – is a 10 tray column, again set up under the usual simplifying assumptions, but this time with a ternary nC5/nC6/nC7 feed. In this case, even though a temperature probe sited near the column ends will 'see' the effects of composition changes, with a ternary feed it has on its own no unique inferential link to the full local tray composition, even at fixed pressure conditions ($n_c = 3$, so two probes are necessary for this).

PERFORMANCE OF THE MEP CONTROL STRATEGY WITH TWO MANIPULATED INPUTS

In each of the three case studies the MEP strategy was configured using the algorithm outlined earlier together with the non-linear and locally linearised versions of the appropriate dynamic model. The measurement set included the profile of temperatures on each column tray and the reboiler. Ideal liquid level and pressure controls were assumed. Manipulated inputs for composition control were $\mathbf{u} = [R X_S]^T$. The simulated operation included unknown random process disturbances (process noise) and temperature measurement errors (standard error 0.0316°C). The weight matrices \mathbf{Q}_{MEP} and \mathbf{Q}_{C} were set as diagonal and identical, with heavy weights of 1e8 on the distillate and bottoms nC5 mole fractions, compared with unity on the other stages (i.e. aiming for tight control of the end product compositions with a deviation of 1e-4 in end product mole fraction being as costly as an average of 0.5 on other trays). \mathbf{R}_{MEP} was set to zero while $\mathbf{R}_{\text{C}} = diag(20 \ 1)$, i.e. making a move of 0.1 in steam valve fraction open as costly as a 0.022 move in reflux ratio *R*. As a performance baseline a two-point conventional (i.e. SISO) temperature control strategy, simulated on a noise free basis, was carefully tuned for accurate control with minimum interaction effects.

Some typical results of applying the MEP control strategy to Case Sudy 1 are shown in Figure 1 where end product composition movements are shown for a sudden step disturbance in feed composition after a quiescent period of near steady operation. Convergence of the EKF-generated state estimates (which takes place typically within 10 minutes) is assumed to have happened at an earlier stage. The performance improvement offered by the 'two manipulated input' strategy (designated as MEP(2) in the results) are evident in comparison with the conventional control case, where, because the 'bottoms' temperature probe must be placed on the lowest column tray (owing to measurement insensitivity in the reboiler), the leverage of the increased nC5 feed content leads, with no offset in the bottom tray temperature, to a steady offset nC5 content in bottoms product. Although the conventional control is quite successful in reducing temperature deviations (within the restriction imposed by interaction between the two SISO loops) its ability to regulate composition is poor compared to the MEP case where

© 2006 IChemE



Figure 1. Case study 1 end product step responses under control (-- conventional; — MEP (2); — MEP(3), - - -set point)

two factors emerge. The MEP strategy has foresight through 'seeing' temperature deviations from the target profile appear on trays close to the column feed point long before significant deviations appear at the ends. In addition the embedded high fidelity model enables more precisely balanced control actions to bring about a smooth, efficient return to steady state as close as is feasible to the normal steady state – and all of this without recourse to use of a composition measurement. The corresponding manipulated variable traces are shown in Figure 2 where the MEP strategy quickly identifies the composition disturbance and moves the inputs into the range to counteract it in the long term while subsequent trimming adjustments come from the LQR in co-ordinating the transient convergence on the target, eventually having to deal only with the background process noise.

Although a large performance gain with the MEP is evident in Figure 1, the size of the gain is better appreciated in Table 1 where the Integral of Absolute Error (IAE) between the end compositions and their optimum steady state values (\mathbf{x}_{OP}) are presented



Figure 2. Control actions for responses in Figure 1 (--- conventional; — MEP (2); — MEP(3))

© 2006 IChemE

| Case study | Control strategy | Distillate composition | Bottom composition |
|--------------------------|-------------------------|------------------------|--------------------|
| 1 (binary with 10 trays) | Conventional | 8.1e-2 | 5.0e-2 |
| | MEP with 2 manip inputs | 3.8e-4 | 1.4e-3 |
| 2 (binary with 27 trays) | MEP with 3 manip inputs | 2.0e-4 | 7.0e-4 |
| | Conventional Control | 8.4e-1 | 2.0e-3 |
| | MEP | 4.8e-6 | 3.8e-4 |

Table 1. IAE values of end product compositions following a binary feed mole fraction step increase of 0.05 in n-C5 for case studies 1 and 2 (see also Figures 1 & 2)

for the same traces and over the same timescale as in Figures 1 and 2. Deviation reductions in the order of 20 to 30 relative to the conventional control are shown.

Application of the MEP strategy in an equivalent fashion for control in Case Studies 2 and 3 produces very similar transient responses to those shown already and with space limited we therefore focus on the more telling IAE values presented in Tables 1 and 2 respectively (note that with a 25 minute time scale the average mole fraction deviation can be found by dividing IAE values by 25). For Case Study 2 (Table 1) a vast improvement in top product quality appears mainly due to the classic problems in high purity distillations owing to the high response non-linearity and the very strong interaction between the SISO loops which limits the tightness of their tuning.

The multi-component feed in Case Study 3 provides an opportunity to demonstrate reconfiguration of the MEP strategy for different control objectives. Two sub-cases are presented. When nC5 must be controlled to tight specifications in both top and bottom products we apply a higher weighting against nC5 end product deviations with weight matrices set exactly as before in Case Studies 1 and 2. This leads to significantly tighter control than with the conventional strategy (see Table 2).

Alternatively, if nC7 must be kept low in the distillate while nC5 must be kept low in the bottoms, elements in the weight matrices were changed ($Q_{MEP} = Q_C = I$, except for

| Case study | Control strategy | Distillate composition n-C5 n-C7 | | Bottom composition n-C5 |
|---------------------------|-----------------------------------|--|--------|-------------------------------|
| 3 (ternary with 10 trays) | Conventional | 1.3e-2 | 2.0e-3 | 0.29 |
| | MEP – target nC5 in xd & xw | 1.5e-3 | 6.8e-4 | 1.1e-3 |
| | MEP – target nC7 in xd, nC5 in xw | 2.5e-1 | 6.4e-6 | 1.1e-3 |

Table 2. IAE values of end product compositions following a ternary feed mole fraction swing of 0.05 from n-C5 to n-C7 in Case Study 3

the diagonal elements acting on mole fractions of nC7 in the distillate and nC5 in the bottoms being set respectively to 5e8 and 5e6). As can be seen for the distillate in Table 2, closeness of approach to the required component composition switches from nC5 to nC7 with a compensating increase in the nC5 distillate composition but no significant change at the bootom.

PERFORMANCE OF THE MEP CONTROL STRATEGY WITH THREE MANIPULATED INPUTS

The inclusion of feed enthalpy H_F as a potential extra manipulated variable for column control is now considered. Use of this idea in conventional control implementations presents difficulties. Firstly, although feed enthalpy clearly affects column operation it has no simple relationship with say a tray temperature sensor near the feed (where feed enthalpy will affect conditions fastest for control purposes). In fact if end compositions must be held tightly, for example in the face of feed composition swings, temperatures in the centre of the column will need to move up or down with the whole profile to accommodate the changes. Secondly, manipulating feed enthalpy for control requires presence of appropriate heat transfer facilities in the feed system. Equipment designed to handle sub-cooling of a liquid feed is not necessarily capable of also handling partial vaporisation and a significantly increased heat load. Henry and Mujtaba (1999) side-stepped both these issues by restricting their approach to feedforward control against feed composition changes, measured with a composition sensor, by manipulating feed preheater exit temperature – significantly they note that the size of changes demanded in feed enthalpy will limit the performance gains.

Here we instead introduce feed enthalpy directly as a third manipulated variable in feedback composition control via the MEP strategy with $\mathbf{u} = [R X_S H_F]^T$ (thus assuming that suitable feed preheat equipment is available). This is a trivial extension to implement in the MEP algorithm, involving appropriate matrix re-dimensioning and setting their additional elements. It was found necessary to limit the size of moves demanded in H_F using the extended weight matrices $\mathbf{R}_{\text{MEP}} = diag(0 \ 0 \ 2e-10)$ and $\mathbf{R}_{\text{C}} = diag(20 \ 1 \ 10)$.

Even with H_F values being large (expressed in kJ/kmol) its \mathbf{R}_{MEP} weight will only moderately limit long term values while the \mathbf{R}_{C} weight more tightly constrains transient moves. Some results of applying this 'MEP with three inputs' strategy to the column in Case Study 1 are presented in Table 1 alongside the equivalent results already described 'with two inputs'. Further reductions in IAE for the end compositions are shown.

Most dramatic however are the very different control moves shown in Figure 1 in R and X_S that are made simultaneously with those in H_F shown in Figure 3 (in terms of feed vapour fraction) where, for the disturbance involved here, H_F steps immediately to a different operating level with only minor subsequent adjustments. The change in vapour/liquid traffic in the column then calls for a smaller compensating shift in R and a moderate increase (rather than the former decrease when H_F was fixed) in X_S . This suggests that feed enthalpy manipulation may offer very significant possibilities in closed loop control of column systems. As for the MEP strategy itself, what it offers here is a viable



Figure 3. Feed vaporisation as a consequence of feed enthalpy as the third manipulated variable(—■ MEP (3), case study 1, see Figures 1 and 2)

framework within which moves in feed enthalpy can not only be defined clearly but can be co-ordinated carefully with actions in the other manipulated inputs. It should be noted that much higher performance improvements than those shown in Table 1 were found when allowing feed enthalpy to move around with less constraint to conditions far beyond what would be practically reasonable but the MEP strategy, via its weight matrices, provided a direct means of enforcing an appropriate level of constraint.

CONCLUSIONS

The potential of the proposed Minimum Error Profile Control strategy to distillation systems has been demonstrated. Within the assumptions set out, including the absence of any process/model mismatch, the strategy delivered significant improvements in regulating end product compositions against feed composition swings in three case study systems which together exhibit many of the difficult characteristics met in distillation processes. Furthermore, these improvements were achieved solely by means of the column's measured temperature profile and without recourse to on-line composition measurement. Extension of the approach, as a basis for examining the novel introduction of feed enthalpy as an extra manipulated variable for column control, proved straightforward. The MEP strategy also proved flexible in keeping feed enthalpy demands within a realistic range and the performance improvements found through its use suggest this may be an approach worthy of further investigation.

NOMENCLATURE

| EKF | Extended Kalman Filter |
|-----|----------------------------|
| IAE | Integral of Absolute error |
| LQR | Linear quadratic regulator |
| MEP | Minimum error profile |

ACKNOWLEDGEMENT

The authors are grateful to CONACyT for their support of M Chew in contributing to the work reported.

REFERENCES

- Chew M. (2006) "Control of processes systems based on temperature profiles", Ph. D. Thesis, University of Nottingham, UK
- Chew-Hernandez M., Jones W.E. and Wilson J.A. (2004) "On control of the whole temperature profile in an autothermal tube-cooled fixed bed catalytic reactor", *ESCAPE-14*, *Computer-Aided Proc Eng*, **18**, Elsevier, 619–624
- Han M. and Park S. (1993) "Control of High Purity Distillation Column Using a Nonlinear Wave theory" *AIChE J*, **39**, 5, 787–796
- Henry R.M. and Mujtaba I.M. (1999) "Distillation Column Control: the use of feed temperature to respond to modest variations in feed composition" *Comp. And. Chem. Eng. Supp*, 23, S265–S268
- Roffel B., Betlem B.H.L., de Blouw R.M. (2003) "A comparison of the performance of profile position and composition estimators for quality control in binary distillation" *Comp. And Chem. Eng.*, 27, 199–210
- Vais, A-M (2002) "Side reboiled distillation columns", Ph. D. Thesis, University of Nottingham, UK
- Wahl T., Jones W.E. and Wilson J.A. (2002) "A scheme for whole temperature profile control in distributed parameter systems", *ESCAPE-12*, *Computer-Aided Proc Eng*, **10**, Elsevier, 577–582
- Wilson J.A., Chew M. and Jones W.E. (2005) 'A fully integrated scheme for control against impurity variations in gas phase fixed-bed catalytic reaction loops', 7th World Congress of Chem Eng, IChemE, CDROM, paper P6-084
- Yu C.C. and Luyben W.L. (1987) "Control of multicomponent distillation columns using rigorous composition estimators" I. Chem. E. Symp. Ser. No. 104, A29–A69