Performance Assessment of Different Control Structures for Generic Reactive Distillation Using Linear and Nonlinear Process Models

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This paper compares the closed-loop performance of three control structures using an approximate linear model to that when a rigorous nonlinear process model is used for a generic reactive distillation. It is shown that an approximate linear model behaves essentially similarly to a nonlinear model in a closed-loop system when the deviation of process variables resulting from the disturbance is within the region of the base steady state. Responses based on the linear model for various control structures show a good agreement when compared to those based on the nonlinear model under the same conditions. It is found that the linear process model could be used to develop a robust control system when the control valves are conservatively designed. However, it becomes inadequate if the system is open-loop pseudostable or unstable. The performance of the linear model is shown to be better in a single-end control system than in a dual-end control system because of the nonlinearity effect, which is more pronounced in the latter.

1. Introduction

The combination of reaction and distillation in a single vessel is an old idea that has attracted renewed attention recently. The importance and application of reactive distillation have captured the imagination of many because of the demonstrated potential for capital productivity improvements, increased reaction conversion, elimination of difficult separation, selectivity improvements, and reduced energy use through direct utilization of reaction heat. Reactive systems where reactant and product volatilities differ considerably are ideally suited for reactive distillation.

An extensive summary of the work on reactive distillation is contained in the book edited by Sundmacher and Kienle.[1] A significant portion of the literature was devoted to open-loop dynamics of reactive distillation with an emphasis on process steady-state multiplicities. Only a limited number of papers have appeared to discuss closed-loop dynamics of a reactive distillation column. Al-Arfaj and Luyben[2] gave a review of publications on the control of reactive distillation up to 2000. In the same paper, they evaluated six alternative control structures for an ideal two-product reactive distillation column via rigorous dynamic simulation. Several new papers have appeared in recent times. Monroy-Loperena et al.[3] proposed a robust proportional−integral (PI) control configuration for a high-purity ethylene glycol reactive distillation column. Al-Arfaj and Luyben[4−7] extended their work to control of various specific chemical systems. Wang et al.[8] applied simple linear control to a reactive distillation column in the kinetic regime for the synthesis of *n*-butyl acetate. However, the performance and application of an approximate linear model in model-based controllers for reactive distillation columns have not been explored.

The main goal of process control is the design and implementation of effective control systems that will maintain the process conditions close to its desired steady-state value. Even though a reactive distillation system is inherently nonlinear, the essence of effective regulatory control is to ensure that deviations from the base steady state will be small, in which case the behavior will be essentially indistinguishable from that of a linear system. It is in this sense that the linear model-based controls could be applicable.

The present availability of computer software and hardware, which has made it possible to utilize a rigorous dynamic model in process control, will tend to pose a question as to why do we need an approximate linear model? The use of a linear model can enhance our understanding on the process observability and controllability. Without proper understanding, it is almost impossible to design a good control structure. The use of a linear model significantly reduces the speed of computation, which becomes very critical when a plant model, for instance, is needed for online control. Simple models are desirable in computer-based control for optimization and advanced regulatory control application, where online implementation limits the use of complex models.

For proper control of reactive distillation, an internal composition needs to be obtained.[2,4,7] Most of the established estimation techniques (i.e., Kalman filter and Luenberger observer) that could be applied to obtain the internal composition use a linear model. Therefore, the use of a linear model in model-based control is needed and will significantly reduce the complexity involved in the design and implementation stages as compared to when a rigorous nonlinear model is used. Even nonlinear estimators such as an extended Kalman filter and an extended Luenberger observer use a linear model approximation in their design procedure.[9,10]

The aim of this paper is to compare the performance of different control structures when implemented on a linearized process model to that when they are imple-

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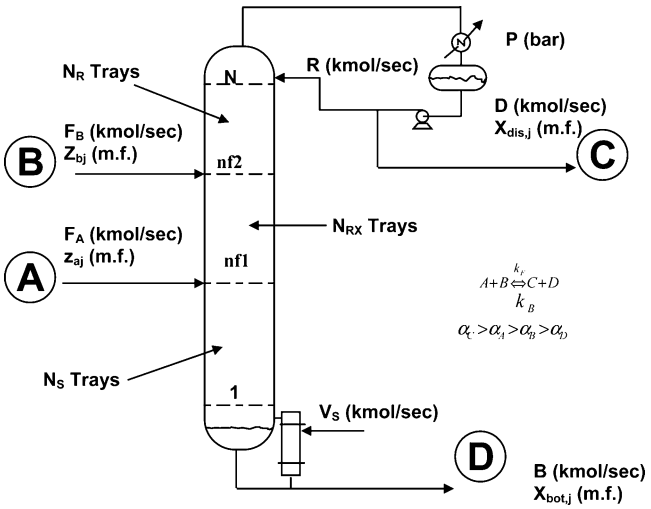

Figure 1. Reactive distillation column.

mented on a nonlinear model for a generic reactive distillation. The idea is to investigate how good of a control can be achieved if a control structure is designed based on an approximate process model. This is an important assessment step before using the linearized model in model-based control applications. In this work, three control structures are implemented to assess the closed-loop performance of a linear process model compared to that of a rigorous nonlinear model. The control structures are dual-end composition control, single-end composition control, and inferential composition control using temperature measurement. All of the control structures use a composition analyzer in the reactive zone to detect the inventory of one of the reactants so that a fresh feed can be manipulated to balance the reaction stoichiometry.

2. Process

In this work, we considered an ideal reactive distillation process proposed by Al-Arfaj and Luyben,[2] as shown in Figure 1. This system contains a single reactive distillation column in which two reactants are fed and two products are produced. The reversible, exothermic liquid-phase reaction occurring in a reactive zone is A + B ↔ C + D.

The reactive distillation column contains nonreactive stripping and rectifying sections with the reactive section in between. Reactants A and B are intermediate boilers, while product C is the lightest and product D is the heaviest. This ensures that high concentrations of reactants A and B are maintained in the reactive zone, which is typical for reactive distillation application.

2.1. Nonlinear Dynamic Model. A rigorous dynamic model for a typical reactive distillation column consists of a large number of nonlinear differential equations and demands much information about the system (compositions, vapor and liquid flow rates, liquid holdup in all stages at every instant, tray hydraulics, energy balances, and vapor−liquid equilibrium data).

However, the system at hand is an ideal generic reactive distillation with simple ideal vapor−liquid equilibrium, reaction kinetics, and physical properties. The model is based on dynamic mass balance, while the energy equations are neglected by assuming a constant molar overflow except in the reactive zone. The vapor flow rate increases through the reactive zone because of the cumulative effect of exothermic reactions in all of the reactive stages

$$V_i = V_s + \frac{\lambda}{\Delta H_v} \sum_{k=1}^{i-N_S-1} R_{N_S+1+k} \tag{1}$$

where V_s is the constant vapor boilup (kmol/s) from the stripping section and V_i is the vapor flow rate (kmol/s) on tray i in the reactive zone. λ is the exothermic heat of reaction (cal/mol), and ΔH_v is heat of vaporization (cal/mol). R_i is the reaction rate (kmol/s) on tray i, which is given by

$$R_i = M_i(k_{F,i}x_{A,i}x_{B,i} - k_{B,i}x_{C,i}x_{D,i}) \tag{2}$$

where M_i is the liquid holdup (kmol) on tray i. $k_{F,i}$ and $k_{B,i}$ are the forward and backward specific rates [kmol/s·kmol] on tray i, which are evaluated according to the Arrhenius equations. The liquid dynamics in the reactive zones are modeled by the Francis−Weir formula. The details of a rigorous dynamic model of the system can be found in work by Al-Arfaj and Luyben.[2] For the purpose of this work, the set of nonlinear equations that describe the reactive distillation system under study are decoupled to separate all-state variables. The decoupled equations are reconstructed into a more compact nonlinear state-space model

$$\mathrm{d}\mathbf{X}(t)/\mathrm{d}t = f[\mathbf{X}(t),\mathbf{U}(t),\mathbf{d}(T);\theta] \tag{3}$$

$$\mathbf{Y} = h[\mathbf{X}(t);\theta] \tag{4}$$

where the vector $\mathbf{X}$ of length $5N$ is of state variables (liquid mole fractions and holdup in all stages including the partial reboiler and total condenser). θ is the model parameter. $\mathbf{U}$ is the vector of manipulated input variables, which could be the vapor boilup, reflux flow rate, reflux ratio, or distillate or bottoms flow rate depending on the control structure in consideration. The sources of disturbance are feed flow rates and compositions. The source of measurable disturbances is the two feed flow rates and compositions, i.e., $\mathbf{d} = (F_A, F_B, Z_a, Z_b)^T$. $\mathbf{Y}$ is a vector of measured output variables.

2.2. Linear Dynamic Model. Because of the complexity, computational burden, and desire to obtain an approximate model for control purposes, it is necessary to develop a linear model that captures the essential elements of the system dynamics. Linearization of nonlinear equations 3 and 4 is carried out by using Taylor series expansion. This implies that the nonlinear equations of reactive distillation are approximated by a truncated Taylor series approximation around the steady-state operating conditions

$$f(\mathbf{X}) = f(\bar{\mathbf{X}},\bar{\mathbf{U}}) + \frac{\partial f}{\partial \mathbf{X}}(\mathbf{X} - \bar{\mathbf{X}}) + \frac{\partial f}{\partial \mathbf{U}}(\mathbf{U} - \bar{\mathbf{U}}) + \frac{\partial f}{\partial \mathbf{d}}(\mathbf{d} - \bar{\mathbf{d}}) \tag{5}$$

$$\mathbf{Y}(\mathbf{X}) = h(\bar{\mathbf{X}}) + \frac{\partial h}{\partial \mathbf{X}}(\mathbf{X} - \bar{\mathbf{X}}) \tag{6}$$

In eq 5, $f(\mathbf{X})$ is a derivative of a $5N \times 1$ vector with respect to a $5N \times 1$ state vector, a $P \times 1$ input vector, and a $m \times 1$ disturbance vector.

The steady-state condition corresponds to $f(\bar{\mathbf{X}},\bar{\mathbf{U}}) = 0$ and $h(\bar{\mathbf{X}}) = 0$. Thus, the deviation variables arise naturally out of the Taylor series expansion. Hence, the

linearized state-space model in terms of deviation variables is

$$\frac{d\hat{x}}{dt} = \mathbf{A}\hat{x} + \mathbf{B}\hat{u} + \mathbf{E}\hat{d} \tag{7}$$

$$\hat{\mathbf{Y}} = \mathbf{C}\hat{x} \tag{8}$$

where the superscript "∧" denotes the change in the variable from the linearization point. Constant matrices **A**, **B**, **C**, and **E** are evaluated at the desired steady-state operating conditions. The detailed formulation of a linearized state-space model for the system in consideration is contained in work by Olanrewaju and Al-Arfaj.[11] Thus, the vector of the state variables can be evaluated by

$$\mathbf{X}(t) = \bar{\mathbf{X}} + \hat{\mathbf{X}}(t) \tag{9}$$

where $\bar{\mathbf{X}}$ is the vector of the state variables at their base steady-state values and $\hat{\mathbf{X}}(t)$ is the solution of eq 7.

3. Base Steady-State Design Data

The kinetics, physical properties, and vapor−liquid equilibrium data for an ideal reactive distillation under consideration can be found in the work of Luyben.[12] Olanrewaju and Al-Arfaj[11] slightly modified the optimum design proposed by Luyben[12] to ensure open-loop stability at the required state when no disturbance is introduced. This work uses that modified optimum design. An equal stoichiometric amount of fresh feed flow rate of 0.0126 kmol/s is used for both reactants A and B. The conversion and purity are fixed at 95%. The initial holdup in each tray is 1 kmol. The column has seven stripping trays, six reactive trays, and seven rectifying trays. The operating pressure is 9 bar.

4. Control Structures

The operation of a multivariable processlike reactive distillation column has to satisfy several control objectives. Typical objectives are to ensure the stability of the process, to produce specified products, and to optimize the operation economically. Because the various objectives may be of quite different importance and normally require different control actions, it is usually desirable to explore a wide variety of control structures in order to meet different objectives.

Three control structures are explored to compare and assess the closed-loop performance of a linearized model with that of a nonlinear model. All structures are single-input−single-output (SISO) structures with PI controllers except in level controls where P-only controllers are used. For each controller, a relay feedback test[13] is employed to obtain the ultimate gain and frequency. The controllers are tuned using the Tyreus−Luyben tuning method.[14] The design of inventory controllers is carried out first. The pressure is controlled by heat removal from the condenser. The assignment of manipulated variables for level controllers is based on the principle of choosing the stream with the most direct impact.[15] The base level is controlled by manipulating the bottoms flow rate, while the reflux drum level could be controlled by manipulating either the distillate flow rate or the reflux flow rate. All of the valves are designed to be half open at the initial steady state. Two measurement lags of 30 s each are used in all composition or temperature loops.

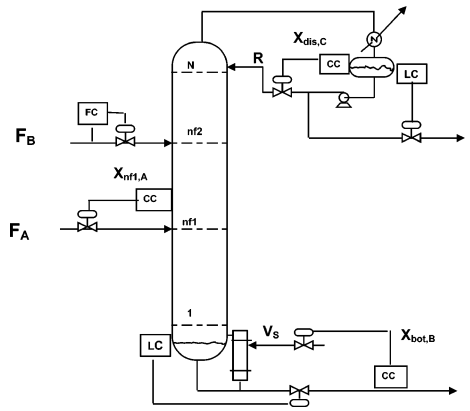

Figure 2. Dual-end composition control structure.

All of the three control structures considered use a composition analyzer in the reactive zone as proposed by Al-Arfaj and Luyben[2] to detect the inventory of one of the reactants so that fresh feed can be manipulated to balance the reaction stoichiometry. The concentration of reactant A on the first tray of the reactive zone (numbered from the bottoms) is controlled by manipulating the reactant A fresh feed flow rate. Three types of disturbances are investigated as follows:

1. Change in feed flow rate of component B (F_B): in this disturbance, F_B is increased by 10% and 20% and decreased by 20%. This disturbance is applied to all of the control structures.

2. Feed composition of reactant B: the reactant B feed is 100% mol of B. This feed composition disturbance will introduce reactant A in the feed composition of reactant B (Z_b). Two magnitudes are used: $\Delta Z_b = 5\%$ (where the feed of reactant B becomes 95% mol of B and 5% mol of A). $\Delta Z_b = 10\%$ (where the feed of reactant B becomes 90% mol of B and 10% mol of A). This disturbance is applied to all control structures.

3. Setpoint changes: in this disturbance, the composition setpoint of the composition controller is changed from 95% mol of D in the bottoms to 92% and 98%. This is applied to the first two control structures (see sections 4.1 and 4.2). For the third control structure (section 4.3), temperature setpoint changes of ±2 K are tested.

4.1. Control Structure I. Figure 2 shows a dual-end composition control structure. The reflux drum level is controlled by manipulating the distillate flow rate. The purity of both products is maintained at 95%. In the distillate products, the composition of component C in the distillate is controlled by manipulating the reflux flow rate from the condenser, while the bottoms composition of component D is controlled by manipulating the vapor boilup.

Various magnitudes of disturbance in the feed flow rate and feed composition are studied to assess the closed-loop performance of this control structure based on linear and nonlinear models. Figure 3 shows the response of the system for −20%, +10%, and +20% changes in the feed flow rate of reactant B (F_B). Two curves are shown in each of the plots comparing the closed-loop performance of this control structure when a linear model is used to that when a rigorous nonlinear model is applied. The results show that this control structure is able to reject the load disturbance effectively with the two models. While the responses of controlled variables in both models show an excellent agreement, the responses of manipulated variables in a linear model show a slight variation from that of a nonlinear model

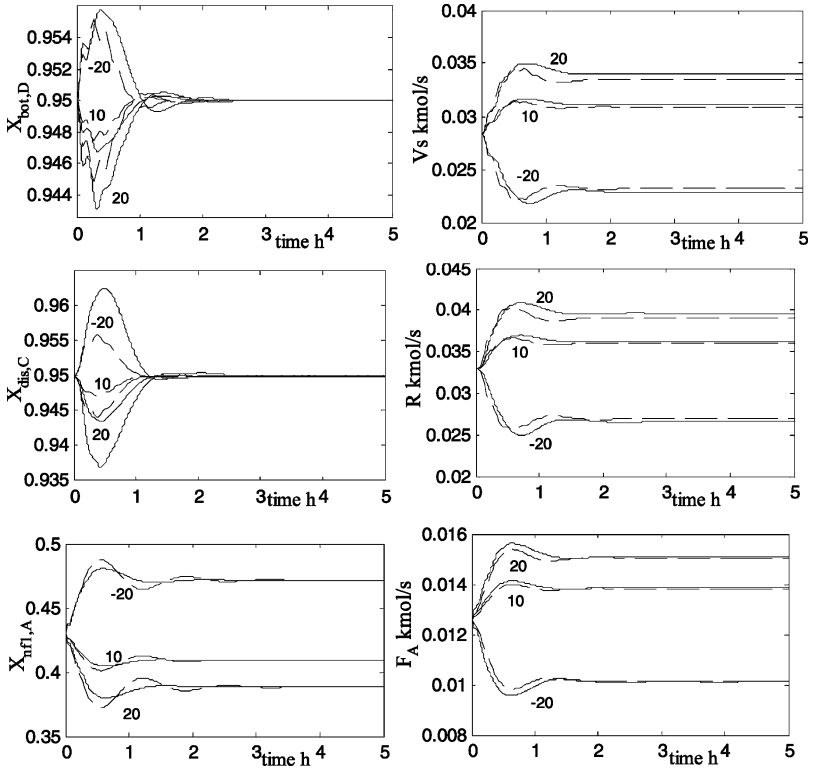

Figure 3. Dual-end composition control responses, −20%, +10%, and +20% F_B: (- - -) linear model; (—) nonlinear model.

in an attempt to satisfy the same control objectives. This variation is seen to increase with an increase in the magnitude of the disturbance.

Under open-loop operation where only level inventories are controlled, the process will drift from the base steady state to a lower conversion state when F_B is decreased with small magnitude and will be unstable at higher magnitude of the disturbance.[16] The linearized model will not predict this drift because it is a nonlinear feature of the process. Even though the drift will not take place in the closed-loop scenario because the controllers will adjust the manipulating variables to maintain product purity, the process dynamics during the transit region will not be properly described in the linear model. The open-loop stability of the nonlinear model must be investigated before the linearized model is used in model-based control applications. The use of a linear model is inappropriate if the system is open-loop pseudostable (drifts to another steady-state region) or unstable under disturbance.

Figure 4 compares the closed-loop performance of a linear model to that of a nonlinear model when 5% and 10% impurities of A are introduced in the feed composition of F_B. Under open-loop operation, introducing reactant A impurities in reactant B feed allows the process to drift sharply to another state at lower impurity magnitudes and destabilizes the process completely at higher magnitudes of impurity.[16] Even though the composition controllers are able to meet the control objective of rejecting the feed composition disturbance, the response of a linear model is seen to be slower than that of a nonlinear model, thus making the time to reach the desired steady state longer than that when the controller is designed based on a linear model. The performance of this structure deteriorates with an increase in the magnitude of the disturbance when a linear model is used. Again, this shows the inapplicability of the use of linear models in control system design when the process is open-loop pseudostable or unstable under certain disturbances where the linear process model could not describe the nonlinear process behavior.

Figure 5 shows the responses of composition controllers with setpoint changes in the composition of component D in the bottoms product for both closed-loop linear and nonlinear models. The results show that setpoint changes by decreasing the bottoms purity from 95% to 92% or increasing the purity from 95% to 98% can be handled. The composition controllers appear to be effective and robust with both linear and nonlinear models.

The results shown in Figures 3−5 point toward an interesting observation. The control system when controllers are designed based on a linear process model can achieve the control objectives but would typically underestimate some or all of the input characteristics (the magnitude, the rate, and the speed of change of manipulated variables) when the process is open-loop pseudostable or unstable under the influence of disturbance. Even though the controlled variable will eventually settle to the required level, the manipulated variable may differ not only in the transit region but also in the amount required to get the controlled variable to the required level. If the resulting manipulated variables from the two models are comparable, then this underestimation in the input characteristics could be overcome by properly designing the control valves to be more aggressive than what would otherwise be designed based on the closed-loop performance of linear models.

4.2. Control Structure II. Although a dual-end composition control structure might have the advantage of energy savings, the additional expenses and the risk associated with designing and operating a more complex control system may not be justified in some systems where a single-end control system is feasible. The single-end composition control loop is a simple SISO system,

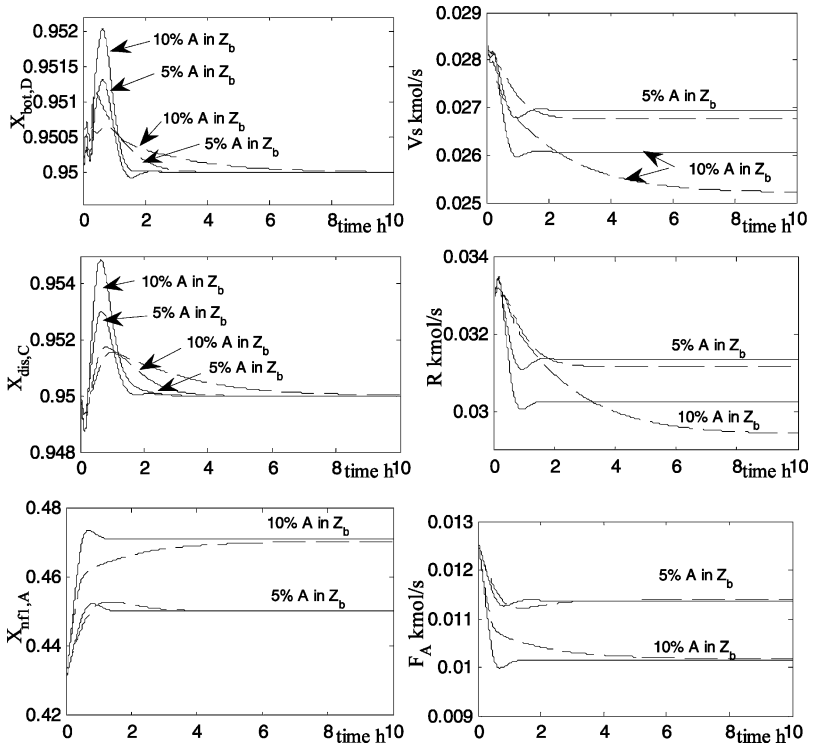

Figure 4. Dual-end composition control responses, 5% and 10% mol of reactant A in Z_b: (- - -) linear model; (—) nonlinear model.

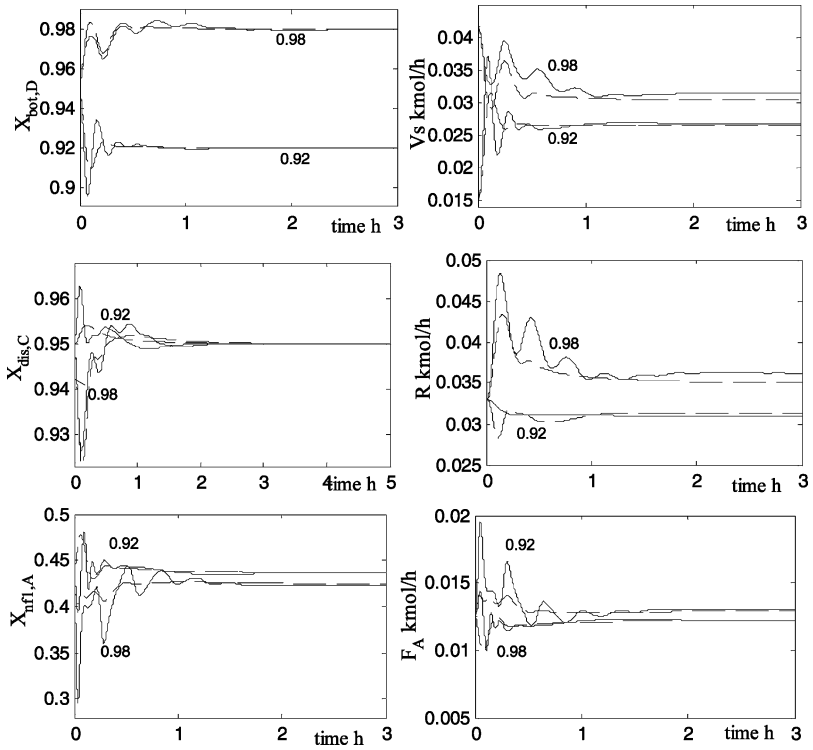

Figure 5. Dual-end composition control responses, setpoint changes $X_{bot,B}$ from 95% to 92% and 98%: (- - -) linear model; (—) nonlinear model.

so it can be easily tuned and give a faster response because of the reduced effect of loop interaction.

To further assess the impact of open-loop stability on the extendibility of control systems designed based on linear models, various control arrangements of the reflux drum level are investigated when the distillate product is not controlled. Three level control schemes are considered as follows:

1. Scheme 1: the reflux ratio is fixed, and the reflux drum level is controlled by the reflux flow rate.

2. Scheme 2: the reflux ratio is fixed, and the reflux drum level is controlled by the distillate flow rate.

3. Scheme 3: the reflux flow rate is fixed, and the reflux drum level is controlled by the distillate flow rate.

As discussed in section 4.1, a reduction on F_B by 20% destabilizes the system under the open-loop operation when both the reflux flow rate and vapor boilup are kept constant. Scheme 3 is mimicking that open-loop scenario because the reflux flow rate is kept constant, while the other two schemes are not because the reflux flow rate

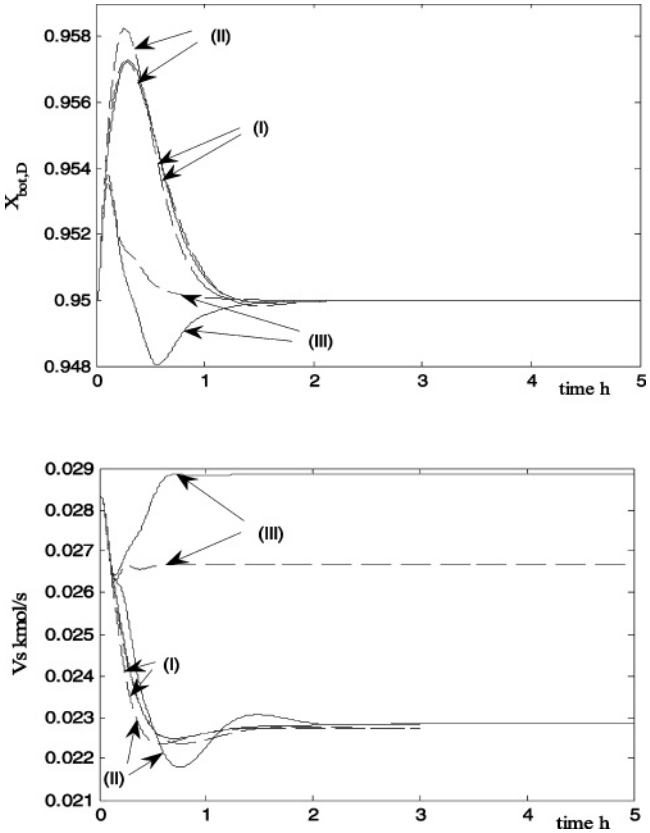

Figure 6. Three alternative control schemes for a single-end control structure: (I) fixed reflux ratio and control level by the reflux flow rate; (II) fixed reflux ratio and control level by the distillate flow rate (D); (III) fixed reflux flow rate and control level by the distillate flow rate.

will vary to fix the reflux ratio. Therefore, it is expected that the linear process model will be useful for schemes 1 and 2 but will not be appropriate to use for scheme 3 because of the open-loop instability.

Figure 6 shows the closed-loop response based on the two process models for the three schemes when a 20% reduction in F_B is introduced. The result in Figure 6 indicates that the process performances under Figures 1 and 2 are essentially similar and the control response of both linear and nonlinear models are close and comparable. Therefore, which of the flow rates is used to control the drum level when the reflux ratio is fixed is not critical. This result also indicates that fixing the reflux ratio is more suitable when single-end control is used because it filters the disturbance impact on the system.

When the reflux flow rate is fixed (scheme 3) instead of the reflux ratio, a different behavior is observed. Fixing the reflux flow rate will not filter the disturbance impact to the system and thus could destabilize the system if the process is operated at a critical region of stability. Similar to the observation in section 4.1 about the impact of open-loop stability on the closed-loop performance based on linear models, it is shown in Figure 6 that the response of the linear system when the reflux flow rate is kept constant is not matching the nonlinear response in the transit region. The prediction of the manipulated variable behavior from the linear model completely misses the trajectory suggested by the nonlinear model. The reason for this behavior is the fact that the system drifts to another state at this disturbance and the nonlinear model will calculate the

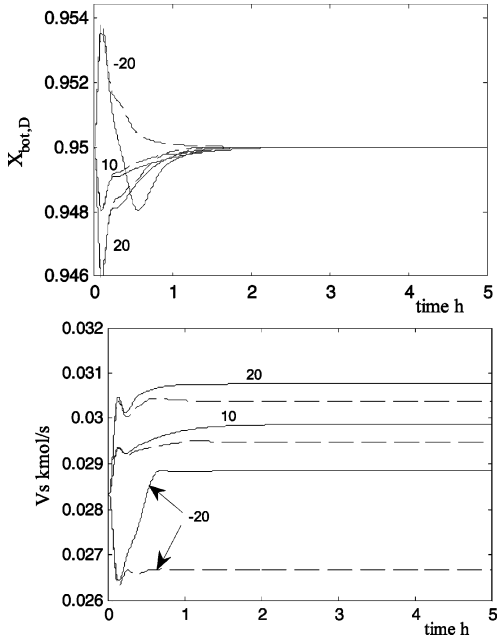

Figure 7. Singe-end composition control responses based on scheme 3 with −20%, +10%, and +20% disturbances in F_B: (- - -) linear model; (—) nonlinear model.

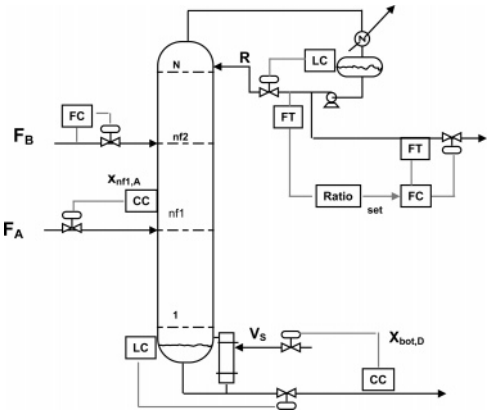

Figure 8. Single-end composition control structure.

required input to get the product purity to the required level from the new state. Because the linear model cannot predict the drift, the trajectory suggested by the linear model does not take this into consideration, which resulted in this inappropriate prediction of the transit behavior. In such a case, we cannot use the linear model as a basis for developing the control system of the process. On the other hand, when the change in F_B is made in the positive direction, the system is open-loop stable even with the fixed reflux flow-rate configuration, and consequently it is expected that the performance based on the linear model will be similar to that based on the nonlinear model. A comparison of the performance based on the two models for this disturbance is shown in Figure 7, which is in line with our expectations.

The scheme 1 configuration is considered in detail to compare the closed-loop performance based on a linear model to that based on a nonlinear model for the single-end composition control structure. Figure 8 shows the single-end composition control structure based on the scheme 1 configuration. The composition of component D in the bottoms product is controlled by adjusting the vapor boilup. Figure 9 shows the performance of this

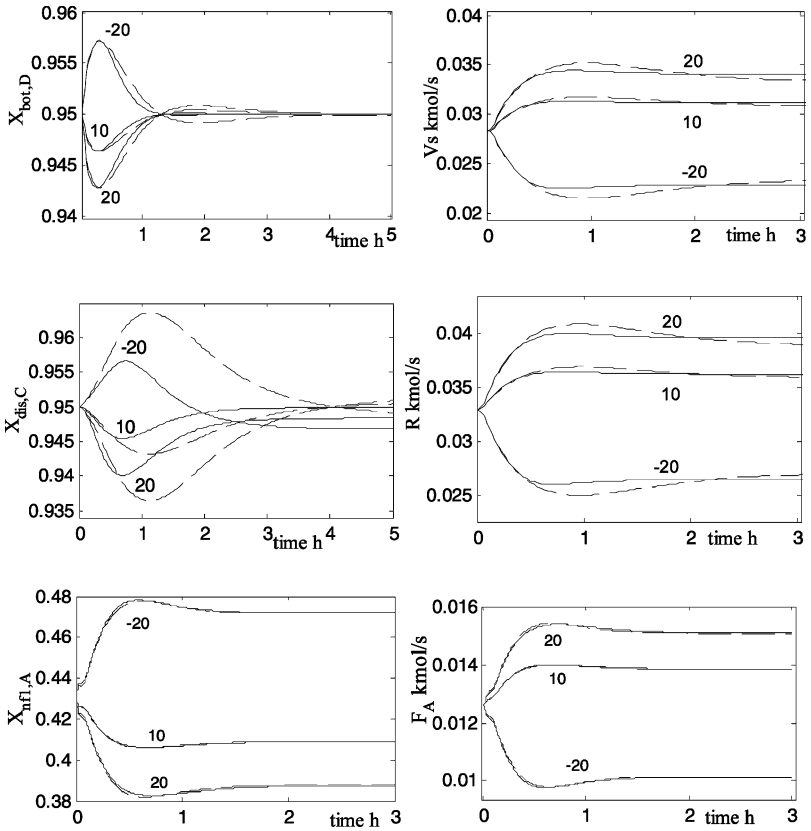

Figure 9. Singe-end composition control responses, −20%, +10%, and +20% F_B: (- - -) linear model; (—) nonlinear model.

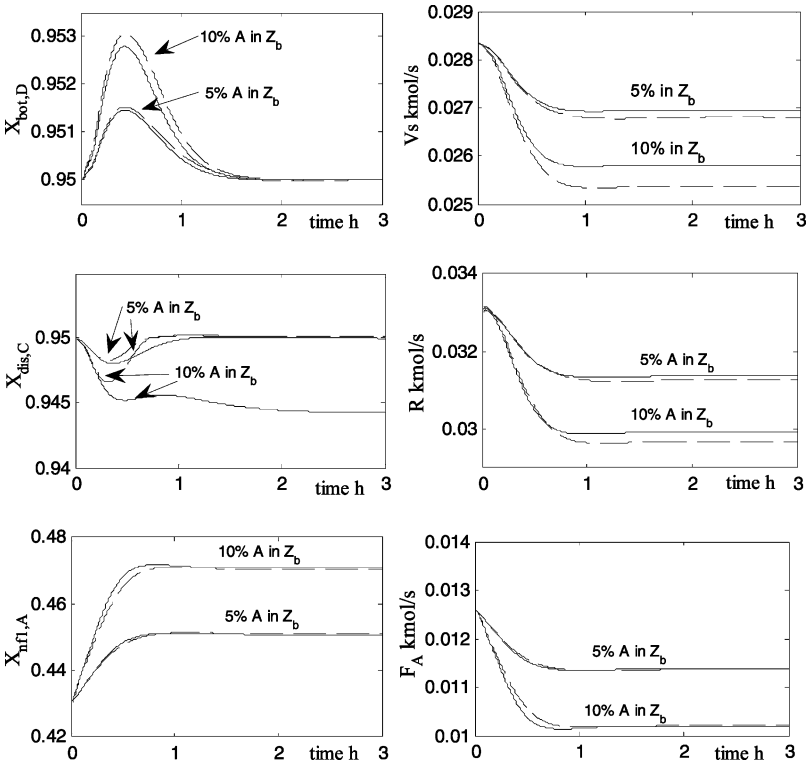

Figure 10. Single-end composition control responses, 5% and 10% mol of A in Z_b: (- - -) linear model; (—) nonlinear model.

control structure when F_B is increased by 10% and 20% and reduced by 20%. The responses from both controlled and manipulated variables when an approximate linear model is used are in agreement with those when a rigorous nonlinear model is used. The results demonstrated that changes in throughput can be handled using a linear model. The response of the distillate product composition of component C exhibits some variation from that of a nonlinear model because it is not controlled, and this difference increases greatly with an increase in the disturbance magnitudes. This is expected because the two models are not identical.

Figure 10 shows that a single-end composition control structure could also provide an effective regulatory

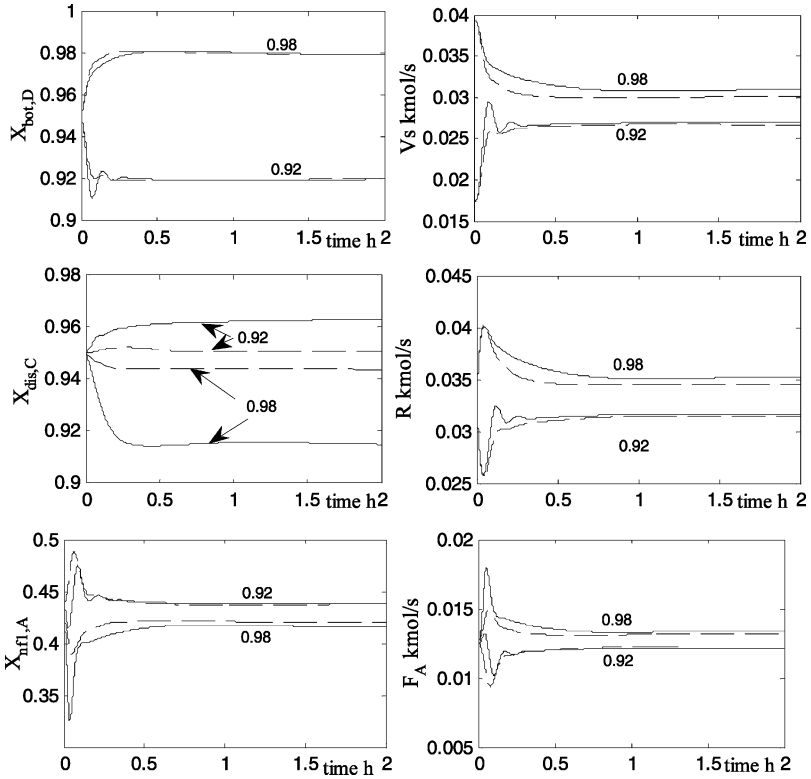

Figure 11. Single-end composition control responses, setpoint changes $X_{bot,B}$ from 95% to 92% and 98%: (- - -) linear model; (—) nonlinear model.

control of the process when impurities of A are introduced in the feed composition of the reactant B stream. The linear process model demonstrates a better performance in feed composition disturbance rejection in the single-end composition control structure than in the dual-end control (compare the results shown in Figure 8 to those shown in Figure 4). Figure 11 compares the closed-loop performance based on the linear and nonlinear models to that based on changes in the setpoint of the bottoms purity specification. The results demonstrate that a very high purity of the bottoms product could be achieved with a single-end controller by changing the setpoint from 95% to 98%.

4.3. Control Structure III. Because the direct composition control structures discussed in the above sections inevitably require the use of an expensive and unreliable composition analyzer, it is important to study how the linear model will behave when a simple temperature control system is used. The temperature sensor is typically fast, inexpensive, and reliable. It could provide an indirect measurement of the composition. Figure 12 shows a single-end temperature control structure. The reflux drum level is controlled by adjusting the reflux flow rate, while the reflux ratio is kept constant by changing the distillate flow rate. Because the control objective of this structure is to maintain the product composition as close as possible to its desired specification, the temperature measurement is placed on the most sensitive tray in the stripping section. The temperature on tray 2 (numbering from the bottoms) is measured and controlled by manipulating the vapor boilup.

Figure 13 compares the closed-loop performance of this control scheme using a linear model to that using a rigorous nonlinear model with different magnitudes of disturbance in the feed flow rate of reactant B. The

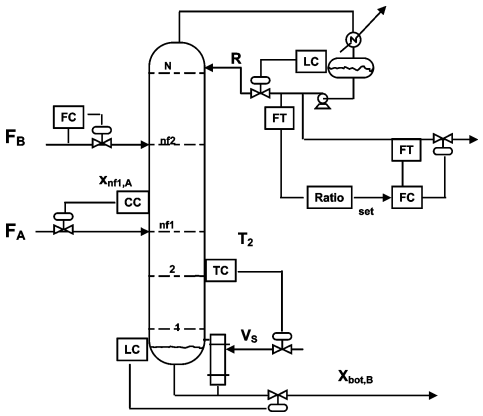

Figure 12. Single-end temperature control structure.

results demonstrate that the temperature control performs well by keeping the purity of the bottoms product as close as possible to the desired value. The system responses under this control structure to feed composition disturbances are shown in Figure 14. Even though the bottoms purity is not maintained exactly at the desired level, this control structure is able to reject feed composition disturbances by keeping the bottoms purity within reasonable bounds using a linear process model. Note that there is a significant difference between the responses of linear and nonlinear process models for component C in the distillate product because it is not controlled. This signifies that the use of a linear model in a single-end control structure could be restricted to a chemical system where the purity of one component is desirable. Alternatively, the process could be designed with a higher uncontrolled product purity to compensate for any inferior control performance.

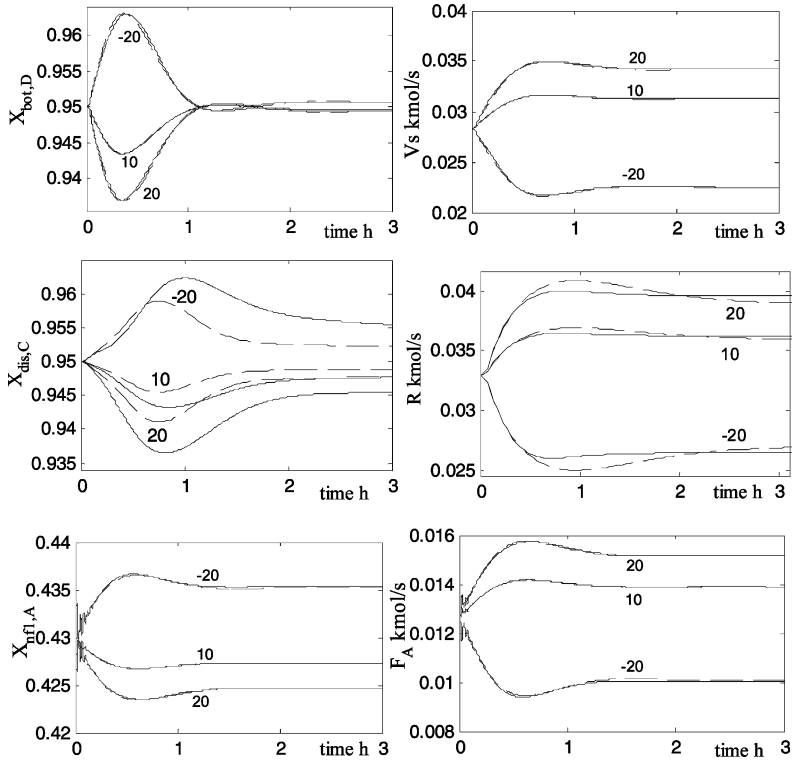

Figure 13. Singe-end temperature control responses, −20%, +10%, and +20% F_B: (- - -) linear model; (—) nonlinear model.

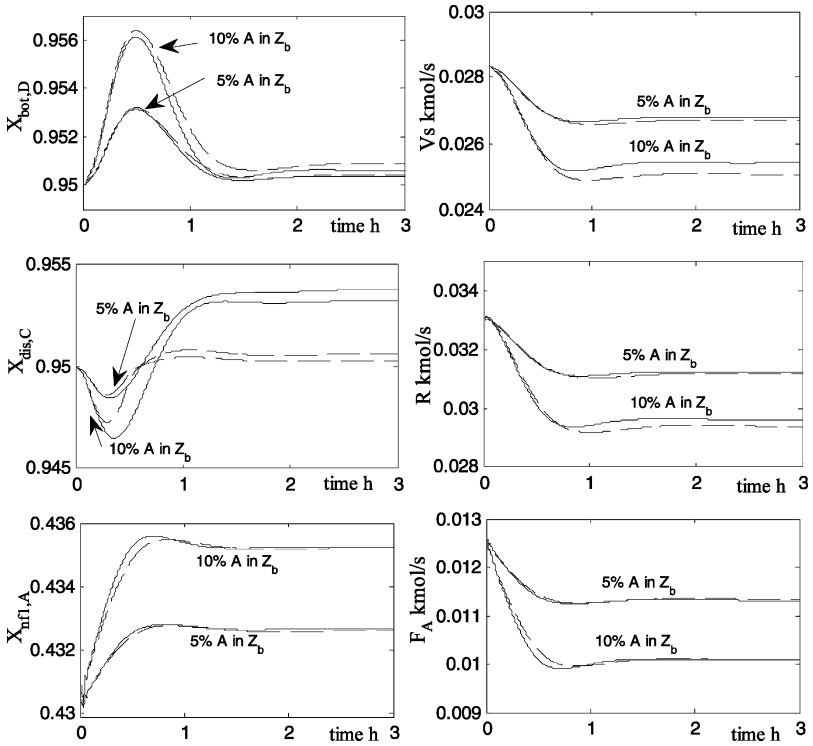

Figure 14. Singe-end temperature control responses, 5% and 10% mol of reactant A in Z_b: (- - -) linear model; (—) nonlinear model.

The dynamic responses of the two models for ±2 K step changes in the temperature are shown in Figure 15. These results demonstrate that the temperature setpoint changes can be easily handled and the system responses of a linear model are comparable to those of a nonlinear model. An increase in the temperature causes the controller to increase the vapor boilup, and more heat is available to overpurify the bottoms product. The distillate purity changes in the opposite direction as expected. On the other hand, a decrease in the temperature results in a decrease in the amount of vapor boilup. The effects are an increase in the impurity in the bottoms and overpurification of the distillate product.

All of the responses of a linear model using this structure show a good agreement when compared to the responses of a nonlinear model under the same control structure. The exception is in the distillate purity, where

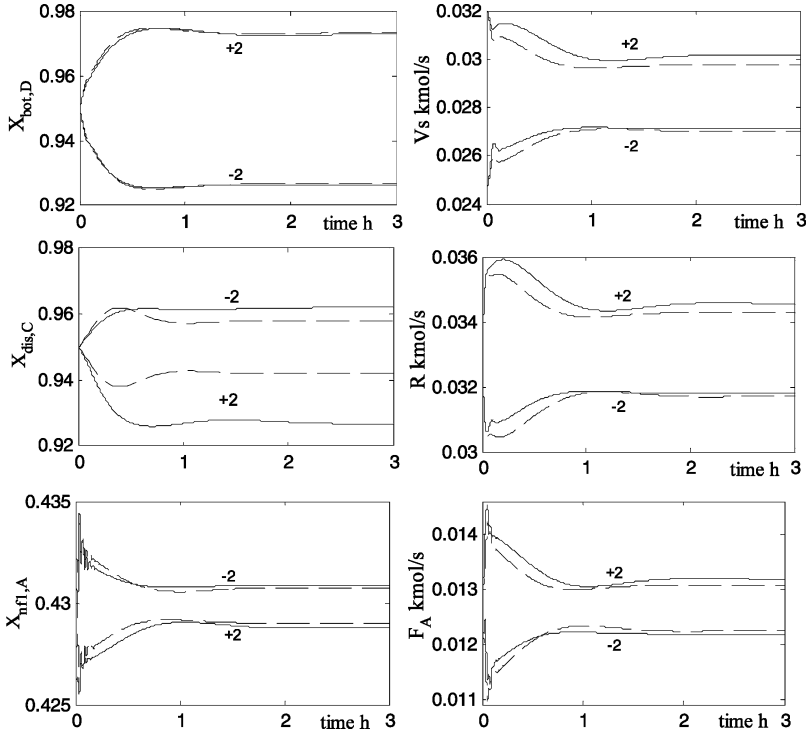

Figure 15. Singe-end temperature control responses, ±2 K changes in temperature on tray 2: (- - -) linear model; (—) nonlinear model.

the difference in the responses of the two models becomes increasingly significant with an increase in the disturbance magnitude because that purity is not controlled.

4.4. General Comparisons and Observations. Probably the most important finding of this work is the robustness and the extendibility of the control system when designed based on a linear process model. It is found that the linear process model could be used to develop a robust control system provided that the control valves are conservatively designed to compensate for the underestimation of the input characteristics by the linear model. That control system will be valid only if it is applied in the operating region where the model is linearized around and if the process is open-loop stable under disturbance. If the process shifts to another operating region for whatever reasons, then the process model must be linearized around the new operating region. This observation would be useful for the model-based control applications.

Comparing the closed-loop performance of linear and nonlinear models in a single-end (composition or temperature) control structure with that of dual-end composition control as discussed in section 4.1 reveals that the use of a linear model in a single-end control structure gives a better agreement with the nonlinear model than when the linear model is used in dual-end composition control. The responses of both controlled and manipulated variables for the two models in single-end control structure are in better agreement when compare to that in dual-end composition control. The responses of the system with single-end control are also faster than the responses of the system with dual-end composition control. This could be due to an increase of nonlinearity in the system with a dual-end control structure, which results from increased loop interactions. The single-end control suffers the ability to precisely control the uncontrolled end, but this could be compensated for by overdesigning the process (design at higher product purity). It is found that fixing the reflux ratio scheme in a single-end control structure provides better disturbance filtration and process dynamics.

5. Conclusion

In this paper, we have compared the closed-loop performance of three control structures when based on an approximate linear process model to that when based on a nonlinear process model for a generic two-product reactive distillation. The control structures examined are dual-end composition control, single-end composition control, and single-end temperature control. All of the structures use a composition analyzer in the reactive zone to detect the inventory of one of the reactants so that the fresh feed can be manipulated to balance the reaction stoichiometry.

It is shown that an approximate linear model behaves reasonably well compared to a nonlinear model in a closed-loop system when a disturbance in the process variables is introduced provided that the system is open-loop stable under that disturbance. Most of the responses of a closed-loop linear model using three alternative control structures show good agreement when compared to the responses of a closed-loop nonlinear model under the same process conditions. It is also shown that the performance of a linear model is better in a single-end control system than in a dual-end control system. It is generally recommended to fix the reflux ratio and not the reflux flow rate in the single-end control schemes. Further studies will focus on the application of a linear model for composition estimation in a model-based control system, which addresses the problem of using an expensive and unreliable composition analyzer in the control of reactive distillation.

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Nomenclature

A = reactant component
A = matrix of state variables of the linearized process
B = matrix of inputs of the linearized process
B = reactant component
B = bottoms flow rate (kmol/s)
C = matrix of outputs of the linearized process
C = product component
d = disturbance variables vector
$\bar{\mathbf{d}}$ = steady-state disturbance variables vector
F_A = fresh feed flow rate of reactant A (kmol/s)
F_B = fresh feed flow rate of reactant B (kmol/s)
K_F = specific reaction rate of the forward reaction (kmol/s·kmol)
K_B = specific reaction rate of the reverse reaction (kmol/s·kmol)
M_i = liquid holdup in all stages (kmol)
N = total number of stages including the reboiler and reflux drum
N_{RX} = number of reactive trays
N_R = number of rectifying trays
N_S = number of stripping trays
nf1 = first tray of the reactive section (entrance of feed F_A)
nf2 = last tray of the reactive section (entrance of feed F_B)
R = reflux flow rate (kmol/s)
T_i = temperature in tray i (K)
R_i = rate of production on tray i (kmol /s)
U = input variables vector
$\bar{\mathbf{U}}$ = steady-state input variables vector
V_i = vapor flow rate from tray i (kmol/s)
V_s = vapor boilup from the reboiler (kmol/s)
$X_{bot,D}$ = composition of D in the bottoms
$X_{dis,C}$ = composition of C in the distillate
$X_{nf1,A}$ = composition of A in tray nf1
$X_{nf1,B}$ = composition of B in tray nf2
$\bar{\mathbf{X}}$ = steady-state values vector
$\hat{\mathbf{X}}(t)$ = state variable at time t
Z_a = composition of fresh feed F_A
Z_b = composition of fresh feed F_B
α_j = relative volatility of component j with respect to the heavy component
ΔH_v = heat of vaporization (cal/mol)
λ = heat of reaction (cal/mol)

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