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Reduced Order Modeling of High Purity Distillation Columns for Nonlinear Model Predictive Control

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***Abstract*— Fundamental dynamic models of distillation columns are not well suited for incorporation into nonlinear model predictive control schemes due to their high state dimension. We investigate two reduced order nonlinear modeling techniques for high purity distillation columns. Compartmental and nonlinear wave models developed for a nitrogen purification column are compared to a rigorous dynamic simulator to assess the relative tradeoffs between prediction accuracy and computational complexity. The utility of each reduced order modeling technique for nonlinear model predictive control of high purity distillation columns is discussed.**

I. INTRODUCTION

Fundamental models of distillation columns are comprised of stage-by-stage mass and energy balances combined with hydraulic relations for the liquid holdup on each stage. Such dynamic models usually are too complex to be utilized for real-time control due to their high dimensionality. A distillation column with N stages and n components is described by $N(n+1)$ differential equations plus algebraic equations for the hydraulic relations. Even under simplifying assumptions such as a binary (or pseudo-binary) mixture, equal molar overflow and constant molar holdup, N differential equations are required to model the column dynamics. For high purity distillation columns such as nitrogen purification columns with 50 stages and ethane/ethylene splitters with 100 stages, the high model dimension is a major obstacle to nonlinear controller design.

Nonlinear model predictive control (NMPC) is an extension of linear model predictive control in which a nonlinear model is utilized to describe the process dynamics [1]. Temporal discretization of the dynamic model equations produces a set of nonlinear algebraic equations that invariably introduce non-convexities in the NMPC optimization problem. Because the control moves are generated by real-time solution of a non-convex nonlinear program at each sampling period, computational effort is inextricably linked to the complexity of the controller design model. While recently proposed solution techniques allow the application of NMPC to column models of moderate complexity [2], there remains considerable motivation to develop reduced order column models that provide a more favorable tradeoff between prediction accuracy and computational effort.

We investigate two techniques that allow the derivation of reduced order distillation column models directly from fundamental models. Nonlinear wave models are based on the premise that the column concentration or temperature profile can be described by a wave front with constant pattern [3], [4], [5], [6]. Column dynamics attributable to disturbances such as feed flow rate and concentration changes are described by the movement of this profile. Mathematical expressions for the wave propagation velocity and the profile shape can be derived from differential material balances for an infinitely long packed column [5]. The derivation requires several simplifying assumptions including equal molar overflow and constant molar holdup. For each column section delimited by feed and withdrawal streams, the model includes a single nonlinear differential equation for the wave position in that section and nonlinear algebraic equations for the wave profile and vapor-liquid equilibrium relations.

Compartmental [7] and aggregate [8] models are based on the assumption that the dynamics of an individual separation stage are significantly faster than the dynamics of a column section comprised of many stages. The column is divided into a number of compartments and the balance equations for one stage in each compartment are replaced with balance equations written for the entire compartment [8]. Through the application of singular perturbation theory [9], this full-order model is reduced to a compartmental model consisting of a single differential equation for each compartment balance and algebraic equations for the individual stage balances. The complexity of the compartmental model is determined by the type of balance equations included in the full order model and the number of compartments utilized.

The remainder of the paper is organized as follows. The nitrogen purification column used as the basis for this study is described in Section II. Nonlinear wave and compart-

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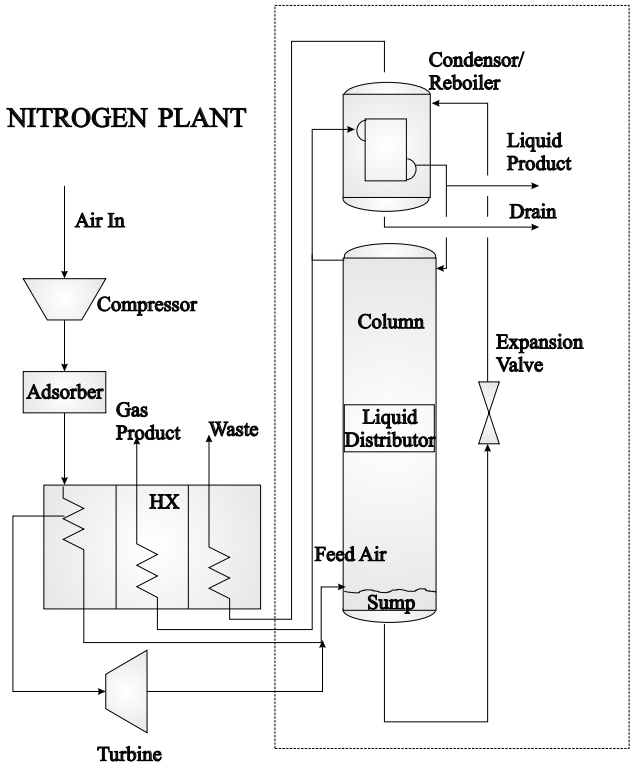

Fig. 1. A typical nitrogen production plant.

mental models developed for this very high purity column are compared to a rigorous dynamic simulator in Sections III and IV, respectively. A summary and conclusions are provided in Section V.

II. NITROGEN PURIFICATION COLUMN

Our research has focused on the nitrogen production plant depicted in Figure 1. The feed air stream is compressed and cooled by column waste and product streams in a multi-pass heat exchanger. A portion of the feed stream is expanded across a turbine to provide additional cooling. The combined feed stream is introduced to the bottom of a packed distillation column with 42 theoretical stages. A liquid distributor located in the middle of the column is used to improve flow characteristics of the descending liquid. The bottom liquid stream is expanded across a valve and partially liquified to produce a two-phase stream with a lower temperature than the overhead stream. In the combined condenser/reboiler the partially liquified bottom stream is vaporized and the nitrogen vapor stream from the top of the column is condensed to produce the reflux stream and liquid nitrogen product stream. A portion of the overhead stream is withdrawn as the gaseous product.

Aspen Dynamics (Aspen Technology) was used to develop a rigorous dynamic simulation of the equipment located inside the dashed line of Figure 1. The Aspen model includes ternary component balances and energy balances as well as hydraulic relations for each of the 42 separation stages. Detailed descriptions of the expansion value and the combined condenser/reboiler also are included. Thermodynamic property data for the major air components (nitrogen, oxygen and argon) were provided by Praxair. Equipment specifications and the nominal operating point were obtained from a typical Praxair nitrogen plant. To evaluate the reduced order models over a range of operating conditions, two other steady states corresponding to feed flow rate changes $\pm$ 10 kmol/hr from the nominal value also were investigated. The Aspen model was used as a surrogate for the nitrogen plant in our simulation studies.

III. NONLINEAR WAVE MODEL

Model Formulation

We previously developed a nonlinear wave model for the nitrogen purification column by augmenting the wave velocity equation with detailed mass and energy balances for the combined condenser/reboiler [10]. A pseudo-binary mixture is obtained by lumping nitrogen and argon into a single component with the thermodynamic properties of nitrogen. The wave model is based on several simplifying assumptions including constant molar overflow, constant molar holdup and constant relative volatility. Only a single differential equation is required to describe the composition wave dynamics, while the remaining seven differential equations account for auxiliary equipment such as the condenser/reboiler system. Although the condenser holdup is approximately 50% of the total column holdup, we recently found that prediction errors introduced by neglecting condenser dynamics are negligible compared to errors caused by the assumptions listed above. By omitting the condenser/reboiler equations, the NMPC design problem is simplified considerably.

The oxygen vapor composition y is described by the wave profile equation [5]:

$$y(z) = y_{min} + \frac{y_{max} - y_{min}}{1 + exp[\gamma(z - s)]} \tag{1}$$

where $z \in [0, 1]$ is the dimensionless distance along the column with z = 0 representing the bottom; s is the wave position; γ is the wave slope; and y_{min} and y_{max} are lower and upper asymptotic limits, respectively. The simplified wave model that results from neglecting the condenser/reboiler dynamics is:

$$\frac{ds}{dt} = \frac{1}{N_t} \frac{-L(x_{in} - x_{out}) + qF(y_{out} - y_{in})}{n_l(x_{in} - x_{out}) + n_v(y_{out} - y_{in})} \tag{2}$$

$$y_{out} = y_{min} + \frac{y_{max} - y_{min}}{1 + exp[-\gamma(1 - s)]} \tag{3}$$

$$y(0) = y_{min} + \frac{y_{max} - y_{min}}{1 + exp(\gamma s)} \tag{4}$$

$$x_{out} = \frac{y(0)}{\alpha - (\alpha - 1)y(0)} \tag{5}$$

$$y_{in} = \frac{\alpha x_f}{1 + (\alpha - 1)x_f} \tag{6}$$

$$0 = Fz_f + Lx_{out} - qFy_{in} - [(1-q)F + L]x_f \quad (7)$$

$$x_{in} = y_{out} \quad (8)$$

where: F, q and z_f are the flow rate, vapor fraction and composition of the feed air stream, respectively; L and qF are the internal liquid and vapor flow rates, respectively; N_t is the total number of equilibrium stages; n_l and n_v are the liquid and vapor holdups of a single stage; x_{in} and x_{out} are the liquid compositions entering and exiting the column, respectively; y_{in} and y_{out} are the vapor compositions entering and exiting the column, respectively; $y(0)$ is the vapor composition in equilibrium with the liquid composition x_{out}; x_f is the feed stage liquid composition in equilibrium with y_{in}; and α is the constant relative volatility.

The simplified wave model is comprised of the wave velocity equation (2), the wave profile equation expressed at the top (3) and bottom (4) of the column, the equilibrium relation expressed at the bottom of the column (5) and the feed stage (6), a steady-state mass balance for the feed stage (7) and the trivial equation (8) for the condenser/reboiler. The fast dynamics of the feed stage relative to the overall column dynamics justifies the steady-state feed stage balance. Manipulation of the algebraic equations (3)–(7) allows the wave model to be reduced to a single differential equation for the wave position s [10]. The relative volatility α was regressed from Aspen vapor-liquid equilibrium data. The nominal wave position s and the wave parameters γ, y_{min} and y_{max} were estimated to minimize the least-squares difference between the steady-state composition profiles of the wave and Aspen models [10].

Simulation Results

Figure 2 shows a comparison of the wave and Aspen models for a +10% step change in the feed flow rate. The nitrogen product composition dynamics in Figure 2a show that the wave model exhibits significantly faster dynamics and a much smaller steady-state gain than the Aspen model. Figure 2b depicts the composition wave dynamics in actual coordinates at three time points (initial steady state, shortly after the step change and final steady state). Reasonable agreement is obtained at the initial steady state due to the estimation described above. However, the wave model yields poor predictions of the composition wave dynamics and the final composition profile. The results in Figure 2c are plotted in terms of the log transformed oxygen composition ($-\ln(y)$) to further illustrate the poor steady-state predictions generated by the wave model. The limited predictive capability of the wave model is attributable to the assumption of constant wave profile shape [10] as well as the small oxygen compositions in the top of the column.

Figure 3 shows a comparison of the two models for a –10% step change in the feed flow rate. Figure 3a shows that the wave model exhibits faster dynamics and a slightly larger steady-state gain for the nitrogen product composition than the Aspen model. The composition wave dynamics depicted in Figure 3b are consistent with those obtained for

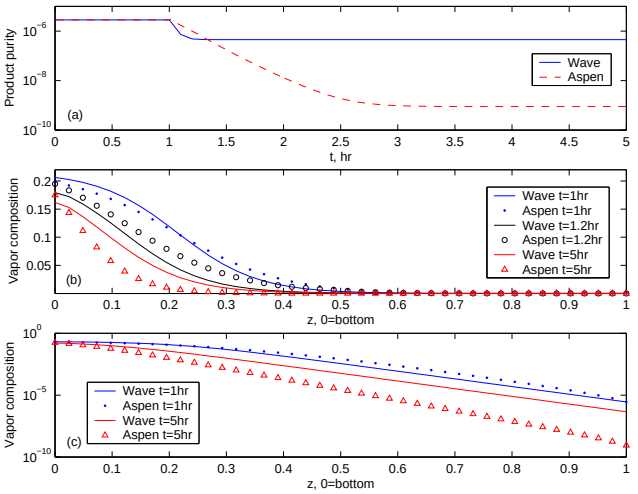

Fig. 2. Comparison of Aspen and wave models for a 10% increase in the feed flow rate.

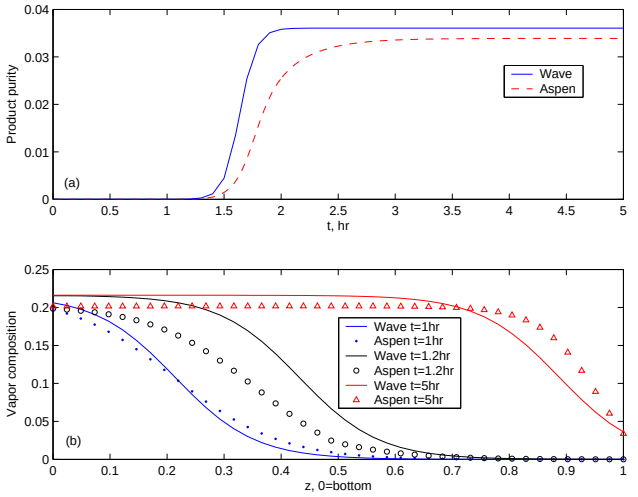

Fig. 3. Comparison of Aspen and wave models for a 10% decrease in the feed flow rate.

the positive feed flow rate change in Figure 2. These results can be explained by noting that the wave model is incapable of accurately predicting separation performance when the wave profile shape changes with operating conditions. Because the assumption of constant profile shape is not easily relaxed, an alternative approach is needed to achieve satisfactory wave model performance. We have developed a combined state and parameter estimation scheme based on extended Kalman filtering to address the limited prediction capabilities of the nonlinear wave model. The proposed method is described in another manuscript [11].

IV. COMPARTMENTAL MODEL

Model Formulation

The first step is to derive a full order model comprised of stage-by-stage mass and energy balance equations. Re-

duced order model accuracy is limited by any simplifying assumptions used in the derivation of the full order model. The next step is to divide the column into a small number of sections [7]. While systematic rules for selecting the number and location of these compartments are not available, a typical strategy is to define separate compartments for both the condenser and reboiler and three equally spaced compartments within the column [8]. The reduced order model is derived from the full order model by applying singular perturbation theory to each compartment. Below the derivation of a compartmental model for a very simple full order model comprised of a single component balance per separation stage is outlined [8].

The component balances for an arbitrary compartment within the column can be written as:

$$\begin{aligned} H\dot{x}_1 &= Lx_0 + Vk(x_2) - Lx_1 - Vk(x_1) \\ &\vdots \\ H\dot{x}_k &= Lx_{k-1} + Vk(x_{k+1}) - Lx_k - Vk(x_k) \\ &\vdots \\ H\dot{x}_m &= Lx_{m-1} + Vk(x_{m+1}) - Lx_m - Vk(x_m) \end{aligned} \tag{9}$$

where: x is the liquid oxygen composition; H is the liquid holdup; L and V are the liquid and vapor flow rates, respectively; $k(x)$ is the vapor-liquid equilibrium relation; the subscript represents the stage numbered from the top of the column; and m is the total number of stages in the compartment. The subscripts 0 and m+1 are used to represent liquid properties from the stage immediately above the compartment and vapor properties from the stage immediately below the compartment, respectively. The holdup H and the flow rates L and V are assumed to be constant across the compartment for simplicity. An overall component balance about the compartment yields:

$$H_c\dot{x}_c = Lx_0 + Vk(x_{m+1}) - Lx_m - Vk(x_1) \tag{10}$$

where the compartment holdup and composition are:

$$H_c \equiv \sum_{i=1}^{m} H_i, \qquad x_c \equiv \frac{\sum_{i=1}^{m} H_i x_i}{H_c} \tag{11}$$

The time scale separation necessary to apply singular perturbation analysis is introduced by replacing the k-th stage component balance (9) with the overall component balance (10). The resulting model can be written in standard singularly perturbed form through the introduction of the parameter $\epsilon = \frac{H}{H_c}$ [8]. By setting $\epsilon = 0$, the compartment dynamics are reduced to a single differential equation representing the overall component balance and m–1 algebraic equations derived from the stage component balances:

$$\begin{aligned} 0 &= Lx_0 + Vk(x_2) - Lx_1 - Vk(x_1) \\ &\vdots \\ H_c\dot{x}_c &= Lx_0 + Vk(x_{m+1}) - Lx_m - Vk(x_1) \\ &\vdots \\ 0 &= Lx_{m+1} + Vk(x_{m+1}) - Lx_m - Vk(x_m) \end{aligned} \tag{12}$$

The reduced-order model is derived by applying this procedure to each compartment and by adding separate compartments for the reboiler and condenser as appropriate.

Pseudo-binary and ternary full order models were derived for the nitrogen purification column. The ternary model was developed by writing mass balance equations for two components (oxygen and argon) analogously to the binary case in (9). Liquid hydraulic effects were modeled as:

$$L_i = K_i H_i \tag{13}$$

where K_i is a constant parameter for the i-th separation stage obtained by averaging Aspen simulation data over several steady states. The assumption of equal molar overflow eliminated the need for energy balances. Binary and ternary relative volatilities with respect to lumped nitrogen and nitrogen, respectively, were determined from Aspen vapor-liquid equilibrium data. An advantage of compartmental modeling as compared to nonlinear wave modeling is that full order model extensions are easily incorporated into the reduced order model. Although more complex than the simple binary model in (9), the binary and ternary models can be placed in singularly perturbed form by following a similar procedure to that outlined above. The reduced order binary model has the same number of equations per compartment as in (12), while the reduced order ternary model has two nonlinear differential equations and 2(m–1) nonlinear algebraic equations for each compartment.

Simulation Results

Figure 4 shows a comparison between the binary and ternary full order models and the Aspen simulator for a +10% step change in the feed flow rate. Figure 4a shows that the ternary model yields substantially more accurate predictions of the oxygen impurity in the nitrogen product than the binary model. The ternary model also provides superior tracking of the oxygen composition wave dynamics as illustrated in Figure 4b. The oxygen composition profiles in Figure 4c show that the ternary model provides significantly improved predictions at the initial and final steady states. The superior performance of the ternary model is attributable to the relatively high concentration of argon relative to oxygen in the middle of the column. At these low feed flow rates, the middle of the column actually separates nitrogen and argon rather than nitrogen and oxygen. The binary model is not appropriate for these operating conditions.

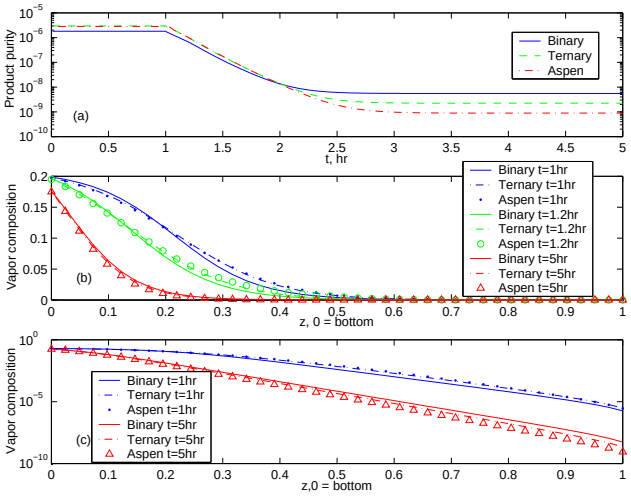

Fig. 4. Comparison of Aspen and full order models for a 10% increase in the feed flow rate.

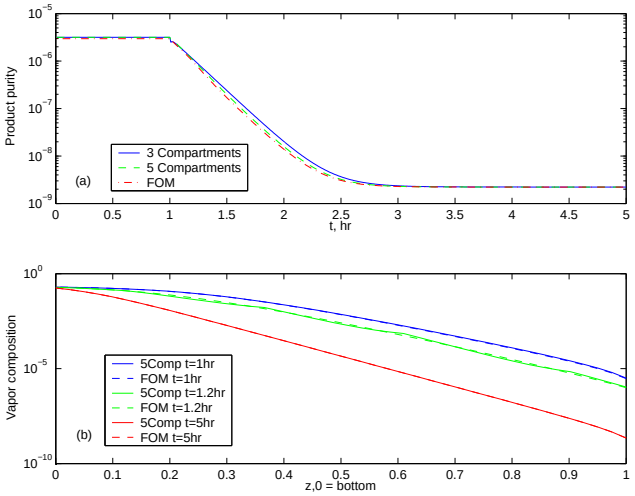

Fig. 5. Comparison of ternary full order and compartmental models for a 10% increase in the feed flow rate.

Figure 5 shows a comparison between the ternary full order model (FOM) and two reduced order models with equally spaced compartments for the positive feed flow rate disturbance. Figure 5a shows that a reduced order model with three compartments yields significant prediction errors in the nitrogen product purity as compared to the FOM. By contrast, a five compartment model yields very close agreement with the FOM. Figure 5b shows that the five compartment model also produces very accurate predictions of the FOM composition wave dynamics. Although small improvements in prediction accuracy can be obtained by including more than five compartments, the increased complexity of the resulting reduced order model does not seem necessary. Slight discontinuities in the transient composition profile produced by the five compartment model occur at the boundaries of the three interior compartments. This behavior is observed immediately after the feed disturbance because the fast dynamics of the individual stages have not yet converged [9].

Figure 6 shows a comparison between the two full order models and the Aspen simulator for a –10% step change in the feed flow rate. Figure 6a shows that the ternary model yields more accurate predictions of the nitrogen product purity than the binary model. The ternary model also provides improved tracking of the oxygen composition wave dynamics as illustrated in Figure 4b. However, the improvement obtained with the ternary model is not as substantial as observed for the negative feed flow rate change because concentration of argon relative to oxygen is relatively low at these higher flow rates.

Figure 7 shows a comparison between the ternary full order model (FOM) and two compartmental models for the negative feed flow rate disturbance. The three compartment model exhibits significant prediction errors in the nitrogen product purity as illustrated in Figure 7a.

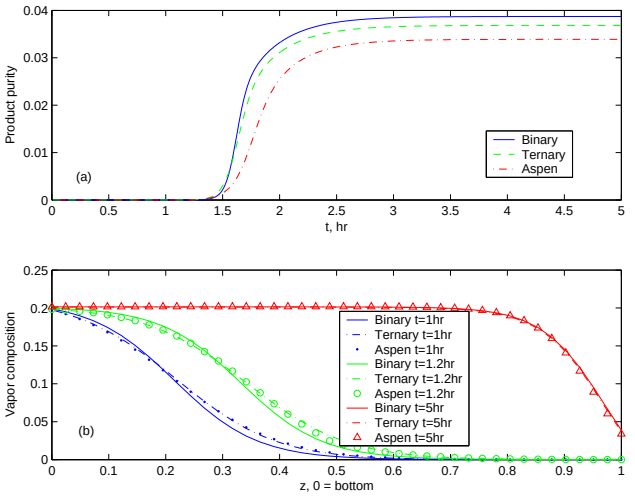

Fig. 6. Comparison of Aspen and full models for a 10% decrease in the feed flow rate.

By contrast, the five compartment model yields excellent predictions of the product purity dynamics. Figure 7b shows that the five compartment model also produces very accurate predictions of the FOM composition wave dynamics. Only small improvements can be obtained by including additional compartments. When taken together, Figures 5 and 7 demonstrate that excellent agreement with the 86-dimensional ternary FOM can be obtained with as few as five compartments (*i.e.*, with ten differential equations).

V. SUMMARY AND CONCLUSIONS

Two reduced order nonlinear modeling techniques were investigated for a high purity nitrogen purification column. A rigorous dynamic simulator was developed to assess the tradeoffs between the prediction accuracy and computational complexity of the reduced order models. Nonlinear

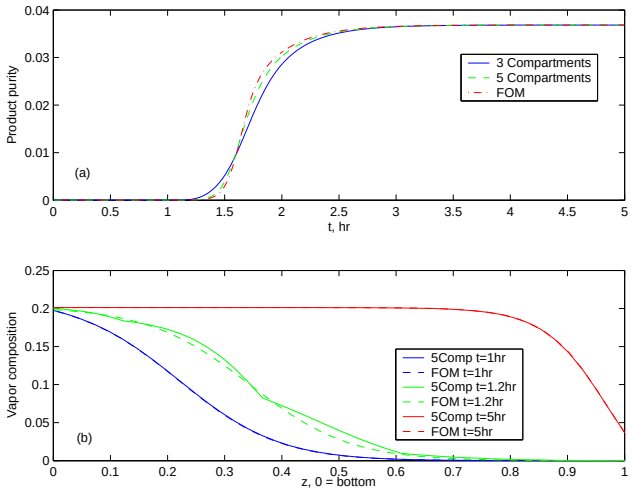

Fig. 7. Comparison of ternary full order and compartmental models for a 10% decrease in the feed flow rate.

wave theory was used to derive a very simple dynamic model comprised of a single nonlinear differential equation for the wave position. While the basic dynamic trends of the Aspen simulator were captured, the wave model was not capable of producing quantitatively accurate predictions over a range of column operating conditions. Wave model predictions were particularly poor for positive changes in the feed flow rate that result in very high nitrogen product purities. The principal limitation of the wave model is the assumption that the wave profile has constant shape. Although not discussed here for the sake of brevity, we have developed a combined state and parameter estimation scheme to address the limited prediction capabilities of the wave model [11]. Assuming the availability of properly placed composition and/or temperature measurements along the column, the adapted wave model can produce composition predictions comparable to those of the compartmental model.

Singular perturbation theory was used to derive compartmental models from full order column models comprised of stage-by-stage component balances and hydraulic relations for the liquid flow. Compartmental models were developed from a pseudo-binary model in which nitrogen and argon were lumped into a single component and from a ternary model that explicitly accounted for the presence of argon. The ternary full order model was shown to provide much better agreement with the Aspen simulator than the binary full order model. The ternary model was particularly advantageous for positive feed flow rate changes which produce a relatively large concentration of argon relative to oxygen in the middle of the column. A reduced order model with five compartments was shown to yield very close agreement with the ternary full order model from which it was derived. The five compartment model comprised of ten differential equations and 76 nonlinear algebraic equations was shown to yield substantially improved predictions of Aspen composition dynamics as compared to the nonlinear wave model without state and parameter estimation.

We have utilized the nonlinear wave model to develop a NMPC controller which manipulates the vapor nitrogen production rate to regulate the nitrogen product purity [11]. While significant improvement is achieved for large feed flow rate changes relative to a conventional regulatory control scheme, the NMPC controller is considerably more complex due to the need for on-line state and parameter estimation. We plan to design a similar NMPC controller from the five compartment model derived from the ternary full order model. Despite the increased complexity of the controller design model, the compartmental model has the potential to yield improved closed-loop performance due to its superior prediction capabilities. The results of this work will be reported in our future publications.

VI. ACKNOWLEDGMENTS

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