2008 American Control Conference
Westin Seattle Hotel, Seattle, Washington, USA
June 11-13, 2008

Improved Crude Oil Processing Using Second-Order Volterra Models and Nonlinear Model Predictive Control

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Abstract— **The petroleum industry operates a wide variety of chemical processes that can benefit from advanced modeling and control methods. Traditional linear control methods can be applied to these systems, but this often results in sub-optimal closed-loop performance. The current work presents modeling and control of a refinery facility simulation using second order Volterra series models and a nonlinear model predictive control formulation. Realistic process data were generated using a dynamic refinery simulation model. The data set from the crude oil separation facility simulation was used to determine an empirical model for use with nonlinear Model Predictive Control (MPC). Results show that a second-order Volterra model can be used to represent the multivariable chemical plant which exhibits both nonlinear gains and nonlinear dynamics. It is demonstrated that the proposed nonlinear MPC formulation tracks setpoints and rejects disturbances better than traditional linear control methods.**

I. Introduction

Model Predictive Control (MPC) has been used extensively for control of refinery operations since MPC can accommodate multivariable systems, actuator constraints, and economic objectives. The original linear MPC method has been extended to include control of nonlinear dynamic systems by a variety of authors [3], [16], [5], [4], [9], [1], [14], [2]. Use of more accurate nonlinear process models potentially results in improved controller performance but also requires solution of a more difficult nonlinear optimization problem. Guaranteed closed-loop stability of nonlinear systems using MPC based methods generally use a terminal state constraint [12], [17], [10] or some sort of backup control system that monitors convergence [11]. The nonlinearity of a refining process and multivariable interacting nature of such systems makes this class of process attractive to nonlinear MPC methods.

When dealing with a multivariable interactive systems, techniques such as Relative Gain Array (RGA) and Singular Value Decomposition (SVD) are useful to obtain a measure of the extent of the influence of process interactions when input u_i is used to control output y_j [13], [18]. Based on the open-loop gains that can be obtained linearization of the input/output model, RGA and SVD analysis can suggest to what extent would a certain type of interacting control be the most efficient to track setpoints and reject disturbances. A process linearization may be accurate near a single operating point. However, for highly nonlinear dynamic systems, linear analysis methods may be insufficient. This is especially true for nonlinear dyanamic systems with input multiplicity, where the system open-loop gain may change sign depending on the current operating conditions.

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II. System Description

A crude oil processing facility model has been developed for the purpose of modeling and nonlinear control. This simulation model uses an atmospheric column to fractionate the crude oil feedstock into its straight run products. The crude column consists of a refluxed absorber with three side strippers and three cooled pump-around circuits. The column flowchart appears in Figure II.

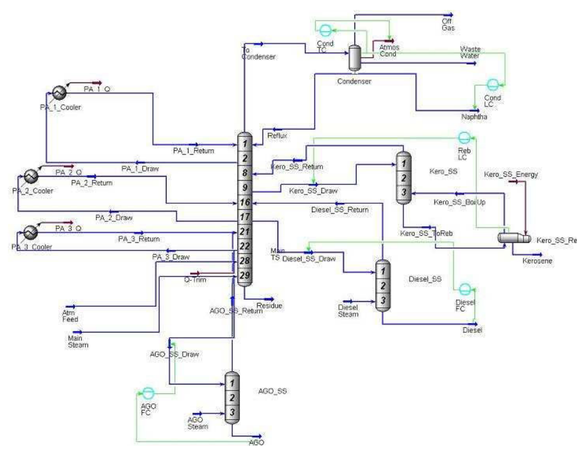

Fig. 1. A dynamic HYSYS distillation plant simulation flow sheet.

The column consists of 29 trays plus a partial condenser. The column feed enters on stage 28, while superheated steam is fed to the bottom stage. In addition, the trim duty is represented by an energy stream feeding onto stage 28. The naphtha product and the waste water

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stream are produced from the three-phase condenser. Crude atmospheric residue is yielded from the bottom of the tower.

Each of the three-stage side strippers yields a straight run product. Kerosene is produced from the reboiled KeroSS side stripper, while diesel and AGO (Atmospheric Gas Oil) are produced from the steam-stripped DieselSS and AGOSS side strippers, respectively. Using HYSYS Dynamic Simulation [6], [7], key control loops were implemented to increase the realism of the model and provide simulation stability by maintaining the condenser level and the products flow rates. The controllers were tuned to rapidly achieve steady state.

Each of the four product streams include three process outputs that may be of interest: flow rate, temperature, and composition. In order to address the nonlinearity of the process, one may analyze the response of these twelve outputs to changes in four different inputs. Inputs for this simulation include the reflux flow rate from the condenser to the column, the heat flow supplied to the reboiler, and both the temperature and flow rate of the feed stream into the column. The first two inputs (reflux flow and reboiler duty) are traditionally treated as manipulated inputs in distillation processes, whereas the feed conditions that can not always be predicted are considered as disturbances.

A series of varying size step changes were introduced to the open-loop system to analyze the nonlinearity of the simulation model. Observing the plots of the steady state output vs. input values and the step response information (normalized by input step size), it is obvious that the response of the temperatures and the flow rates of the products may be considered linear. However, significant nonlinearity was observed in the case of molar compositions variables. This was expected. Therefore, the four product compositions were used as the only control variables of interest for the purpose of this work resulting in a *4x2* (4 outputs, 2 inputs) multivariable modeling and control problem.

Figure 2 presents the steady state product compositions deviated with respect to the original steady state values for inputs and outputs. Observing the slopes of the compositions in Figure 2 it is clear that the open-loop process gains of naphtha (y_1), kerosene (y_2), diesel (y_3), and AGO (y_4) exhibit input multiplicity with respect to the Heat Duty. Additionally, the reflux ratio significantly influences the maximum attainable value for the four compositions. This means that the zero gain operating point may potentially change location depending on the value of the reflux ratio. The nonlinearity observations are confirmed by the normalized output plots (Figures 3 and 4). Here, nonlinear dynamics are apparent as the dynamic response obviously depends on the size of the input change. Additionally, input multiplicity is also obvious in the normalized step response plots, as some outputs show both positive and negative steady state values.

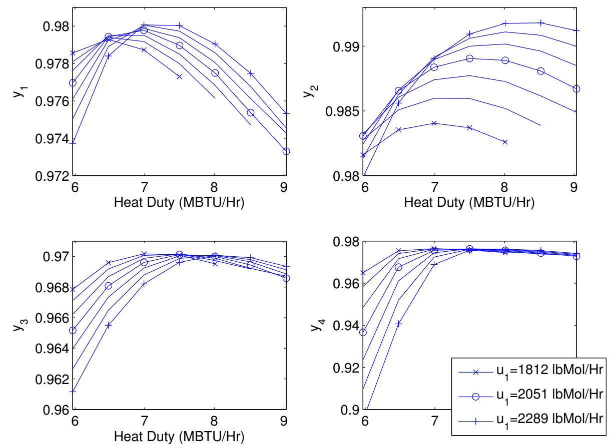

Fig. 2. Steady states values showing deviations from the original steady state values.

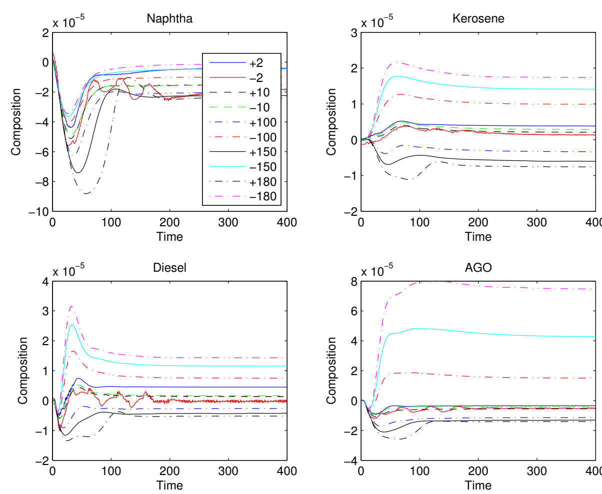

Fig. 3. Normalized output response for Reflux flow step changes.

III. Model Identification

Despite the fact that significant advances have been made with regard to the theory and practice of Model Predictive Control as a control system design methodology, developing and evaluating appropriate models still remains an important and time-consuming step in the implementation of nonlinear MPC. For complex chemical processes (such as distillation columns), fairly accurate first principle models are usually difficult and/or very time consuming to obtain. Using plant data, empirical models may be determined. The models considered for control in this work are the second order Volterra

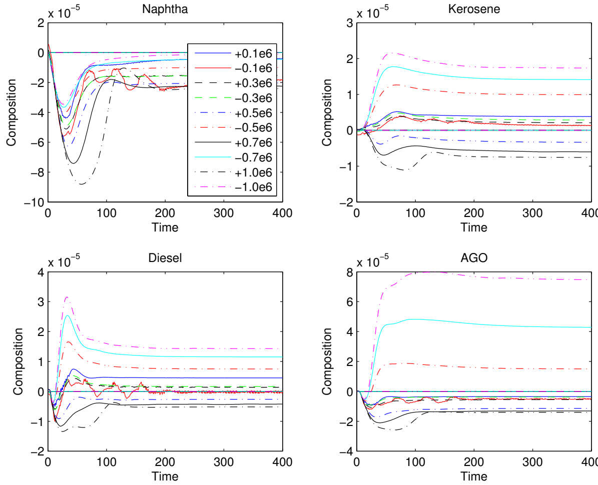

Fig. 4. Normalized output response for Reboiler duty step changes.

Series models of the form

$$y_j(k+M) = \sum_{i=1}^{n_u} \sum_{l=k}^{k+M-1} \left(\alpha_{j,i}(l)\, u_i(l) + \beta_{j,i}(l)\, u_i(l)^2\right) + \sum_{\substack{i=1 \\ ii=i+1}}^{n_u,n_u} \sum_{l=k}^{k+M-1} \gamma_j(l)\, u_i(l)\, u_{ii}(l)$$

$$\forall j \in n_y, \forall k \in [1, D-M] \quad (1)$$

where n_y is the number of outputs, n_u is the number of inputs, M is the number of past input values used in the model, and D is the total number of available data points. Note that linear models are a subset of the nonlinear models above when $\beta_{j,i}= 0$ and $\gamma_j= 0$ with the coefficients γ_j corresponding to the cross input terms $u_1 \times u_2$, in the case of only two inputs.

The actual values for the inputs u_i and the outputs y_j are obtained from the generated process data using the dynamic refinery model. Using a vector notation and linear algebra nomenclature, the above model can be presented as

$$b_j = A\, x_j \quad (2)$$

where for each output j vector b_j = $(D\times 1)$ represents the generated output values y_j, vector x_j = $(2Mn_y\times 1)$ contains the modeling coefficients, and a matrix A = $(D\times 2Mn_y)$ is the actual generated input data. The task of model identification is to obtain the coefficients $\alpha_{j,i}$, $\beta_{j,i}$ and γ_j. It is reduced to finding a solution

$$x_j = A^{\dagger}\, b_j \quad (3)$$

where $A^{\dagger}$is a pseudo-inverse (Moore-Penrose generalized inverse) of a matrix A.

One may identify linear models ($\beta_{j,i} = 0, \gamma_j = 0$), simple nonlinear models ($\beta_{j,i} \neq 0, \gamma_j = 0$) and full nonlinear models ($\beta_{j,i} \neq 0, \gamma_j \neq 0$). The modeling results are compared with the actual generated output data by finding a sum of squared errors throughout the available D data points, $k = 1$ to $k = D-M$. A portion of the data can be used to evaluate the model fit. After finding the model coefficients using a set of data, a different set of data can be used to validate the model. Figures 5-6 show the actual open-loop generated outputs presented in deviation form around the steady state values. The model data outputs obtained in the first 80 percent of the range D (D=16,512) and the models were validated for the remaining 20 percent. This is shown for both the linear (Figure 5) and the nonlinear with the cross terms (Figure 6) cases. A five minute sample period was used. The inputs and outputs were put in deviation form and scaled for modeling and control purposes.

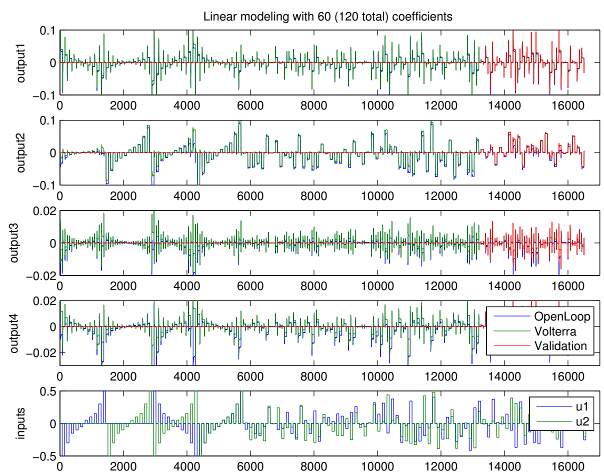

Fig. 5. Linear model with validation.

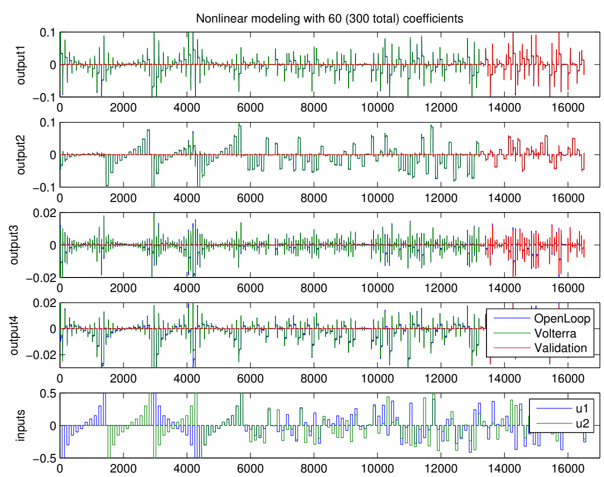

Fig. 6. Volterra based nonlinear modeling with validation.

The sum of squared errors (SSE) over the range $[D_1, D_2) \in D$ defined for each output j as

$$SSE^{(j)}_{D_1,D_2} = \frac{1}{D_2 - D_1} \sum_{i=D_1}^{D_2} \left[y_{j,model}(i) - y_{j,actual}(i) \right]^2 \tag{4}$$

are summarized in Table I for M=60 (number of terms used in the model). Note that the total number of model coefficients for one output is Mn_un_t+$n_{ct}Mn_u(n_u-1)/2$. The second term includes the binary variable n_{ct}which represents the inclusion or exclusion of cross terms. For this work, $n_u = 2$ is the number of inputs, n_t is the order of the model, and n_{ct} accounts for the presence or absence of input cross terms. Therefore, in the linear case ($n_t = 1$, $n_{ct} = 0$) and the total number of the model coefficients is 120, whereas in the nonlinear case ($n_t = 2$) the total number of the model coefficients is 240 without cross terms ($n_{ct} = 0$) and 300 with the input cross terms ($n_{ct} = 1$), respectively.

Model Identification			
Type of model	Linear	Volterra	W/Cross
# model coeffs	120	240	300
y_1	0.1997	0.1360	0.1114
y_2	0.5743	0.3418	0.2209
y_3	0.1535	0.0830	0.0326
y_4	0.3996	0.2160	0.0824
Model Validation			
y_1	0.878	0.600	0.5038
y_2	2.495	1.458	0.9559
y_3	0.677	0.352	0.1456
y_4	1.758	0.908	0.3481

TABLE I
SUM SQUARED ERRORS (X 10^{-4}) FOR LINEAR AND VOLTERRA MODELING, M = 60.

IV. CONTROLLER FORMULATION

The nonlinear MPC model with M terms, n_u inputs, n_y outputs, moving horizon m, and predicting horizon p, is formulated using the second-order Volterra series in the following model:

$$\begin{aligned} y_j(k)\big|_{k\in[1,p]} &= d_j + \textstyle\sum_{i=1}^{n_u} \sum_{l=0}^{M-1} \alpha_{j,i}(l)\, u_i(k-M+l) \\ &+ \textstyle\sum_{i=1}^{n_u} \sum_{l=0}^{M-1} \beta_{j,i}(l)\, u_i(k-M+l)^2 \\ &+ \textstyle\sum_{i=1,ii=i}^{n_u,n_u} \sum_{l=0}^{M-1} \gamma_j(l)\, u_i(k-M+l)\, u_{ii}(k-M+l) \end{aligned} \tag{5}$$

In the above equation, $u_i(k-M+l)$ is the input i at the given sample time, $y_j(k)$ is a predicted value of output j at time k, and the update d_j is defined as:

$$d_j = y_{j,m}(0) - y_{j,p}(0) \tag{6}$$

where for each output j, $y_{j,m}(0)$ and $y_{j,p}(0)$ are the measurement at the current time and the predicted value of the output at the current time, respectively. In this model, values for u_i before time k are known and values for times greater than $k+m$ are fixed to $u(k+m)$.

This formulation chooses a sequence of input moves over the move horizon (m) that minimizes the cost function. A 2-norm is used in the MPC objective function in this work to avoid performance issues associated with the 1-norm formulations [15]. The 2-norm objective function takes the form

$$\phi = \sum_{j=1}^{n_y} \sum_{k=1}^{p} \Gamma_{y,j}(k)\, e_j(k) + \sum_{i=1}^{n_u} \sum_{l=1}^{m} \Gamma_{u,i}(l)\, \Delta u_i(l) \tag{7}$$

where $e(k)$ is the squared value of error predicted for the k^{th} time step into the future. The error (e) is defined as

$$e_j(k)|_{k\in[1,p]} = (y_{p,j}(k) - y_{sp,j}(k))^2 \tag{8}$$

Here, $y_{p,j}(k)$ is the predicted value of output j at time k, updated based upon process model mismatch at the current time. The term Δu_i defines changes in input i movements,

$$\Delta u_i(k)|_{k\in[1,m]} = (u_i(M+k-1) - u_i(M+k))^2 \tag{9}$$

$\Gamma_{y,j}(k)$ and $\Gamma_{u,i}(l)$ are weighting factors used to define the relative importance of each objective function term in Equation 7. The move horizon limits changes in u_i after m steps such that

$$\Delta u_i(l-1) = 0 \quad \forall l > m \tag{10}$$

In this formulation, the optimization problem to be solved at each time step includes only hard constraints on the actual inputs of the process:

$$u_i^l \leqslant u_i \leqslant u_i^u \tag{11}$$

In MPC formulations, the prediction horizon (p) can be chosen as a large value to promote stability. Stability can also be ensured through the use of a hard constraint which drives the terminal state error to zero. This theoretical guarantee for nominal stability fails in cases where an unreachable setpoint is provided, as the optimization problem is infeasible [8].

V. CLOSED-LOOP RESULTS

Comparison between the proposed Volterra-based Nonlinear Model Predictive Control (NMPC) formulation and a traditional linear PID control was considered for a 2x2 system of kerosene-diesel compositions. In both cases the reflux molar flow rate and the reboiler duty were used as the process inputs. The RGA analysis, in addition to the obtained open-loop steady state distribution and the normalized gain plots, suggested that this combination of manipulated inputs to be used to control the compositions of the pair kerosene-diesel be avoided.

Indeed, a traditional PID control failed to adequately handle the nonlinear interacting pairing of outputs (y_2, y_3). This is shown in Figure 7. Note the oscillatory nature of the closed-loop response and the very slow settling time. No attempt was made to develop a 2x2 decoupling control system for this process, although improved controller performance would be expected.

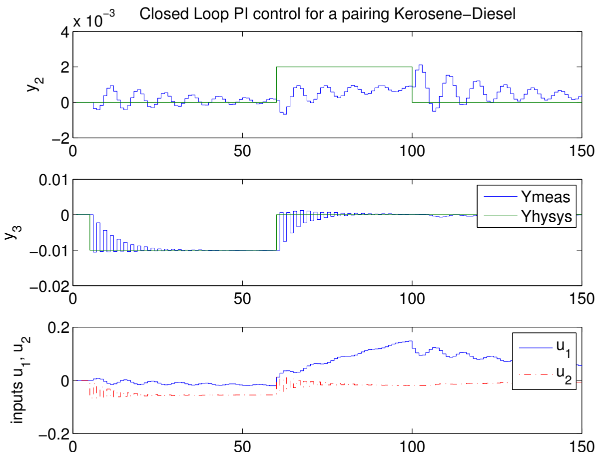

Fig. 7. PI control of a nonlinear interacting pairing (kerosene-diesel).

The proposed nonlinear MPC formulation based on Volterra modeling was implemented on the entire 4x2 system. The closed-loop results appear in Figure 8. Taking into account the complexity and a very sensitive nature of the process, as well as the multivariable interactions, it was anticipated that it would be impossible to control all four process outputs by manipulating the two inputs. This is obvious, as process outputs 3 and 4 fail to track the setpoint.

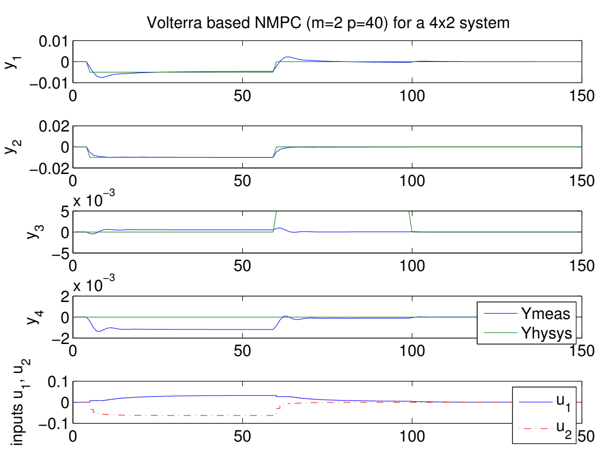

Fig. 8. Nominal nonlinear MPC closed-loop control showing setpoint tracking. m=2, p=40, Γ_y= [10 10 10 10], $\Gamma_{\Delta u}$= [1 1].

The MPC controller was compared to the 2x2 PI control simulation. The nonlinear MPC results are much better than the obtained results using traditional PI control methods. These results for the pair kerosene-diesel are shown in Figures 9 and 10 for disturbance rejection and setpoint tracking, respectively. The control system could track the setpoints and reject small disturbances despite the strong nonlinear dynamics that were associated with this pair of process outputs. Note that the PI control system required relatively small setpoint changes in order to maintain stability and avoid input saturation. Nonlinear MPC allows for a wider range of operating conditions. Eventually, soft constraints based on a prioritized list of control objectives will be developed for this nonsquare system.

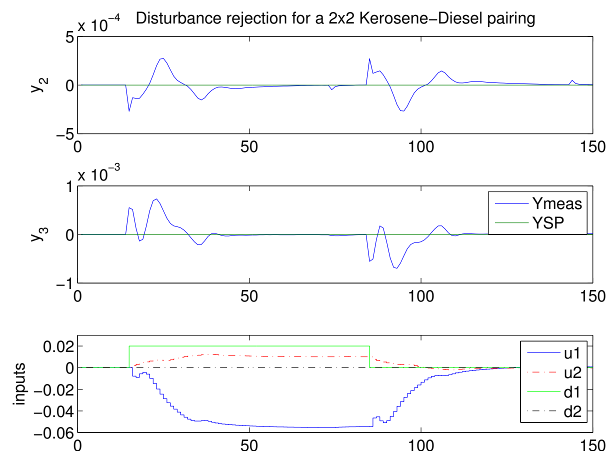

Fig. 9. Disturbance rejection for a 2x2 control, normalized Kerosene and Diesel compositions

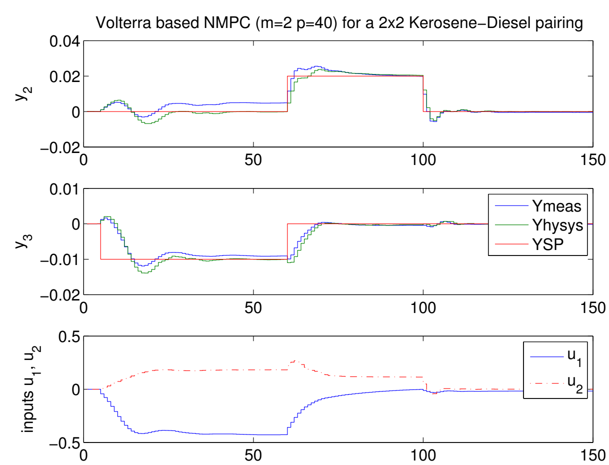

Fig. 10. Closed-loop nonlinear MPC 2x2 control, normalized Kerosene and Diesel compositions

VI. Conclusions

This work considered improved dynamic modeling and control of nonlinear dynamic systems. The modeling and control methods are tested using data from a high fidelity dynamic simulator. The results of the work indicate that a multivariable chemical process such as a distillation operation demonstrates a clear nonlinear behavior and can be empirically modeled using the second-order Volterra series models to closely match the data obtained from the plant dynamic simulation. As expected, the Nonlinear Model Predictive Control formulation used in this work has produced better control results comparing to those obtained with a traditional PI control. In particular, the proposed control formulation was able to track setpoints in those 2x2 interacting loops in which the more traditional PI tuning method failed or caused significant input saturation. Situations where the inputs saturate or reach their critical values are not desired and could potentially be very harmful to a plant or a process, in general, affecting both safety and costs due to the energy intensive nature of distillation operation. Additionally, the nonsquare formulation can be used with soft penalty constraints to maintain adequate operation when limited actuation is available.

ACKNOWLEDGMENTS

The authors would like to acknowledge financial support from National Science Foundation CAREER Award CTS-0238663 as well ACS PRF Grant 47261-AC9. Additionally, the authors recognize useful conversations with Professor Vincent Van Brunt.

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