On-line Parameter Estimation and Control for a Pilot Scale Distillation Column

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Abstract

A dynamic model developed in the HYSYS process simulator was validated using experimental data obtained from a pilot scale cyclohexane / n-heptane distillation. The resulting model was linked to the pilot unit's DeltaV (Emerson Process Management) process control software. This link allowed non-measured parameter estimation to occur in parallel with the operation and control of the pilot plant column. To enhance the model's accuracy, a novel model reconciliation methodology was implemented using output from the controller interface. A virtual sensor was also developed which predicted product compositions based on measured column parameters. Linear and non-linear multivariable control strategies were implemented and tested.

Keywords: Control, Distillation, Model Reconciliation, Model Predictive Control.

Introduction

Distillation is the most common separation technique employed in industry and one of the most energy consuming. Improving the process efficiency is an on-going goal of the chemical industries. This paper presents simulation development and experimentation results for the binary distillation of cyclohexane / n-heptane in a column at the Separation Research Program at the University of Texas. A dynamic model of the process was developed using HYSYS (Aspentech) and validated with experimental data. The model was connected to the process online and used to estimate parameters where process data was not available. The process was controlled using DeltaV from Emerson Process Management.

Pilot Plant Description

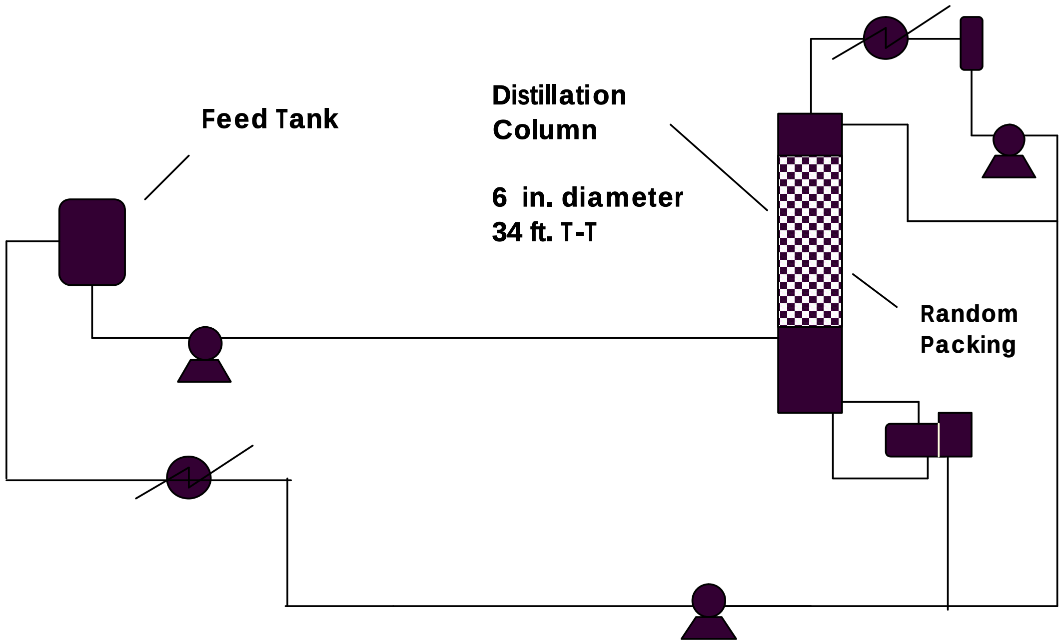

Figure 1. Process configuration

The process configuration and equipment description are presented in Figure 1 and Table 1 respectively. The fully instrumented process was operated continuously while distillate and bottom products were recycled back to the feed tank increasing the time to steady state and adding difficulty to the modeling effort.

Table 1. Equipment Description

	Diameter	Total Height	Packing Height	Packing Type
Column Characteristics	6 in	34 ft	30 ft	Nutter Rings (Metal, random) No. 0.7

	Volume
Feed Tank	50.72 ft3
Accumulator	1.05 ft3
Reboiler (Design maximum)	130 KBTU/HR

Process Simulation

Steady state and dynamic state models for binary distillation were developed using Aspen Plus and HYSYS from Aspentech. To adequately predict the process dynamics in the HYSYS model, the column template was represented by components shown in Figure 2.

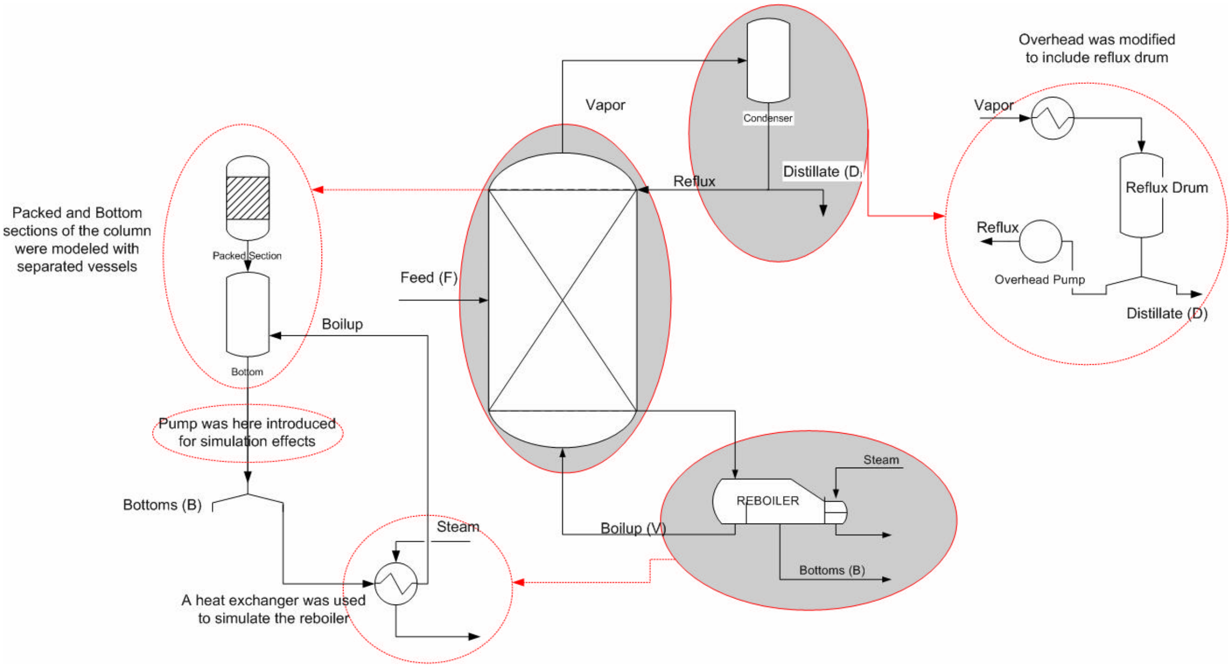

Figure 2. Block diagram of Column Internals and Bottom Configuration.

All the control loops where implemented with PID controllers. Initially, for the simulation in HYSYS, composition control was not implemented. An initial simulation was conducted to determine the most responsive column temperatures that could be employed in the model predictive composition control in DeltaV.

Twenty four equilibrium stages (condenser and reboiler not included) were used in the column dynamic simulation. Using the physical location of the temperature measurements, it was determined that these measurements corresponded to stages 6, 8, 9, 11, 13, 15, 16, 21 and 22. Based on the simulation, temperatures from stages 9 and 16 were selected for control.

Experimental Results

Steady State Data

Table 2 presents a comparison between the simulated data from the steady state model developed in Aspen Plus and the experimental results.

Table 2. Steady State Data

Process Variable	Experimental Data	Simulated Data
Reboiler Duty	59,359.0 BTU/hr	28,124.4 BTU/hr
Column Pressure Drop	7.99 psig	8.3 psig
Overhead Pressure	2.406 inH20	0 inH20
Feed Flow Rate	90.11 PPH	90.11 PPH
Bottoms Flow Rate	45.47 PPH	48.05 PPH
Distillate Flow Rate	45.55 PPH	42.06 PPH
Reflux Flow Rate	94.1PPH	94.1PPH
Feed Temperature	203.71 F	221.75 F
Reflux Temperature	54.8 F	60 F
Distillate Composition C6	0.86	0.8649
Distillate Composition C7	0.14	0.1351
Bottom Composition C6	0.105	0.1055
Bottom Composition C7	0.895	0.8945
Feed Composition C6	0.46	0.46
Feed Composition C7	0.54	0.54

The steady state simulation was configured to match the compositions of feed, distillate and bottoms streams. The results were very close to the experimental data, it is estimated that there are heat losses of 31,234.6 BTU/hr (53 percent of the reboiler input).

Dynamic State Data

HYSYS was selected for the simulation because it allows dynamic simulation and has a DCS interface with the DeltaV control system. This facilitates linking the model to the process. HYSYS has an object-oriented design with event-driven graphical operating environment. Although it is a simulation package with pre-built operation units, it allows the user to customize the modules or add supplement code by interfacing it with visual basic.

Based on the simulation results, experiments were performed in the real plant. The data collected during the experiments were used to improve and validate the model. The model and controller configuration is described by Figure 3.

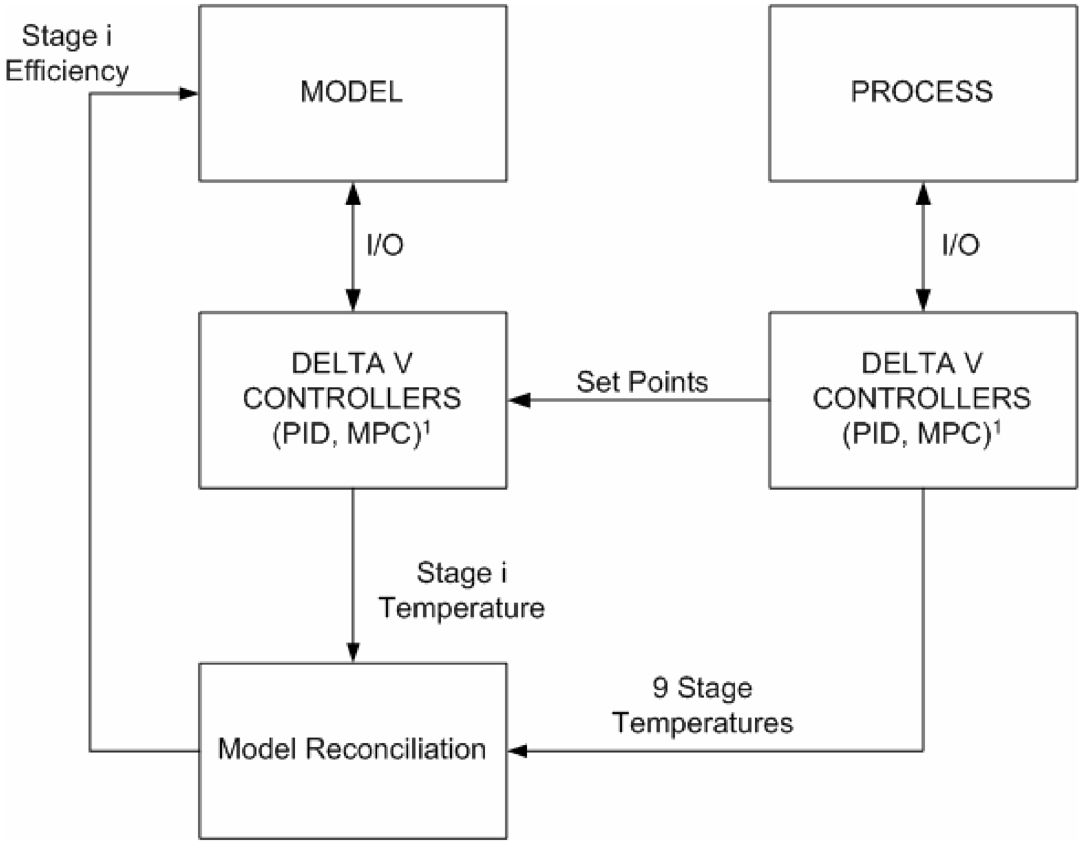

Figure 3. Model and data acquisition configuration.

The range of operating conditions was determined by the equipment limitations and combined with simulation to identify the ranges in the manipulate variables. A summary of the variable operating ranges is presented on Table 3.

Table 3. Operating Conditions.

Feed Flow Rate (lb/hr)	Feed Temperature (F)	Steam Flow Rate (lb/hr)	Steam Temperature (F)	Steam Pressure (psia)	Reflux Flow Rate (lb/hr)	Reflux Temperature (F)	Column Level (in)	Accumulator Level (in)
90-105	200-210	65-80	340-343	124-127	90-115	52-63	9-14	8-12

Control configuration

The operating objectives for the binary distillation experiment were to hold constant the level in the accumulator and bottom of the column constant and to maintain the pressure of the column while producing distillate and bottom products at the desired concentrations. The pairing of manipulate variables with controlled variables is described in Table 4.

Table 4. Pairing of Manipulate Variables with Controlled Variables.

Manipulated Variables	Controlled Variables	Control Strategy
Feed flow valve position	Feed Flow	PID
Steam flow valve position	Feed Temperature	PID
Nitrogen flow valve position	Pressure	PID
Distillate Flow	Accumulator Level	PID - Cascade
Bottom Flow	Bottom Level	PID – Cascade
Reflux Flow	Temperatures at top and bottom of the column	Multivariable control
Steam Flow		Multivariable control

The process control configuration included separate PID loops for column pressure, feed temperature and steam, reflux, distillate, bottoms and feed flow rates. Column and accumulator hold-ups were configured with master PID loops whose manipulate variables were bottom and distillate flow rate respectively. The two point composition control was perform indirectly with model predictive control, reflux and steam flow rate were manipulated to control the temperatures at the top and bottom of the column. Since pressure was held constant, temperature could be used to control composition.

Multivariable Control

Multivariable control was implemented by the configuration of a model predictive control strategy, where, as stated in Table 5, the manipulated variables were reflux and steam flow rate and the control variables were the temperatures from stages 9 (top of the column) and 16 (bottom of the column). The controller configuration included one measured disturbance, one constrained variable, and one optimized variable. The control strategy is illustrated in Figure 4.

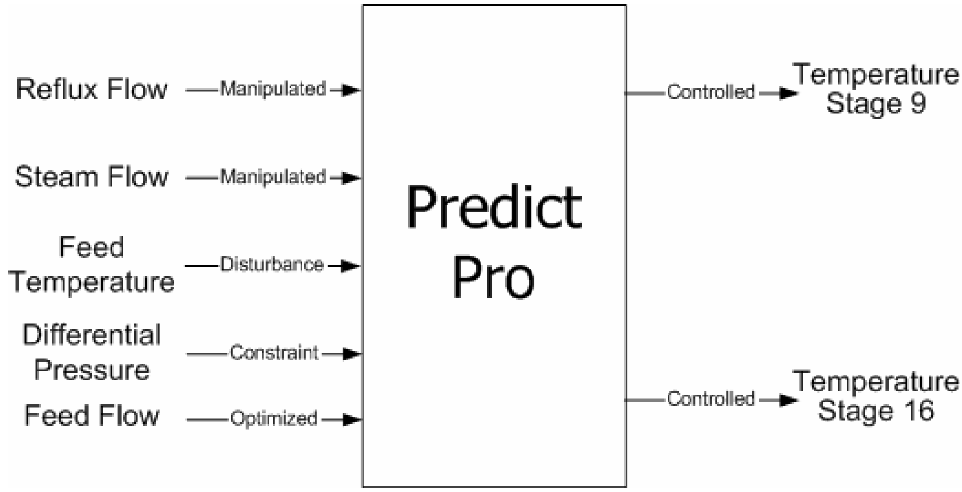

Figure 4. Model Predictive Control Configuration

Model Reconciliation

To reconciliate the model with the real data, efficiencies from the column model were modified to match readings from the process column temperatures with the temperature readings from the model. Since there were only nine column temperature measurements, the column efficiencies from the stages without process measurement were modified at the same time as the closest stage with measurement. The configuration is illustrated in Figure 5.

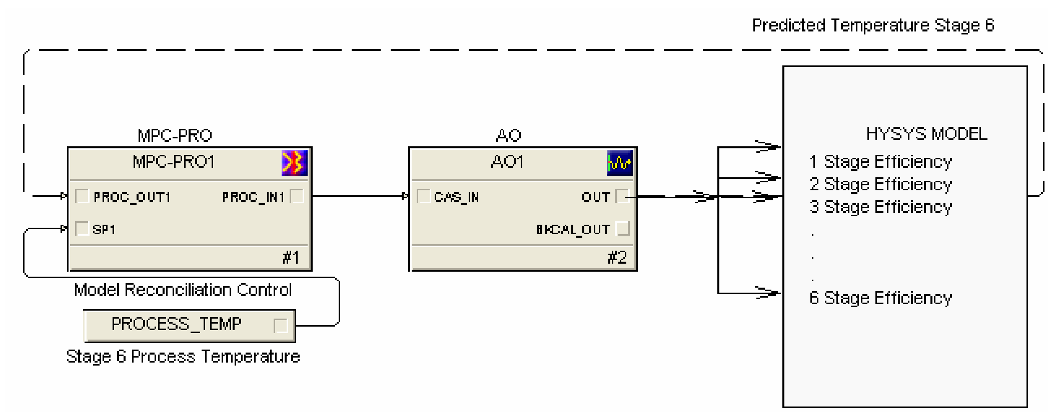

Figure 5. Stage efficiency manipulation for model reconciliation.

The model efficiencies were modified by a model predictive control whose control variables where the model temperatures from stages 6, 8, 9, 11, 13, 15, 16, 21, and 22. The controller set points were given by the readings collected from the process temperatures.

Initially the approach to equilibrium of each stage was assumed to be the same, and this parameter was adjusted to match the real process data. At the start this was done manually and then a parameter estimator was used to modify the efficiencies online using feedback from the process. The stage efficiency used in HYSYS is a modified Murphree stage efficiency [1]. It is described by Equation 1.

$$E_n = \frac{(V_n * y_n) - (V_{n+1} * y_{n+1})}{(V_n * K_n * x_n) - (V_{n+1} * y_{n+1})} \qquad (1)$$

Where:

E = efficiency
Vn = total vapor molar flow leaving stage n
yn = vapor mole fraction on tray n
xn = liquid mole fraction on tray n
n = tray number (measured top down)

If the vapor flow is constant (i.e. Vn = Vn+1; Constant molar overflow), then Equation 1 reduces to the standard Murphree stage efficiency.

Figures 6 to 9 compare the model predictions and the process data over an operating region for a step test in the reflux flow rate from 90 to 150 lb/h. The r-squared fit is used as a measure of agreement between the model and the real data.

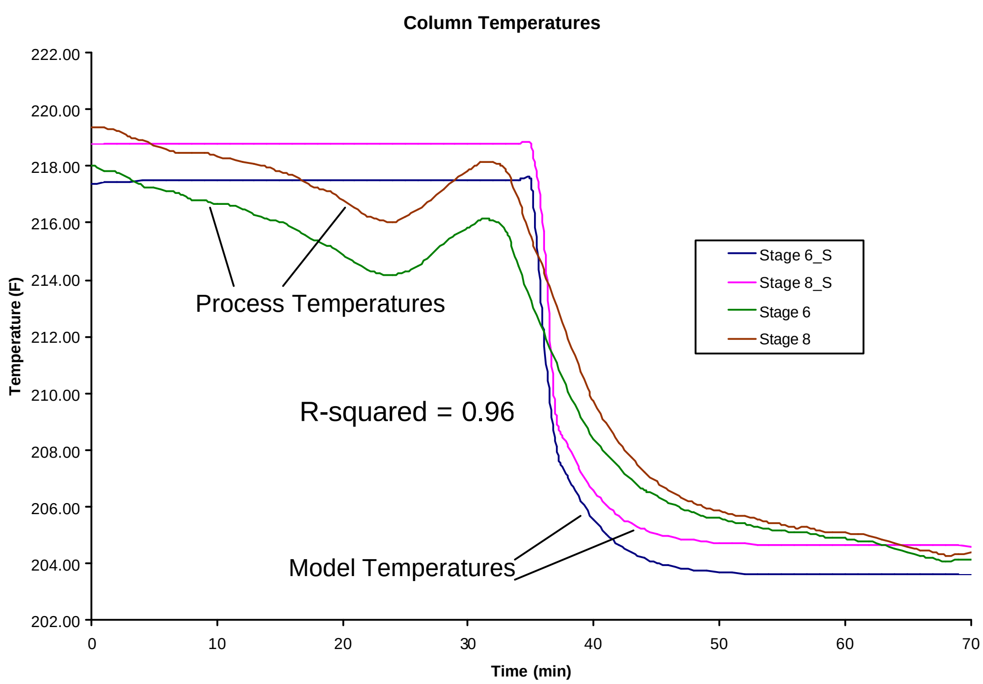

Figure 6. Simulated and actual temperature profiles for stages 6 and 8 during a positive step change in the manipulated variable rate (reflux flow 90 lb/hr -115 lb/hr).

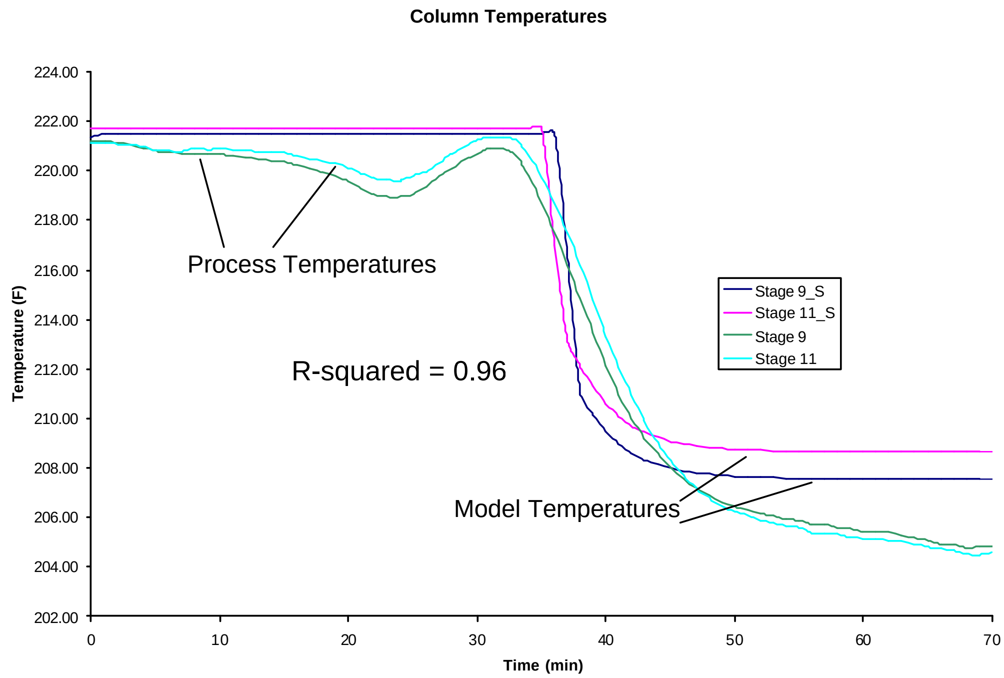

Figure 7. Simulated and actual temperature profiles for stages 9 and 11 during a positive step change in the reflux manipulated variable rate (reflux flow 90 lb/hr -115 lb/hr).

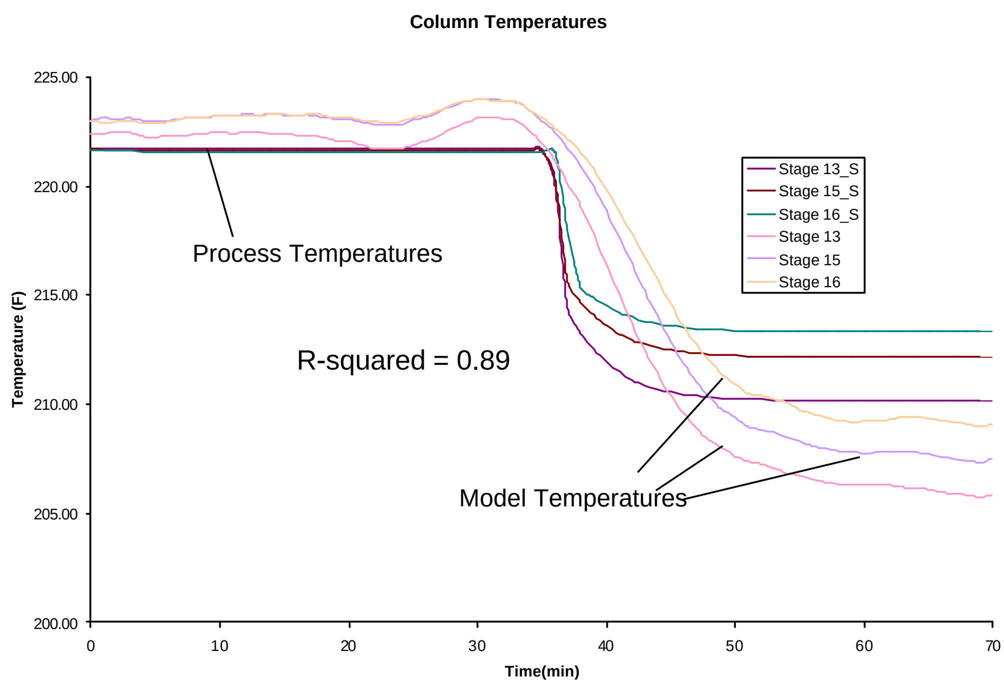

Figure 8. Simulated and actual temperature profiles for stages 13, 15 and 16 during a positive step change in the manipulated variable rate (reflux flow 90 lb/hr -115 lb/hr).

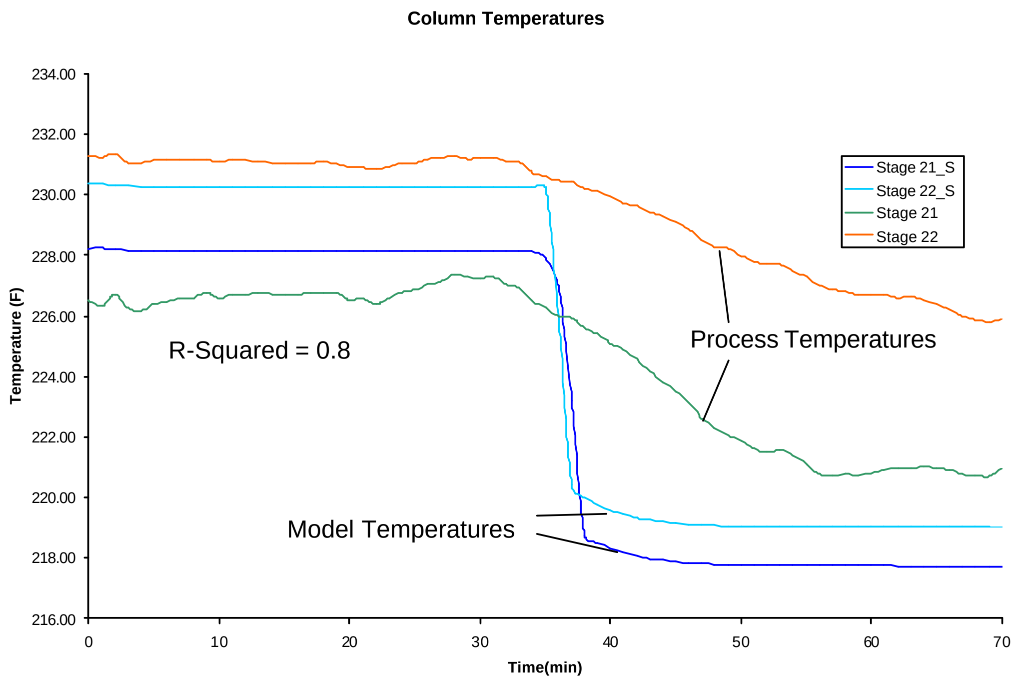

Figure 9. Simulated and actual temperature profiles for stages 21 and 22 during a positive step change in the manipulated variable rate (reflux flow 90 lb/hr -115 lb/hr).

After the model was reconciled in the operating region, experimental and simulated data were used to identify a first order model plus dead time model relating reflux flow rate and temperatures from stages 9 and 16. These models were used by the model predictive controllers to control composition in the model and process. The results are summarized in Table 5.

Table 5. FOPDT models for simulated and real data. Manipulated variable: Reflux flow rate.

	Reflux Flow Rate Negative Step Change			
	Stage 9		Stage 16	
	Simulation	Pilot Plant	Simulation	Pilot Plant
Process Gain	-0.4294	-1.94	-0.421	-1.6
Overall Time Constant	0.2337	6.48	0.1	5.33
Dead Time	0.1347	7.69	1	2.87
Sum of Squared Error (SSE)	0.4474	35.17	8.74	20.4
Goodness of Fit (R2)	0.9983	0.9915	0.9651	0.9931
	Reflux Flow Rate Positive Step Change			
	Stage 9		Stage 16	
	Simulation	Pilot Plant	Simulation	Pilot Plant
Process Gain	-0.5861	-0.6881	-0.3544	-0.6489
Overall Time Constant	1	7.49	1.5	8.86
Dead Time	0.9505	1.55	0.4685	4.55
Sum of Squared Error (SSE)	10.24	887.35	3.82	150.17
Goodness of Fit (R2)	0.9983	0.8784	0.9982	0.9651

The analysis indicated close agreement in the model gains and limited agreement in the time constants and delays. This effect is due to the fact that the model does not account for all the process characteristics as pipe lengths, valve stiction, etc. The overall model agreement was very satisfactory. The highest disagreement found during a change in the reflux flow rate was indicated by stage 21, were the feed temperature disturbance had more influence. With the model reconciliation configuration, the model fit was improved to an r-squared fit of 0.84 – manual mode. Figure 10 illustrates the stage temperature response with the feed temperature influence.

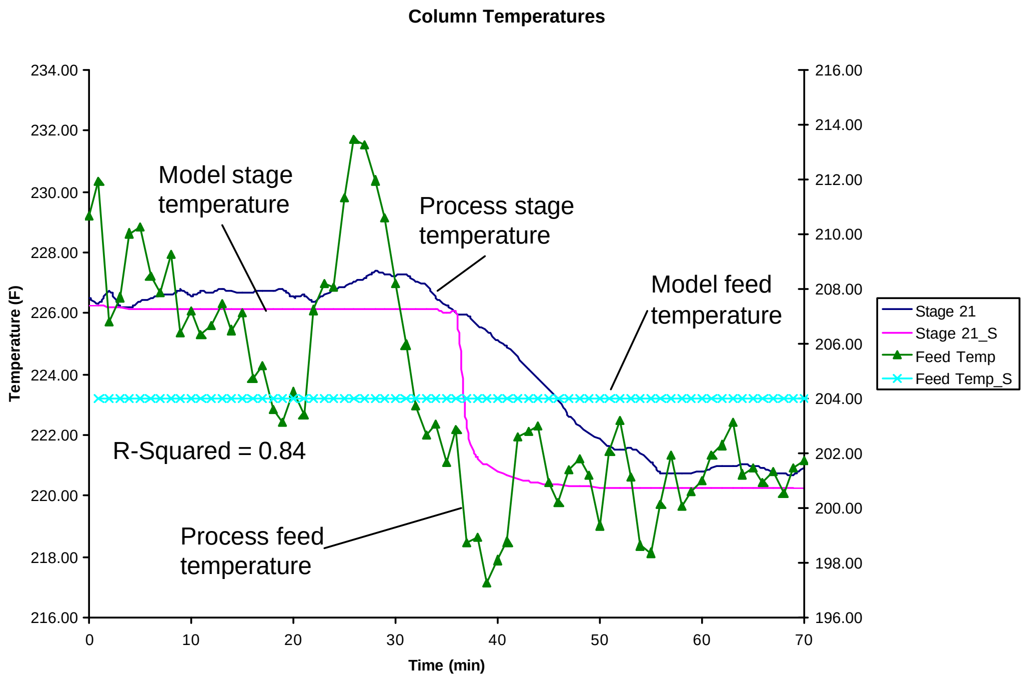

Figure 10. Simulated and actual temperature profile for stage 21 and feed during a positive step change in the reflux flow rate (90 lb/hr -115 lb/hr).

As can be seen in Figure 10, the model response does not reflect all the feed temperature disturbances introduced to the process. The process feed temperature control is writing the set point to the model feed temperature control which holds the temperature at a constant value since the model does not account for the ambient and steam flow variations. Instead of complicating the model to account for every disturbance in the process, temperature from stage 16 was selected for control and temperatures from stages 21 and 22 were left as indication and not considered in the control strategy.

Offline, the model predictive control used in the model was modified to use the same FOPDT used by the model predictive control used in the process. Online, the model predictive control in the model was overriden and the set point of the manipulated variables set up by the process controllers directly. The same analysis was repeated for the other manipulated variable, reboiler duty. The summary of the FOPDT models is given in Table 6.

Table 6. FOPDT models for simulated and real data. Manipulated variable: Reboiler Duty. Controlled Variable: Stage Temperature.

	Reboiler Duty Negative Step Change			
	Temperature Stage 9		Temperature Stage 16	
	Simulation	Pilot Plant	Simulation	Pilot Plant
Process Gain	0.062	0.4925	0.0357	0.175
Overall Time Constant	0.1146	10.88	0.1	0.6143
Dead Time	0.113	1	0.9991	1.66
Sum of Squared Error (SSE)	0.0191	22.5	0.0794	11.23
Goodness of Fit (R2)	0.9925	0.9448	0.9037	0.8845
	Reboiler Duty Positive Step Change			
	Temperature Stage 9		Temperature Stage 16	
	Simulation	Pilot Plant	Simulation	Pilot Plant
Process Gain	0.0621	1.25	0.0356	1.01
Overall Time Constant	0.75	5.23	0.1	3.93
Dead Time	0	4.91	0.651	0.5401
Sum of Squared Error (SSE)	0.0342	181.06	0.0336	89.78
Goodness of Fit (R2)	0.9969	0.9781	0.9911	0.9811

The results from the FOPDT models indicated that the model performed very well to changes in the reflux flow rate but still needed improvement to responses to duty changes.

Development of a Composition Estimator

The pilot plant does not have online composition measurement, for this reason it was necessary to develop an online composition estimator for distillate and bottom products. Additionally, the plant is configured to recycle the products back to the feed tank constantly changing the feed composition. For this reason, a feed composition estimator was also needed.

Three complete runs of 36 hours were performed to collect the data to develop the composition estimators. During the first two runs data was collected to develop the models, and once the models were developed a third run was performed to validate them. The compositions used to train the feed composition predicting module were from the actual samples collected during the experiments. Two validations of the feed module were performed. One used as input the prediction from the distillate and bottom composition estimators. To eliminate additional error the other used the measured distillate and bottom compositions. The bottom and feed modules had very good performance which was verified by comparing the prediction with actual data. Since the variations were higher in the distillate composition, the distillate module displayed lower agreement between the prediction and the real data. This experience pointed out the relation between the number of data points used to train the neural net and the output range of variation.

Conclusions

In this work, a virtual sensor to measure composition, an online model reconciliation technique, and a multivariable control strategy were tested experimentally using a cyclohexane

/ normal-heptane binary distillation system. A neural net was used for the virtual sensor and increasing the range of variation in the measured variable introduced error to the prediction. The proposed model reconciliation approach displayed good results in the multivariable nonlinear system. In future work disturbances could be added to the model to improve its performance.

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