COMPARISON OF ADVANCED DISTILLATION CONTROL METHODS

First Annual Report

By

James B. Riggs

Work Performed Under Contract No. DE-FC04-94AL98747

Prepared:
U.S. Department of Energy
Office of Industrial Technologies
Washington, D.C.

Prepared:
Texas Tech University
Lubbock, Texas

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PREFACE

This report documents the technical progress made on the project "Comparison of Advanced Distillation Control Methods" the time period April 1994 through March 1995. Cost sharing for this study is being supplied by Texas Tech University and the Texas Tech Process Control and Optimization Consortium. Charles Russomann is the Program Manager for the DOE Office of Industrial Technologies. Ken Lucien is Technical Manager for the DOE Albuquerque Operations Office. Chuck Quinn and Frank Childs, the Project Technical Monitors are on the staff of Scientech, Inc. Professor James B. Riggs is the Principal Investigator and is the author of this report along with post-doctoral researcher and current PhD candidates and technician.

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Abstract

A detailed dynamic simulator of a propylene/propane (C_3) splitter, which was bench-marked against industrial data, has been used to compare dual composition control performance for a proportional-integral (PI) controller and several advanced controllers. The advanced controllers considered are dynamic matrix control (DMCTM), nonlinear process model based control, and artificial neural networks. Each controller was tuned based upon setpoint changes in the overhead product composition using 50% changes in the impurity levels. Overall, there was not a great deal of difference in controller performance based upon the setpoint and disturbance tests. Periodic step changes in feed composition were also used to compare controller performance. In this case, oscillatory variations of the product composition were observed and the variabilities of the DMC and nonlinear process model based controllers were substantially smaller than that of the PI controller. The sensitivity of each controller to the frequency of the periodic step changes in feed composition was also investigated.

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INTRODUCTION

Distillation in the refining and chemical industries consumes 3% of the total U.S. energy usage (Humphrey et al, 1991) which amounts to approximately 2.4 quad of energy annually. In addition, distillation columns usually determine the quality of final products and many times determine the maximum production rates.

Unfortunately, many times industry over-refluxes their columns in order to insure that the product purity specifications are met. That is, they use more energy than necessary to meet the product specifications. As a result, industry many times uses 30 to 50% more energy than necessary to produce their products. It has been estimated that an overall average 15% reduction of distillation energy consumption could be attained if better column controls were applied (Humphrey et al, 1991).

While there are many options for applying conventional and advanced distillation controls, industry does not know how to compare the various options. As a result, whether or not to apply advanced distillation control, what type of advanced control to apply, and how to apply it are usually determined based upon internal company politics and hearsay. In fact, when industry discusses advanced control, they refer to taking a "leap-of-faith." Because it is not understood, it may be applied where it is not needed or not applied where it should be applied. When improvements in distillation control performance are obtained, there is a tendency for industry to be satisfied not realizing that further improvements in control may be even more economically important. The bottom line is that industry does not have a consistent basis with which to compare the various options for distillation control.

1.1 Research Approach

The objective of the research is to develop the necessary information for the refinery and chemical industries to be able to make economic-based advanced control decisions.

The challenge to meeting these objectives is that as the particulars of a column change, the relative performance among proportional integral (PI) controls, and the advanced control options are likely to change. For example, it is likely that for some columns that are relatively easy to control there are not likely to be significant performance improvements over PI-controls. And for more difficult problems, the differences are expected to be substantial. Therefore, we must be able

identify what makes a distillation column more or less difficult to control. In addition, there are general classifications of distillation cases (highly non-ideal separations, columns with multiple sidestreams, etc.) that must be considered as well.

As a result, the approach used to meet the objective is to use detailed dynamic simulators of a range of distillation columns with varying degrees of control difficulty to assess the control performance of the various control options. It is well known that dynamic models of distillation columns contain the same control difficulties as real distillation columns (nonlinearity, coupling, and nonstationary behavior) when properly applied; therefore, column simulations offer an efficient means to make controlled comparisons of the various control approaches over a range of columns design and operating conditions. In fact, the simulators offer a degree of control in comparing distillation control methods that a real column cannot provide.

Distillation columns encompass a wide range of applications. In order to develop advanced control comparisons that will be useful, a range of columns must be considered.

The following factors should be considered in selecting representative columns:

- binary vs multicomponent separations
- hydrocarbon vs highly non-ideal separations
- high pressure vs. vacuum columns
- component separations vs. product cuts (e.g., crude columns)

Based upon these factors the following types of columns would be studied:

- a high reflux ratio binary column (e.g. a propylene/propane column)
- a multicomponent refinery column (e.g a depropanizer)
- a non-ideal binary column (e.g. a methanol/water column)
- a binary vacuum column (e.g a toluene/xylene column)
- a column with product cuts (e.g. a main fractionator)

Finally, there is the question of credibility. If the results of this study are to have an impact upon the practice of process control of distillation, industry must believe the results of the study and be willing to use them.

CASE STUDY AND SIMULATOR - C₃ SPLITTER

A simulation of an industrial C₃ splitter has been used as a test case to compare a conventional PI controller and several advanced controllers for dual composition control. Table 1

contains the design conditions for the C_3 splitter. The overhead composition is 99.7 mole % propylene, the bottoms composition in 2 mole % propylene, and the feed composition is 70 mole % propylene. There are 234 trays with a Murphree tray efficiency of 85% and an operating pressure of 18 atm. The modeling assumptions used in developing the dynamic model of the C_3 splitter are listed in Table 2.

The dynamic column model is based upon dynamic mole balances on propylene for each tray. A hydraulic time constant is used to model the liquid dynamics for the trays with one value of the hydraulic time constant for the entire column. The equimolal overflow assumption is used to calculate the flow rate of vapor leaving each stage. The vapor/liquid equilibrium was described using a relative volatility which was modeled as an explicit function of pressure and composition (Hill., 1959). As a result, each tray had its own relative volatility. Product composition analyzers and feed composition analyzers (when used) were assumed to have five minute cycle times.

The test column simulator has the (L, B) configuration implemented on it. See Table 3 for configuration definition. Gokhale(1994) evaluated nine possible column control configurations and found that the (L,B) configuration yielded the best performance for diagonal PI dual-composition control. When the simulation was equipped with perfect level control, the control performance of the (D,B) structure was found to be equivalent to the performance of the (L, B) configuration.

The dynamic model equations were integrated using an Euler integrator (Riggs., 1994) with a step size of 0.3 seconds. A fifty to one ratio of simulated time to CPU was obtained for a 66 MHz 486 PC using Microsoft FORTRAN 5. 1.

The dynamic model was bench-marked against dynamic step test data from an industrial C_3 splitter. The industrial data was based upon the (L,B) configuration. The (L,B) configuration is also used industrially (O'Conner, 1993). First, the simulator was found to provide the same general behavior as the industrial plant data (O'Conner, 1993) for open loop step changes in the manipulated variables and the feed rate. Then based upon response times, the hydraulic time constant of each tray was adjusted to match the industrially observed response times as closely as possible. For example, the overhead composition was observed to have an open loop response time of approximately 7 hours for a 0.5% change in the reflux rate. In addition, for a 1% change in the bottom flow rate, the response time for the bottom composition was approximately 25 hours (O'Conner, 1993). A hydraulic time constant of 3 seconds was found to provide the best overall dynamic match.

The following test scenarios were used to test the composition controllers.

1. Setpoint change to 99.85% propylene in the overhead product at $t = 100$ minutes followed by a setpoint changed to 99.5% at $t = 1000$ minutes
2. A ramp change in pressure from 211 to 226 psia from $t = 100$ minutes to $t = 160$ minutes followed by a step change in feed composition to 65% at $t = 1000$ minutes.
3. Negative and positive 5% step changes in feed composition with changes applied every 250 minutes. At time (t) equal to 250 minutes, the feed composition (z) was decreased to 65% propylene. At $t = 500$ minutes, z was set to 70%. At $t = 750$ minutes, z was set to 75%, at $t = 1000$ minutes, z was changed to 70%. At $t = 1,250$ minutes, z was set to 65%, etc.

Each controller was tuned for scenario 1 and tested on scenarios 2 and 3. Controller performance was evaluated by considering the variability in the propylene product while keeping the bottom product in the vicinity of 2% propylene.

IMPLEMENTATION APPROACH FOR EACH CONTROLLER

Conventional PI control, Dynamic Matrix Control (DMCTM), nonlinear Process Model Based Control (PMBC), and Artificial Neural Network (ANN) control were applied to the simulator of the C_3 splitter for dual composition control. The PI and nonlinear PMBC controllers were applied using the (L/F, B/F) configuration and DMC was applied using the (L,B) configuration but each controller was tuned for test scenario 1 based upon the overhead composition control performance. Setpoint changes using 50% changes in impurity were chosen for controller tuning in order to provide a consistent tuning procedure that is likely to be robust for a wide range of upsets.

The diagonal PI composition controllers were tuned using Auto Tune Variation tests (ATV; Astrom and Agglund, 1988) with on-line determination of the overall detuning factor. ATV tests were used to identify the ultimate gain and ultimate period for the overhead and bottoms. The Ziegler-Nichols (Ziegler and Nichols, 1942) PI settings were then calculated. Both controllers were detuned to provide minimum IAE (integral absolute error) for setpoint changes in the overhead product using 50% impurity changes (test scenario 1). Detuning was accomplished by dividing both controller gains and multiplying both reset times by the detuning factor. The diagonal PI controllers were also tuned using pulse tests for identification of transfer function models followed by the application of the BLT tuning procedure (Luyben, 1986) as a comparison to the ATV tuning

procedure. The control performance of the controllers tuned by each procedure were found to be essentially equivalent. Since the ATV test, with online detuning, was easier to implement and is more realistically applied in an industrial setting, it was chosen as our PI tuning procedure.

A lead-lag feed forward element for the PI controllers was developed for feed composition changes for the composition control loop on the bottom of the column and for the top. The feedrate used in the L/F and B/F manipulated-variable configurations was dynamically compensated using a dead time plus a lag. The tuning setting for the PI controllers and the feed forward controllers are listed in Table 4.

The DMC™ controller was provided to us by the Dynamic Matrix Control Corporation. The step response models for the DMC controllers were developed for each input (z, F, L, B)/output (x, y) pair. The output for the overhead product was log transformed in an effort to linearize the overall process behavior:

$$y^l = \log(1-y) \quad (1)$$

At least 12 independent step tests were conducted for each input variable. Identification software (DMI™ provide by DMC Corporation) was applied to all the step test data in order to develop the step response models for each input/output pair used by the DMC™ controller. The step response models were supplied to the DMC™ controller and the final controller tuning was performed for test scenario 1. Because impurity level in the overhead is 6.67 times lower than the bottoms and because it is more important to minimize the variability of the overhead product, the deviations in the overhead product were weighted to be 15 times more important than the bottoms product. A move suppression factor of 1.0 for the reflux and 0.1 for the bottoms flow were selected for the DMC™ controller.

The nonlinear PMBC controller using the tray-to-tray binary model was applied using the approach presented by Riggs et al, 1993. The control law calculates target setpoints (x_{ss} , y_{ss}) based upon proportional and integral feedback.

$$x_{ss} = x + K_{11}(x_{sp} - x) + K_{21} \int (x_{sp} - x) dt \quad (2)$$

$$y_{ss} = y + K_{12}(y_{sp} - y) + K_{22} \int (y_{sp} - y) dt \quad (3)$$

Then, the values of x_{ss} and y_{ss} are used by the tray-to-tray binary model to calculate the reflux rate. Since Equations (2) and (3) can result in values of y_{ss} that are negative and values of y_{ss} that are greater than 1.0, limits are used to restrict the maximum and minimum values of x_{ss} and y_{ss} .

An overall material balance was used to calculate the value of the bottoms flow rate. Because the column responds much faster to energy changes (e.g., reflux flow) than to material balance changes (e.g., bottoms flow), the target product compositions (y_{ss} and y_{ss}) are amplified by K_{MB} according to the following equations in an effort to improve the response of the bottom product composition.

$$x_{MB} = x_{sp} + K_{yMB}(x_{ss} - x_{sp}) \quad (4)$$

$$y_{MB} = y_{sp} + K_{yMB}(y_{ss} - y_{sp}) \quad (5)$$

Then

$$\frac{B}{F} = \frac{y_{MB} - z}{y_{MB} - x_{MB}} \quad (6)$$

The feedrate and the feed composition used by the model were each dynamically compensated using a first order lag and a deadtime. When a feed compensation analyzer is not available, the product purities and product flow rate are used to calculate an estimate of the feed composition. This back calculated feed composition is filtered and the filtered value is used as the feed composition by the tray-to-tray steady state model. When Equations (2) and (3) are used for setpoint changes, the resulting changes in the manipulated variables are much too sharp; therefore, a filter on the setpoint changes was used to stabilize the controller for setpoint changes. The nonlinear PMBC controller was tuned for test scenario 1 based upon minimizing the IAE for the

overhead product. Table 5 contains the tuning settings for the nonlinear PMBC controller.

The tray-to-tray steady-state controller model used by the nonlinear PMBC controller used the relative volatility modeled as a function of liquid composition and pressure, but used a stagewise tray efficiency while the dynamic simulator used a Murphree tray efficiency. At the base case, the controller model required a stagewise efficiency of 92% to match the simulator-state conditions with a 85 % Murphree efficiency.

An ANN steady-state model was used to replace the tray-to-tray steady-state binary model used by the nonlinear PMBC controller. The ANN model considers x_{ss} , y_{ss} , z and, P , as input and calculates the reflux rate as its output. Then, the bottoms flow rate was calculated by material balance in a manner similar to the nonlinear PMBC controller. Because the ANN model did not always match the simulator at steady-state, a filtered bias was used to keep the ANN model in agreement with the process (dynamic column simulator). That is, for the reflux, the difference between the measured reflux flow and the value calculated by the ANN model was filtered on-line. When control calculations were required, the values of x_{ss} , y_{ss} , Z_i and P were fed to the ANN model and the resulting reflux flow rate was added to the current value of the filtered bias. A similar procedure was used for calculating an on-line bias for the bottom flow rate. The ANN model was trained over the expected range of inputs using 700 steady state data sets from a tray-to-tray steady-state simulator. The ANN model based controller was tuned for test scenario 1, and the resulting controller setting are listed in Table 6.

RESULTS - C₃ SPLITTER

For the C₃ splitter column, Figures 1 and 2 show the control results for the PI, nonlinear PMBC, and DMCTM controllers for setpoint changes in the overhead product (test scenario 1). Each controller was tuned for this test based upon optimizing the performance of the overhead composition and the resulting tuning parameters remained unchanged throughout the remainder of the tests. From Figure 1, the nonlinear PMBC and DMCTM had essentially equivalent performances while the PI controller performed well but was somewhat slower settling than the multivariable controllers. There is a slight glitch in the DMCTM performance at about 700 minutes and 1600 minutes. This resulted because the model horizon in the DMCTM controller (600 minutes) was significantly smaller than the actual process settling time of about 1800 minutes. We used version

4.0 of DMCTM which limits the number of model coefficients to 120 while the more recent release (version 5.0) has up to 600 coefficients which would have easily eliminated the glitch. Figure 2 shows the performance of each controller for the control of the bottom product composition during the setpoint changes on the overhead. Note that the nonlinear PMBC controller had the shortest settling times. Overall considering Figure 1 and 2, there is not a great deal of difference between the controllers although the multivariable controllers did out perform the PI controller. Figures 3 and 4 show the reflux and bottoms flow rates for each controller for test scenario 1. The nonlinear PMBC controller clearly shows the smoothest use of the manipulated variables.

The nonlinear PMBC controller that used the ANN steady-state model is compared with the nonlinear PMBC controller that used the tray-to-tray steady-state model in Figures 5 and 6 for test scenario 1. The ANN controller actually performed slightly better for the overhead composition control but it was quite sluggish with greater deviations from setpoint for the bottom composition control.

Figures 7 and 8 show the control results for the PI, nonlinear PMBC, and DMCTM controllers for test senairo 2 with no feed composition analyzer readings available. Note that each controller seemed to handle the column pressure changes more or less with the same proficiency for the overhead composition while the multivariable controllers showed smaller maximum deviation from setpoint for the step change in feed composition. For the bottoms composition, the nonlinear PMBC controllers demonstrated tighter control than the DMCTM and PI controllers.

Figures 9 and 10 show the control results for the PI, nonlinear PMBC, and DMCTM controllers for test scenario 3 with no feed composition analysis available. For the overhead product, the multi-variable controllers had variabilities that were about two and a half times lower than the PI controller. For the bottom composition, the PI and DMCTM controllers had very nearly equivalent performance while the nonlinear PMBC controller performed considerably better.

Figures 11 and 12 show the control results for the PI, nonlinear PMBC, and DMCTM controllers for test scenario 3 using a feed composition analyzer. The results improved for the PI and DMCTM controllers but worsened for the nonlinear PMBC controller. This was because the feedforward controllers for the PI and DMCTM were adjusted for the overhead and bottoms products separately, but the nonlinear PMBC controller had only one feed composition which is filtered. Moreover, the top and bottom behave quite differently dynamically which significantly penalized

the nonlinear PMBC controller. The bottoms composition control for the DMC and PI controllers seemed to benefit the most from the addition of feedforward of the feed composition analyzer.

Figure 13 shows the average total variation in the overhead product for each controller as a function of hold time for the periodic feed composition changes (test scenario 3). The DMCTM controller showed significant variability reduction over the PI-controller for the full range of hold times with variability reductions ranging between 4/1 to 2/1. The nonlinear PMBC controller showed results equivalent to the DMCTM controller up to a hold time of 300 minutes, but above 300 minutes the results of the PMBC controller approached those of the PI controller. The deteriorating performance of the nonlinear PMBC controller at larger hold times was probably due to the lack of flexibility of this controller and the dynamic difference between the overhead and bottom of the C₃ splitter. Figure 14 shows the average total variation in the bottoms product for each controller as a function of hold time for test scenario 3. The PI and DMC controllers exhibited essentially equivalent performance while the results from the nonlinear PMBC controller were consistently better.

CONCLUSION

Although the difference in performance for the PI and the multivariable controllers for setpoint changes and step changes in disturbances was not large, significant improvement in performance was observed for the multivariable controllers over the PI controller for a periodic variation in feed composition. In fact, the variability reduction observed in the simulation study for nonlinear PMBC over PI controls are similar to those observed industrially (Riggs et al, 1993).

The periodic variation in disturbances resulted in a product variability with characteristics similar to the product variabilities observed industrially (Riggs et al, 1993). Usually industrial feed composition upsets involved some variation in feed composition with respect to time, but are not well-represented as step changes. Industrial disturbances are likely to have an amplitude/frequency distribution that would combine with the frequency sensitivity of the controller to produce the resulting overall product variability performance. Periodic variation of disturbances (preferably sine wave disturbances) are proposed here as a more critical analysis of controller performance than classical step tests particularly if the frequency of the disturbance is changed.

NOMENCLATURE

B - bottom product flow rate

F - column feed rate

K_1 - the proportional gain in the GMC control law (Equations 2 and 3)

K_2 - the integral gain in the GMC control law (Equations 2 and 3)

L - reflux flow rate

x - the mole fraction of propylene in the bottoms product

y - the mole fraction of propylene in the overhead product

y^1 - the log transformed value of y

z - the mole fraction of propylene in the feed

SUBSCRIPTS

MB - material balances

SP - setpoint

SS - steady state target

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Table 1
Design Specifications for Propylene/Propane Splitter

Number of Trays	232
Feed Tray Location (From Bottom)	64
Feed Flow rate	13.44 kg/sec (106,400#/HR)
Feed Comp. (mole %)	
Light Key	C ₃ = - 70
Heavy Key	C ₃ - 30
Factor times minimum reflux for design	1.3
Column Diameter	3.96 m (13 ft)
Overhead Pressure	15.0 atm (221 PSIA)
Overhead Product Impurity	C ₃ - 0.3 mole%
Bottoms Product Impurity	C ₃ - 2.0 mole %
Overhead Flow rate	9.21 kg/sec (73,100 #/HR)
Overhead Temperature	34.7°C (94.4 °F)
Bottom Flow rate	4.21 kg/sec (33,400 #/HR)
Bottom Temperature	42.3°C (108.1 °F)
Reboiler Vapor flow rate	131.24 kg/sec (1,041,165 #/HR)
Reflux Ratio	12.6
Feed Quality	Saturated

Table 2
Modeling Assumptions for Propylene/Propane Splitter

Liquid Dynamic	Hydraulic time constant
Negligible Vapor/Holdup	yes
Value dynamic on all flows	no
Accumulation and reboiler level control	PI
Analyzer delays on product composition	5 minutes
Eqimolal overflow	yes
Residence time in reboiler	5 minutes
Residence time in accumulator	5 minutes
Heat transfer dynamics modeled	no
Saturated liquid feed	yes
Subcooled reflux	no
Pressure dynamics modeled	no
Perfect mixing of liquid on trays	yes
Ideal Vapor Liquid Equilibrium	no

Table 3

Combinations for 9 Control Configurations

Top

L = Reflux Flow Rate

D = Distillate Flow Rate

L/D = Reflux Ratio

Bottom

V = Blow Up Rate

B = Bottom Flow Rate

V/B = Boil Up Ratio

Table 4
Controller Settings for PI Controllers

<u>Feedback Only Controller</u>	<u>Overhead Control Loop</u>	<u>Bottom Control</u>
<u>Loop</u>		
K _c	232.15 #mole/mole% -sec	1.7 #mole/mole% -sec
T _I	75 minutes	400 minutes
<u>Feedback with Feedforward</u>		
K _L	309.#mole/mole% -sec	4.53 #mole/mole% -sec
T _I	56.3 minutes	150 minutes
<u>Feedforward Controller</u>		
<u>For Feed Composition Changes</u>		
Gain	5.08 #mole/mole% -sec	-0.71 #mole/mole% -sec
Deadtime	20 minutes	10 minutes
Lead	120 minutes	600 minutes
Lag	240 minutes	450 minutes
<u>Dynamic Compensation for Feedrate</u>		
Deadtime	5 minutes	20 minutes
Lag	100 minutes	150 minutes

Table 5
Controller Settings for Nonlinear PMBC Controller

Feedback Controller

	Overhead Control Loop	Bottoms Control Loop
K_1	3.0	3.0
K_2	0.0	0.0
Material Balance Gain (K_{yMB} and K_{xMB})	10.0	6.0

Feedforward Controller

Filter factor on feedrate	0.04
Deadtime on feedrate	10 minutes
Filter factor on z	0.10
Deadtime on z	5 minutes

Filters

For model efficiency parameterization	0.025
For back calculated feed composition	0.025
For setpoint changes for overhead	0.085
For setpoint changes for bottom	0.10

Table 6

Controller Settings for ANN Controller

Feedback Controller

	<u>Overhead Control Loop</u>	<u>Bottoms</u>	<u>Control</u>	<u>Loop</u>
K_1	3.0	4.0		
K_2	0.0	0.0		
Material Balance Gain (K_{yMB} and K_{xMB})	10.0	6.0		

Feedforward Controller

Filter factor on feedrate	0.04
Deadtime on feedrate	10 minutes
Filter factor on z	0.10
Deadtime on z	5 minutes

Filters

For model efficiency parameterization	0.02
For back calculated feed composition	0.001
For setpoint changes for overhead	0.085
For setpoint changes for bottom	0.10

Figure 1. Comparison of overhead composition control for test scenario no. 1

Figure 2. Comparison of bottoms composition control for test scenario no. 1

Figure 3. Reflux flow rate for various controllers for test scenario no.1

Figure 4. Bottoms flow rate for various controllers for test scenario no. 1

Figure 5. Comparison of overhead composition control for nonlinear PMBC and ANN controllers for test scenario no. 1

Figure 6. Comparison of bottoms composition control for nonlinear PMBC and ANN controllers for test scenario no. 1

Figure 7. Comparison of overhead composition control for test scenario no. 2 without a feed composition analyzer

Figure 8. Comparison of bottom composition control for test scenario no 2 without a feed composition analyzer

Figure 9. Comparason of overhead composition control for nonlinear PMBC, DMC, and PI controllers for test scenario no. 3

Figure 10. Comparison of bottoms composition control for test scenario no. 3 without a feed composition analyzer

Figure 11. Comparison of overhead composition control for test scenario no. 3 without a feed composition analyzer

Figure 12. Comparison of bottoms composition control for test scenario no. 3 with a feed composition analyzer

Figure 13. Variation in overhead product composition as a function of hold time for test scenario no. 3 without an feed composition analyzer

Figure 14. Variation in bottoms product composition as a function of hold time for test scenario no. 3 without a feed composition analyzer