

CHAPTER 7
DYNAMIC DATA RECONCILIATION
OF AN ACETYLENE HYDROGENATION PROCESS

7.1 Introduction

This chapter presents the procedure of dynamic data reconciliation. All case studies are computer simulation studies. The dynamic data reconciliation application and the results are discussed in this chapter.

7.2 Dynamic data reconciliation simulation of an acetylene hydrogenation process

The chosen method of dynamic data reconciliation is based on weight least square principle. This method is described in the efficient data reconciliation and estimation for dynamic process using nonlinear programming techniques paper by Liebman and friends (Liebman *et. al.*, 1992) and is presented in the thesis in Chapter 3. The dynamic data reconciliation objective function of this application is

$$\min_{y_{est}} \sum_{i=1}^N s^2 [(y_m)_i - (y_{est})_i]^2 \quad (7.1)$$

where y are the all components and temperature
subject to the constrains

1. The overall mole balance equation and the component balance equation

mole fraction balance equation: inlet bed I

$$[F_{Ac}]_{in} + [F_{Eth}]_{in} + [F_{H2}]_{in} + [F_{MA}]_{in} + [F_{PD}]_{in} + [F_{CO}]_{in} + [F_E]_{in} + [F_{Pr}]_{in} + [F_{Me}]_{in} + [F_{Inert}]_{in} - 100 = 0 \quad (7.2)$$

mole fraction balance equation: outlet bed III

$$[F_{Ac}]_{out} + [F_{Eth}]_{out} + [F_{H2}]_{out} + [F_{MA}]_{out} + [F_{PD}]_{out} + [F_{CO}]_{out} + [F_E]_{out} + [F_{Pr}]_{out} + [F_{Me}]_{out} + [F_{Inert}]_{out} - 100 = 0 \quad (7.3)$$

mole balance of acetylene

$$[mole_{Eth}]_{in} + [mole_{Ac}]_{in} - [mole_{Ac}]_{out} - [mole_{Eth}]_{out} - [mole_E]_{out} + [mole_E]_{in} = 0 \quad (7.4)$$

mole balance of propene

$$[\text{mole}_{\text{MA}}]_{\text{in}} - [\text{mole}_{\text{MA}}]_{\text{out}} + [\text{mole}_{\text{PD}}]_{\text{in}} - [\text{mole}_{\text{PD}}]_{\text{out}} - [\text{mole}_{\text{Pr}}]_{\text{out}} + [\text{mole}_{\text{Pr}}]_{\text{in}} = 0 \quad (7.5)$$

mole balance of hydrogen

$$[\text{mole}_{\text{H}_2}]_{\text{in}} - [\text{mole}_{\text{H}_2}]_{\text{out}} - [\text{mole}_{\text{Pr}}]_{\text{out}} + [\text{mole}_{\text{Pr}}]_{\text{in}} - [\text{mole}_{\text{E}}]_{\text{out}} + [\text{mole}_{\text{E}}]_{\text{in}} = 0 \quad (7.6)$$

mole balance of methane

$$[\text{mole}_{\text{Me}}]_{\text{in}} - [\text{mole}_{\text{Me}}]_{\text{out}} = 0 \quad (7.7)$$

2. The overall energy balance equation

$$\begin{aligned} & [\text{Cp}_{\text{average}} * (\text{total mole}) * T]_{\text{in}} + (\Delta\text{Hr}_{\text{Ac}} * ([\text{mole}_{\text{Ac}}]_{\text{in}} - [\text{mole}_{\text{Ac}}]_{\text{out}})) + \\ & (\Delta\text{Hr}_{\text{Eth}} * ([\text{mole}_{\text{E}}]_{\text{out}} - [\text{mole}_{\text{E}}]_{\text{in}})) + (\Delta\text{Hr}_{\text{MA}} * ([\text{mole}_{\text{MA}}]_{\text{in}} - [\text{mole}_{\text{MA}}]_{\text{out}})) + \\ & (\Delta\text{Hr}_{\text{PD}} * ([\text{mole}_{\text{PD}}]_{\text{in}} - [\text{mole}_{\text{PD}}]_{\text{out}})) + (\Delta\text{Hr}_{\text{CO}} * ([\text{mole}_{\text{CO}}]_{\text{in}} - [\text{mole}_{\text{CO}}]_{\text{out}})) - \\ & [\text{Cp}_{\text{average}} * (\text{total mole}) * T]_{\text{out}} - Q = 0 \end{aligned} \quad (7.8)$$

$$\begin{aligned} Q = & [(\text{water flow rate}) * \text{Cp}_{\text{H}_2\text{O}} * (T_{\text{out}} - T_{\text{in}})]_{\text{inter cooler I}} + \\ & [(\text{water flow rate}) * \text{Cp}_{\text{H}_2\text{O}} * (T_{\text{out}} - T_{\text{in}})]_{\text{inter cooler II}} \end{aligned} \quad (7.9)$$

and inequality constrains is

$$[\text{Fr}_{\text{Ac}}]_{\text{out}} < 0.1 \quad (7.10)$$

the estimation function of y_{est} is

$$y_{\text{est}} = Ay_m + B \quad (7.11)$$

Note : The steps for the dynamic data reconciliation is presented in chapter 3.

The dynamic data reconciliation program are test with the measurement of outlet acetylene concentration (ppm) that are simulated at time steps of 0.01 and 0.0025 hours by adding Gaussian noise (random noise with normal distributed graph and zero mean) to the true values obtained from the model. The measurements are simulated with a measurement error standard deviation of 5% and 10% of the corresponding reference value. The created data reconciliation algorithm is applied with history horizons (H) of 5, 10, and 15 time steps to investigate the effect of changing H on the performance of the method. The data reconciliation are proceeded with the different conditions summarized in the Table 7.1

Table 7.1 Simulation condition summaries

Case	Feed condition	Noise adding to measured data	History horizon
1	constant	5%	5
2	step change	5%	5
3	constant	5%	10
4	step change	5%	10
5	constant	5%	15
6	step change	5%	15
7	constant	10%	5
8	step change	10%	5
9	constant	10%	10
10	step change	10%	10
11	constant	10%	15
12	step change	10%	15

Table 7.2 The descriptions of the Figure 7.1-7.12

Figure number	History horizon	Noise %	Simulation condition	Computation-time	%Sd reduction
1	5	5	constant feed	1.54	83.21
2	5	5	step change in feed	2.82	83.22
3	10	5	constant feed	5.23	90.38
4	10	5	step change in feed	5.79	90.72
5	15	5	constant feed	6.51	93.01
6	15	5	step change in feed	7.1	92.41
7	5	10	constant feed	1.58	80.37
8	5	10	step change in feed	2.9	80.84
9	10	10	constant feed	5.31	89.11
10	10	10	step change in feed	5.83	89.52
11	15	10	constant feed	6.51	92.79
12	15	10	step change in feed	7.02	92.8

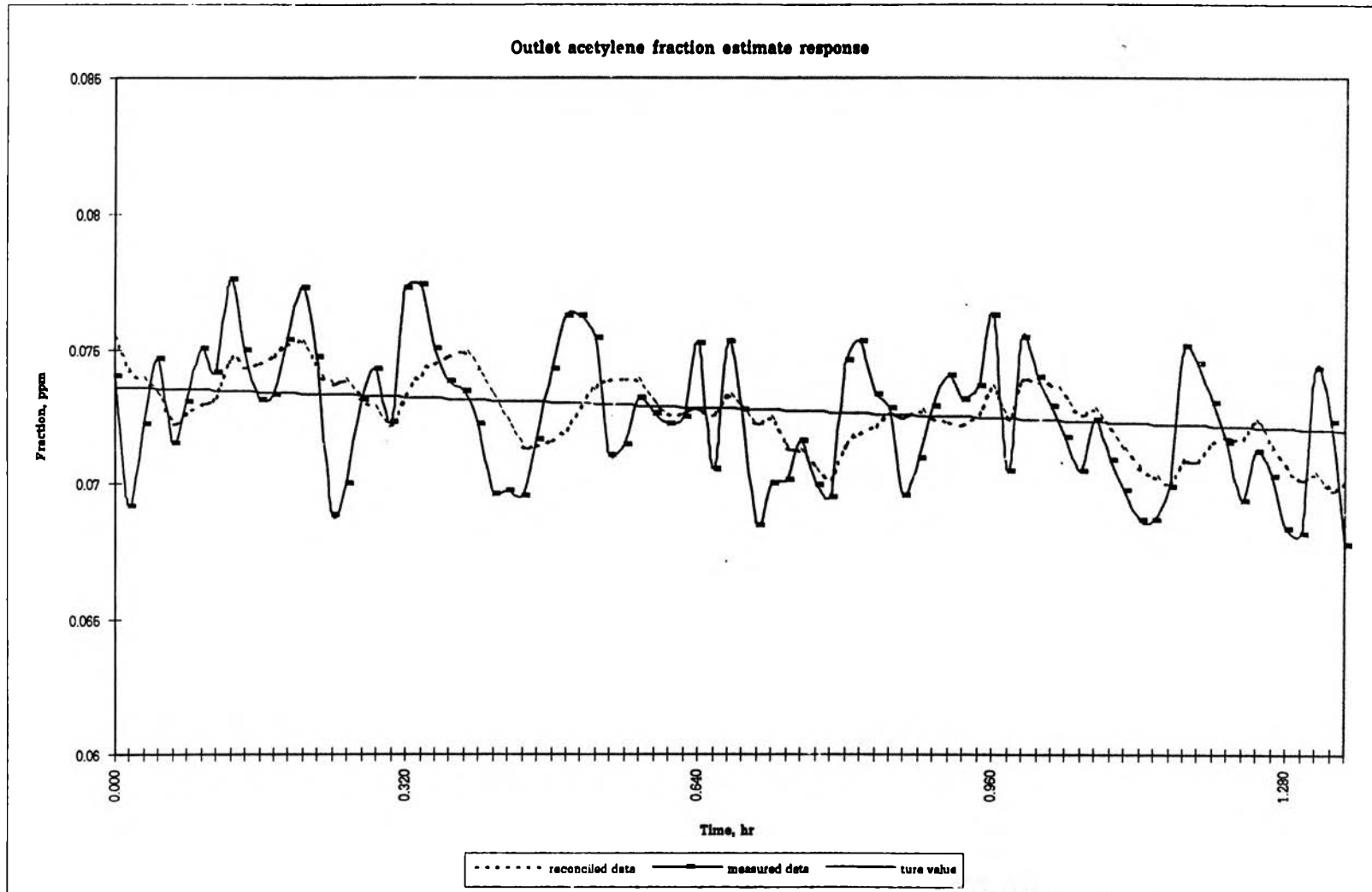


Figure 7.1 Outlet acetylene estimate response through 5% noise measured data with $H = 5$

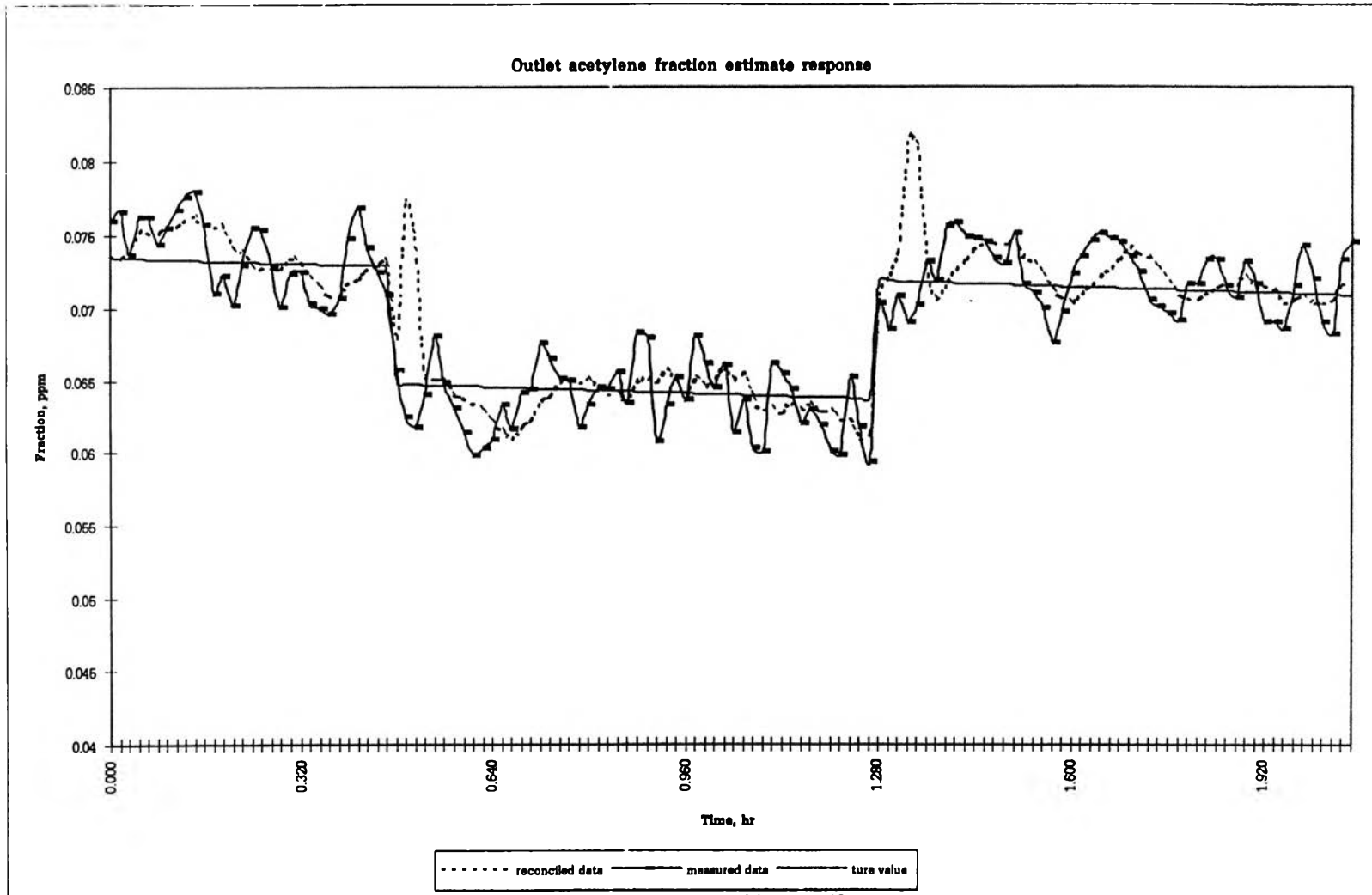


Figure 7.2 Outlet acetylene estimate response to step change in feed concentration through 5% noise measured data with $H = 5$

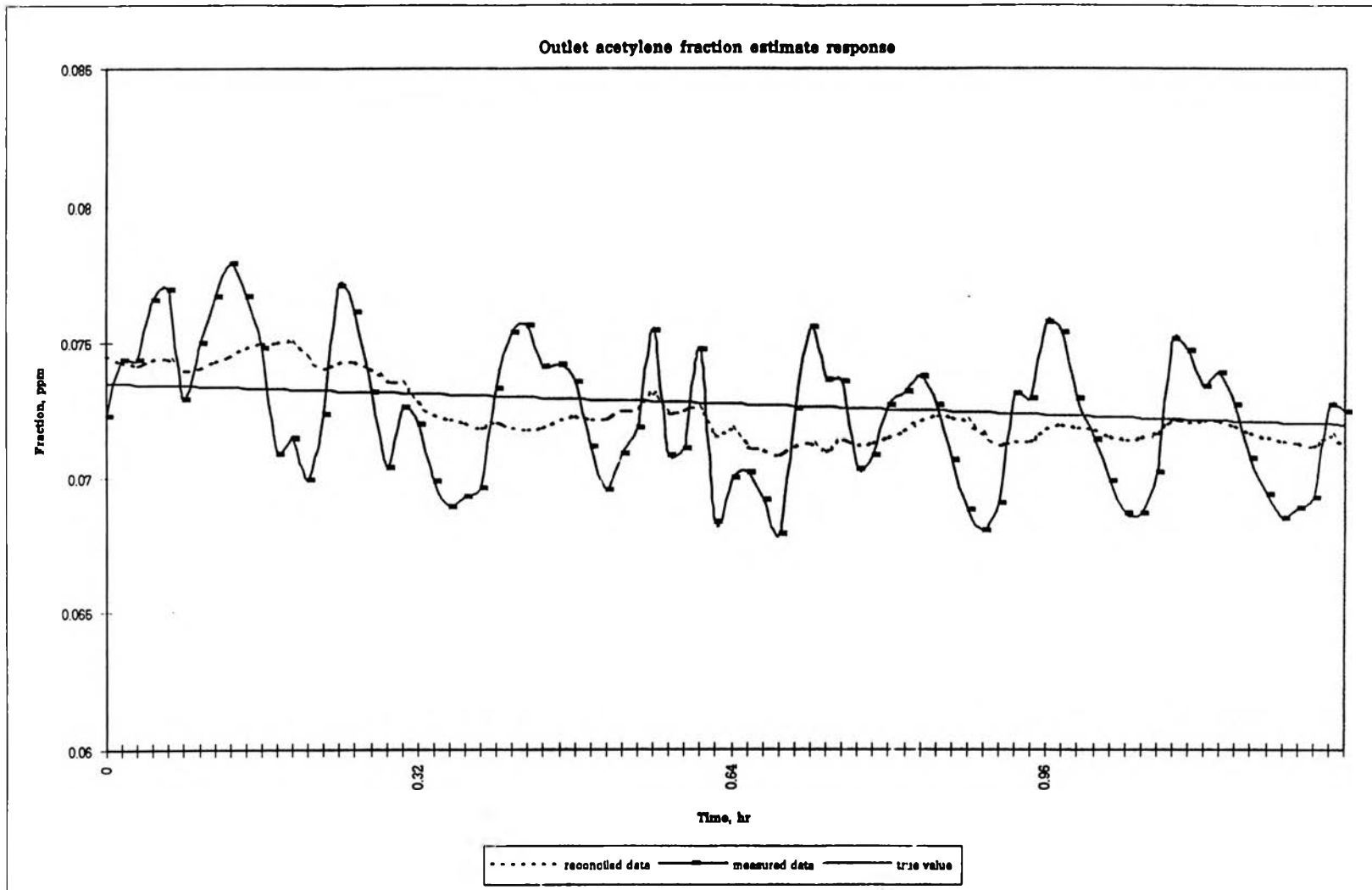


Figure 7.3 Outlet acetylene estimate response through 5% noise measured data with $H = 10$

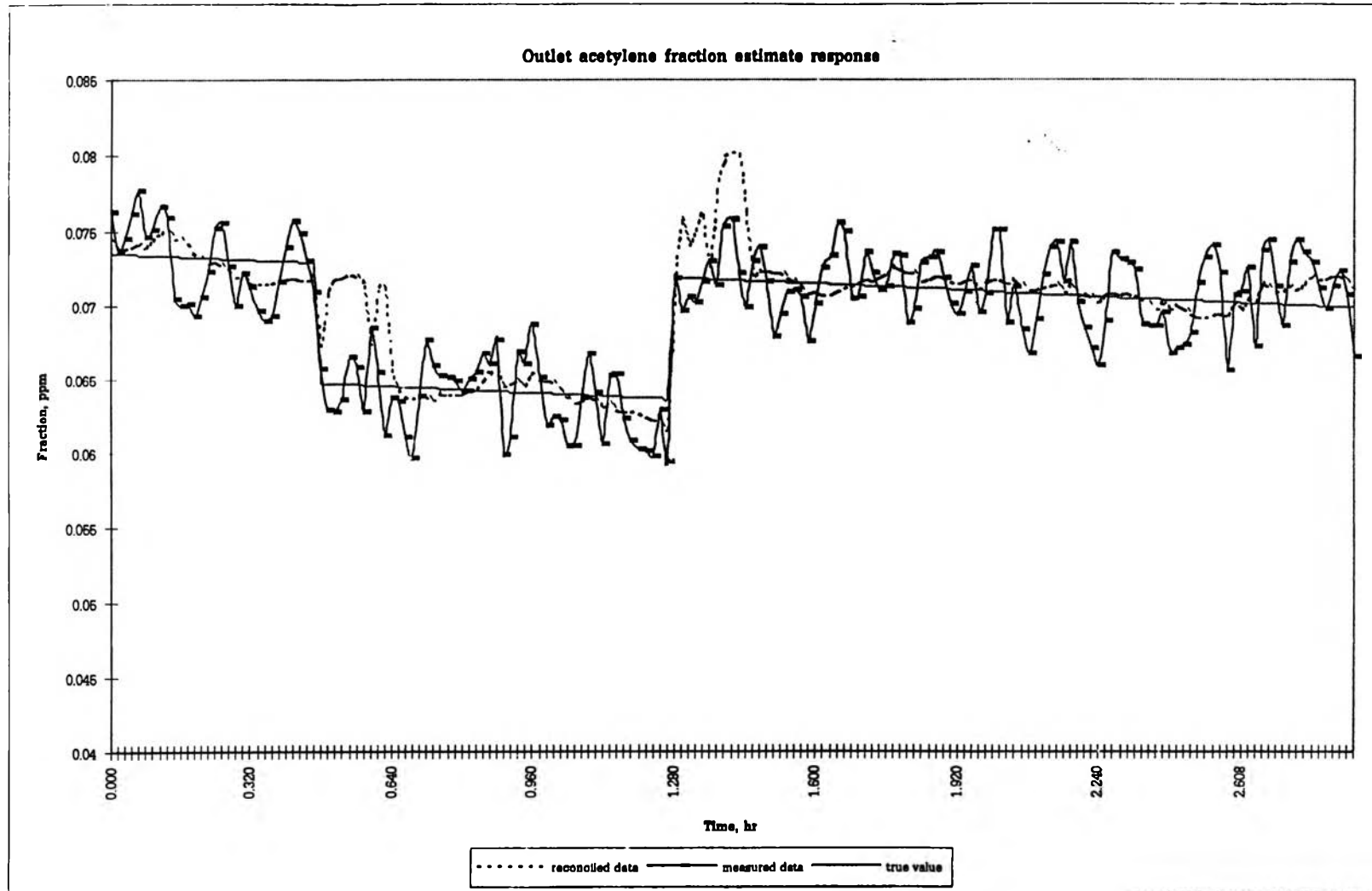


Figure 7.4 Outlet acetylene estimate response to step change in feed concentration through 5% noise measured data with $H = 10$

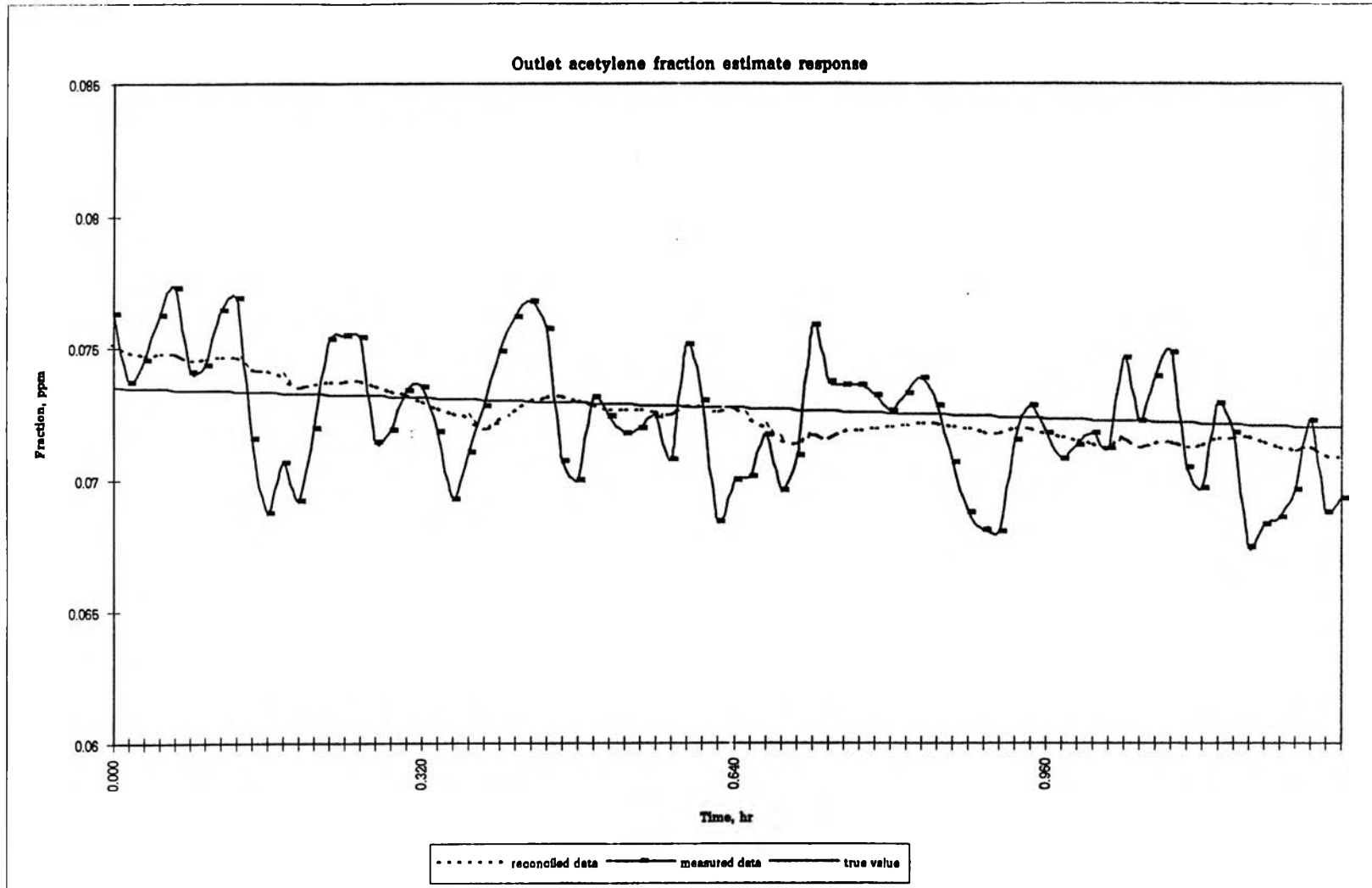


Figure 7.5 Outlet acetylene estimate response through 5% noise measured data with $H = 15$

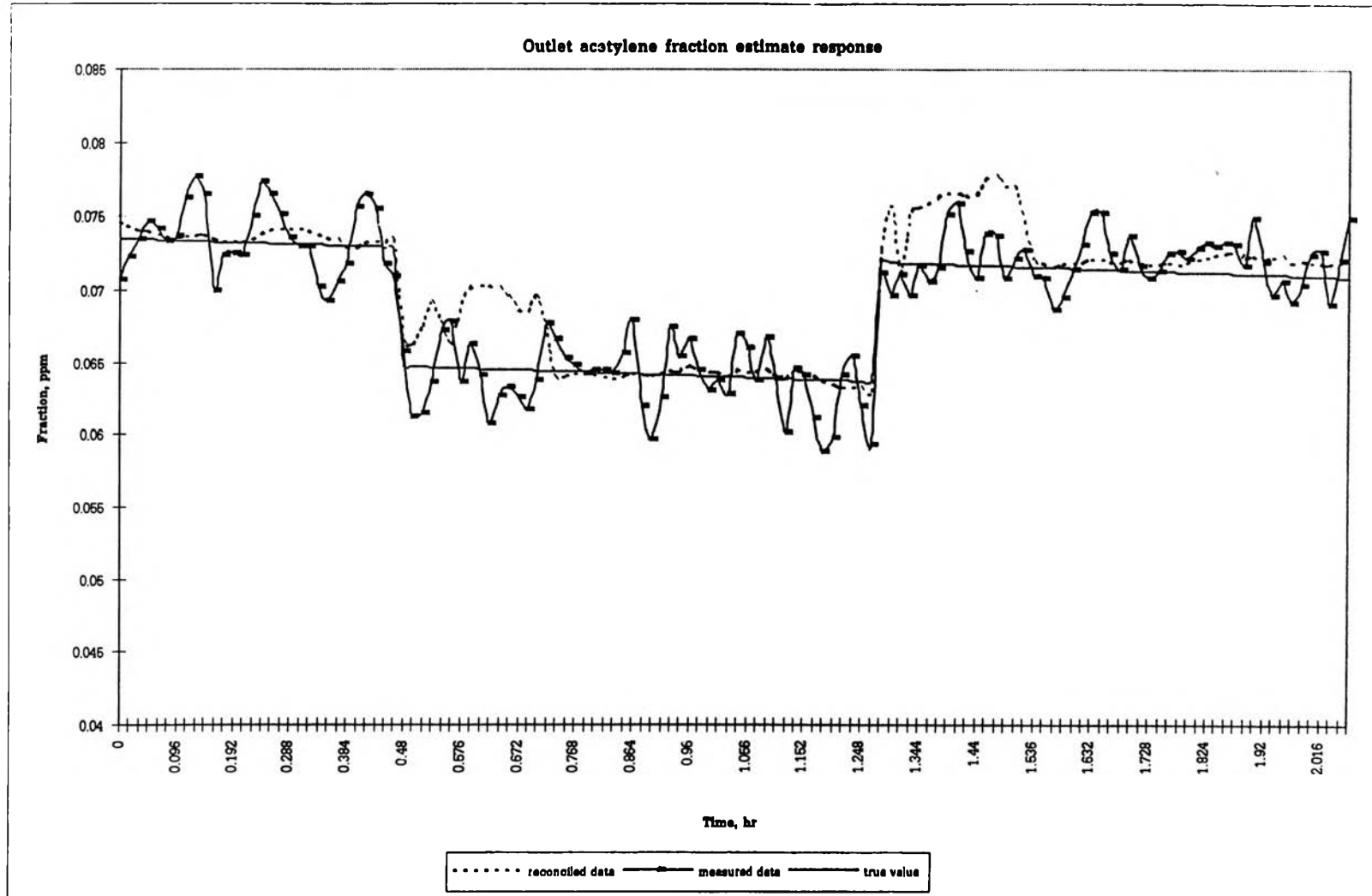


Figure 7.6 Outlet acetylene estimate response to step change in feed concentration through 5% noise measured data with $H = 15$

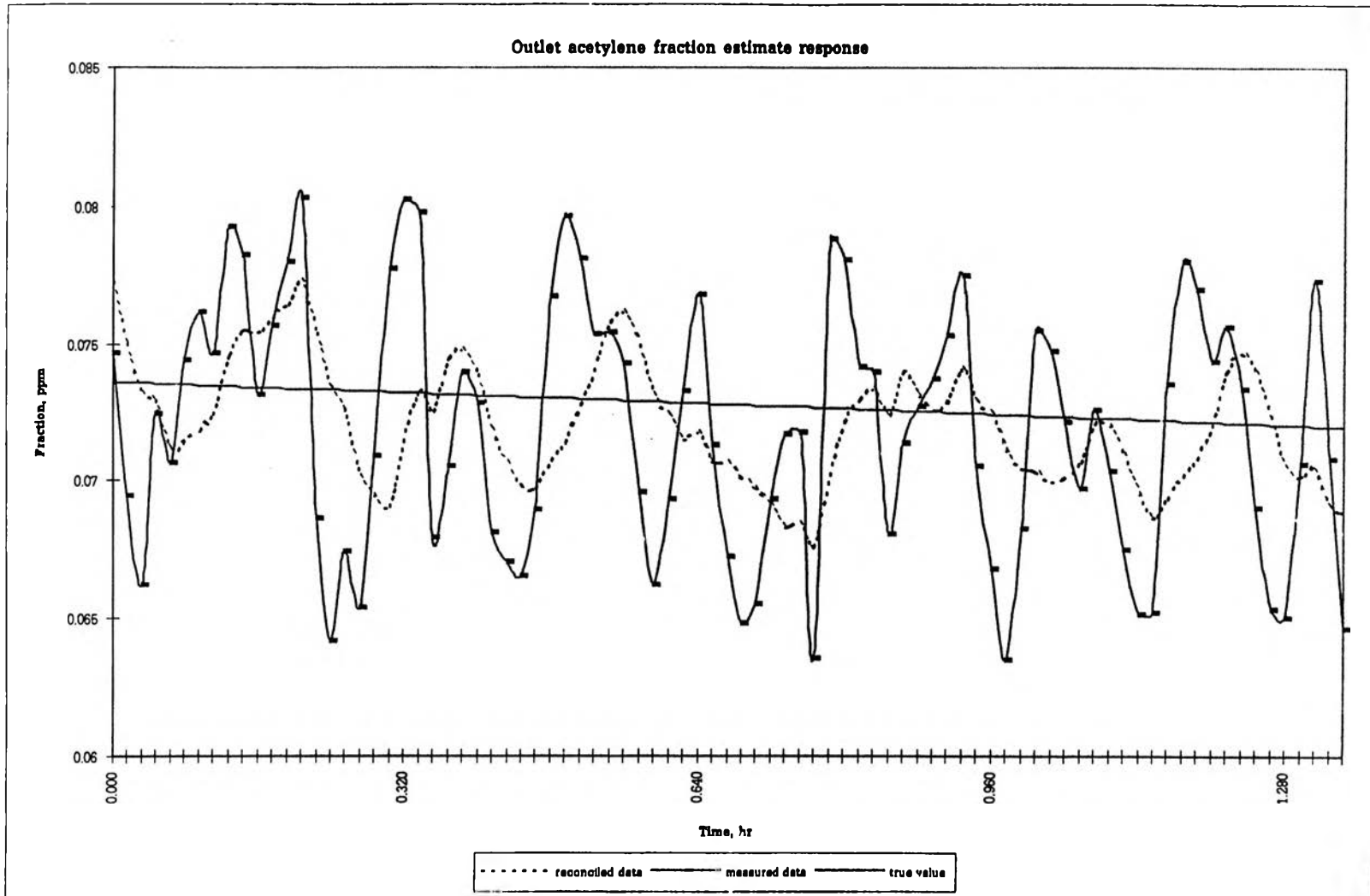


Figure 7.7 Outlet acetylene estimate response through 10% noise measured data with $H = 5$

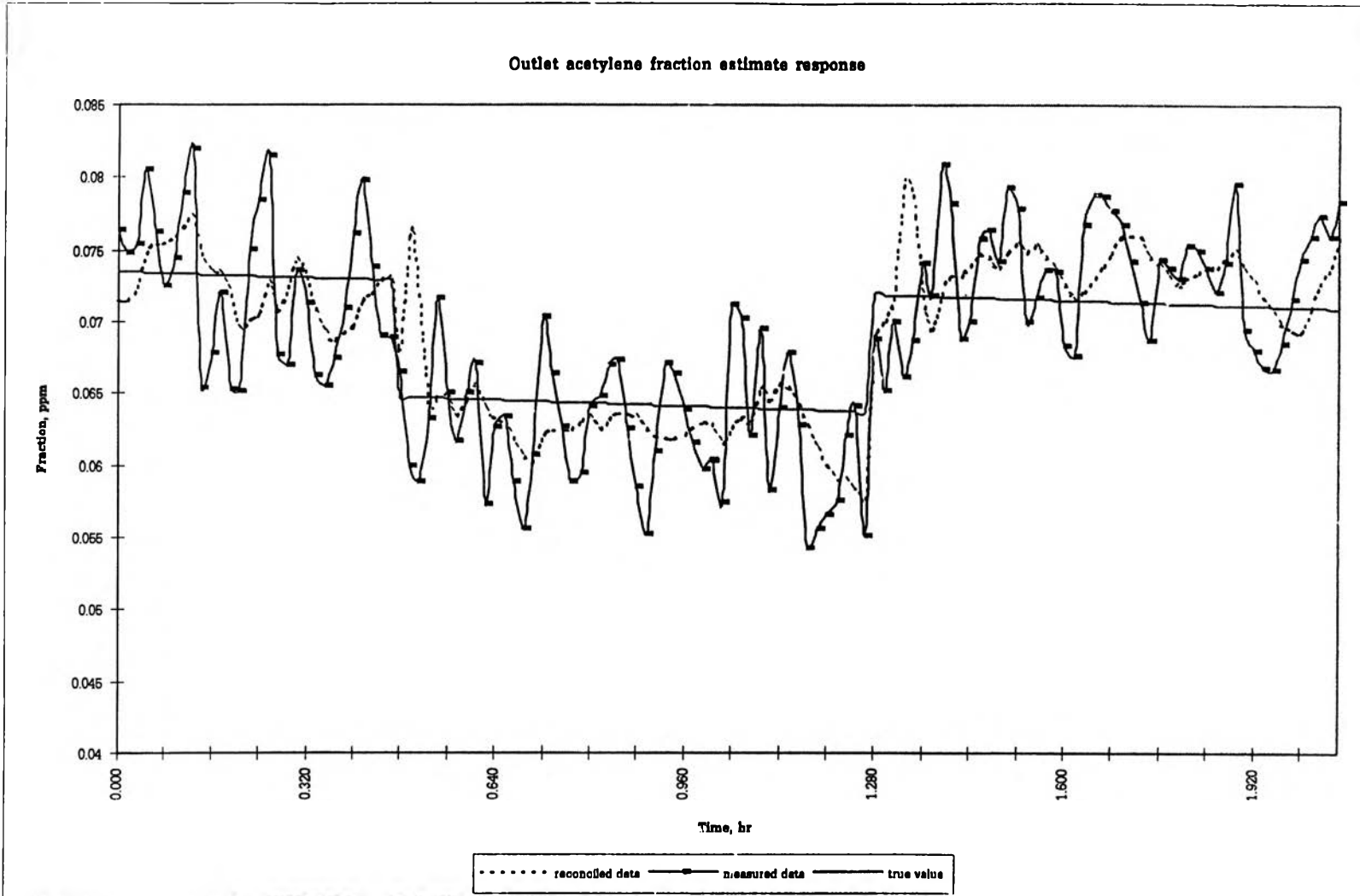


Figure 7.8 Outlet acetylene estimate response to step change in feed concentration through 10% noise measured data with $H = 5$

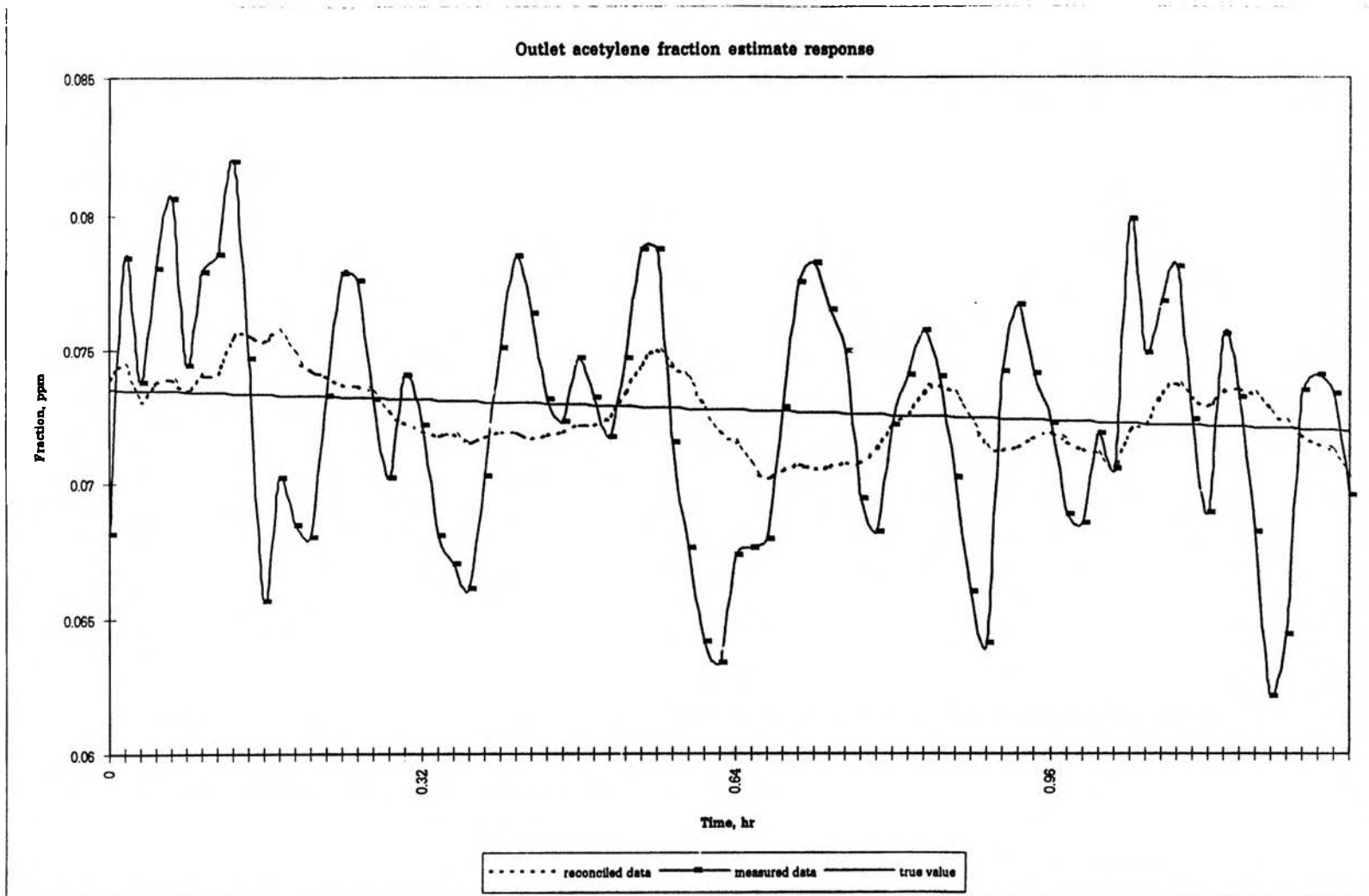


Figure 7.9 Outlet acetylene estimate response through 10% noise measured data with $H = 10$

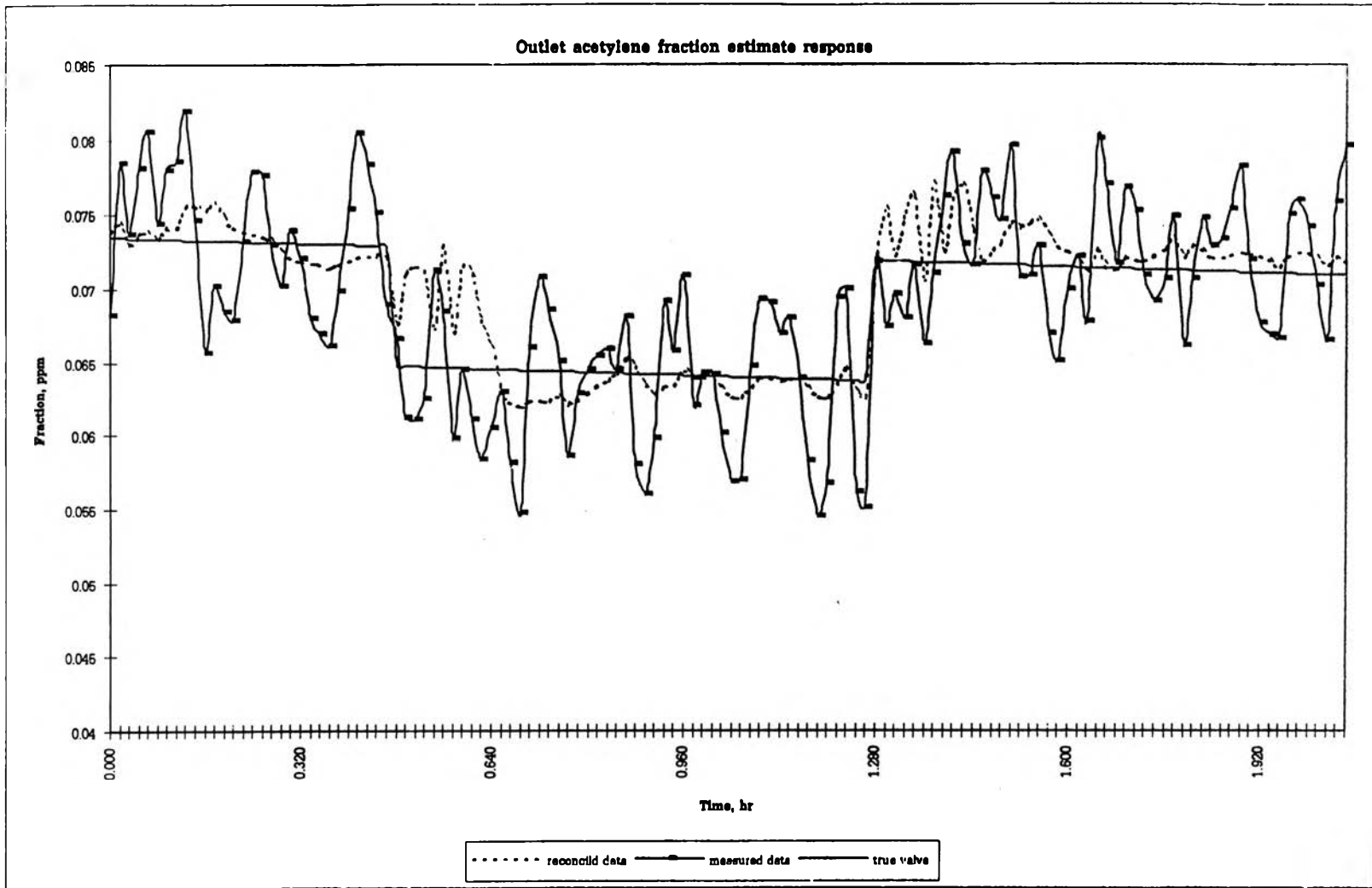


Figure 7.10 Outlet acetylene estimate response to step change in feed concentration through 10% noise measured data with $H = 10$

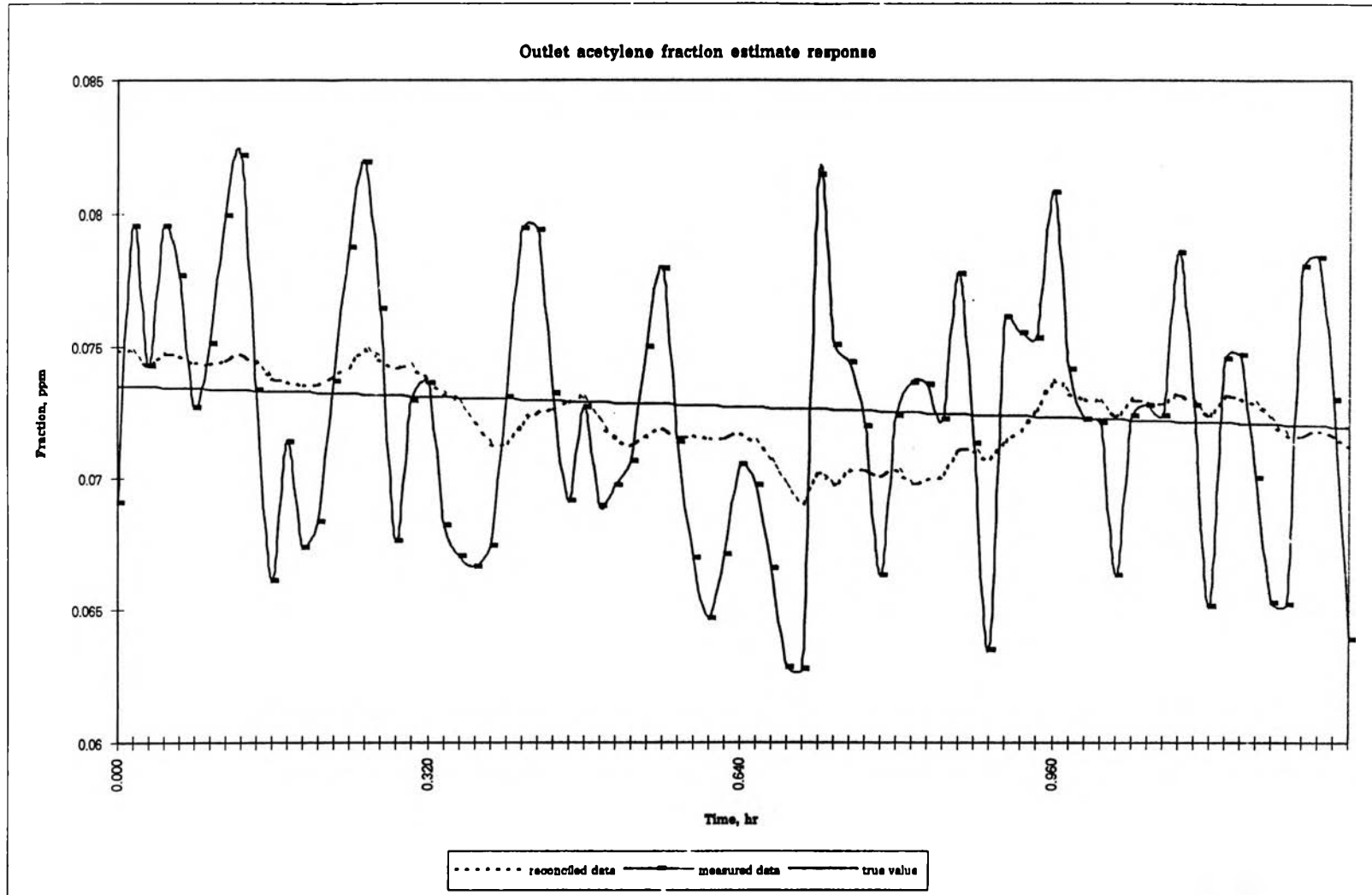


Figure 7.11 Outlet acetylene estimate response through 10% noise measured data with $H = 15$

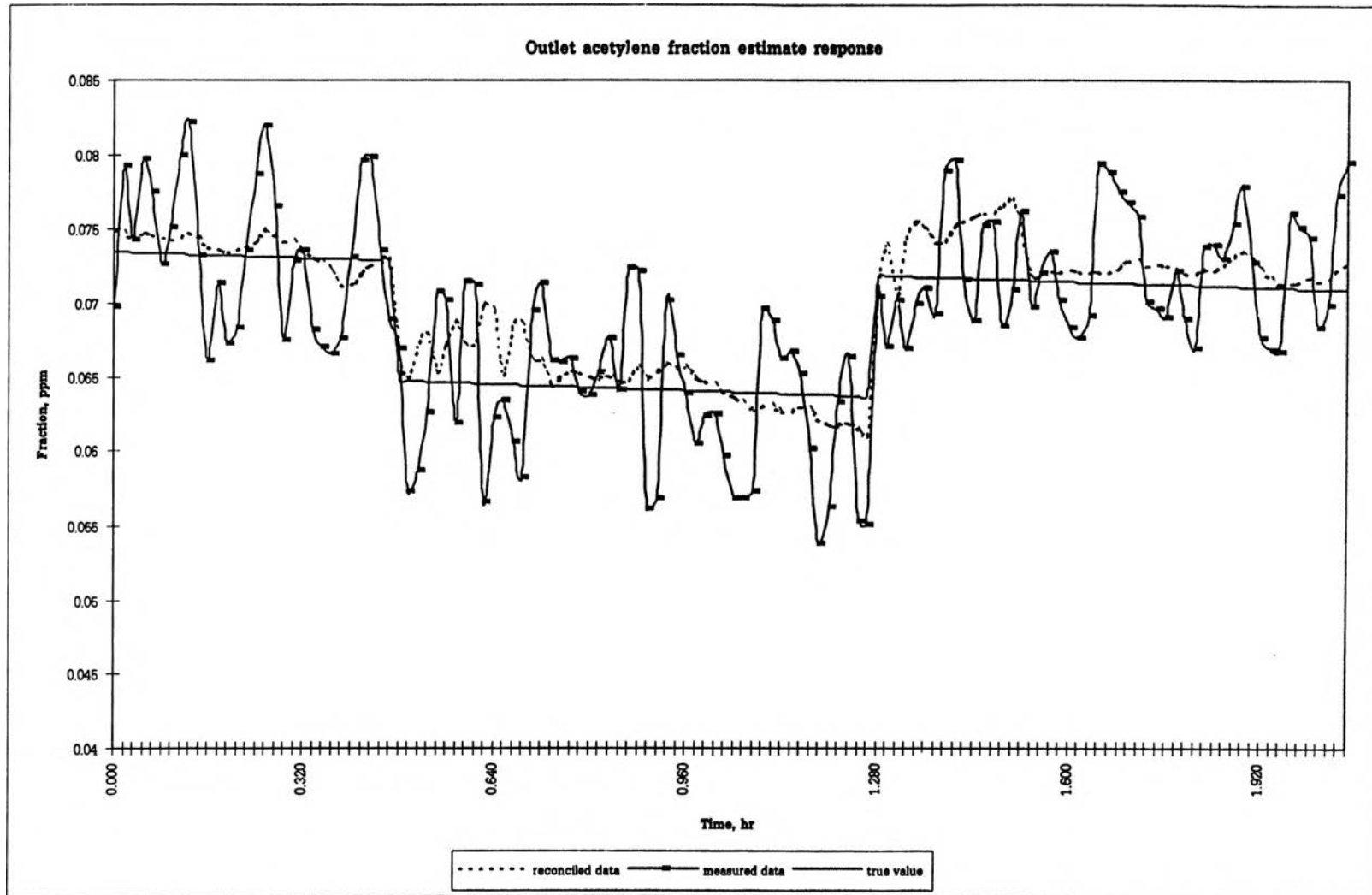


Figure 7.12 Outlet acetylene estimate response to step change in feed concentration through 10% noise measured data with $H = 15$

The results from the simulation are shown in Figure 7.1-7.12. The comparison of the texture of the data among the three forms of data are shown. For all of the Figures, the straight line is illustrated the true simulated data that used to be the base values for comparison. The straight line with square points is illustrated the simulated data with random noise and the discrete straight line is illustrated the reconciled data of the simulated data with random noise.

As shown in Figure 7.1 to Figure 7.12, the reconciled values for outlet acetylene fraction appeared to be significantly smoother than the corresponding the simulated data with random noise or simulated measurements and be closely to the true simulated data more than the simulated measurements. A quantitative comparison between the estimates and the measurements confirming the qualitative results mentioned above is presented in Table 7.3. The estimate error standard deviation is reduced about 80-93% from the measurement error.

The developed dynamic data reconciliation program with $H = 5$ can reduce the standard deviation of the data to about 82%, with $H = 10$ can reduce the standard deviation of the data to about 90%, and with $H = 15$ can reduce the standard deviation of the data to about 93%.

Table 7.3 The data reconciliation results

History horizon	Noise %	Standard deviation		%SD reduction
		data + noise	reconciled data	
5	5	2.204e-3	3.686e-4	83.2%
	10	5.112e-3	9.92e-4	80.6%
10	5	2.183e-3	2.05e-4	90.6%
	10	4.922e-3	5.163e-4	89.3%
15	5	2.515e-3	1.835e-4	92.7%
	10	5.114e-3	3.715e-4	92.8%

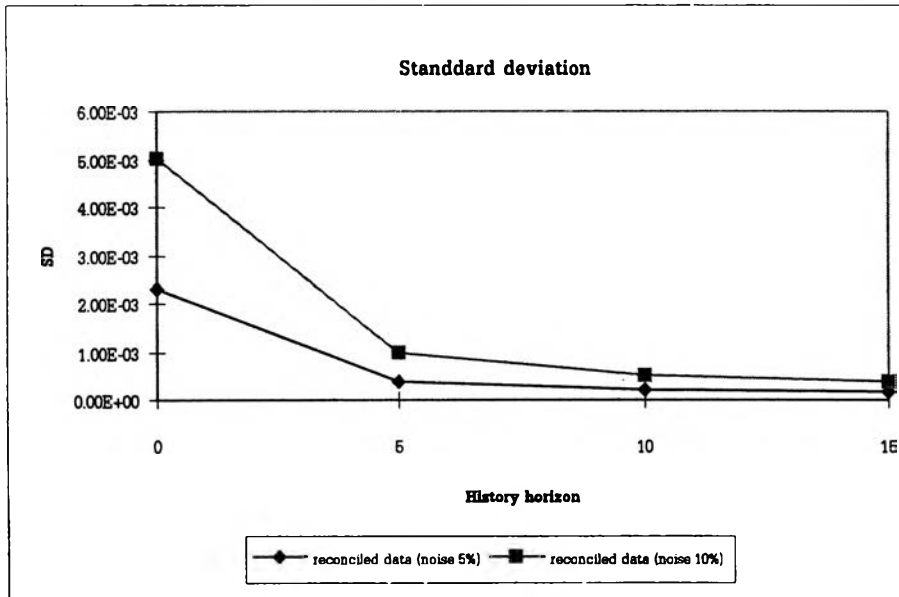


Figure 7.13 Standard deviation corresponding to history horizon

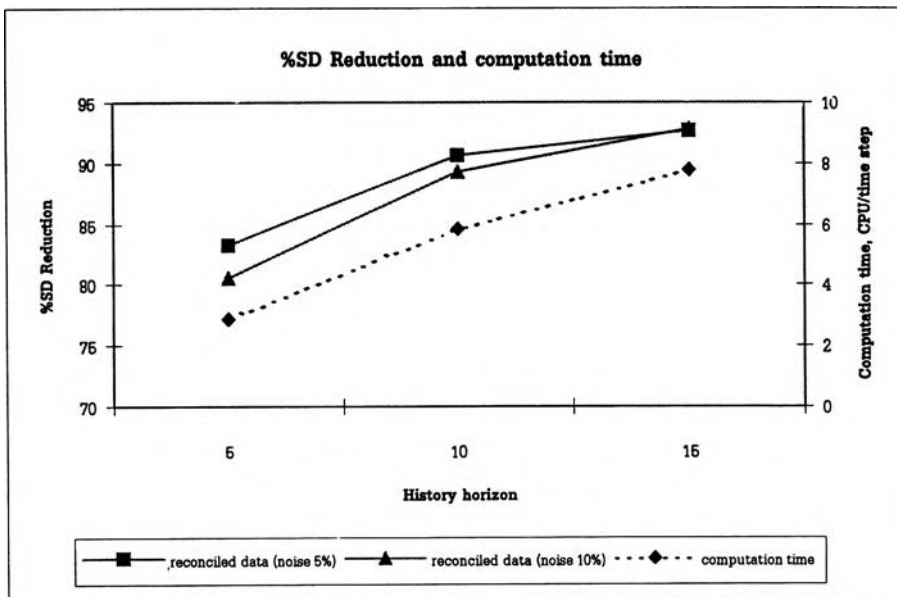


Figure 7.14 %SD reduction and computation time corresponding to history horizon

The effect of increasing the history horizon H can be seen by comparing the texture of the data that is illustrated in Figure 7.1, 7.3, and 7.5, or comparing the texture of the data that is illustrated in Figure 7.2, 7.4, and 7.6, or seen Figure 7.13 and 7.14.

The reconciled data obtained with $H = 5$ are more oscillatory than those obtained by using $H = 10$ and $H = 15$. In the same way, the reconciled data obtained with $H = 10$ are little more oscillatory than those obtained using $H = 15$.

The quantitative comparison is demonstrated in Figure 7.13. The increasing of the value of the history horizon makes the decreasing of the standard deviation of the data to be greater. The slope of graph at range $H = 0$ to 5 is very bigger than the slope at range $H = 5$ to 10 and range $H = 10$ to 15. In the other hand, the slope of graph at range $H = 5$ to 10 is close to the slope at range $H = 10$ to 15. The percent decreasing of the standard deviation at the bigger H value is smaller than at the smaller H value.

Table 7.4 Computation time for the data reconciliation

CPU per time step	H = 5	H = 10	H = 15
constant feed	1.56	5.27	6.51
step change in feed	2.86	5.81	7.06

Moreover, according to Figure 7.14,. The increasing of H causes the computation time increase as shown in Table 7.4 or in Figure 7.14. All range of H , the percent increasing of the computation time is similar.

Due to all the discussions above, The suitable history horizon value for dynamic data reconciliation program is 10 because it can be reduce the standard deviation of the data as same as the program with $H = 15$ but it take the sorter computation time. The other results from dynamic data reconciliation with $H = 10$ for the other variables are shown in Figure 7.15 - 7.21. The meaning sign of lines are the same as the illustrated in Figure 7.1 to Figure 7.12. The performance of the results are the same as the result of the outlet acetylene fraction.

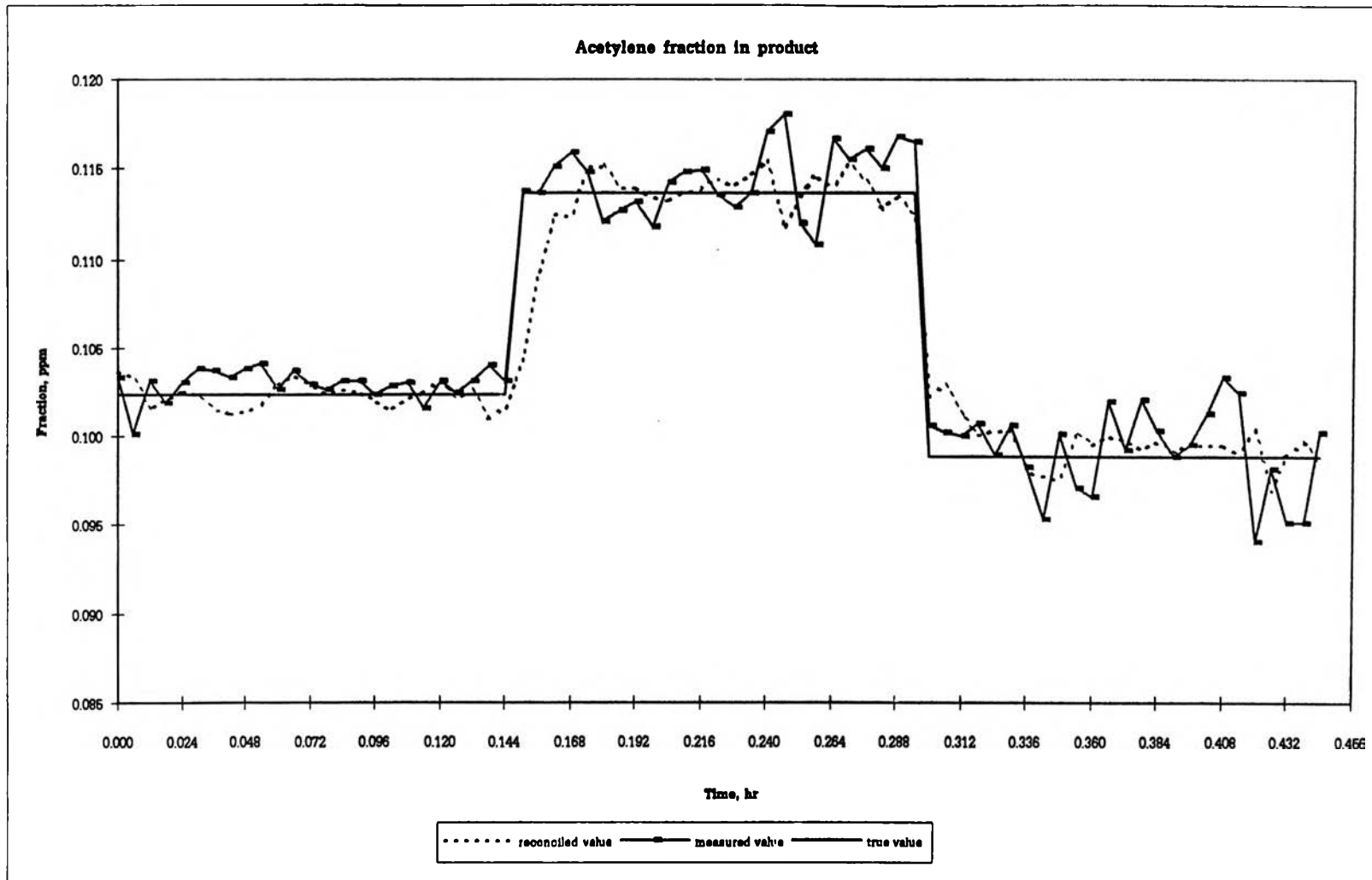


Figure 7.15 Acetylene fraction estimation response

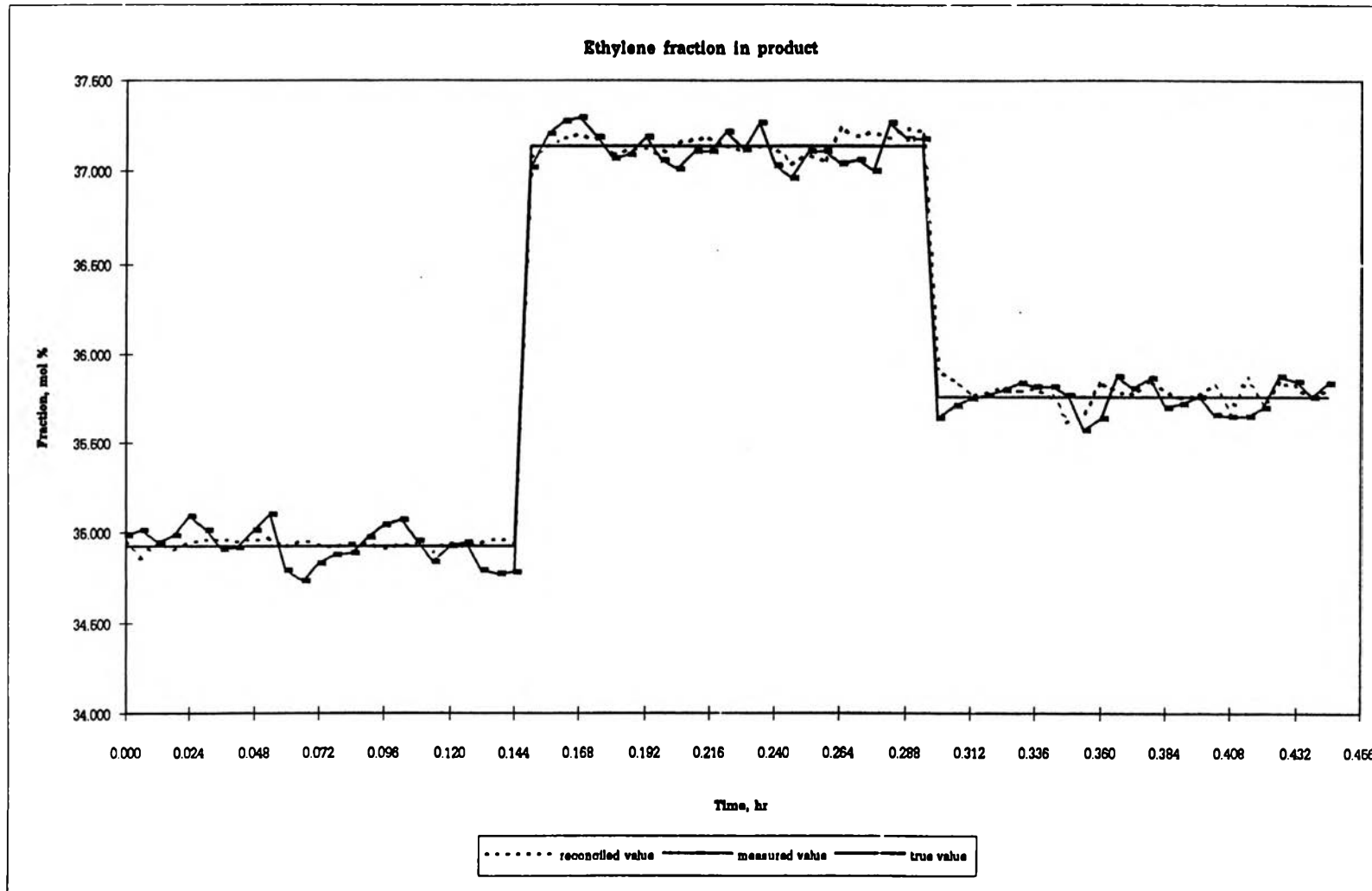


Figure 7.16 Ethylene fraction estimation response

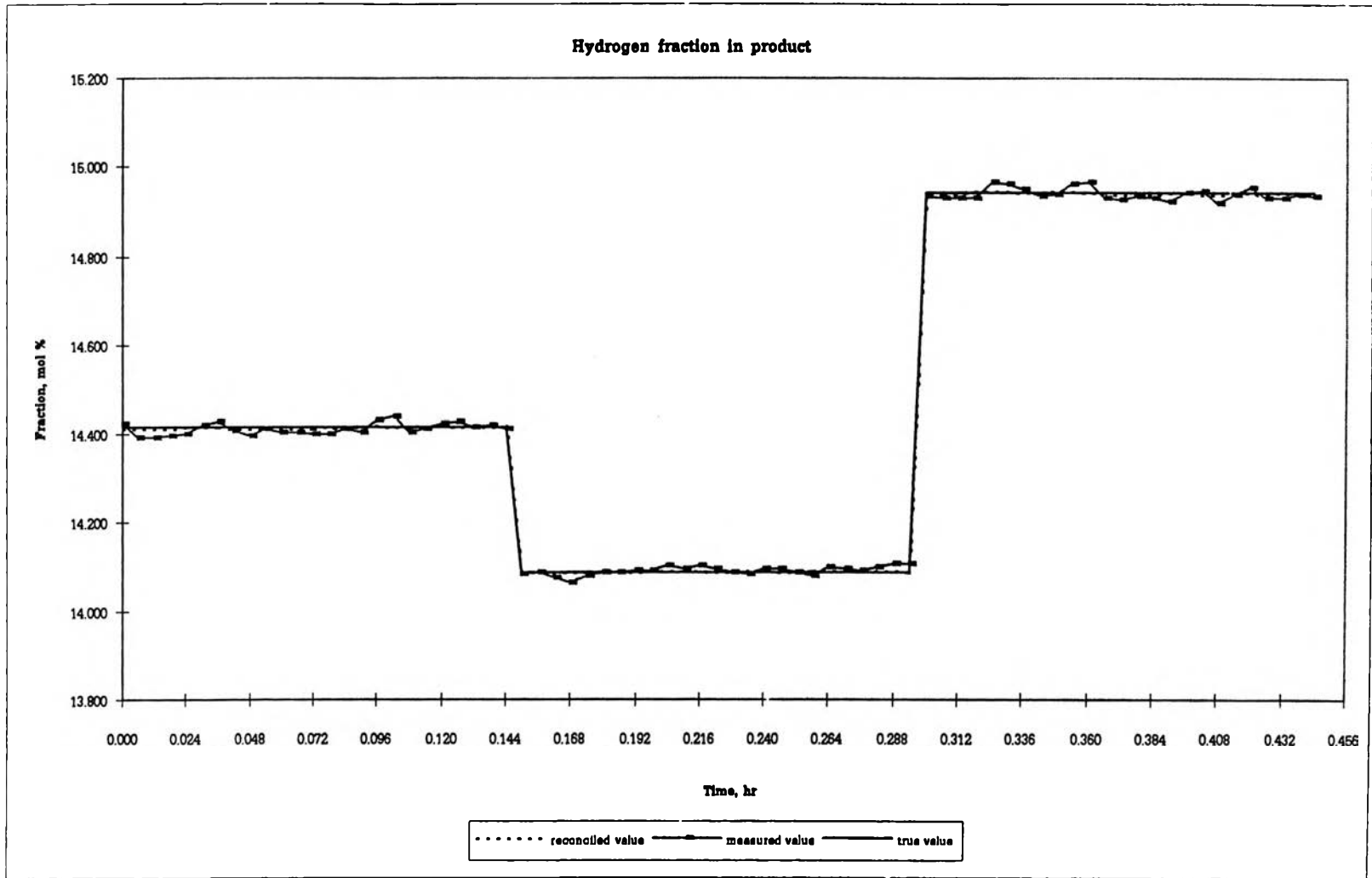


Figure 7.17 Hydrogen fraction estimation response

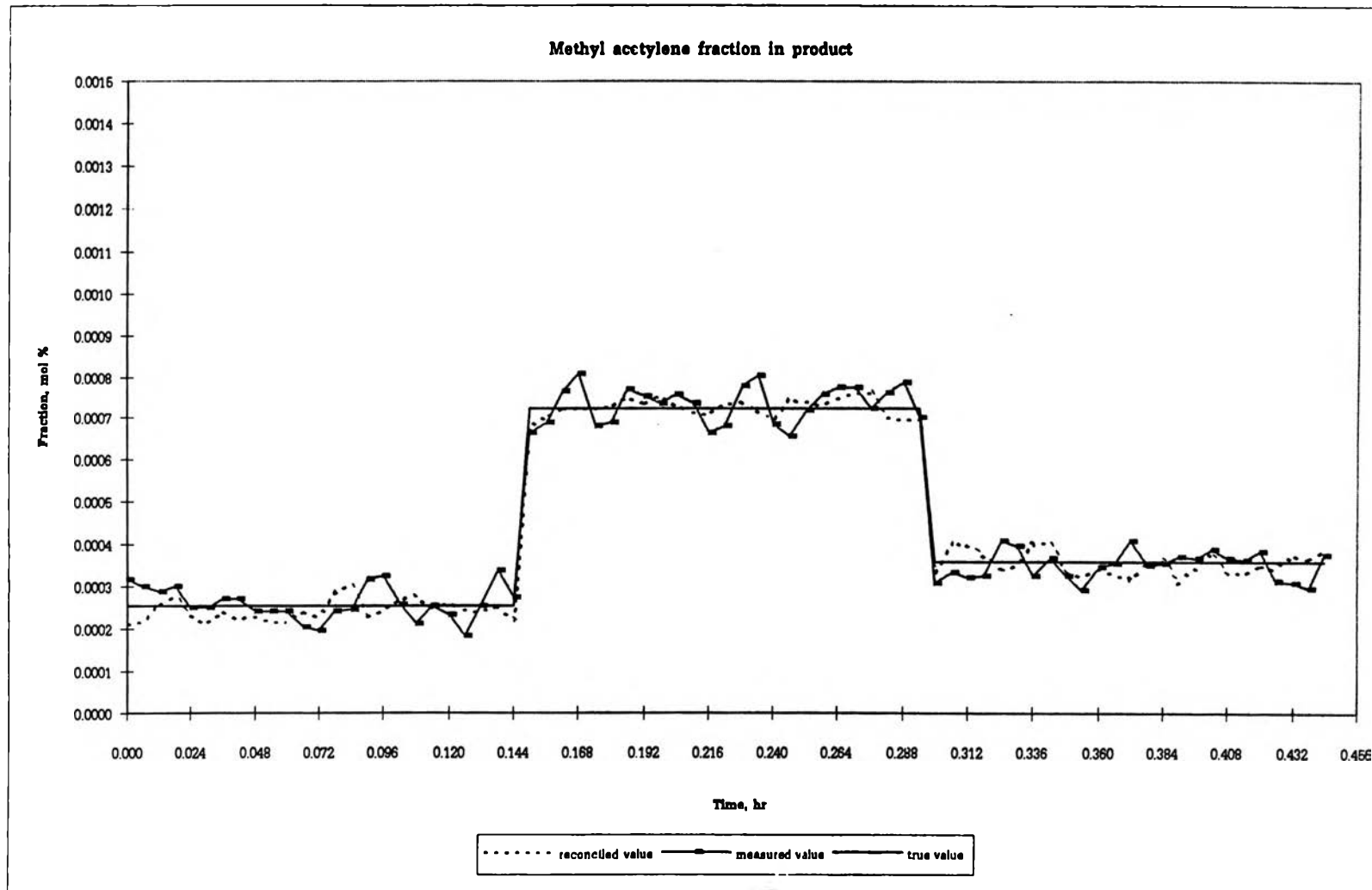


Figure 7.18 Methyl acetylene fraction estimation response

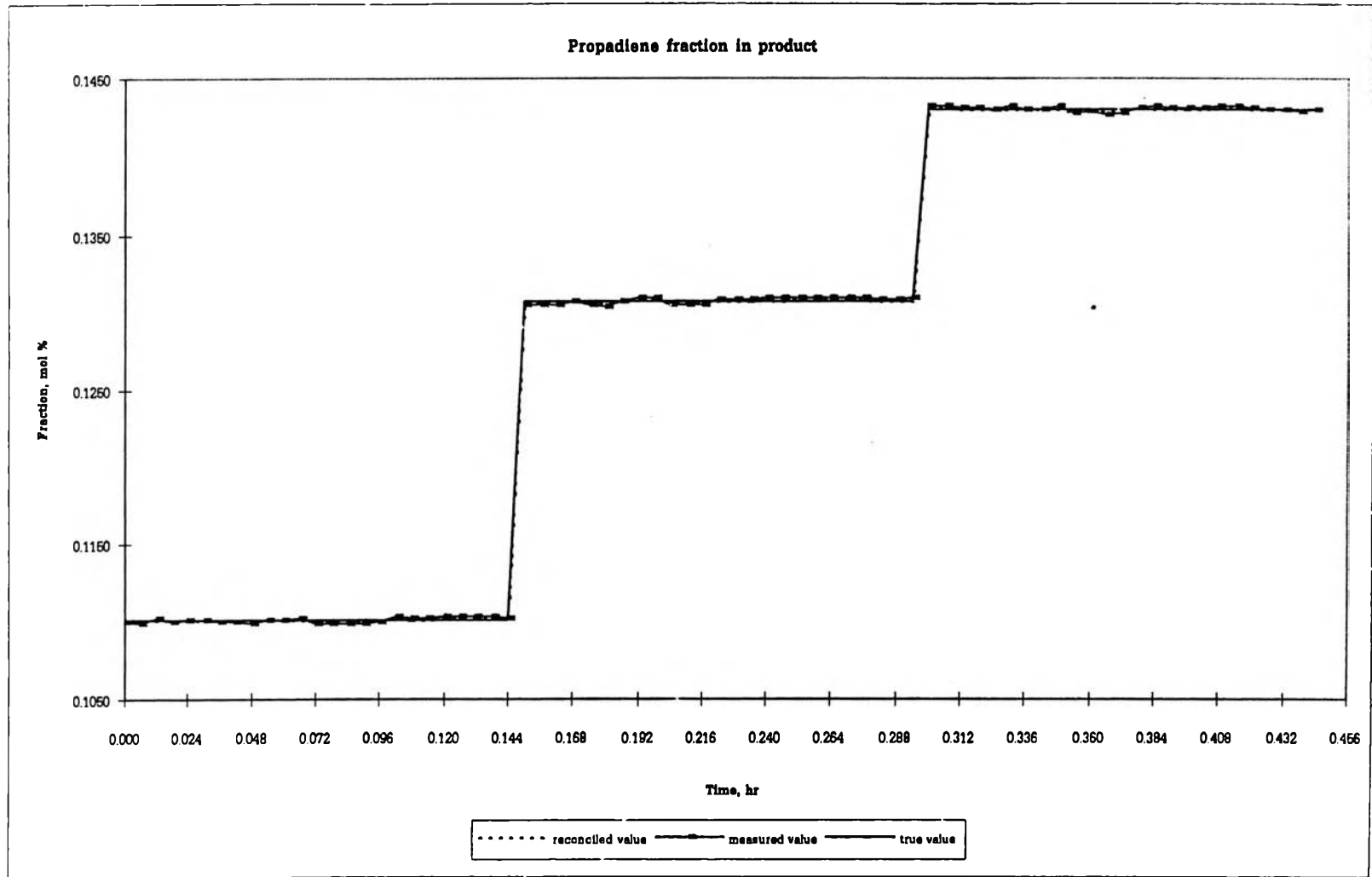


Figure 7.19 Propadiene fraction estimation response

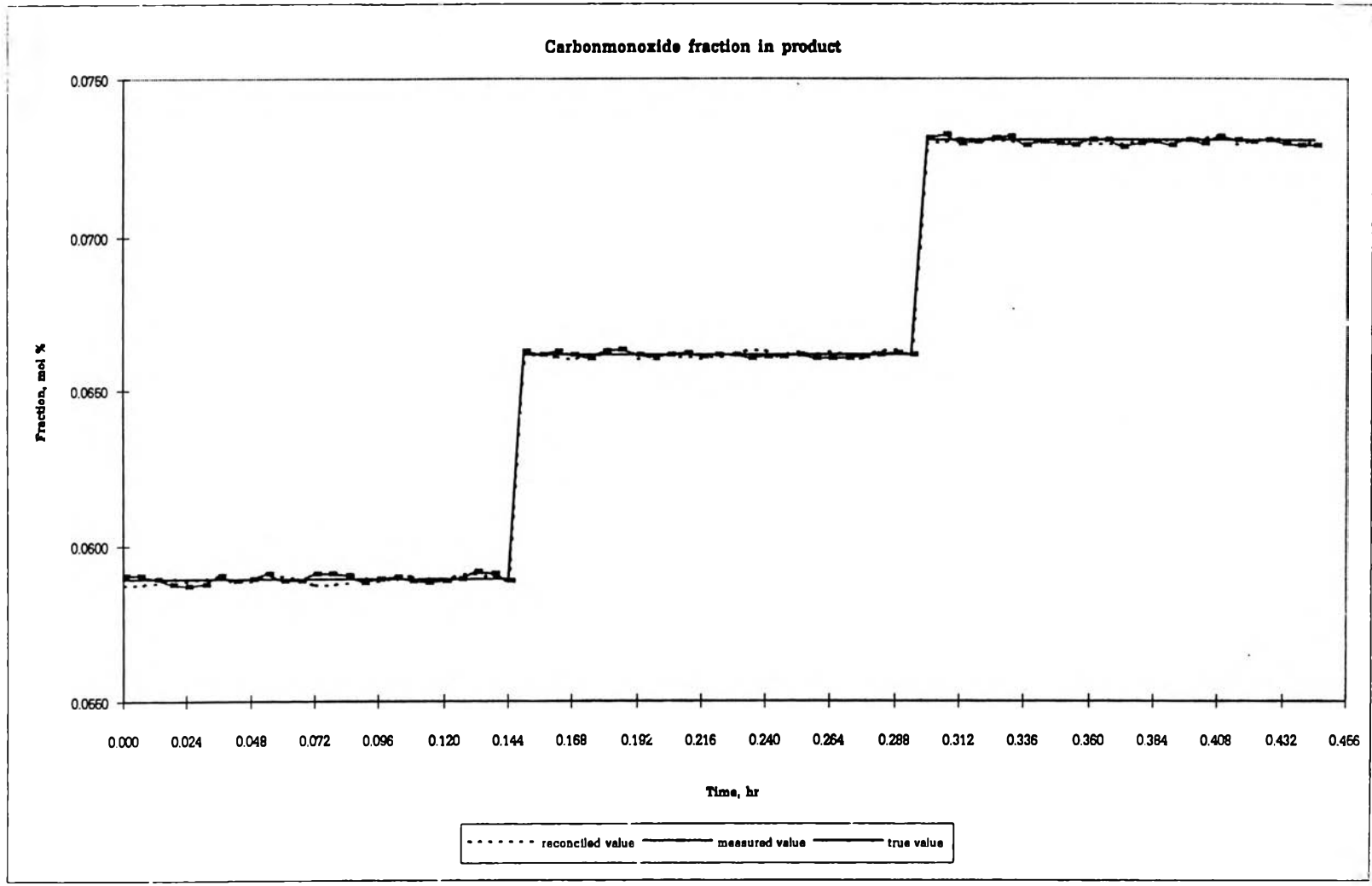


Figure 7.20 Carbonmonoxide fraction estimation response

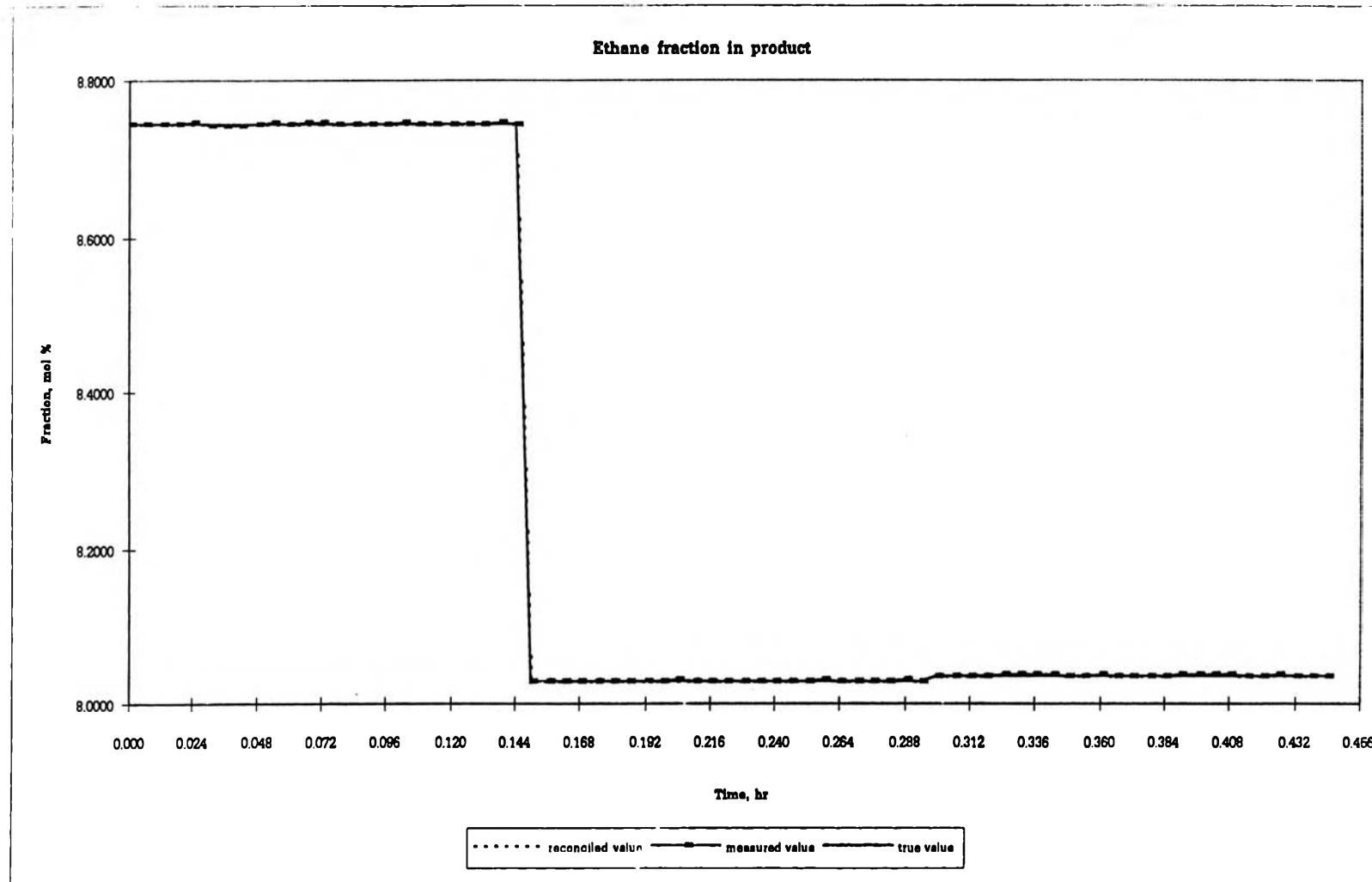


Figure 7.21 Ethane fraction estimation response

The actual data at date September 9, 1997-November 12, 1997 are reconciled before used to estimate the rate constant values of the model. All of the actual data are reconciled by using the developed dynamic data reconciliation program with the ten time step history horizon.

The results of the dynamic data reconciliation with the actual data are shown in figure 7.22-7.30.

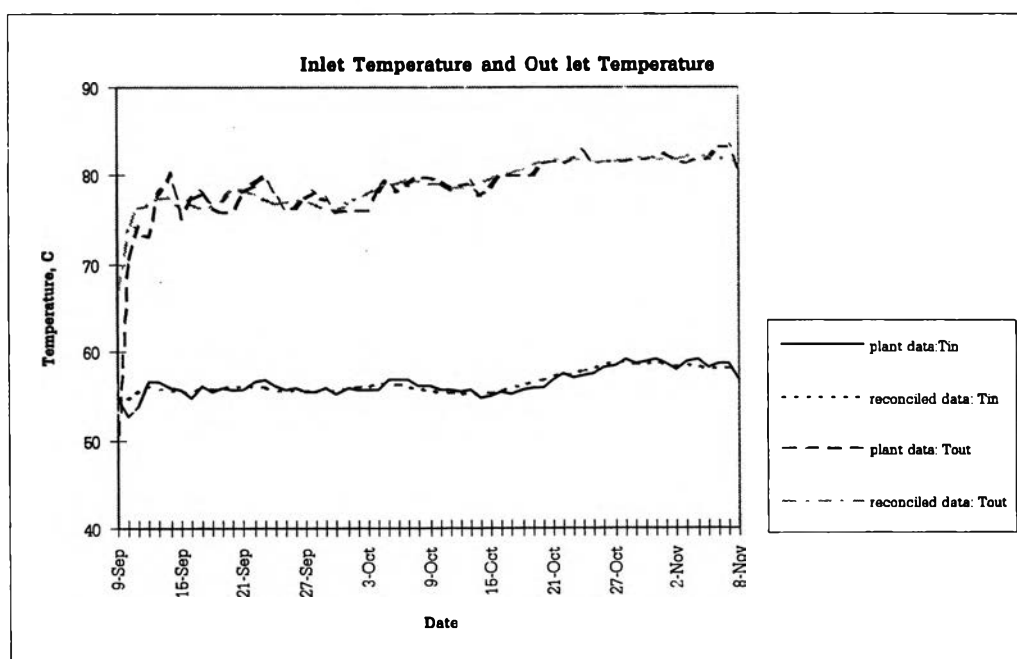


Figure 7.22 The comparison between the actual data and the reconciled data of the inlet temperature data and the outlet temperature data.

The reconciled data of the temperature data is smoother than the actual data as show in Figure 7.22. The standard deviation of the inlet temperature data is reduced by 49.31%. The standard deviation of the outlet temperature data is reduced by 54.611%. Similar to the temperature data, the reconciled of other variables are smoother than the corresponding actual data. The standard deviation of the inlet methane data is reduced

by 64.41%. The standard deviation of the inlet hydrogen data is reduced by 62.05%. The result is shown figure 7.23.

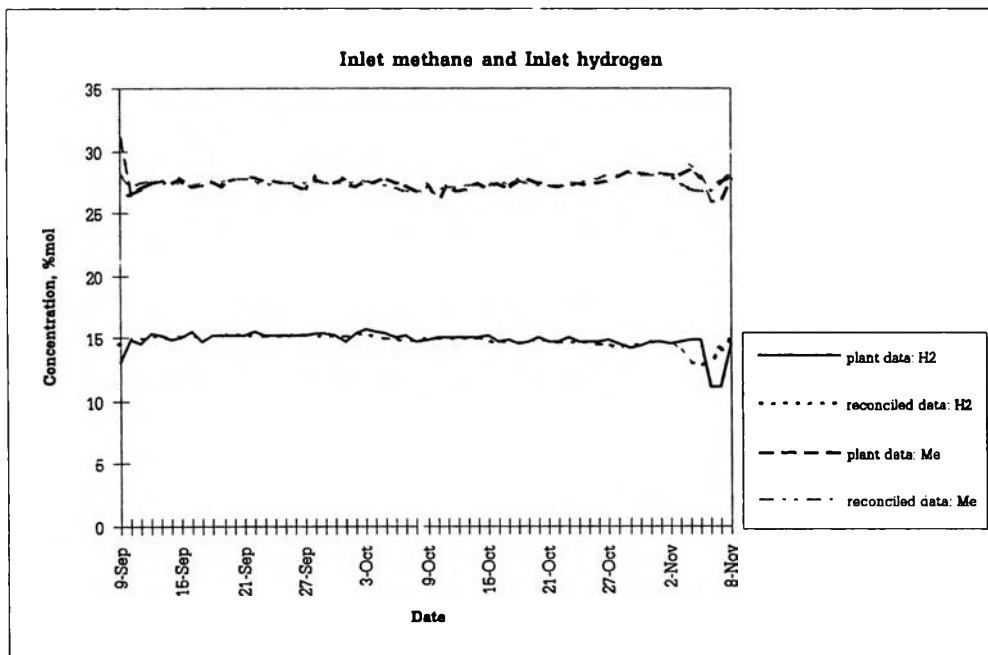


Figure 7.23 The comparison between the actual data and the reconciled data of the inlet methane data and the inlet hydrogen concentration data.

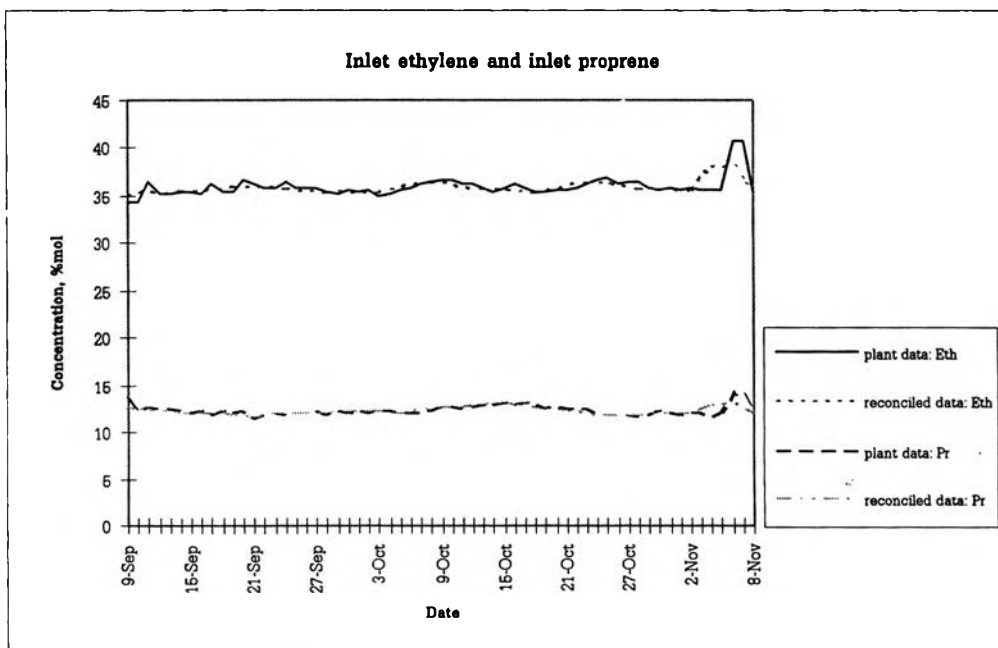


Figure 7.24 The comparison between the actual data and the reconciled data of the inlet ethylene and the inlet propene concentration data.

The standard deviation of the inlet ethylene data is reduced by 58.41%. The standard deviation of the inlet propene data is reduced by 45.61%. The result is shown in Figure 7.24. The standard deviation of the inlet acetylene data is reduced by 43.27%. The standard deviation of the inlet methyl acetylene data is reduced by 61.44%. The result is shown in Figure 7.25.

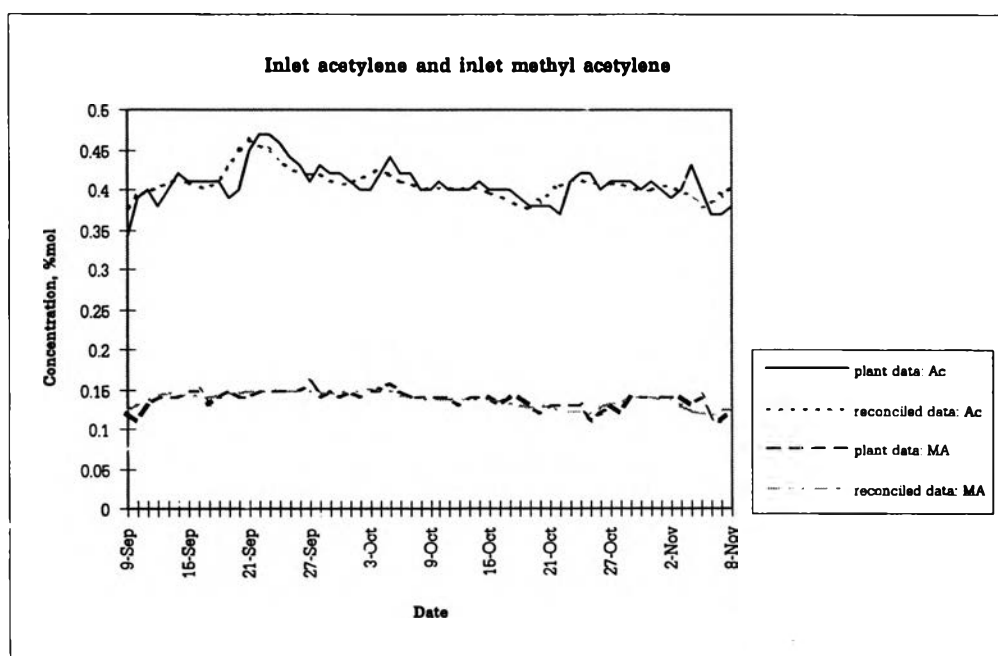


Figure 7.25 The comparison between the actual data and the reconciled data of the inlet acetylene and the inlet methyl acetylene concentration data.

The standard deviation of the inlet ethane data is reduced by 48.01%. The standard deviation of the inlet propadiene data is reduced by 51.87%. The result is shown in Figure 7.26. The standard deviation of the outlet methane data is reduced by 44.3%. The standard deviation of the outlet hydrogen data is reduced by 63.28%. The result is shown in Figure 7.27 The standard deviation of the inlet ethylene data is reduced by 59.24%. The standard deviation of the outlet propene data is reduced by 60.05%. The result is shown in Figure 7.28

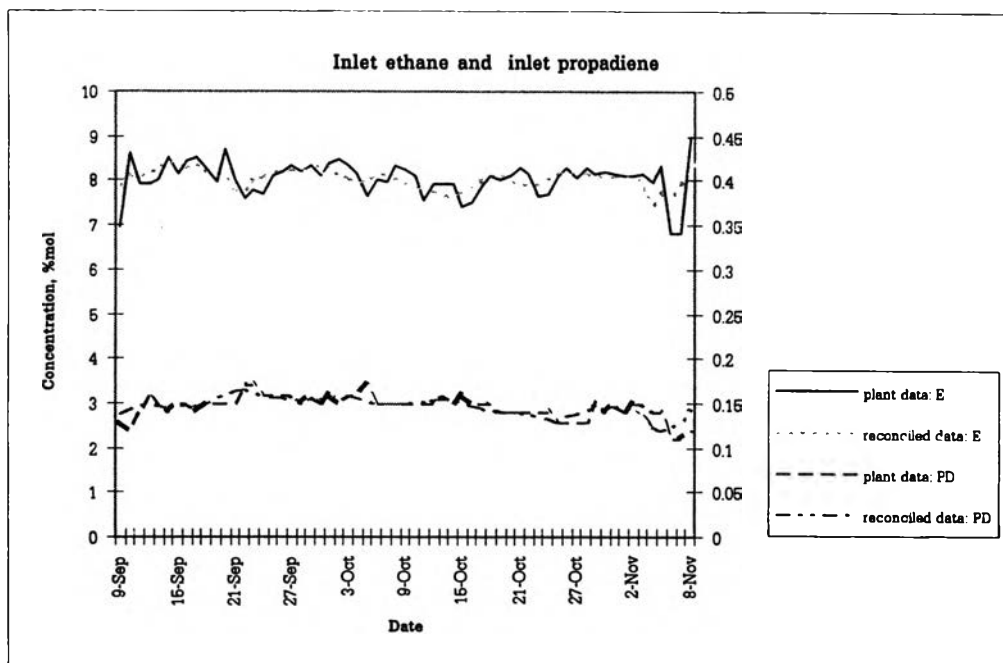


Figure 7.26 The comparison between the actual data and the reconciled data of the inlet ethane and the inlet propadiene concentration data

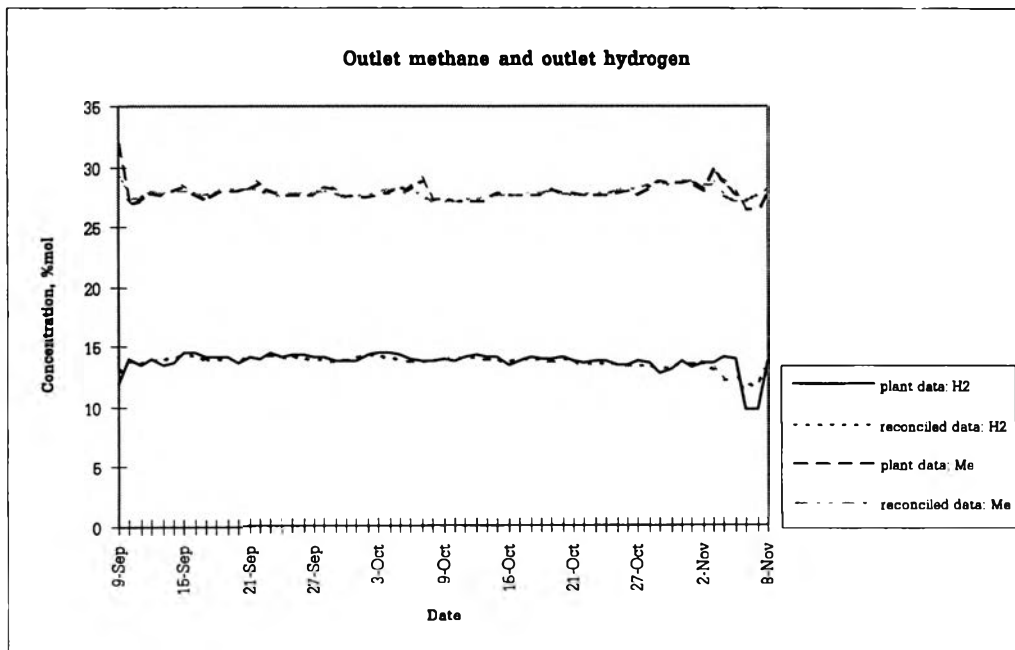


Figure 7.27 The comparison between the actual data and the reconciled data of the outlet methane and the outlet hydrogen concentration data

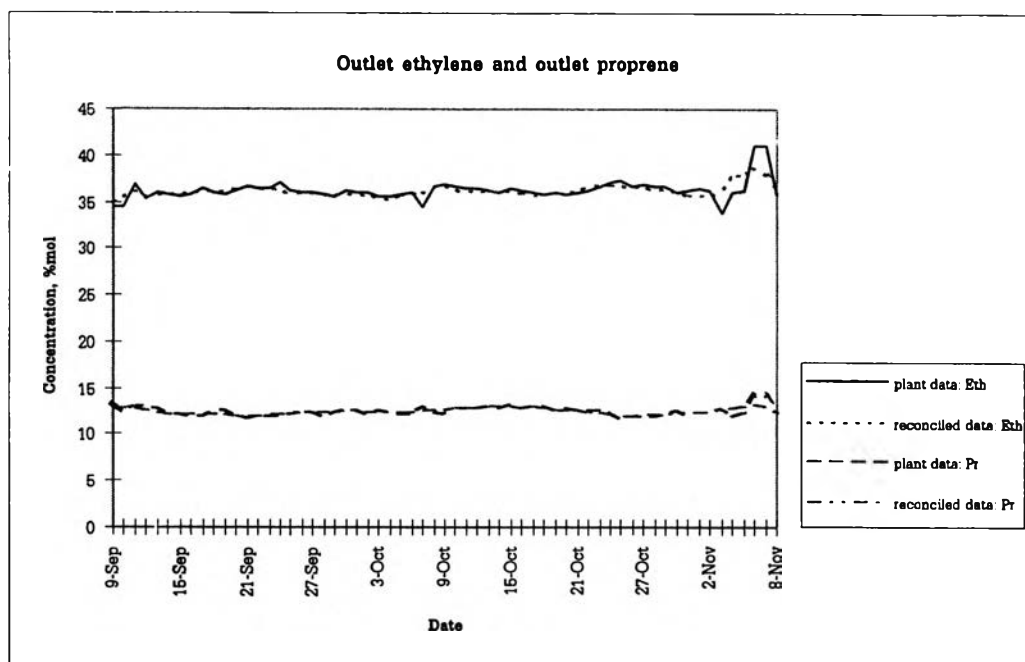


Figure 7.28 The comparison between the actual data and the reconciled data of the outlet ethylene and the outlet propene concentration data

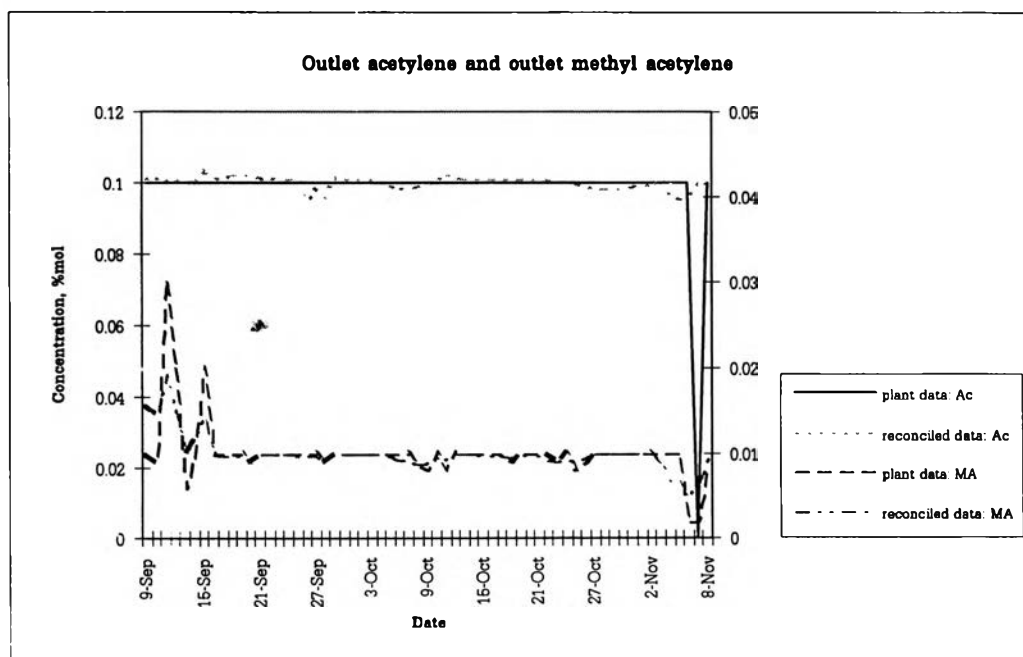


Figure 7.29 The comparison between the actual data and the reconciled data of the outlet acetylene and the outlet methyl acetylene concentration data

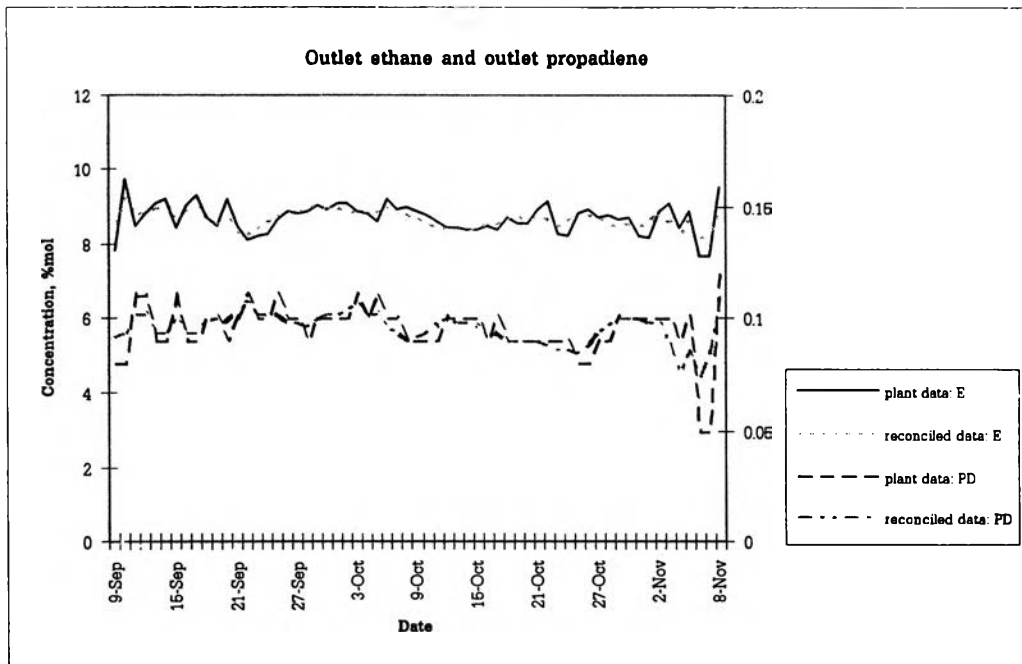


Figure 7.30 The comparison between the actual data and the reconciled data of the outlet ethane and the outlet propadiene concentration data.

The standard deviation of the outlet acetylene data is reduced by 76.08%. The standard deviation of the outlet methyl acetylene data is reduced by 62.26%. The result is shown in Figure 7.29.

The standard deviation of the outlet ethane data is reduced by 52.83%. The standard deviation of the outlet propadiene data is reduced by 41.38%. The result is shown in Figure 7.30.

The developed dynamic data reconciliation program can improve the accuracy of the actual data. All of the results that shown in Figure 7.22-7.30 can be indicated that capability. The developed dynamic data reconciliation program can reduce the standard deviation of the actual data by 40-70%. The reconciled data of the actual data can satisfy the material and energy balance equations of the process. Then, the reconciled data is used to estimate the rate constant parameters of the model. The certain rate constant values can be obtained by using the reconciled data.

7.3 The benefit of the dynamic data reconciliation

The dynamic data reconciliation program is very helpful in order to reduce the measurement error as discussed above. Moreover, the dynamic data reconciliation program can be improve the model accuracy by the more correctly estimated parameters from the reconciled data. To confirm this mention, the experimental tests are done with the following proceeding.

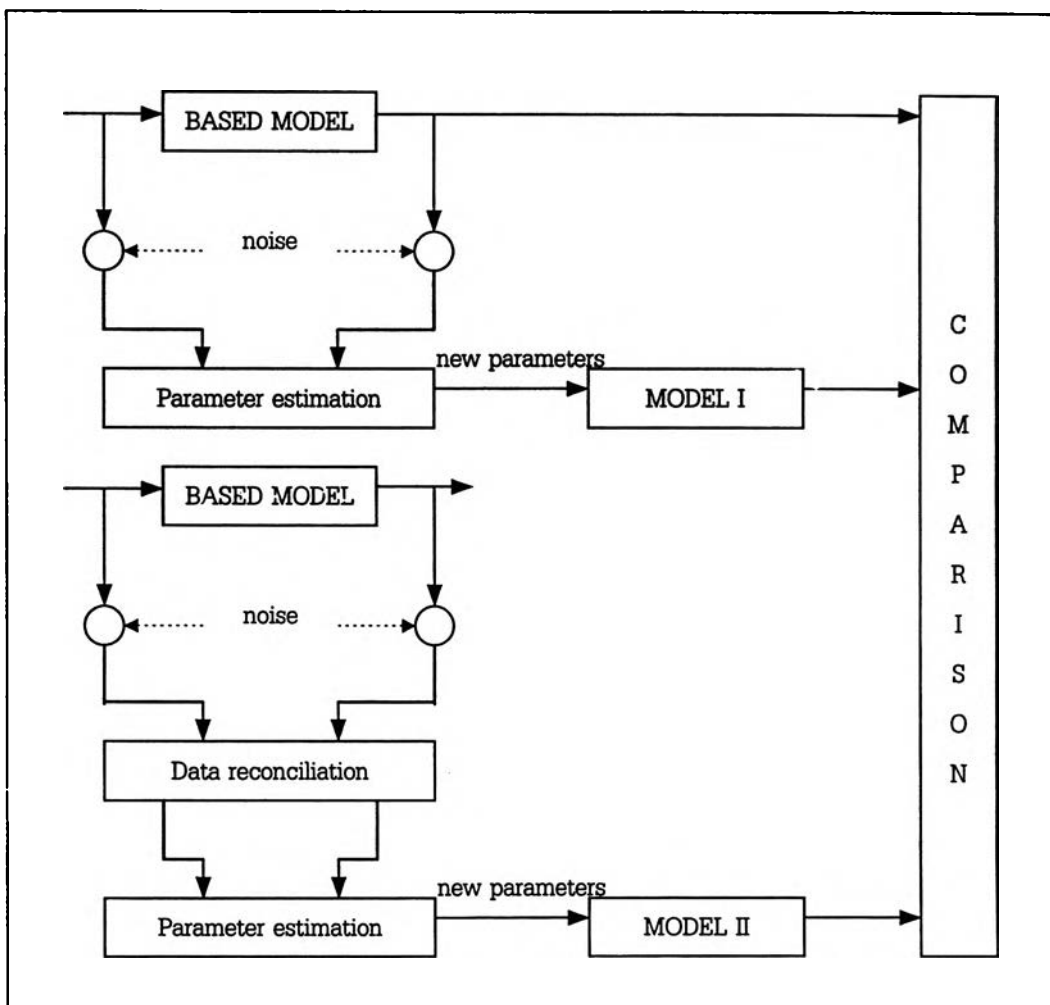


Figure 7.31 The diagram of the test proceeding.

1. Simulate the based model and add noise signal in the variables signal that is assumed to be measurement signal.

2. Estimate the new parameter values of the model from the measurement signal that has noise. The new model names MODEL I.
3. Before estimate the new parameter values, the measurement signal is reconciled. Then the reconciled data is used to estimate the new parameters of the model. The new model names MODEL II.
4. Simulate the both of MODEL I and MODEL II and compare the predicted results with the results of the based model.

The results of the test proceeding are shown in Figure 7.32 - 7.45. All of the Figures show the comparison of the predicted results from the MODEL I, MODEL II, with the results from the based model. The results from the based model is illustrated by the straight line with delta points, the results from the MODEL I is illustrated by the discrete straight line with circle points, and the results from the MODEL II is illustrated by the discrete straight line with square points.

Figure 7.32-7.38 show the predicted results of each model to the steps change in total mass flow.

Figure 7.39-7.45 show the predicted results of each model to the steps change in feed temperature.

The last test is the capability to erase the bias of the data reconciliation program and the result is shown in Figure 7.46.

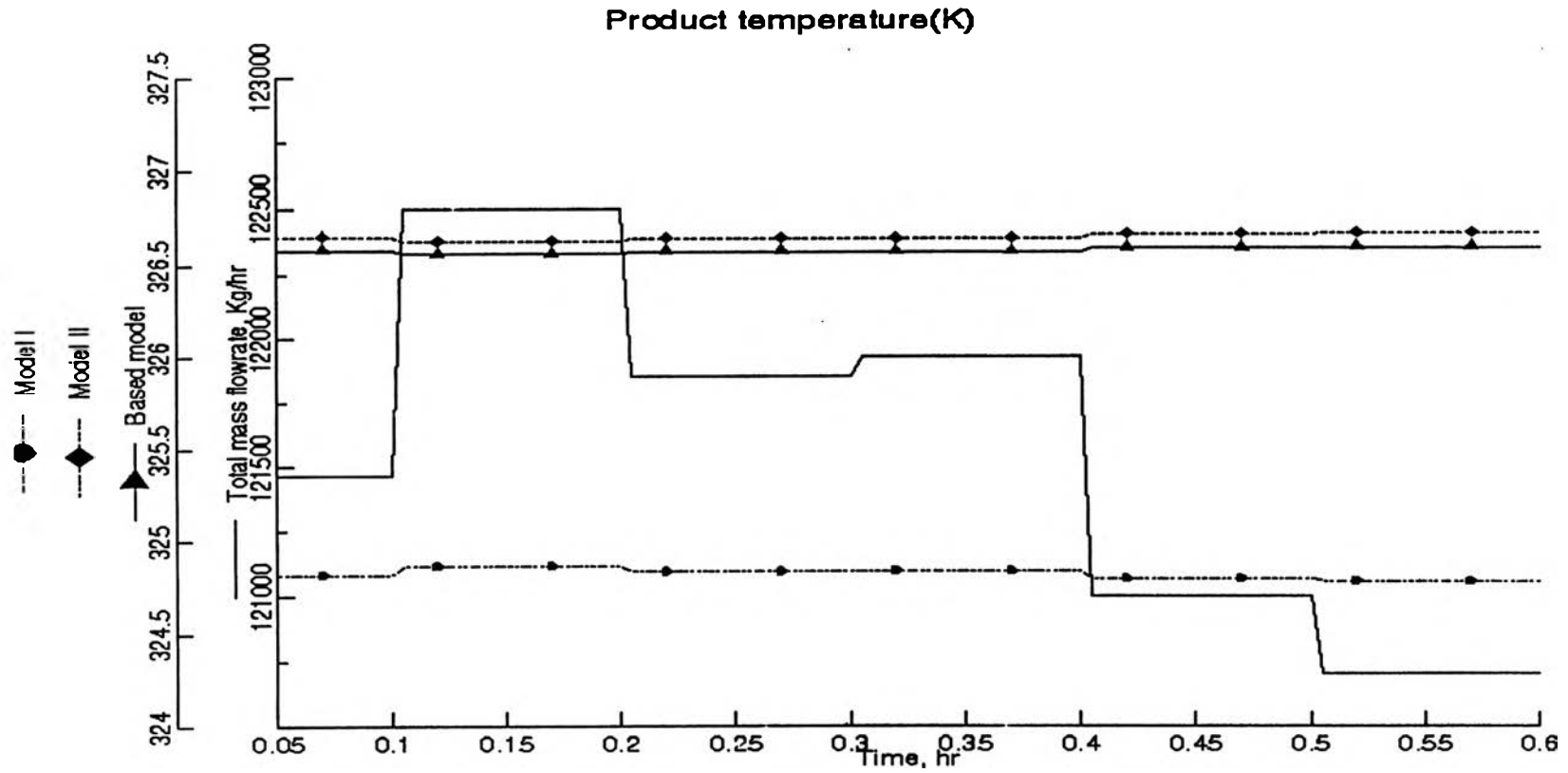


Figure 7.32 Comparison of the predicted product temperature corresponding to step change in total mass flowrate

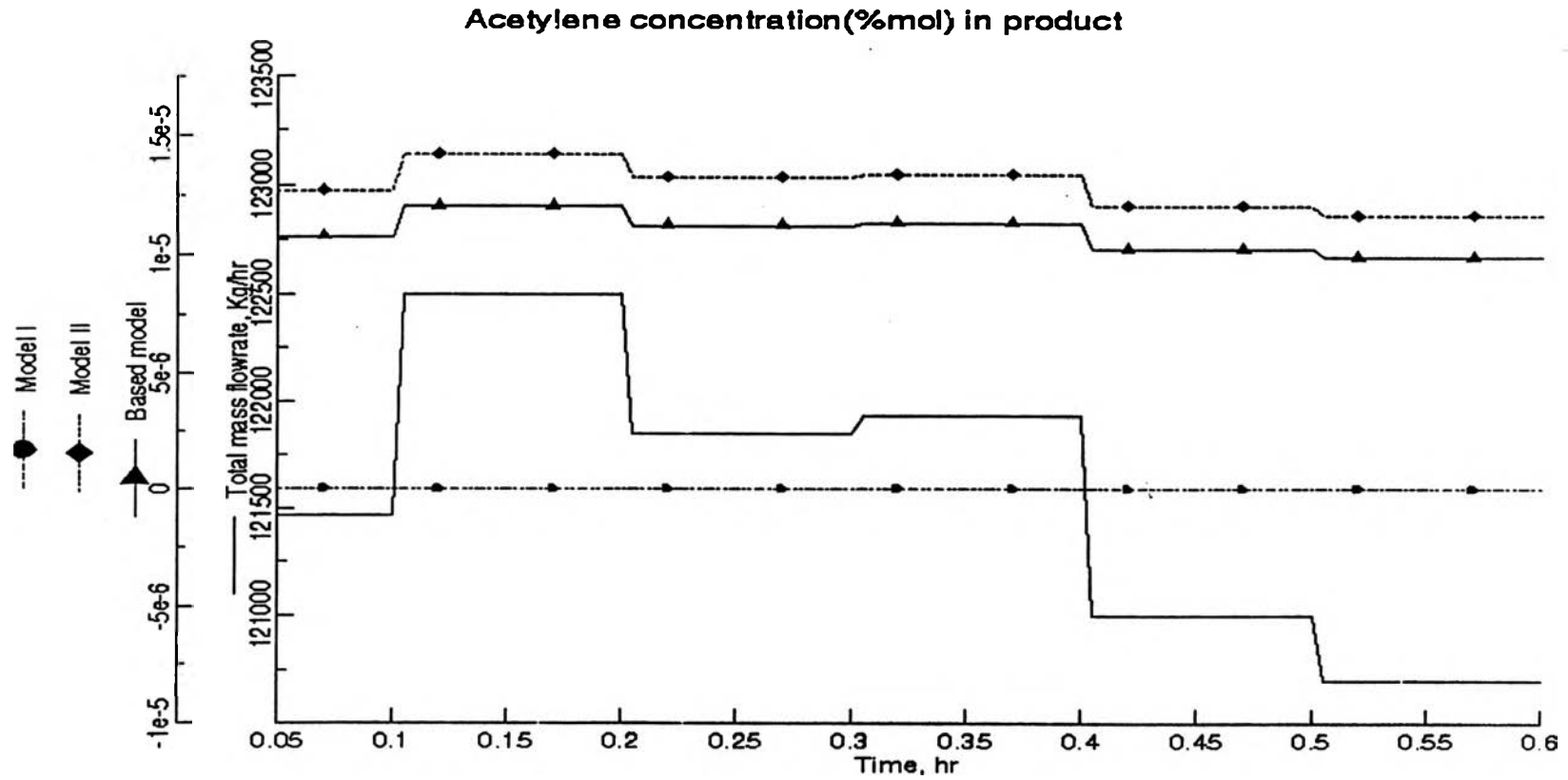


Figure 7.33 Comparison of the predicted outlet acetylene corresponding to step change in total mass flowrate

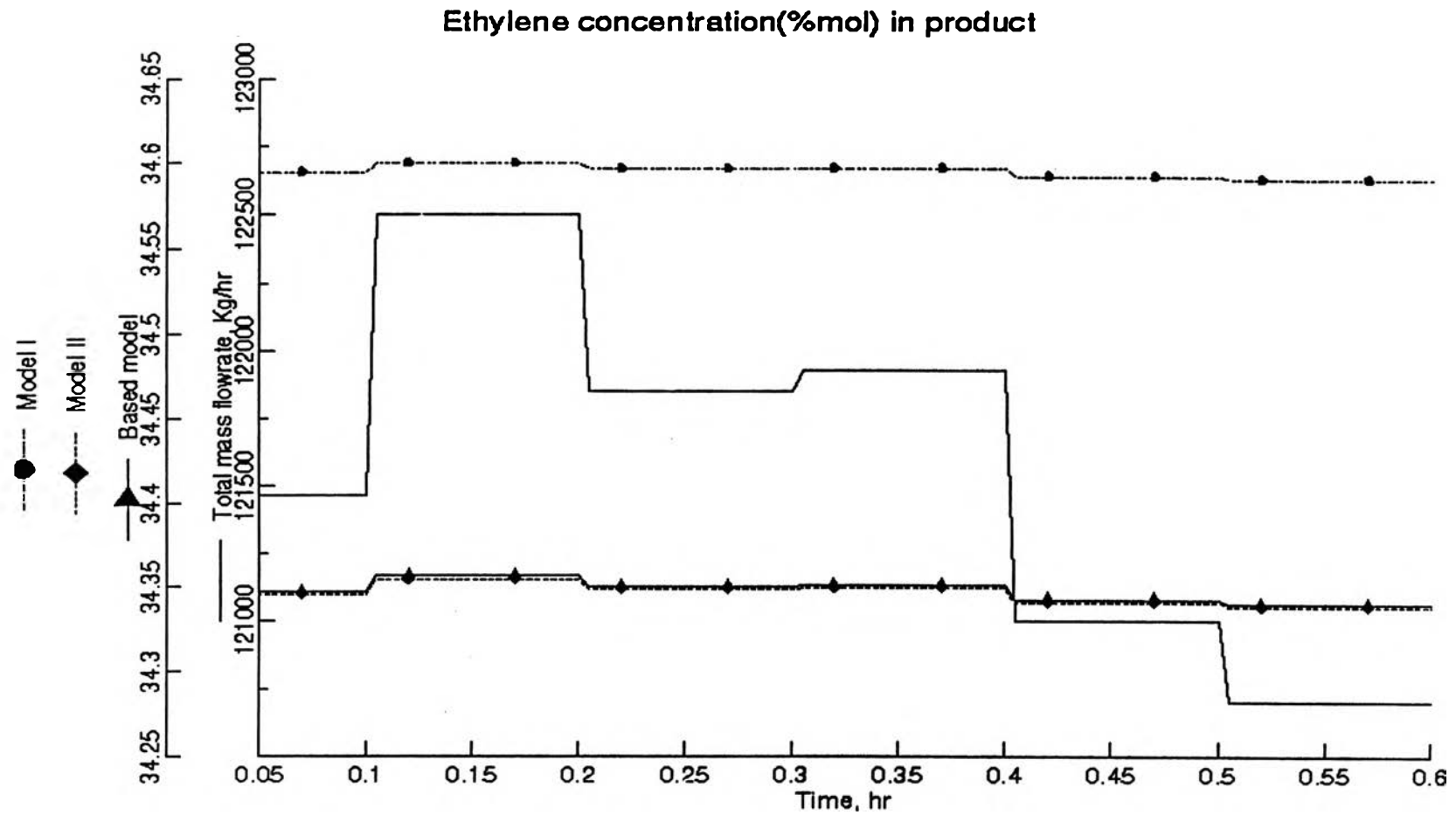


Figure 7.34 Comparison of the predicted outlet ethylene corresponding to step change in total mass flowrate

Hydrogen concentration(%mol) in product

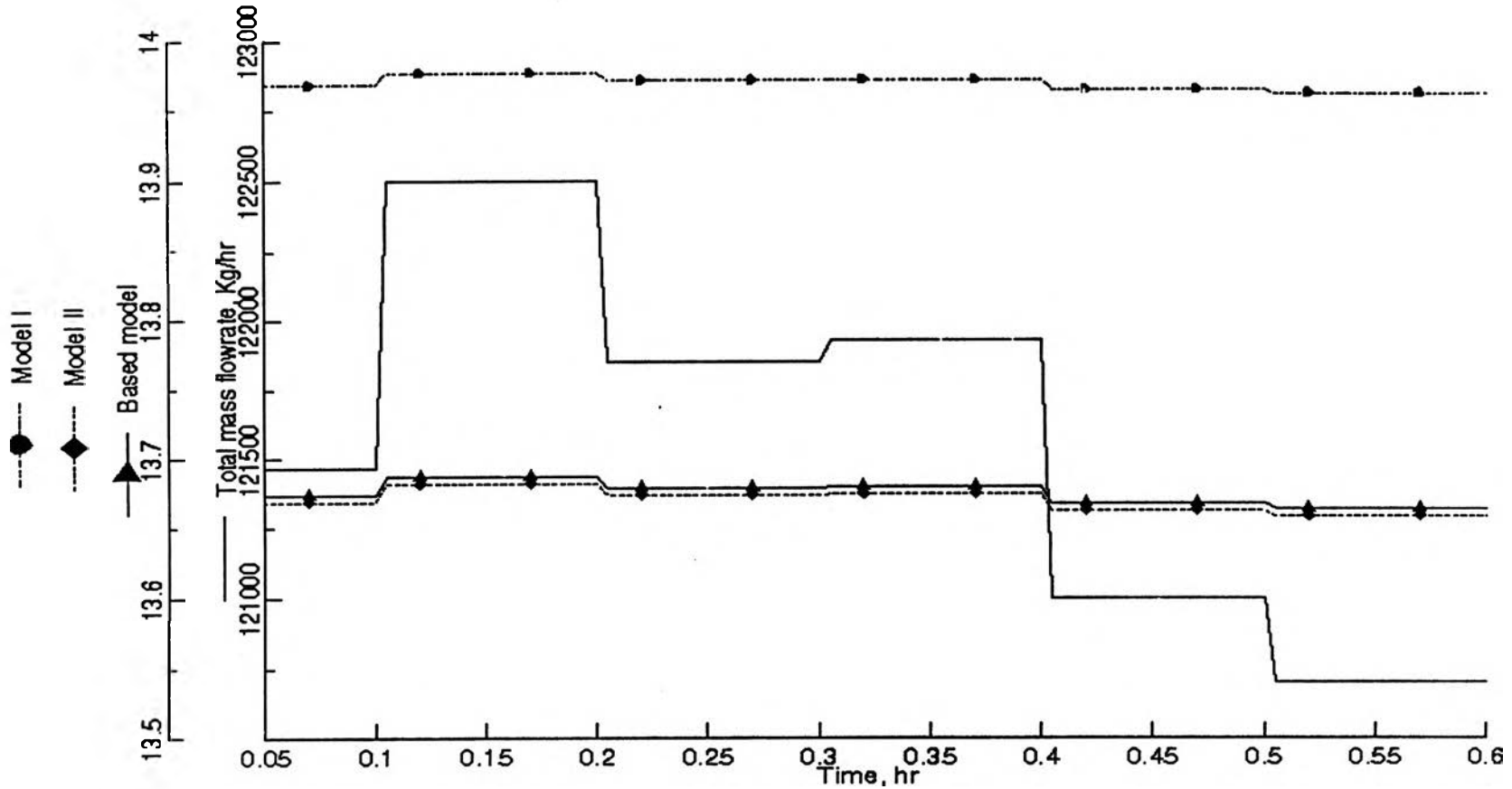


Figure 7.35 Comparison of the predicted outlet hydrogen corresponding to step change in total mass flowrate

Methyl acetylene concentration(%mol) in product

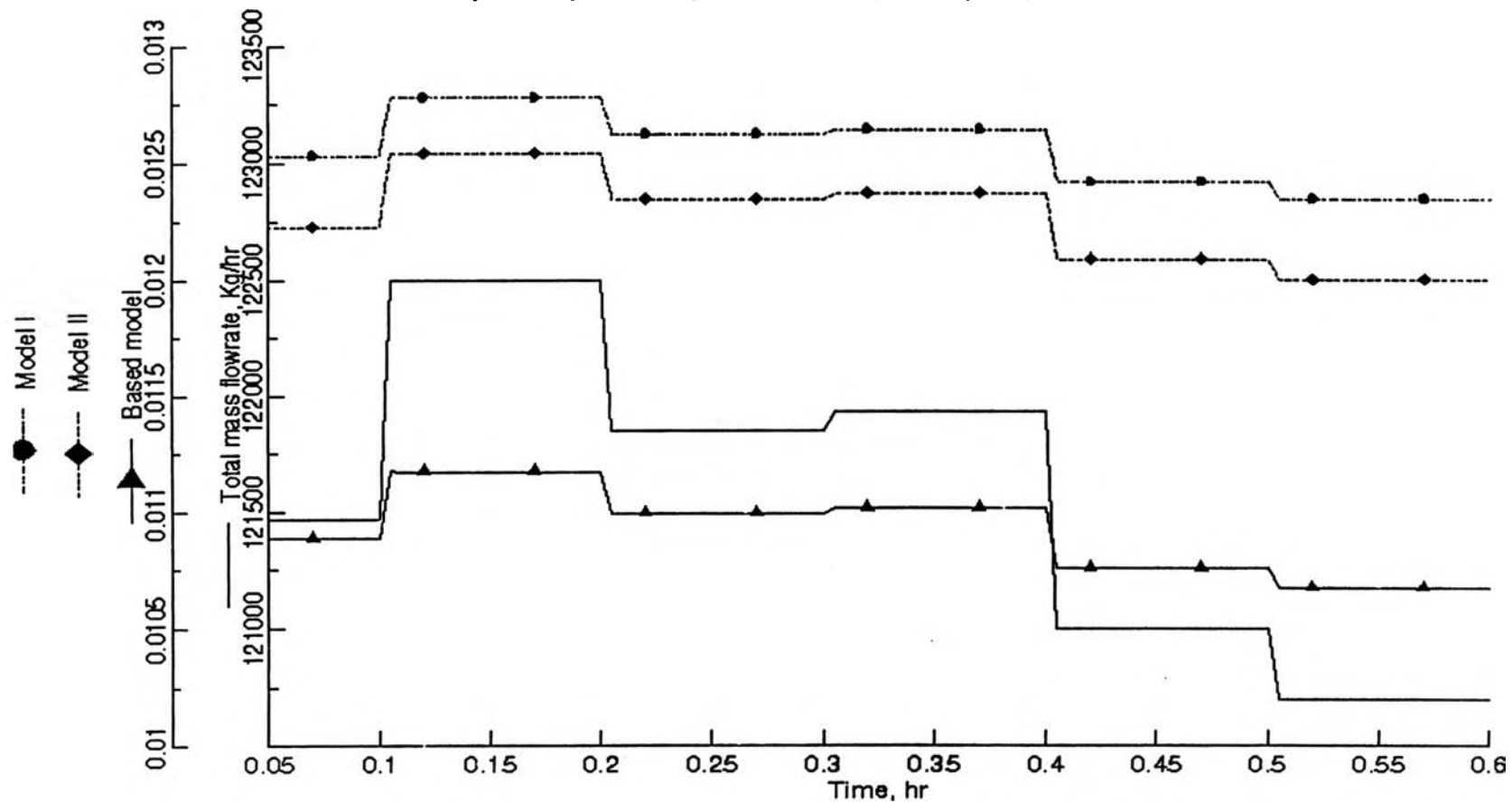


Figure 7.36 Comparison of the predicted outlet methyl acetylene corresponding to step change in total mass flowrate

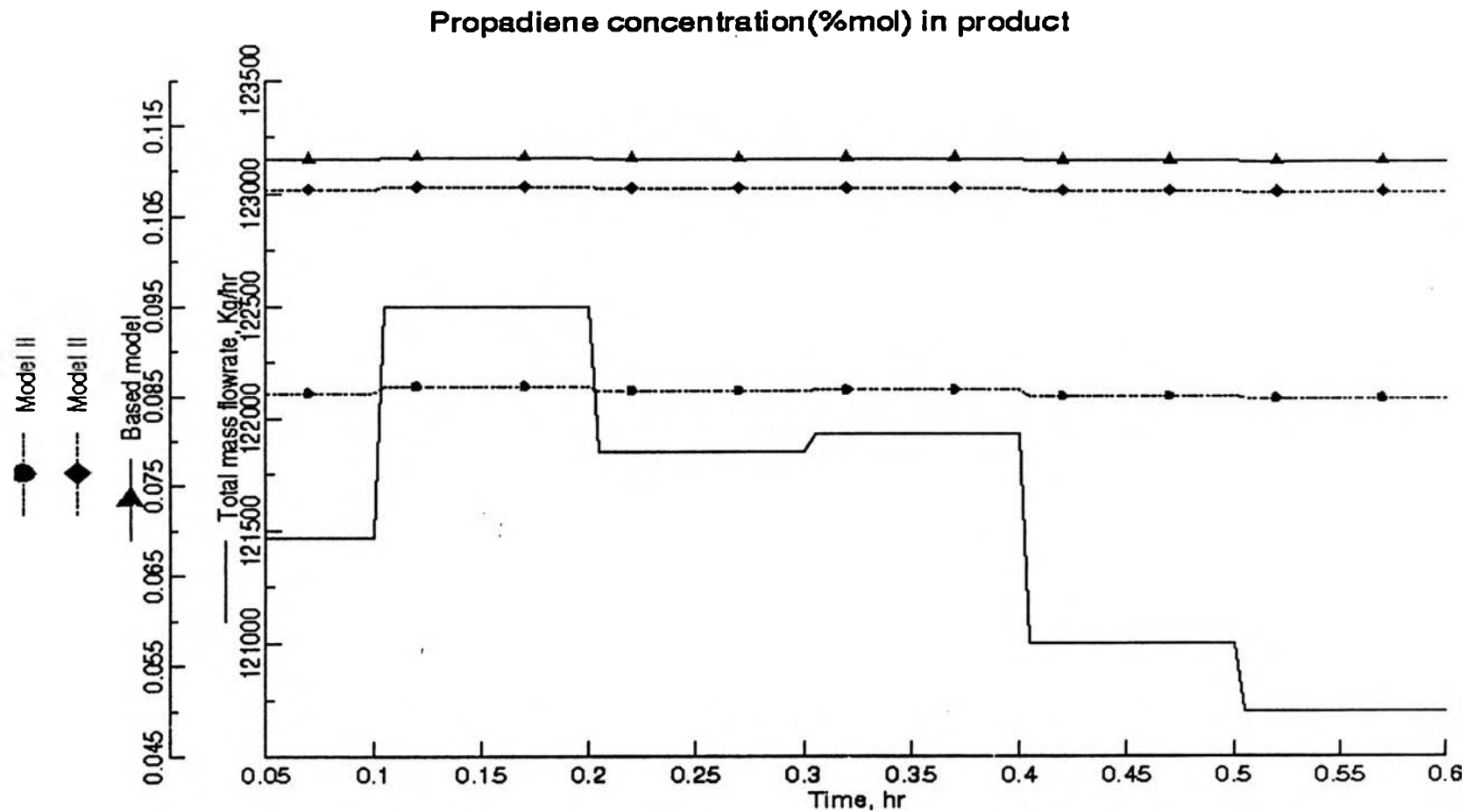


Figure 7.37 Comparison of the predicted outlet propadiene corresponding to step change in total mass flowrate

Methane concentration(%mol) in product

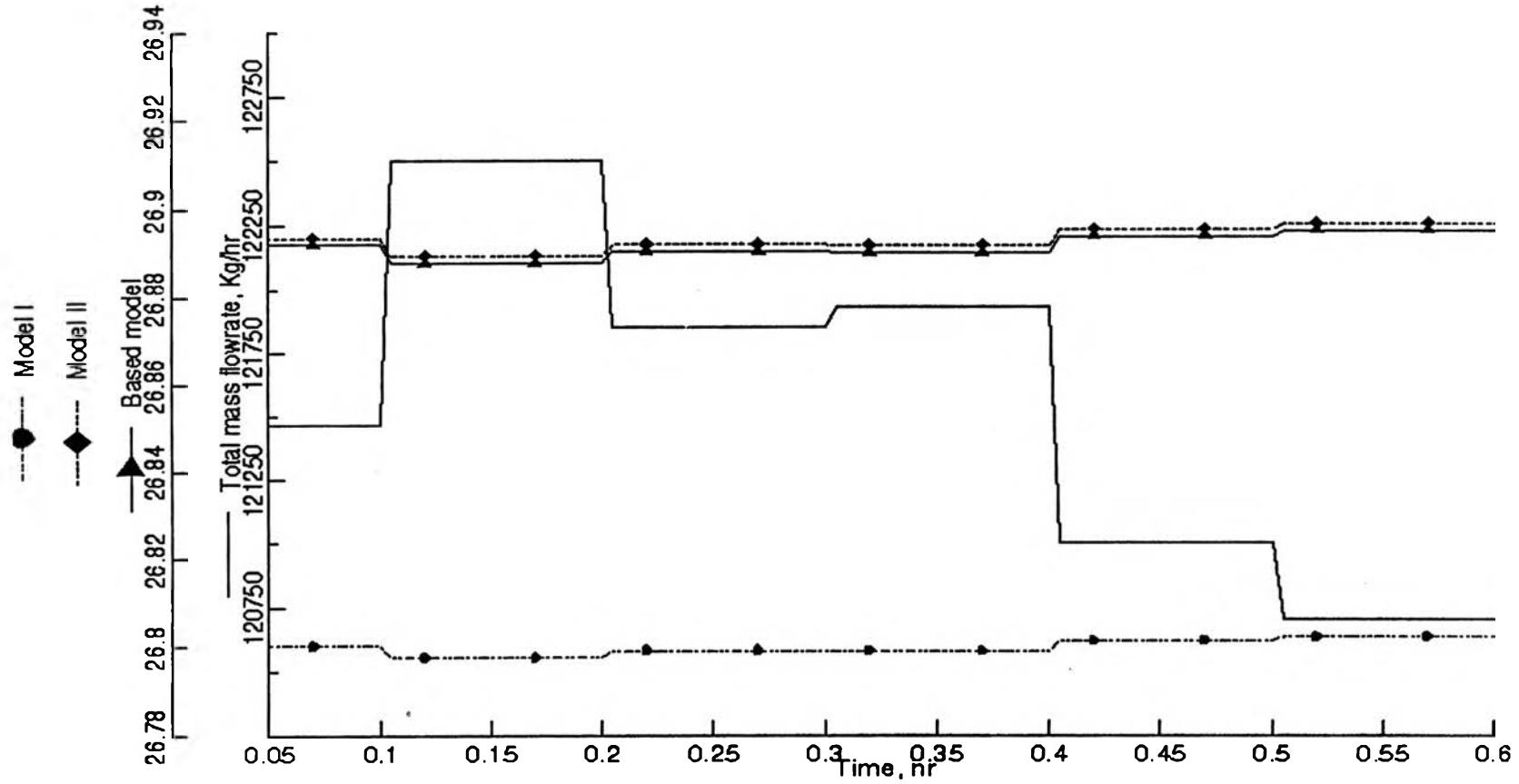


Figure 7.38 Comparison of the predicted outlet methane corresponding to step change in total mass flowrate

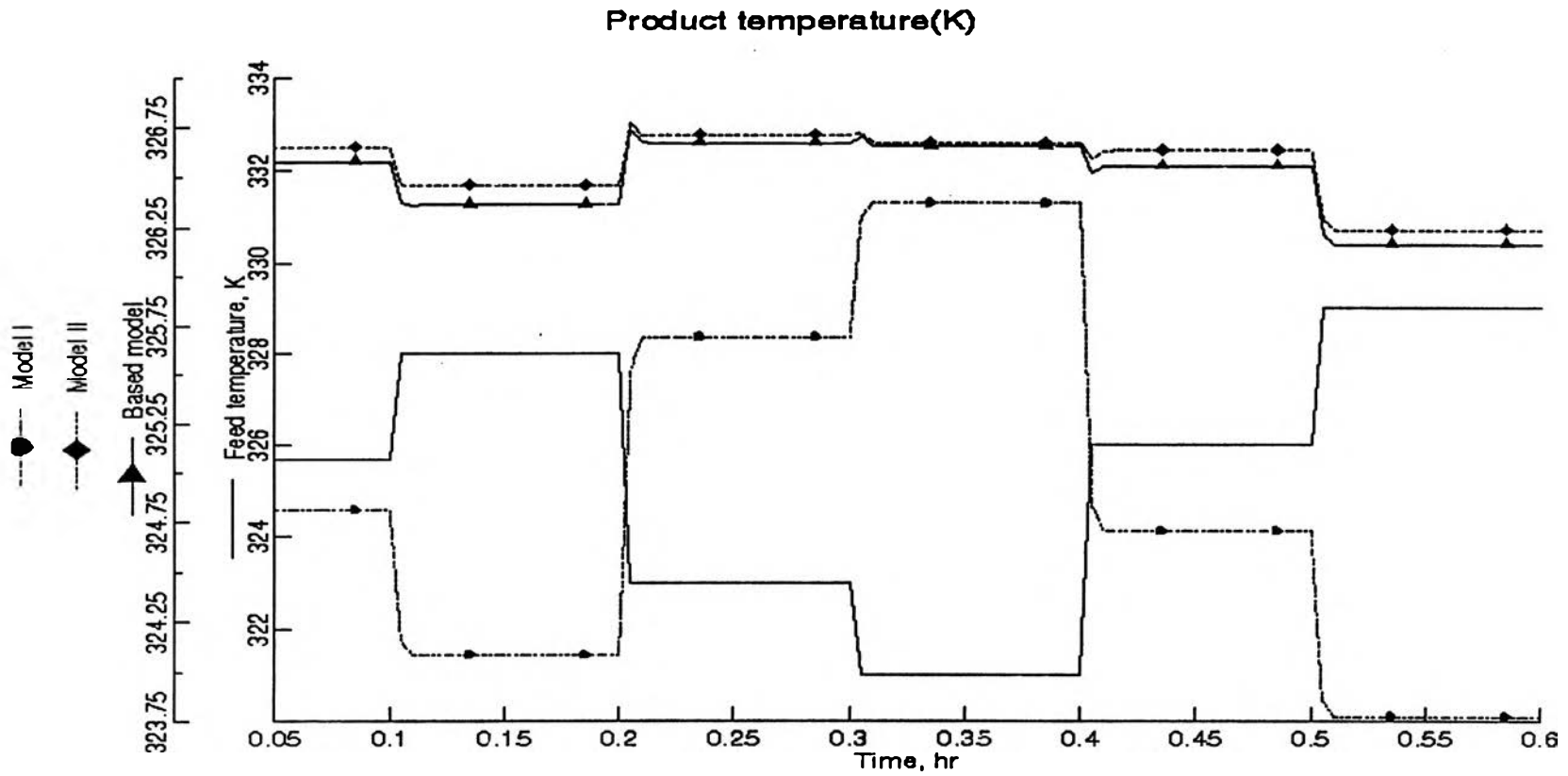


Figure 7.39 Comparison of the predicted product temperature corresponding to step change in feed temperature

Acetylene concentration(%mol) in product

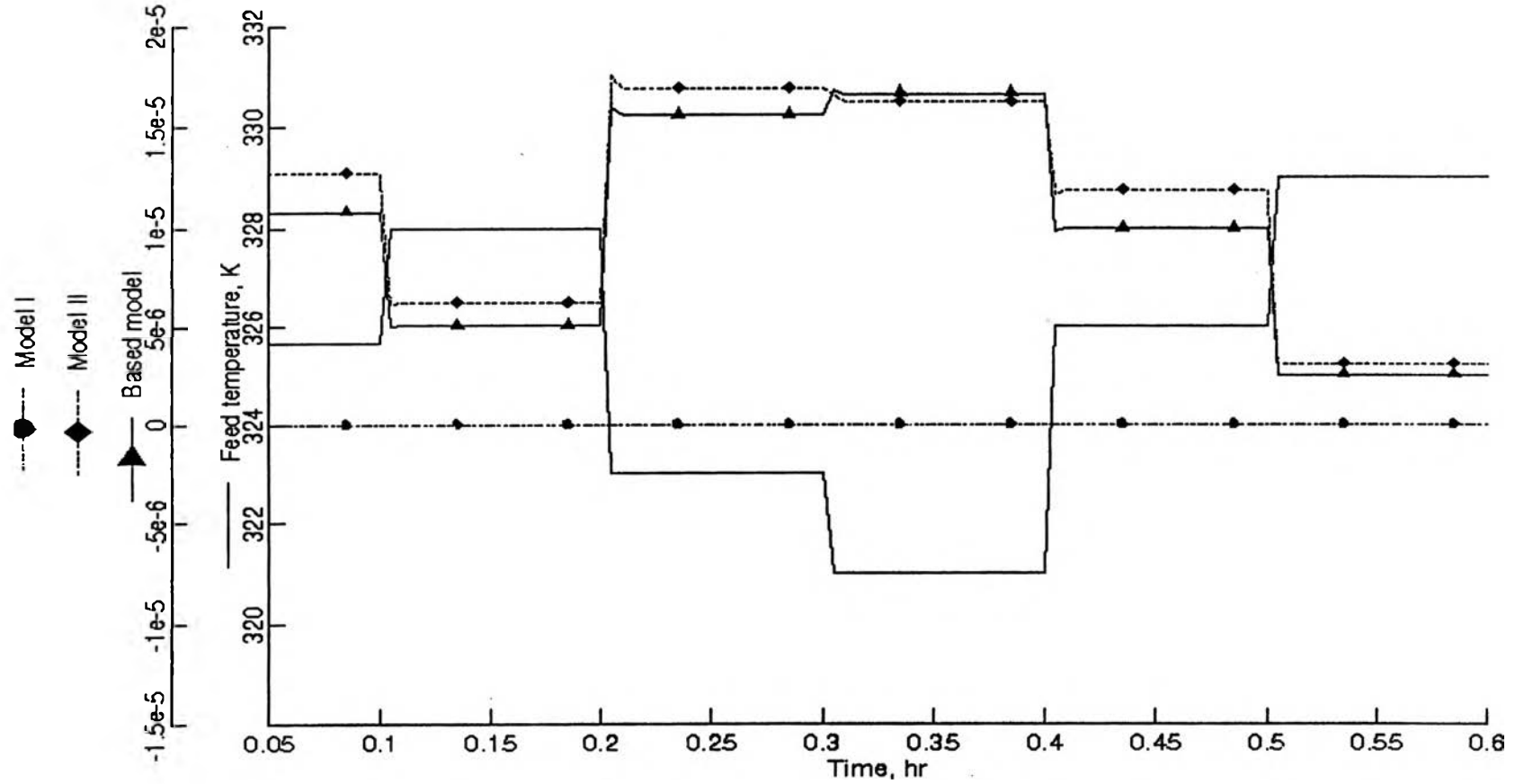


Figure 7.40 Comparison of the predicted outlet acetylene corresponding to step change in feed temperature

Ethylene concentration(%mol) in product

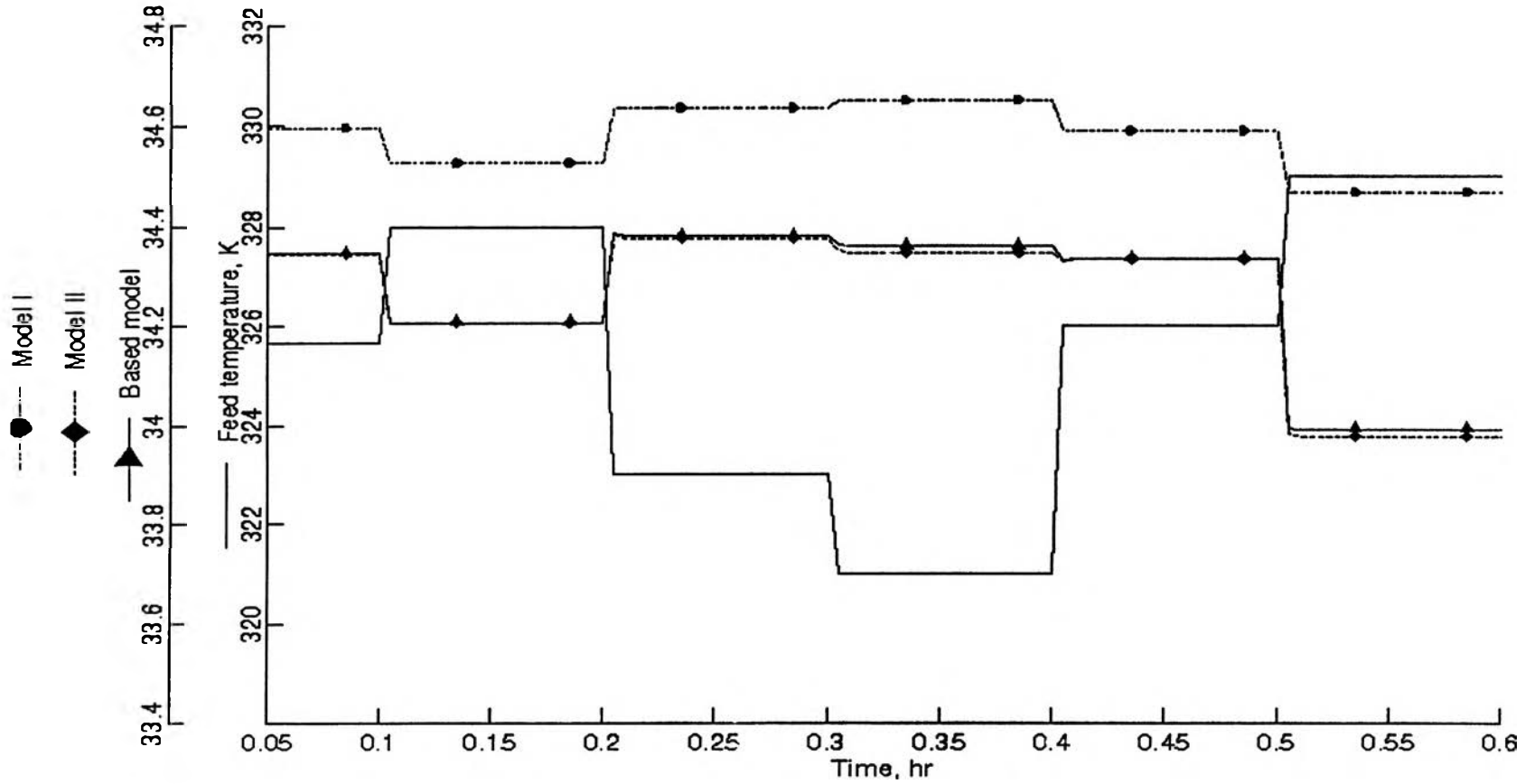


Figure 7.41 Comparison of the predicted outlet ethylene corresponding to step change in feed temperature

Hydrogen concentration(%mol) in product

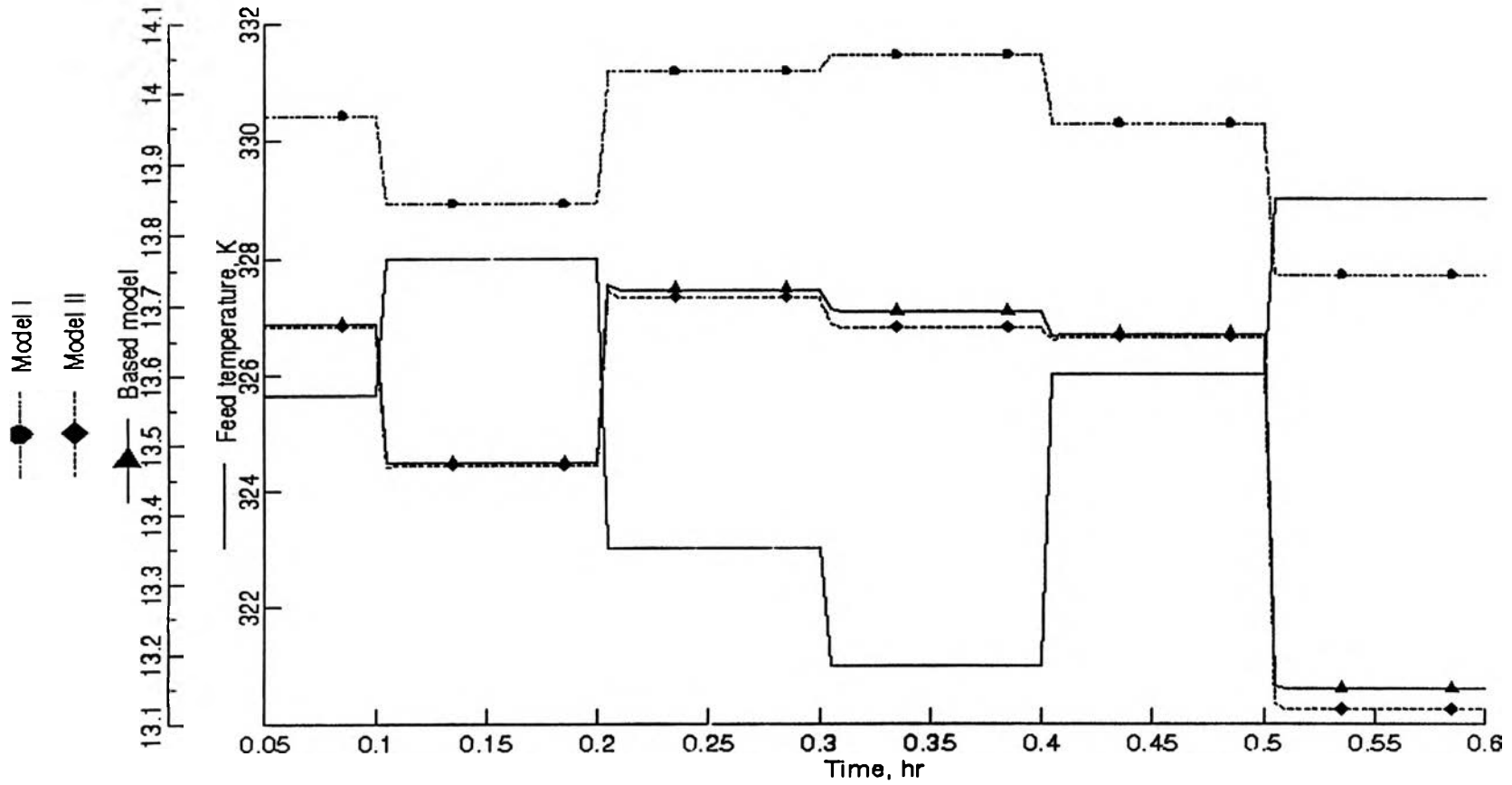


Figure 7.42 Comparison of the predicted outlet hydrogen corresponding to step change in feed temperature

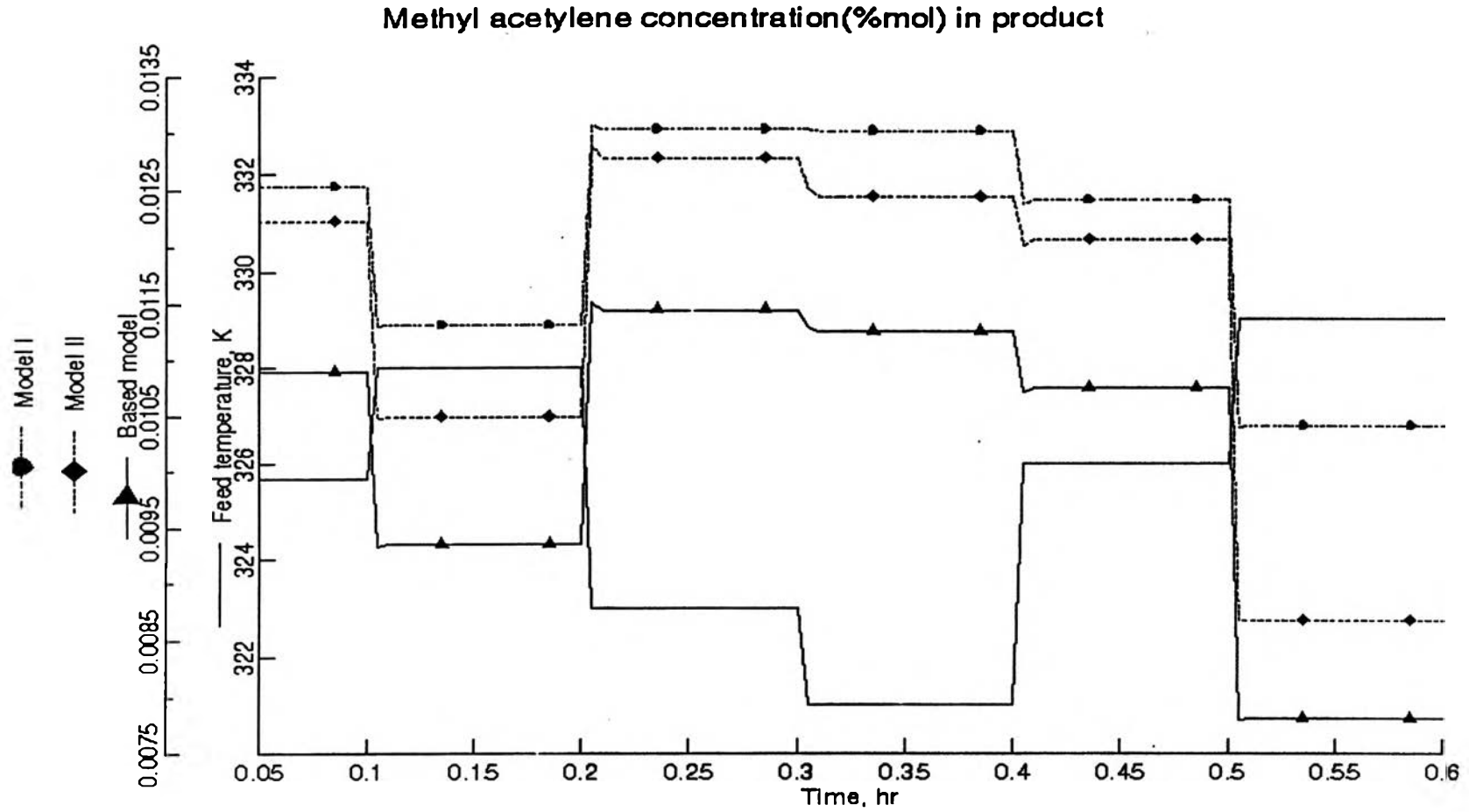


Figure 7.43 Comparison of the predicted outlet methyl acetylene corresponding to step change in feed temperature

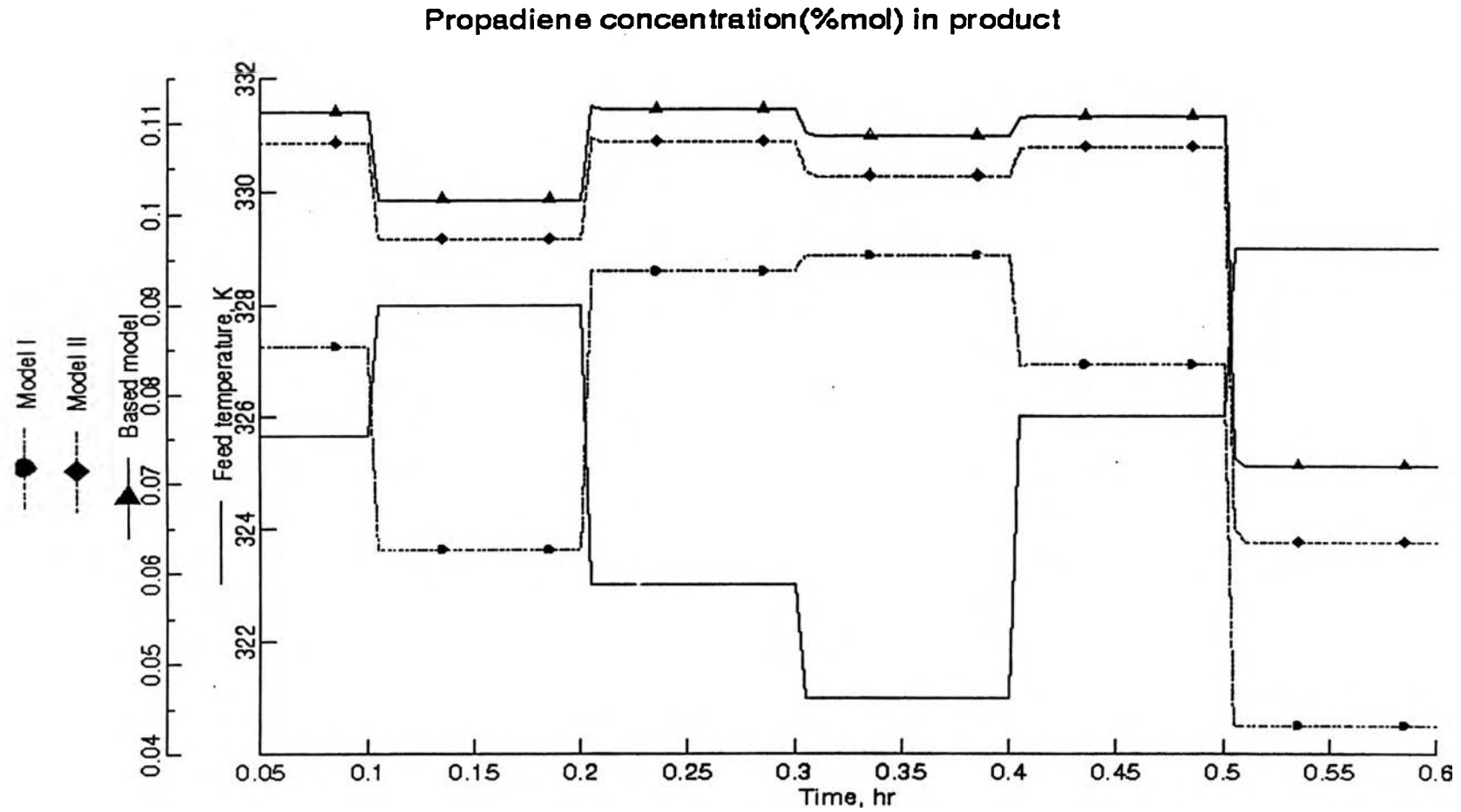


Figure 7.44 Comparison of the predicted outlet propadiene corresponding to step change in feed temperature

Methane concentration(%mol) in product

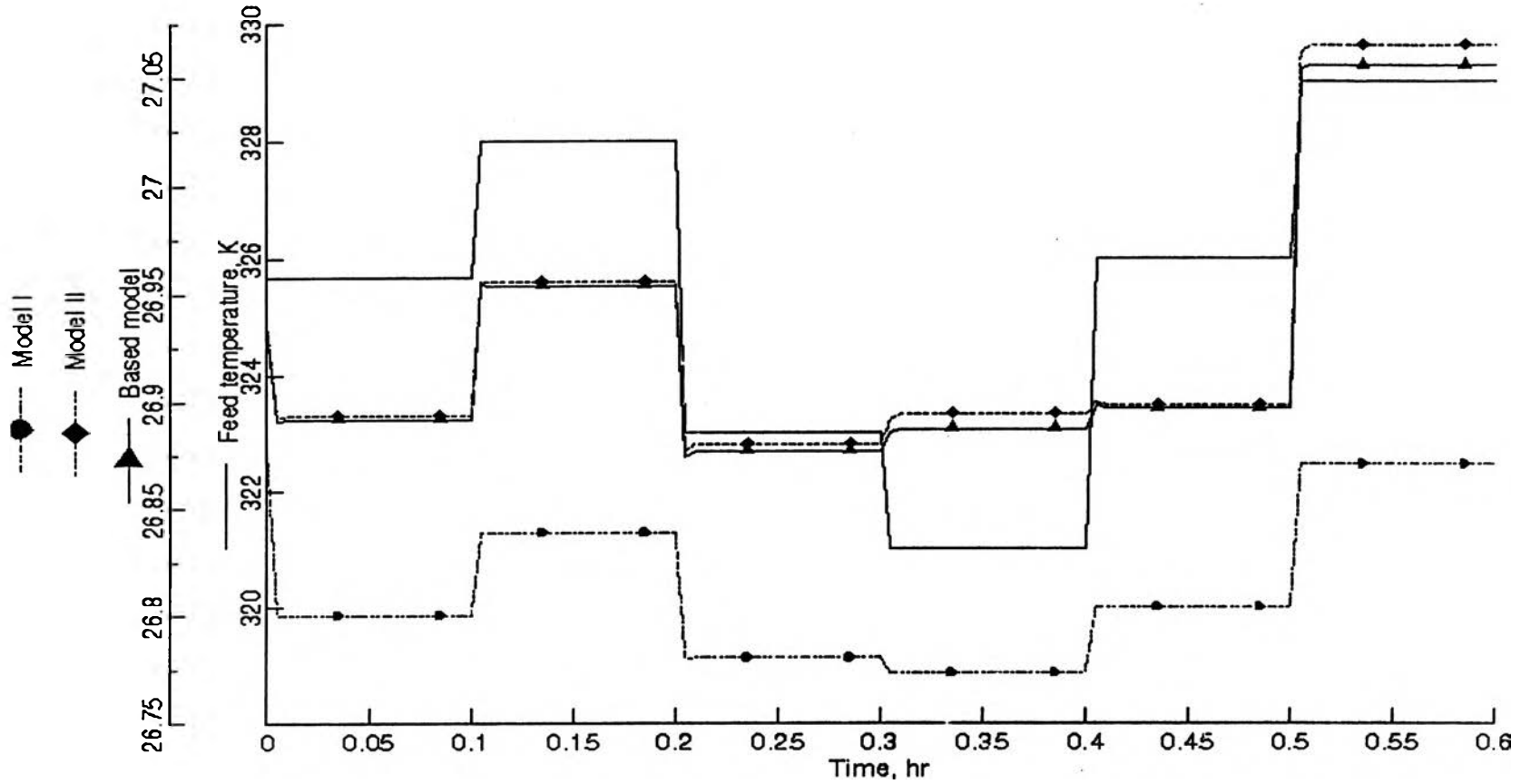


Figure 7.45 Comparison of the predicted methane corresponding to step change in feed temperature

Comparison of Outlet Acetylene Concentration(PPM)

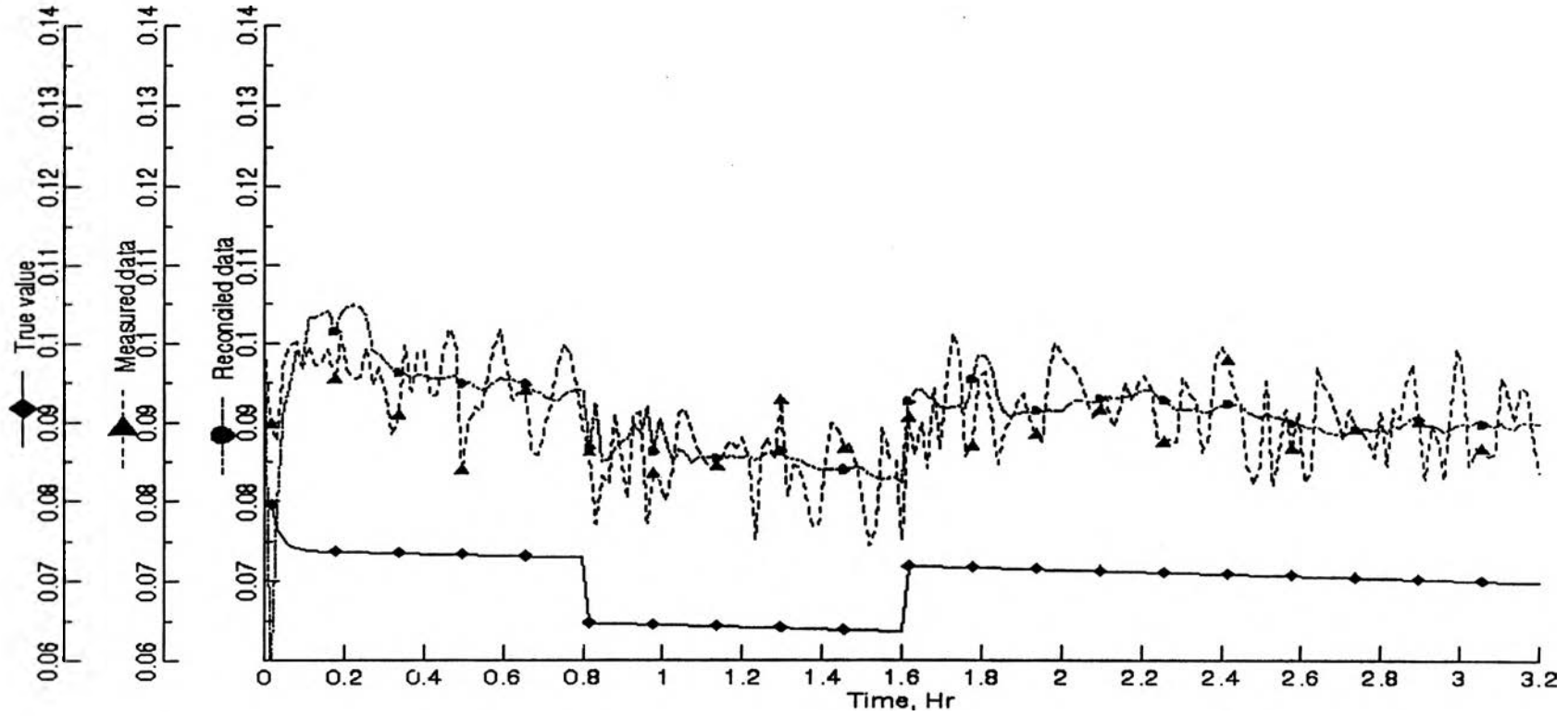


Figure 7.46 The capability to erase the bias of measurement data

According to Figure 7.32 to 7.45, it very clear to say that the data reconciliation can improve the model accuracy because of the accurate reconciled data of the measured data. The MODEL II that contained the rate constant values from the reconciled data can predict the output variables that is very close to the output from the based model.

However, the data reconciliation cannot eliminate the measurement bias as shown in Figure 7.46. The Figure 7.46 shows the comparison among the true value, the simulated measured data, and the reconciled data of the simulated measured data. The true signal value signal is added with the random noise and bias to from the simulated measured data. The measured data is passed to the dynamic data reconciliation. The reconciled data contains the bias as same as the measured data.

7.4 Summary

The dynamic data reconciliation program that developed for an acetylene hydrogenation process is based on the weighted least square sense. The objective function of the program is to minimize the sum of square error between the measured data and the reconciled data, and the reconciled data must satisfy the material and energy balance equations of the process. The method that used to solve the objective function under the constraints is the Lagrange Multiplier method.

The suitable history horizon is ten-step of sampling time. The developed dynamic data reconciliation program can reduce the standard deviation of the simulated measured data decreasingly by 90%, can reduce the standard deviation of the actual plant data decreasingly by 40-70%, but cannot eliminate or reduce the bias. To eliminate the bias, the bias estimator must be added and eliminate the bias from the measured data before passing the data to the dynamic data reconciliation step.

The dynamic data reconciliation subject is completed in this chapter. The next chapter is covered with the DMC controller design for an acetylene hydrogenation process.