CHAPTER VI

RESULTS AND ANALYSIS

This Chapter collects all the simulation results of controlling sulphur content remain from hydro-desulphurisation process. Simulation in this thesis composes of Hydro-desulphurisation process simulations in item 6.1 and plant mismatch simulation by program MATLAB in item 6.2.

6.1 Hydro-desulphurisation Process Simulations

6.1.1 Model Identification

The process model parameters were fit with the real plant data, which the reactor inlet temperature setpoint was stepped between 347 °C to 352 °C, 6 times with 2-hour period. The data were collected every 1-minute. The model was identified by using the first half of the data and verified by the second half of the data. The result of fit can be seen in figure 6.1A and 6.1B and the verification fit can be seen on figure 6.2A and 6.2B. The error of the model is as below table:

Table 6.1 ISE and RMSE between process model and plant data

	Identification		Verification	
	ISE	RMSE	ISE	RMSE
Reactor inlet temperature, T_{ri}	19.689	0.10456	68.517	0.19505
Reactor outlet temperature, T_{ro}	77.413	0.20732	145.3	0.28403

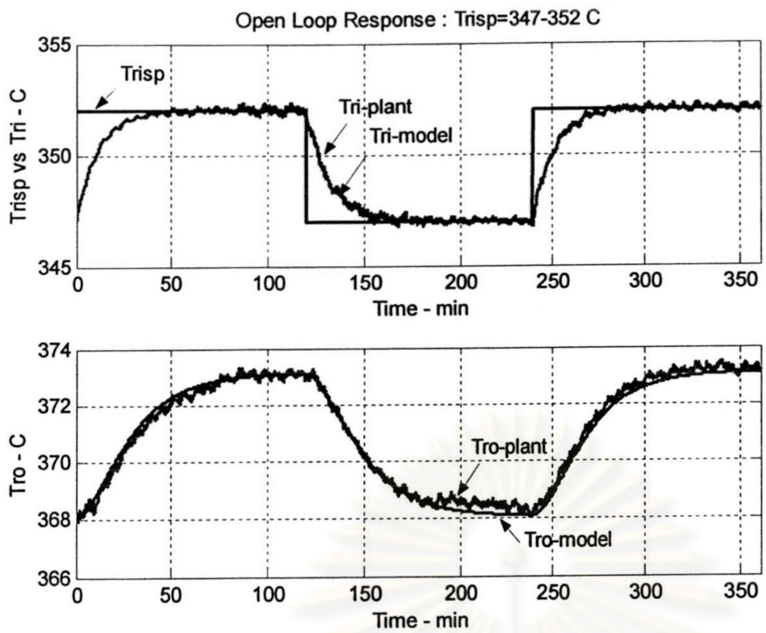

Figure 6.1A The relation graph between the reactor inlet temperature setpoint and the response.

Figure 6.1B The relation graph between the real reactor outlet temperature and model reactor outlet temperature.

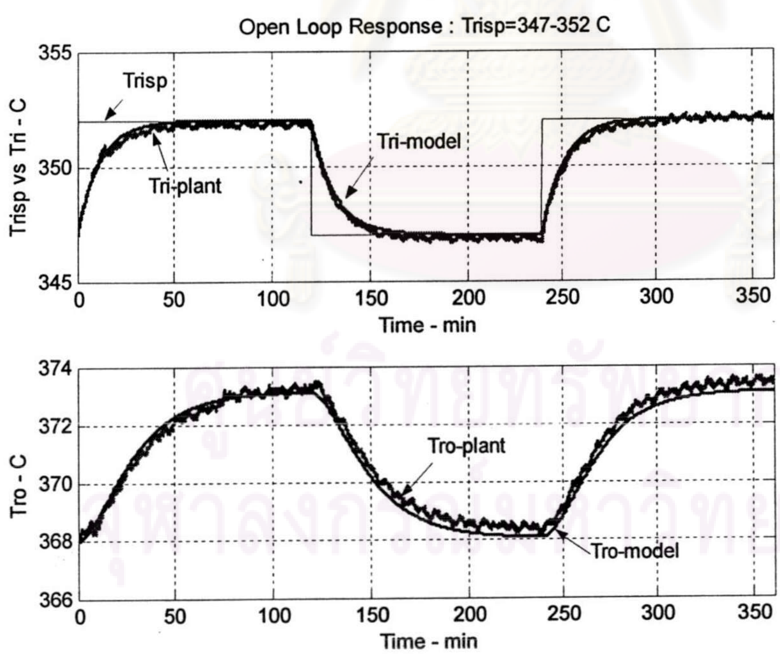

Figure 6.2A The relation graph between the reactor inlet temperature setpoint and the response of verification data set.

Figure 6.2B The relation graph between the real reactor outlet temperature and model reactor outlet temperature of verification data set.

Mean while of plant step testing, the product samples were taken at each steady state step. The lab results for sulphur content in product is as in table 6.2 and 6.3 for learning and verification data set, respectively.

Table 6.2 Sulphur content comparisons for identification data set

Sulphur content	Time=100	Time=220	Time=330
Model	0.044	0.043	0.042
Sample	0.040	0.042	0.041

Table 6.3 Sulphur content comparisons for verification data set

Sulphur content	Time=100	Time=220	Time=330
Model	0.044	0.043	0.042
Sample	0.041	0.044	0.040

6.1.2 Open Loop Simulation

For open loop simulation, the temperature setpoint for reactor inlet temperature was changed from steady state temperature 347 °C to 352 °C. This simulation study the dynamic response of reactor inlet temperature, outlet temperature and effluent sulphur content

The results of open loop simulation can be seen in figure 6.3A, 6.3B, 6.3C and 6.3D. From the response, found that, to reach steady state, the process took about 50 minute. As the result, the process time horizon for controller must be more than 50 minute. To be able to characterize the process, the scan can be either 1 minute or less. In the thesis, 0.2 was chosen.

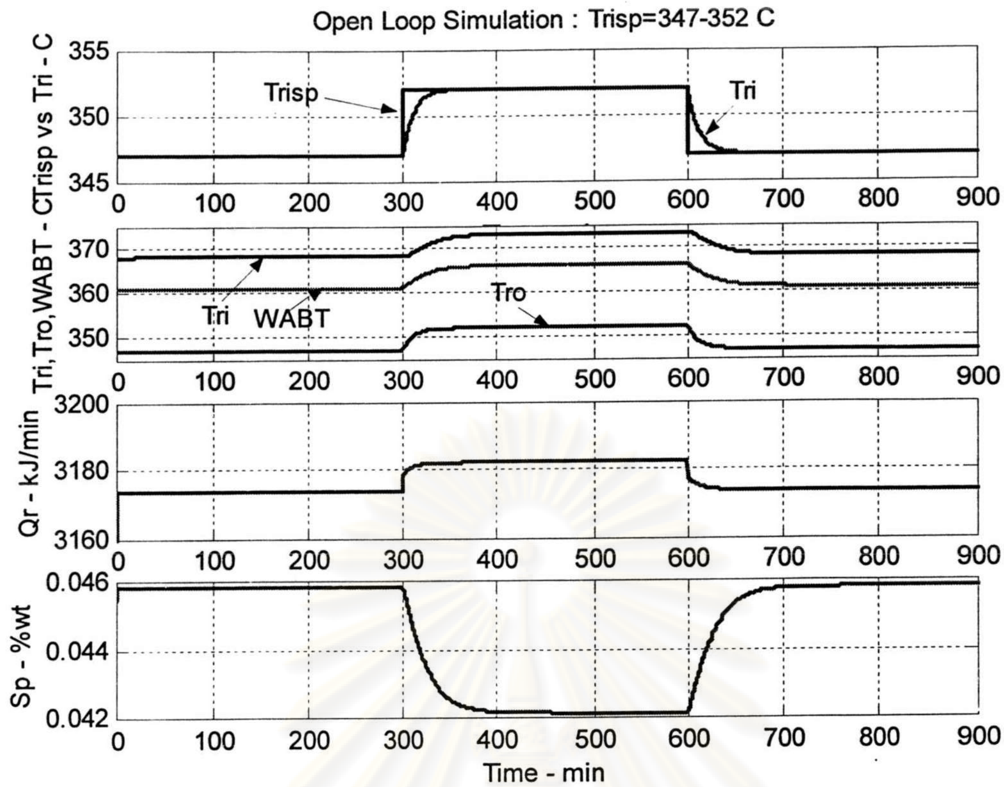

Figure 6.3A Relation between reactor inlet temperature setpoint and reactor inlet temperature measurement.

Figure 6.3B Step response of reactor inlet & outlet temperature and calculated WABT

Figure 6.3C Step responds of model reaction heat energy released

Figure 6.3D Step response of effluent sulphur content from reactor

6.2 State Variable Estimation

6.2.1 Sulphur Content Prediction

Because the process feed stock contains a lot of components with could make model mismatch for sulphur contest estimation just by the identified model in item 6.1.1, a simple linear model which could be able to be updated by lab results for this thesis is proposed. The linear model was identifying by a simple regression data between WABT and the lab result. This was based on the assumption that the sulphur content in feed and the space velocity in the reactor were constant.

To be able to simulate, the sulphur in product from model was modified. The result of the linear model prediction with out lab result update is shown in figure 6.4A, 6.4B, 6.4C and 6.4D. The ISE between the prediction and emulated sulphur in product is 0.1355 with RMSE=0.0058.

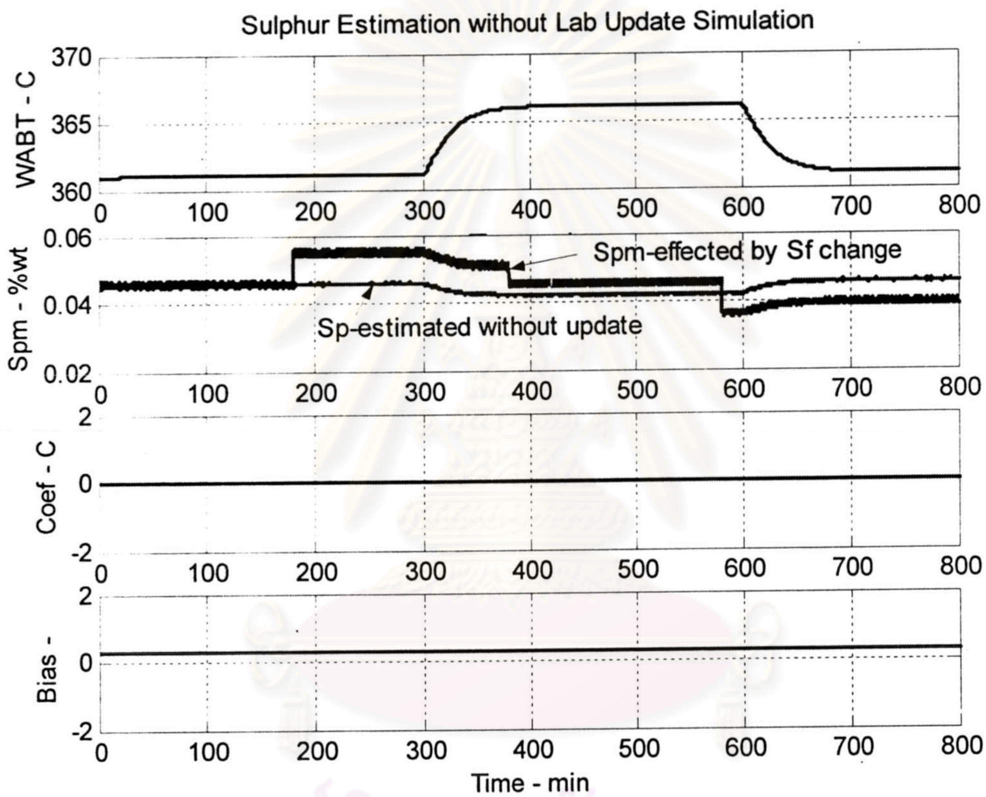

Figure 6.4A WABT response from reactor inlet temperature setpoint changed

Figure 6.4B Comparison between Sulphur content in product when the sulphur in feed changed 1.2, 0.9 and 0.8 times at time 900, 1900 and 2900, respectively and sulphur in product estimation without lab update mechanism

Figure 6.4C Without lab update mechanism; WABT coefficient sulphur estimator is constant.

Figure 6.4D Without lab update mechanism; bias term of sulphur estimator is constant.

To simulate the lab updating results, assumed that the lab results were taken at every time x100. The result of prediction of prediction trends can be seen in figure 6.5A, 6.5B, 6.5C, and 6.5D. From the result, found that by using Kalman filter technique, the coefficient and bias could be identified every lab result. By using this technique, the ISE reduced to 0.0196 with RMSE=0.0022. Kalman filter tuning parameters are shown in table 6.4.

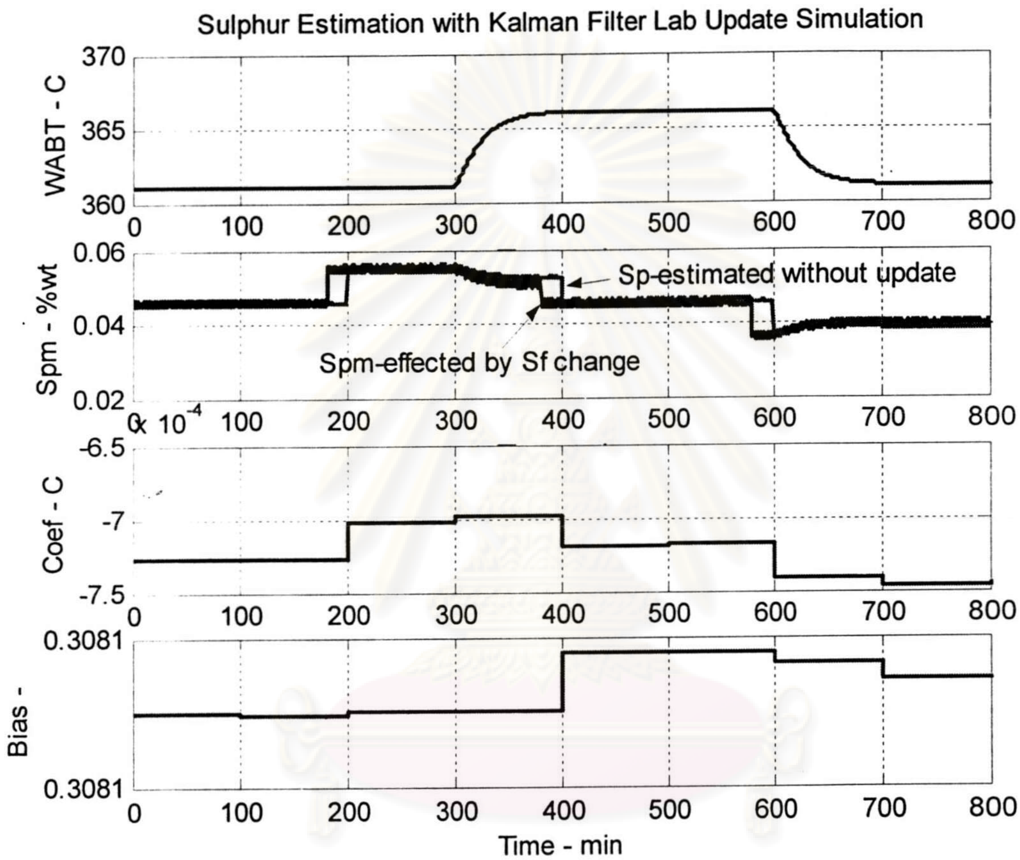

Figure 6.5A WABT response from reactor inlet temperature setpoint changed

Figure 6.5B Comparison between Sulphur content in product when the sulphur in feed changed 1.2, 0.9 and 0.8 times at time 900, 1900 and 2900, respectively and sulphur in product estimation with lab update mechanism

Figure 6.5C With lab update mechanism, WABT coefficient sulphur estimator is updating.

Figure 6.5D With lab update mechanism, bias term of sulphur estimator is updating.

Table 6.4 Kalman filter tuning parameters for sulphur prediction model

P	Q	R
P(1,1)=1 P(2,2)=1	Q(1,1)=1e-3 Q(2,2)=1e-3	R(1,1)=1e-2

6.2.2 Process State Variable Estimation

In the thesis, Kalman filter technique was used for state variable estimations. Especially with sulphur content in product, which was estimated by a simple process model. In figure 6.6 is before Kalman parameter tuning and in figure 6.7 is after Kalman parameter tuning. The results of error are shown in table 6.5.

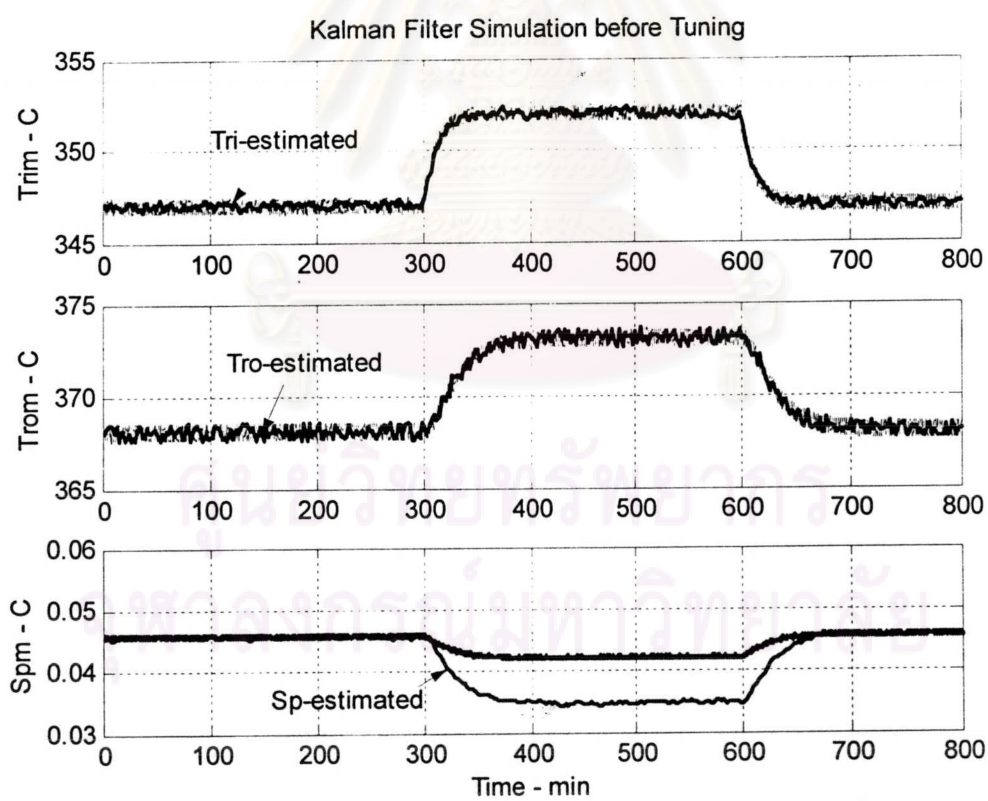

Figure 6.6 State variable estimations for reactor inlet & outlet temperatures and sulphur content in product before Kalman filter tuning.

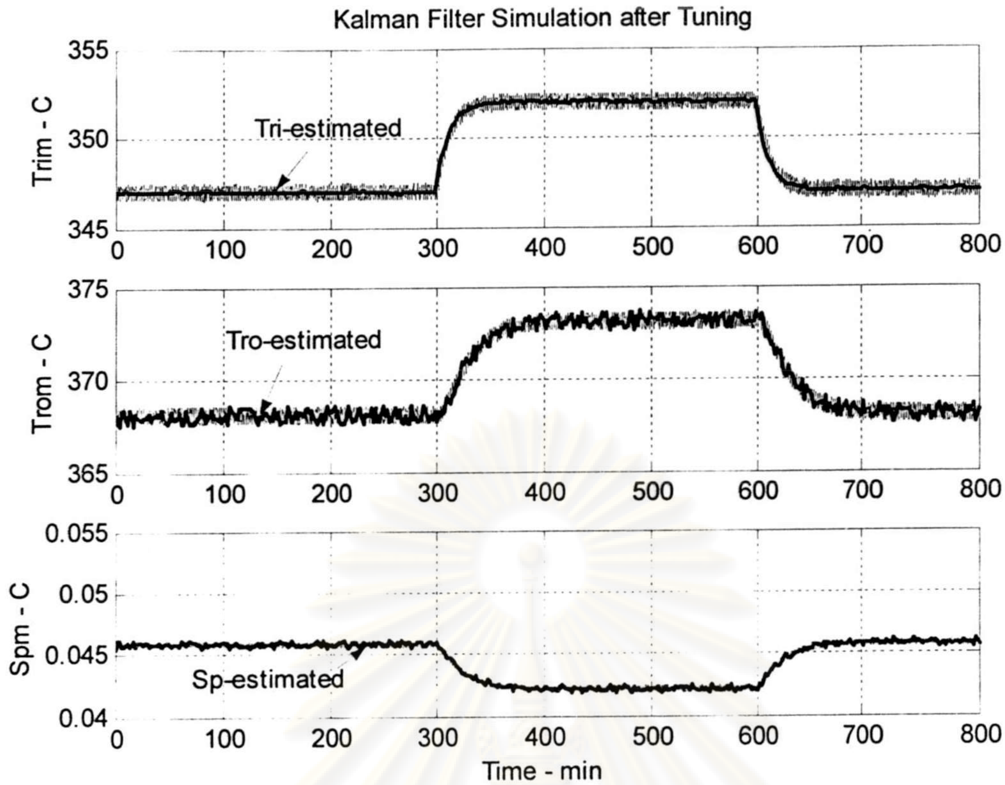

Figure 6.7 State variable estimations for reactor inlet & outlet temperature and sulphur content in product after Kalman filter tuning.

Table 6.5 Kalman filter parameters and error comparison

		ISE	RMSE	Parameters
Before tuning	Inlet Temp.	10.1041	0.1585	Q(1,1)=1,Q(2,2)=1, Q(1,1)=1 R(1,1)=1, R(2,2)=1, R(3,3)=1
	Outlet Temp.	31.5085	0.2800	
	Sulphur content	0.0075	0.0043	
After tuning	Inlet Temp.	4.6194	0.1072	Q(1,1)=1e-1,Q(2,2)=1, Q(3,3)=1 R(1,1)=1, R(2,2)=100, R(3,3)=0.5e-2
	Outlet Temp.	30.7950	0.2768	
	Sulphur content	9.8423e-006	1.5647e-004	

6.3 MPC and GMC with Kalman Filter Simulations

Just just a simple controller like PID could not easily control sulphur content in product because the controller could not know the nonlinear behavior of process. Therefore, in this thesis, model predictive controller was used and was compared with generic model controller. Both controllers are the control system that based on a process model in order to find the manipulated variable values. By using with Kalman filter state variable estimators, the results can be seen in figure 6.8 with tuning parameters sated in table 6.6.

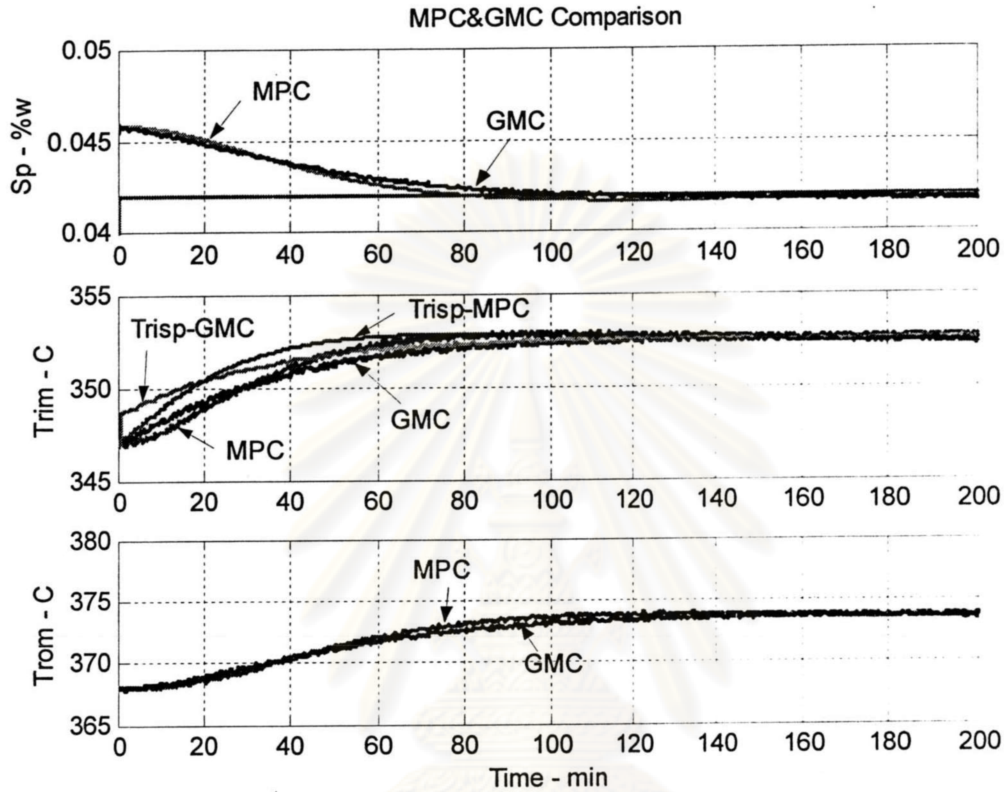

Figure 6.8 Comparison of GMC and MPC control results

Table 6.6 Tuning parameters for controllers and state variable estimators

GMC	K1=0.667, K2=1.11e-3
MPC	Qc(1,1)=10, Qc(2,2)=1e-3, Qc(3,3)=1e-3 Rc(1,1)=1e5, M=30, P=50
Kalman Filter	Q(1,1)=1e-1 Q(2,2)=1 Q(3,3)=1 Q(4,4)=1 R(1,1)=100 R(2,2)=5e-3

From experiments, the ISE was used as a performance index for sulphur content in product compared with sulphur content reference point in product. In the simulation, the sulphur content in product reference point was decreased from 0.046 %w to 0.042%w. found that, the ISE of MPC was 1.883e-3 and the ISE of GMC was 3.867e-4. From figure 6.8 found that both controllers moved the reactor inlet temperature rapidly during early period and slowly down to it target temperature without any overshoots either in sulphur content in product or both reactor temperatures. This was the result of being able to estimate sulphur content in product and having a process model to estimate the state variables i.e. reactor inlet and outlet temperature and sulphur content in product. If we notice carefully, we would see that the reactor inlet temperature setpoint moved by MPC has less vibration than GMC. The reason is because the MPC predicted the manipulated variable data set ahead for M steps and optimizes both manipulated variable and state variables. This leads MPC to produce the proper manipulated variable for M steps.

6.4 MPC with Mismatch Model Simulations

Because the real hydro-desulphurisation process has more parameters than the created simplified model, adjusting the manipulated variable to the real process might not get the expected results as in the model. Therefore these next simulations study about the performance of handling model mismatch both GMC and MPC for hydro-desulphurisation process.

6.4.1 Heat of Reaction Mismatch Simulation

The heat of reaction is a variable that could be mismatch from the real heat of reaction in the process, which is the result from thermodynamic. Heat of reaction change could also be from non-true heat value or there were other side reactions in the reactor, etc. The heat of reaction has highly effect in controlling the reaction temperature and the sulphur content in product. In this thesis, we simulate the robustness of heat of reaction mismatch by using higher heat of reaction values than the model. The result can be seen in figure 6.9 and table 6.7.

Table 6.7 Performance index when heat of reaction mismatch

Heat of Reaction (%)	ISE x 10^{-4} Sulphur Content Control		ISE x 10^{-6} Sulphur Content Estimation	
	MPC	GMC	MPC	GMC
110	1.239	1.405	2.765	2.653
120	1.001	1.013	2.674	2.941
130	6.477	7.251	3.591	3.614
140	4.960	5.454	4.899	6.089
150	4.472	4.799	8.077	12.22

From figure 6.9, we can see that when the heat of reaction in the real process is higher than the heat of reaction in the model, the reactor outlet temperature would increase faster. This leads to sulphur content in product decrease faster than the model prediction. As a result, we can see from sulphur in product trend that sulphur content was decreased lower than the setpoint a little bit and brought back to its setpoint by decreasing reactor inlet temperature. However, from table 6.7, we can see that even the heat of reaction has 50% mismatch, both controllers still can perform their control actions. In term of sulphur prediction, the performance does not really change much.

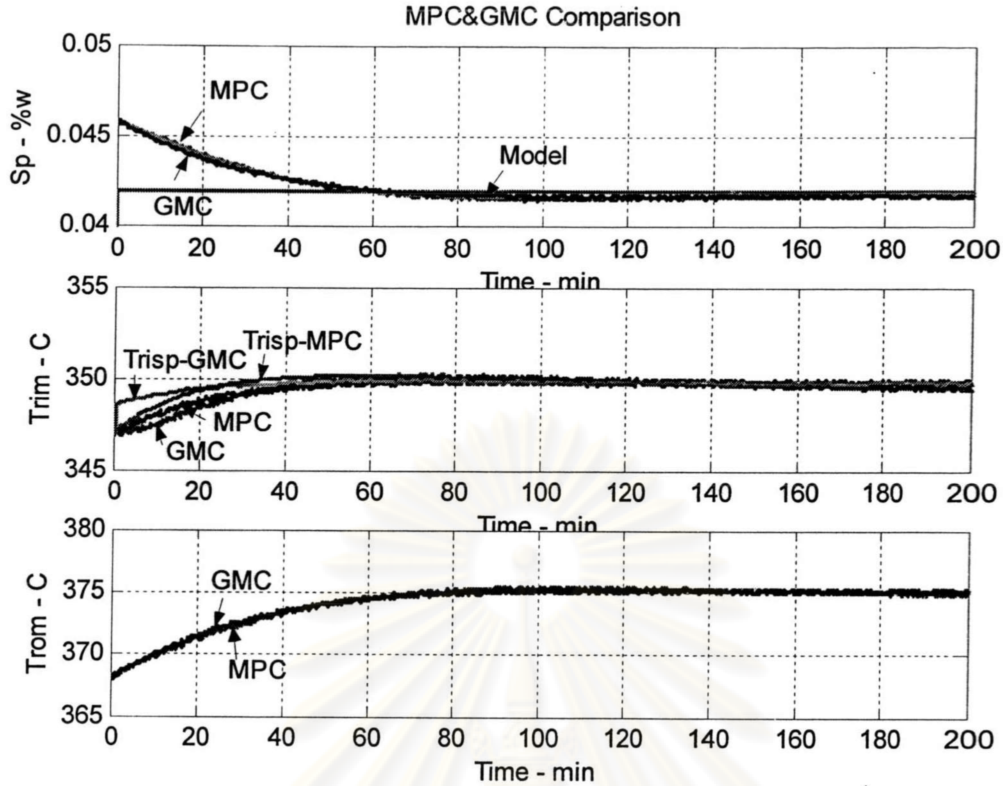

Figure 6.9 GMC and MPC comparison when heat of reaction increased 20%

6.4.2 Rate of Reaction Mismatch Simulation

The rate of reaction could be mismatch from laboratory. Especially, in this thesis the rate of reaction was adjusted to fit the real plant data. The effect of higher rate of reaction leads to higher heat from reaction releasing than usual. The simulation result can be seen in figure 6.10 and table 6.8.

Table 6.8 Performance index when rate of reaction mismatch

Rate of Reaction (%)	ISE x 10^{-4} Sulphur Content Control		ISE x 10^{-2} Sulphur Content Estimation	
	MPC	GMC	MPC	GMC
110	1.958	2.564	0.381	0.376
120	2.868	2.373	1.341	1.329
130	14.440	13.095	2.675	2.654

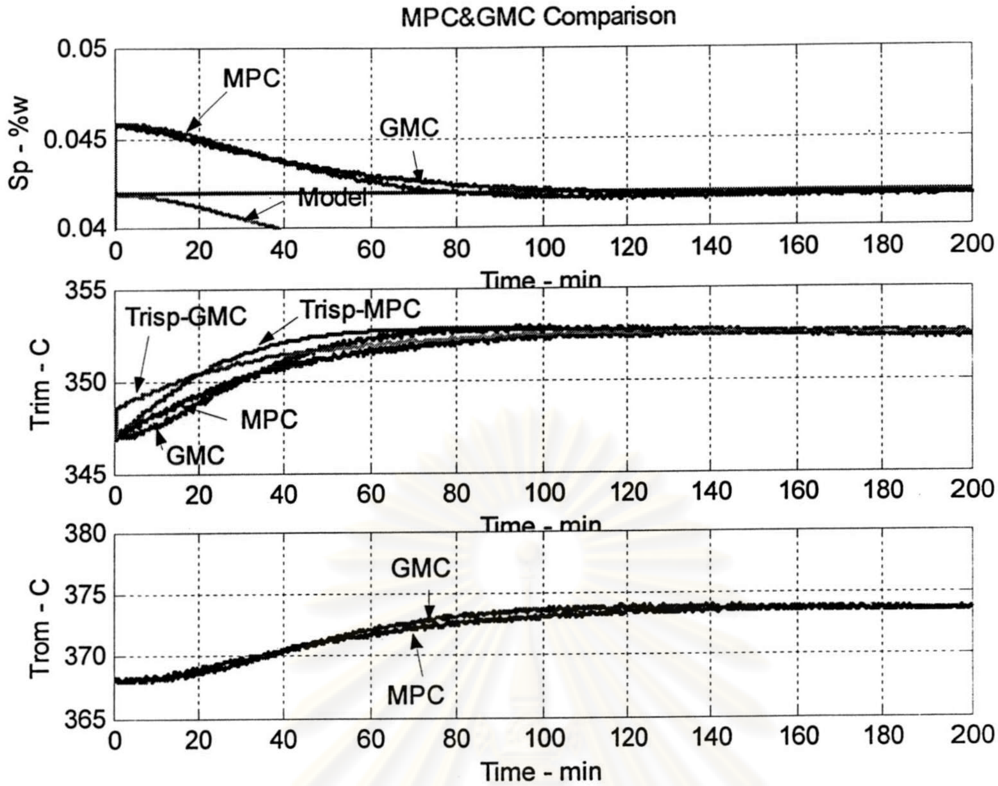

Figure 6.10 GMC and MPC comparison when rate of reaction increased 20%

From simulation found that, when the rate of reaction changed, it had direct effect to the actual sulphur content in product. In other word, it had no effect to sulphur prediction and control in the model even the actual sulphur was beyond the limit. This is because the rate of the reaction was not a state variable for control. This problem can be actually solved by sulphur prediction model lab update method as explained in 6.2.1.

6.4.3 Sulphur Content in Feed Mismatch Simulation

The sulphur content in feed can vary depending on the crude type. The sulphur content in feed can be mismatch from the fixed sulphur content in feed used in the model. The effect of higher sulphur content in feed could lead to lower total reaction rate than usual. The simulation result can be seen in figure 6.11 and table 6.9.

Table 6.9 Performance index when sulphur content in feed mismatch

Sulphur in Feed (%)	ISE x 10^{-3} Sulphur Content Control		ISE x 10^{-3} Sulphur Content Estimation	
	MPC	GMC	MPC	GMC
110	4.312	4.597	4.312	4.504
120	7.754	8.162	16.914	16.937
130	11.830	12.283	36.052	36.048

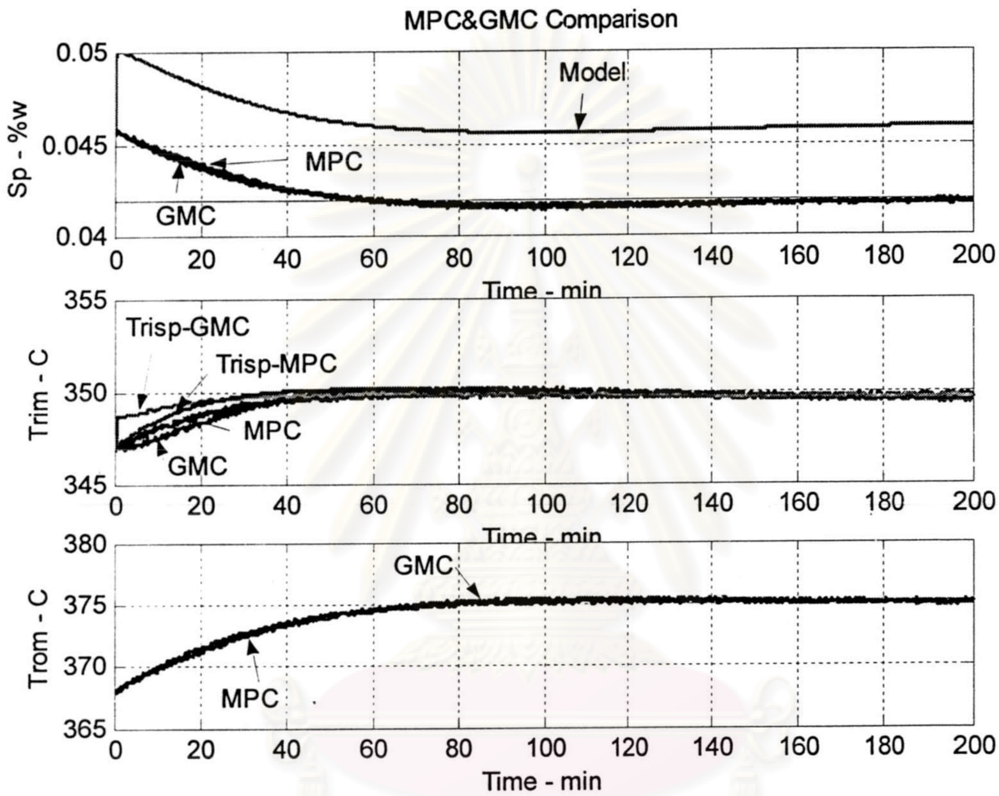

Figure 6.11 GMC and MPC comparison when sulphur content in feed increased 20%

When the sulphur content in feed was increased, we can see from the graph that major effect was the sulphur content in product. The slight effect happened with predicted sulphur content in product control. When the sulphur content in feed increased, the actual reactor outlet temperature was also slightly increased. For both controllers to be able to control the sulphur content in product at their target, the reactor inlet temperature was reduced. In term of controller and prediction performance between GMC and MPC are not really much difference. But the performance decreased along the change of sulphur content in feed incremental. For the move of reactor inlet temperature MPC did smoother move compared with GMC.

6.4.4 Feed Flow Mismatch Simulation

The feed flow has direct effect to the reaction time, the reverse of space velocity, in the reactor. The effect of the higher feed change leads to lower reaction time and consequently, the higher sulphur content in product. In this thesis, the assumption for model was made on fixed feed flow. The simulation result of the feed mismatch can be seen in figure 6.12 and table 6.10.

Table 6.10 Performance index when feed flow mismatch

Feed Flow (%)	ISE x 10^{-3} Sulphur Content Control		ISE x 10^{-3} Sulphur Content Estimation	
	MPC	GMC	MPC	GMC
110	4.934	5.315	4.234	4.256
120	9.571	10.259	16.098	16.116
130	15.508	16.467	34.526	34.620

From figure 6.13, we can see that when the feed flow increase, it increase the sulphur content in product but it has no effect with control because the feed flow is not a state variable in the model for control or predictions. Using sulphur content in product prediction with lab update mechanism can solve this problem.

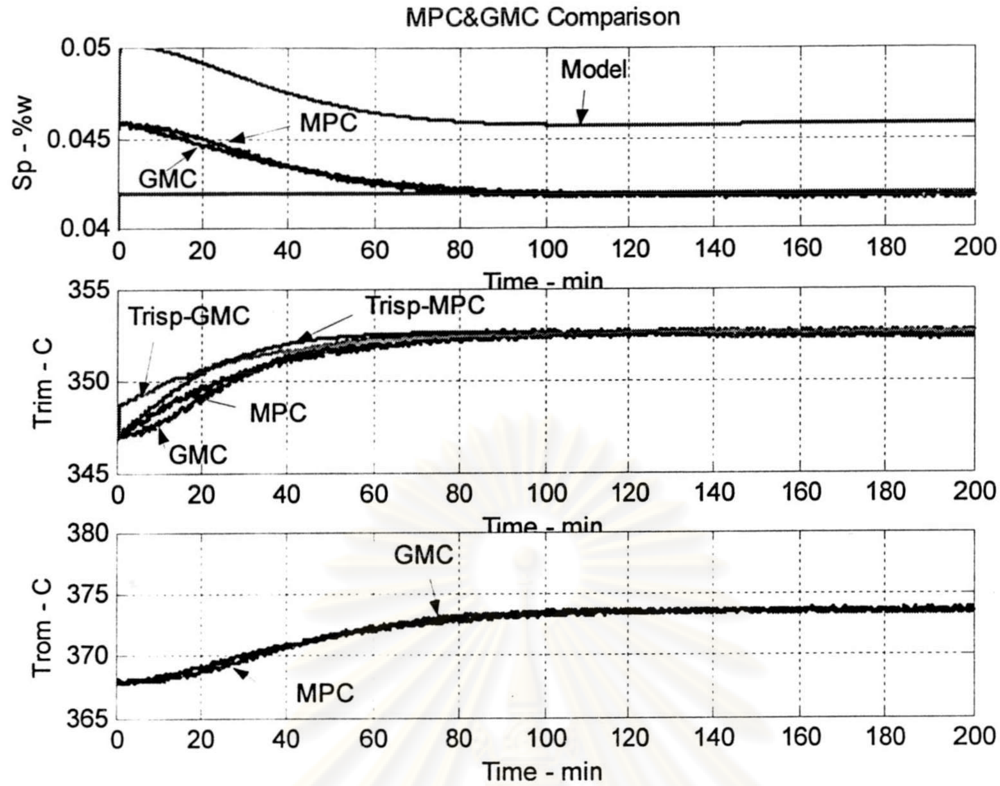

Figure 6.12 GMC and MPC comparison when feed flow increased 20%