CHAPTER IV

HYDRODEALKYLATION PROCESS

4.1 Process Description

4.1.1 Modeling HDA Process

The hydrodealkylation of toluene (HDA) process is used extensively in the book by Douglas (1988) on conceptual design . Figure 4.1 shows the nine basic unit operations of HDA process as described in Douglas: reactor, furnace, vapor-liquid separator, recycle compressor, two heat exchangers, and three distillation columns. Two raw materials, hydrogen and toluene, are converted into the benzene product, with methane and diphenyl produced as by-products. The two vapor-phase reactions are

$$\text{Toluene} + H_2 \rightarrow \text{benzene} + CH_4$$
$$2\text{Benzene} \longleftrightarrow \text{diphenyl} + H_2$$

The kinetic rate expressions are functions of partial pressures (in psia) of toluene p_T , hydrogen p_H , benzene p_B , and diphenyl p_D , with an Arrhenius temperature dependence. Zimmerman and York (1964) provided the following rate expressions:

$$r_1 = 3.6858 \times 10^6 \exp(-25{,}616/T)\, p_T\, p_H^{1/2}$$
$$r_2 = 5.987 \times 10^4 \exp(-25{,}616/T)\, p_B^2 - 2.553 \times 10^5 \exp(-25{,}616/T)\, p_D p_H$$

where r_1 and r_2 have units of lbmol/(min.ft^3) and T is the absolute temperature in kelvin. The heats of reaction given by Douglas (1988) are –21,500 Btu/ lbmol of toluene for r_1 and 0 Btu/ lbmol for r_2.

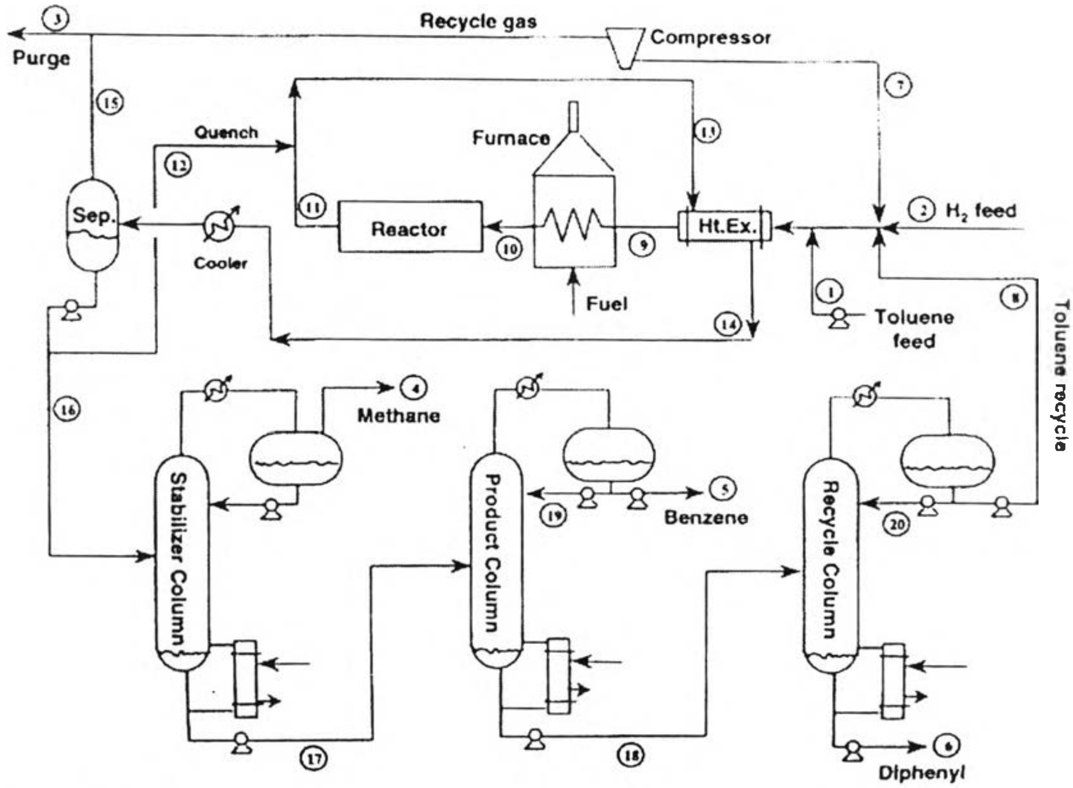

Figure 4.1 HDA process

The effluent from the adiabatic reactor is quenched with liquid from the separator. This quenched stream is the hot-side feed to the process-to-process heat exchanger, where the cold stream is the reactor feed stream prior to the furnace. The reactor effluent is then cooled with cooling water, and the vapor (hydrogen, methane) and liquid (benzene, toluene, diphenyl) are separated. The vapor stream from the separator is split. Part is purged from the process to remove the methane byproduct and the remainder is sent to the compressor for recycle back to the reactor

The liquid stream from the separator (after part is taken for the quench) is fed to the stabilizer column, which has partial condenser and removes any remaining hydrogen and methane gas from the liquid components. The bottoms stream from the stabilizer is fed to the product column, where the distillate is the benzene product from the process and the bottoms is toluene and diphenyl fed to the recycle column. The distillate from the recycle column is toluene that is recycled back to the reactor and the bottoms is the diphenyl byproduct.

Makeup toluene liquid and hydrogen gas are added to both the gas and toluene recycle streams. This combined stream is the cold-side feed to the process-to-process heat exchanger. The cold-side exit stream is then heated further up to the required reactor inlet temperature in the furnace, where heat is supplied via combustion of fuel.

4.1.2 Steady-State Modeling

First, a steady-state model is built in HYSYS.PLANT, using the flowsheet and equipment design information, mainly taken from Douglas (1988); Luyben et al. (1998). Table 4.1 presents the data and specifications for the equipment employed other than the three columns. For our simulation, Peng-Robinson model is selected for physical property calculations because of its reliability in predicting the properties of most hydrocarbon-based fluids over a wide range of operating conditions. The reaction kinetics of both reactions are modeled with standard Arrhenius kinetic expressions available in HYSYS.PLANT, and the kinetic data are taken from Luyben et al. (1998). Since there are four material recycles, four RECYCLE operations are inserted in the streams, Hot-In, Gas-Recycle, Quench, and Stabilizer-Feed (Fig.4.1). Proper initial values should be chosen for these streams, otherwise the iterative calculations might converge to another steady-state due to the non-linearity and unstable characteristics of the process.

Table 4.1 Equipment data and specifications

Reactor	
Length	57 ft
Diameter	9.53 ft
Furnace	
Tube volume	300 ft^3
FEHE	
Shell volume	500 ft^3
Tube volume	500 ft^3
Condenser	
Volume	150 ft^3
Separator	
Volume 2.27 m3	80 ft^3

When columns are modeled in steady-state, besides the specification of inlet streams, pressure profiles, numbers of trays and feed tray, two specifications need to be given for columns with both reboiler and condenser. These could be the duties, reflux rate, draw stream rates, composition fractions, etc. We chose reflux ratio and overhead benzene mole fraction for the stabilizer column. For the remaining two columns, bottom and overhead composition mole fractions are specified to meet the required purity of products given in Douglas (1988). The detailed design data and specifications for the columns are summarized in Table 4.2. This table also includes details of trays, which are required for dynamic modeling. The tray sections of the columns are calculated using the tray sizing utility in HYSYS, which calculates tray diameters based on Glitsch design parameters for valve trays. Though the tray diameter and spacing, and weir length and height are not required in steady-state modeling, they are required for dynamic simulation.

Table 4.2 Column specifications

	Stabilizer column	Product column	Recycle column
Number of theoretical trays	6	27	7
Feed tray	3	15	5
Diameter (ft)	1	5.7	2.5
Reboiler volume (ft^3)	250	293	36
Condenser volume (ft^3)	7.5	316	46
Reflux ratio	1.57	3	0.32
Specification 1	Benzene fraction in overhead = 0.042	Toluene fraction in distillate = 0.0003	Diphenyl fraction in distillate_0.00002
Specification 2	Methane fraction in bottom = 1 ppm	Benzene fraction in bottom = 0.0006	Toluene fraction in bottom = 0.00026

Figure 4.2 shows the simulated HDA process at steady-state by HYSYS.PLANT. Results from steady-state simulation are found to be consistent with those in Luyben et al. (1998) However, there are also some differences: for example, flow rates of reflux stream in product columns in our case is smaller than those in Luyben et al. (1998) and flow rates of reflux stream in recycle columns is

larger than those in the earlier study. The possible reasons for these differences may be that: in Luyben et al. (1998), vapor-liquid equilibrium behavior was assumed to be ideal and the stabilizer column was modeled as a component splitter and tank; but our simulation employs Peng-Robinson equation of state and the stabilizer column is modeled rigorously. The operating pressure for this column is chosen as more than the design information in Luyben (1998). Thus the pressures for the streams around stabilizer column are different.

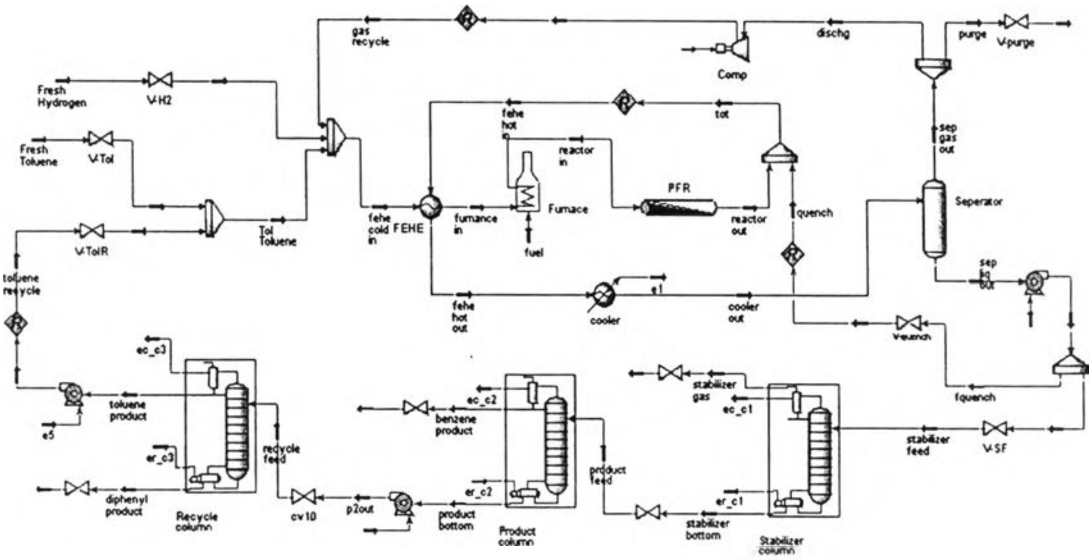

Figure 4.2 Flowsheet of simulated HDA process by HYSYS.PLANT

4.1.3. Dynamic Modeling

In the integrated steady state and dynamic simulation environment provided by HYSYS.PLANT, the dynamic model shares the same physical property packages and flowsheet topology as the steady-state model. Thus it is easy to switch from steady-state to dynamic mode. All flowsheet information from the steady-state simulation case transfers easily to the dynamic simulation environment. On the other hand, the dynamic model uses a different set of conservation equations that account for changes occurring over time. Besides the normal material and energy balances, an advanced method is provided to calculate the pressure and flow profiles. In this method volume balances and resistance equations are set-up, and the required number of pressure-flow (P-F) specifications is given by the user. These equations are solved simultaneously to find unknown pressure or flow rates. The general rule for the number of P-F specifications is 'one P-F specification per flowsheet boundary stream' except for the Column Sub flowsheet .

Before the transition from steady-state to dynamic mode, the flowsheet should be set up so that a definite pressure drop exists across the plant and, if necessary, valves and pumps should be added to the flowsheet. P-F specifications should be selected properly for the P-F solver to converge. Besides the proper sizing of the equipment, removal of redundant logical operations, and addition of controllers to increase the realism and stability of the model should also be considered as outlined below. Valves and pumps are added to the reflux streams in the column sub-flowsheet. For a more rigorous dynamic modeling of columns, condenser part of the column should be changed to a cooler followed by an accumulator. In our case, linear valve type is chosen and the valves are all sized with a 50% valve opening for nominal steady-state flow rates. The valve parameters are sized with the sizing function in HYSYS.PLANT. All the vessels including the separator, condensers and reboilers are initiated with 50% liquid level. In the dynamic mode, RECYCLE operation is redundant because the pressures and flows are calculated simultaneously, and so the four RECYCLE blocks in the steady-state model are removed

The HDA process is an open loop unstable system, and is caused by heat integration (i.e. recycle of energy) via feed-effluent heat exchanger (FEHE). This phenomenon is referred as external instability by Luyben (1998). Also, multiple steady-states exists for this process, and is described by Luyben et al. (1998). From dynamic simulation, we find that closing the reactor inlet temperature with furnace duty loop, the system becomes stable. Further, there are seven levels in the whole plant that need to be controlled due to their integrating characteristics. Initially, all these loops are implemented with the control scheme suggested by Luyben et al. (1998). Since these controllers are set for stability, a proportional (P) only controller is adopted. The model is now ready for switching from steady-state to dynamic mode. Figure 4.3 shows the simulated HDA process at dynamic mode and adding controllers by HYSYS.PLANT. Before activating the integrator to run the dynamic simulation, one P-F specification is given for each flowsheet boundary stream and the strip charts are set up to monitor the response of process variables of interest. After initiating the run, the responses eventually settle, after some initial transients, at the operating values obtained from steady-state simulation.

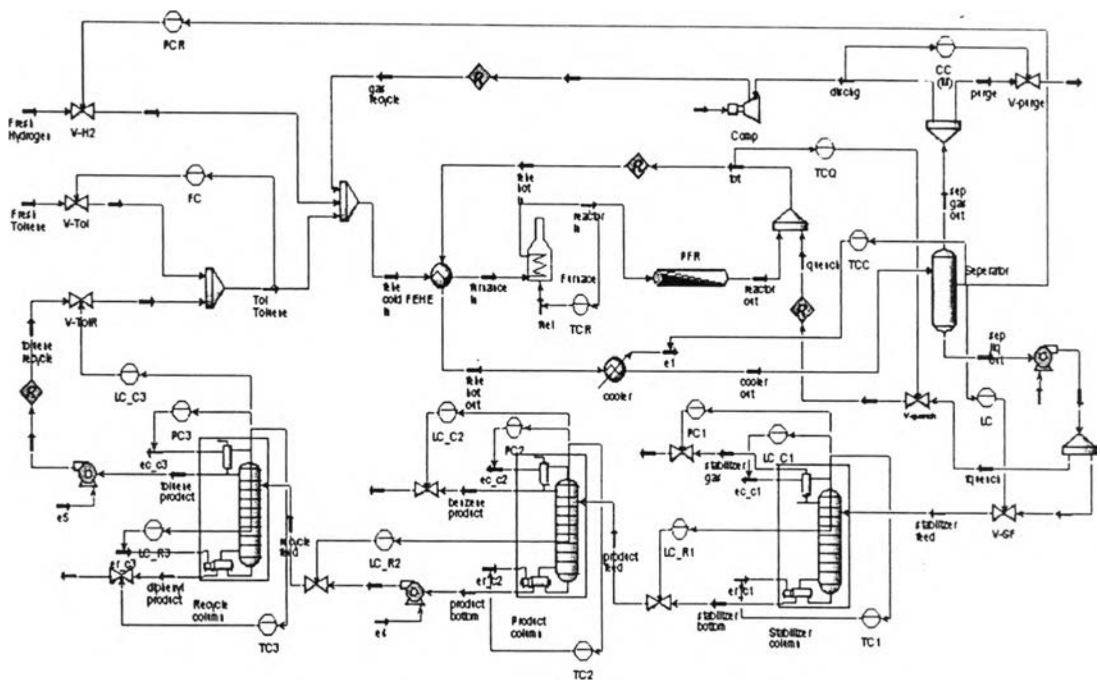

Figure 4.3 Flowsheet of simulated HDA process at dynamics mode and adding controller.

Since dynamic modeling is a complex procedure, it is very important to perform model validation carefully. Each of the transient responses obtained to various set point changes and load disturbances is first verified for their directionality and general characteristics through qualitative reasoning. This is exemplified in Fig. 4.4, where, with the reactor inlet temperature loop closed, a step change in set point of controller is made from 1150 to 1151 °F. As the inlet temperature increases, more toluene converts to benzene and methane. Thus we could see from Fig. 4.4 that the flow rates of benzene product ,diphenyl product and purge streams increase, while the flow rate of Tol-Recycle stream decreases. When the reactor inlet temperature increases, it also causes the reaction rate to go up. Thus the toluene is used to convert to these products so that Tol-Recycle stream go down. The FC-controller must to control flow of total toluene at set point so that the fresh toluene stream rise. Similar checks are made for other loops as well. A rigorous dynamic model of HDA process is thus developed. The process has 23 controlled variables, which is well suited for the study of plant-wide control according to Fig. 4.3

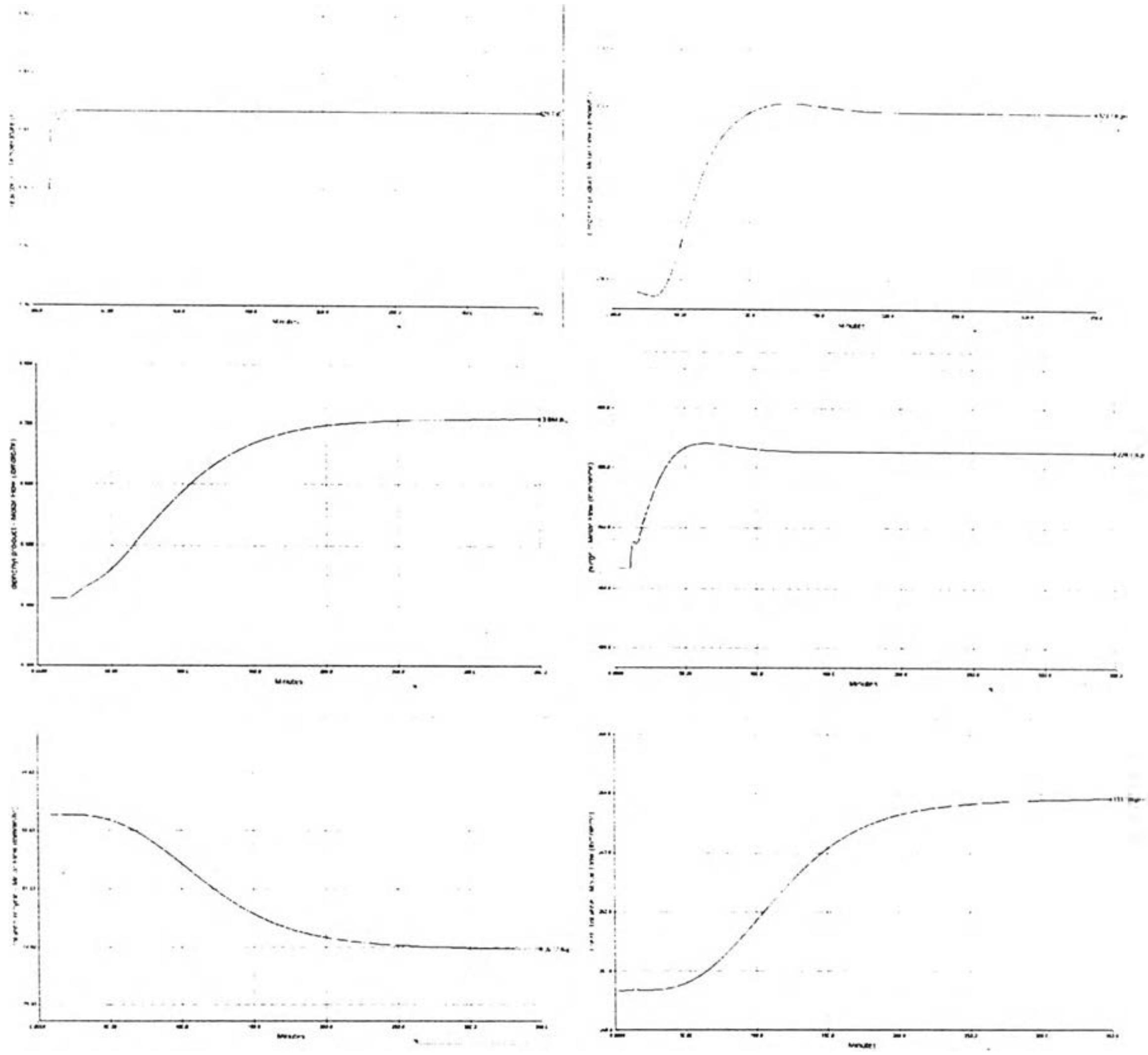

Figure 4.4 Responses of process variable to a step change in Reactor Inlet Temp. from 1150 to 1151 °F

To study the plant-wide control problem, transient responses from open loop tests on the process are often required. However, we faced some difficulties to obtain these from the model developed in HYSYS.PLANT. To get proper transient responses, it is required to close the condenser levels in columns. Thus, the model is only suitable for studying the plant-wide control problem after these level loops are closed.

The flowsheet of HDA process in Fig. 4.1 indicates that this process could be separated into two parts:

1. The reaction part contains reactor, separator, FEHE and gas recycle, etc.
2. The separation part includes the three distillation columns.

The separation part affects the reaction part only by the nearly pure toluene recycle stream. The reduced model effectively assumes that the distillation part is under good control. It is meaningful to study plant-wide control based on this reduced model because (1) distillation columns serve only as separating units, and hence the difficulties for plant-wide control such as manipulation of product rates and handling recycle streams and heat integration are not often present in the separation part, and (2) the control loops of distillation columns are usually built within the unit operation, and the control of distillation columns has been widely studied. Very little toluene leaves the distillation system in methane, benzene and diphenyl product streams (Fig. 4.1). Almost all of the toluene entering this part recycles back to the reaction part, and purity of Tol-Recycle stream is high (99.94%). This approximation, however, will not provide results on the effect of disturbances and control strategies on benzene product purity, recycle composition and toluene inventory.

4.2 Control Objective

The control system that we design must meet certain control objectives within the prescribed operational constraints.

For the HDA process, several control objectives and constraints accord to Luyben (1998). These include: achieving a specified production rate of essentially pure benzene while minimizing yield losses of hydrogen and diphenyl; achieving a ratio of hydrogen to aromatics greater than 5:1 in the reactor feed; and quenching reactor effluent to a temperature of 1150 ^{o}F to prevent coking. Besides these, the control system should be able to handle several disturbances such as set point changes for the base case and load disturbances.

For this study, we consider only the reaction part in according to the prior reason presented. And as we apply the method to compare between the reference control structure designed by Luyben (1998) with the two control structures purposed by Kietawarin (2003). Thus each control structure has 7 loop. For reference control structure designed by Luyben the manipulated variables and control variables are listed in Table 4.3; see also Fig 4.5 .For the first alternative control structure, the manipulated variables and control variables are listed in Table 4.4; see also Fig 4.6 and the manipulated variables and control variables of the second one are listed in Table 4.5; see also Fig 4.7

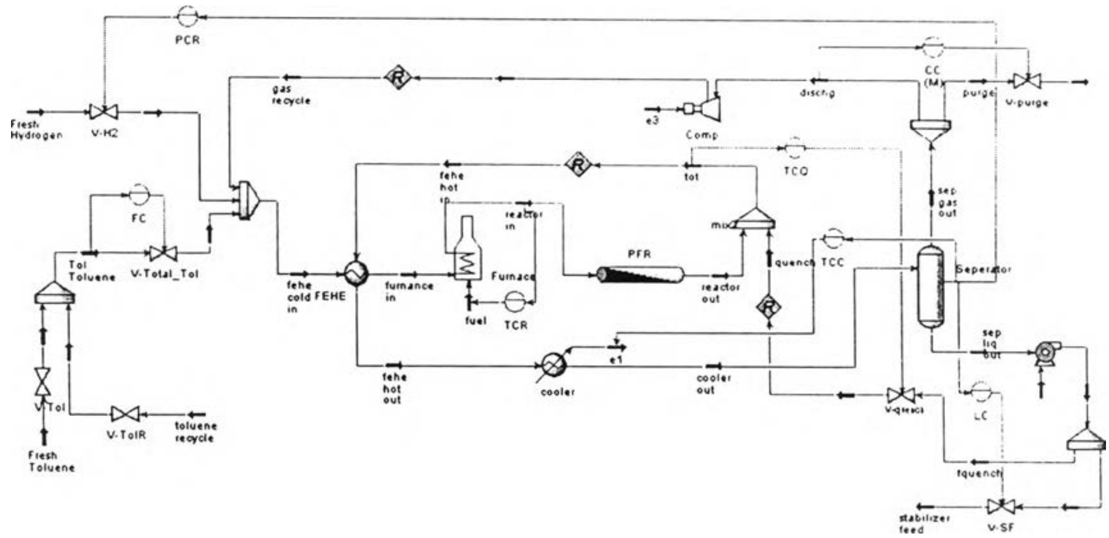

Figure 4.5 Flowsheet of the HDA process with the 7x7 reference control structure

Table 4.3 Manipulated and process variables for reference control structure of the HDA process

Manipulated variables		Process variables	
Symbol	Variable name	Symbol	Variable name
u_1	Fresh feed H2	y_1	Sep. Pressure
u_2	Tol-Total flow rate	y_2	Tol-Total flow rate
u_3	Q_{fuel}	y_3	Reactor inlet temperature
u_4	Quench flow	y_4	FEHE Hot-in Temp.
u_5	Qcooling	y_5	Sep. Temp.
u_6	Stabilizer feed flow	y_6	Separator level
u_7	Purge flow	y_7	Methane in purge

The reference control structure used the total flow of toluene to control the flow rate to reactor (recycle plus fresh). That is difference with the others, the first control structure is applied from the reference control structure as the first one is to measure the toluene flow rate in the process in order to adjust the fresh toluene feed flow rate.

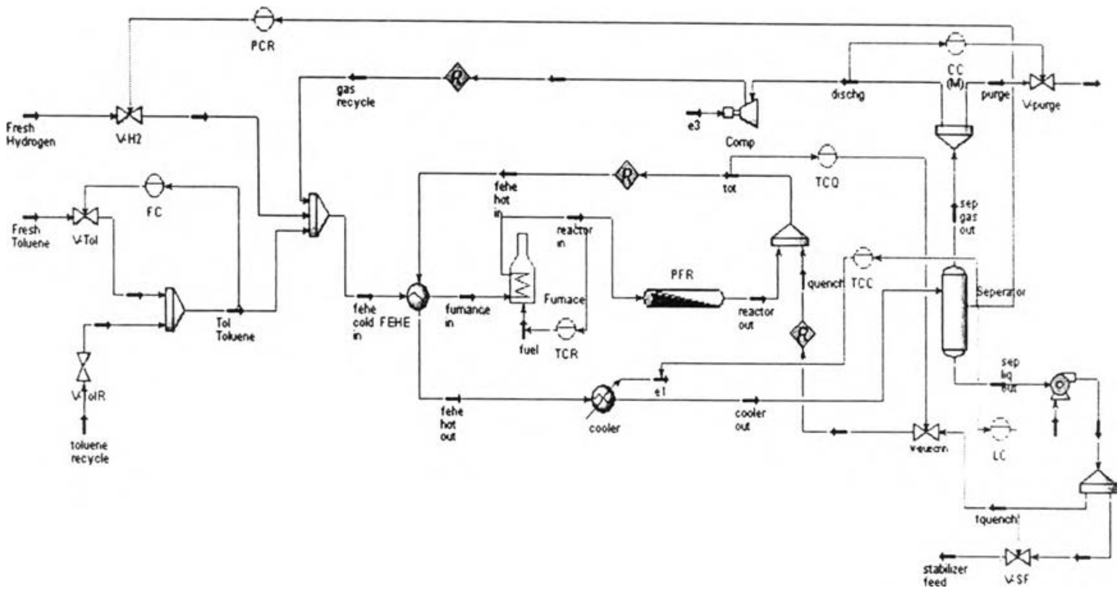

Figure 4.6 Flowsheet of the HDA process with the 7x7 control structure1

Table 4.4 Manipulated and process variables for control structure1 of the HDA process

Manipulated variables		Process variables	
Symbol	Variable name	Symbol	Variable name
u_1	Fresh feed H2	y_1	Sep. Pressure
u_2	Fresh feed Toluene	y_2	Tol-Total flow rate
u_3	Q_{fuel}	y_3	Reactor inlet temperature
u_4	Quench flow	y_4	FEHE Hot-in Temp.
u_5	Qcooling	y_5	Sep. Temp.
u_6	Stabilizer feed flow	y_6	Separator level
u_7	Purge flow	y_7	Methane in purge

The first alternative control structure, quench stream is used to control temperature of the outlet from the reactor. For the second alternative control structure differs from the reference structure and the first one as cooling unit is added to control the outlet temperature from reactor, instead of using internal process flow. Hence there are two differences between the three control structures Those are u_2 in the reference control; total toluene flow with u_2 in the two control structures and u_4 in the reference structure and first control structure; Quench flow with u_4 in the second one; Qcooling2.

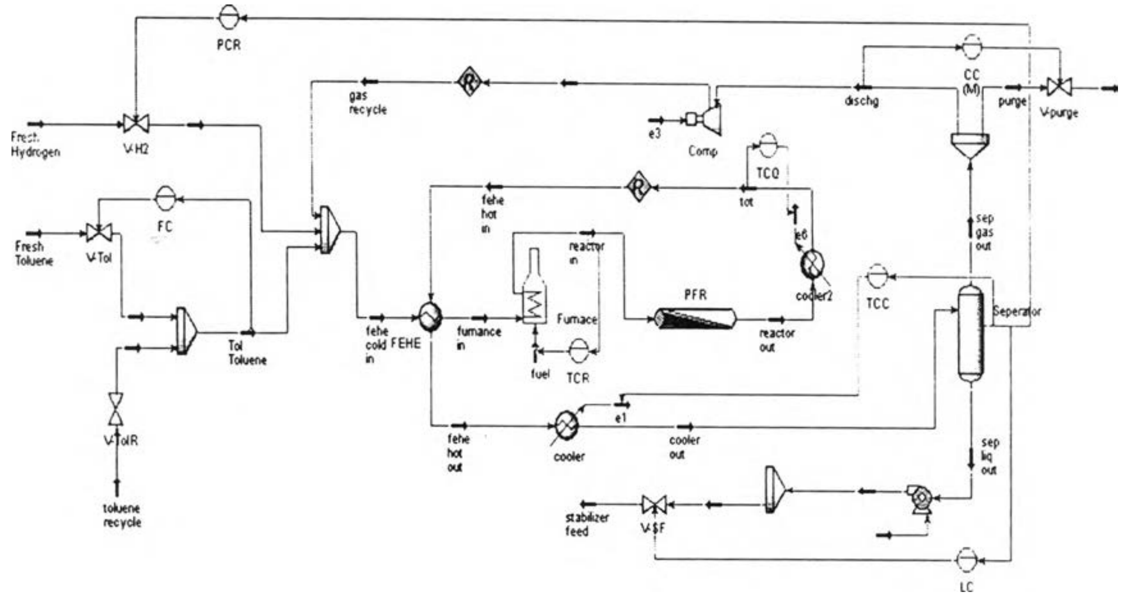

Figure 4.7 Flowsheet of the HDA process with the 7x7 control structure2

Table 4.5 Manipulated and process variables for control structure2 of the HDA process..

Manipulated variables		Process variables	
Symbol	Variable name	Symbol	Variable name
u_1	Fresh feed H2	y_1	Sep. Pressure
u_2	Fresh feed Toluene	y_2	Tol-Total flow rate
u_3	Q_{fuel}	y_3	Reactor inlet temperature
u_4	Qcooling2	y_4	FEHE Hot-in Temp.
u_5	Qcooling	y_5	Sep. Temp.
u_6	Stabilizer feed flow	y_6	Separator level
u_7	Purge flow	y_7	Methane in purge

A major disturbances are typical load disturbances which represent fluctuations in fresh feed streams by environmental conditions or other factors. A first disturbance is Temperature of Fresh feed toluene (T_{FFtol}), simulated here by a step variation . A maximum disturbance of 20 ^{o}F is considered. A second significant disturbance is P_{FFH2}, Pressure of Fresh feed H_2. A maximum disturbance of 20 psi is considered by a step variation.

4.3 Steady-State Controllability Analysis

From extensive steady-state simulations a scaled gain matrix G is generated according to the relation y = Gu, where y are the scaled plantwide control variables and u are the scaled manipulated variables. With the scaled disturbances d, a scaled disturbance gain matrix G_d is generated, according to the relation y = G_dd. The introduction of scaled variables allows reformulation of in section 3.2.5.

4.3.1 Static Gains

Table 4.7 and Table 4.8 show the scaled static gains for the control structure1 and the control structure2, respectively. The output, Sep. Level, has been influenced on all of the manipulated variables both of the two control structures. However, a one-by-one investigation is not able to quantify the effects of interactions. Therefore, it is necessary to perform a RGA analysis.

Table 4.6 Static gain matrix for reference control structure.

	u_1	u_2	u_3	u_4	u_5	u_6	u_7	T_{Tol}	P_{H2}
y_1	-0.900	-0.265	0.876	0.463	-0.887	-0.748	-0.845	0.154	0.592
y_2	1.296	0.737	-1.053	-0.421	1.000	0.749	1.557	-0.340	-0.921
y_3	-0.428	-0.383	0.660	0.411	-0.673	-0.610	-0.483	0.026	0.063
y_4	-0.452	-0.414	0.672	0.431	-0.683	-0.638	-0.524	0.025	0.059
y_5	-0.604	0.289	0.774	0.464	-0.802	-0.719	-0.918	0.089	0.063
y_6	3.953	1.554	-1.492	0.384	1.492	1.388	11.166	-0.991	-0.992
y_7	-0.820	-0.666	0.888	0.520	-0.860	-0.872	-1.374	0.145	-0.020

Table 4.7 Static gain matrix for alternative control structure1.

	u_1	u_2	u_3	u_4	u_5	u_6	u_7	T_{Tol}	P_{H2}
y_1	-0.922	-0.597	0.917	0.703	-0.931	-1.315	-0.906	0.073	0.270
y_2	1.227	0.985	-1.017	-0.641	0.966	1.188	1.429	-0.343	-0.902
y_3	-0.431	-0.409	0.671	0.559	-0.681	-1.052	-0.579	0.027	0.065
y_4	-0.427	-0.400	0.640	0.552	-0.648	-1.032	-0.689	0.024	0.058
y_5	-0.593	-0.495	0.772	0.650	-0.801	-1.214	-0.976	0.088	0.053
y_6	3.697	1.644	-1.495	-0.366	1.495	2.227	8.999	-0.994	-0.996
y_7	-0.804	-0.648	0.886	0.763	-0.860	-1.466	-1.389	0.145	-0.033

Table 4.8 Static gain matrix for alternative control structure2.

	u_1	u_2	u_3	u_4	u_5	u_6	u_7	T_{Tol}	P_{H2}
y_1	-0.598	-0.210	0.781	0.167	-0.794	-0.821	-0.673	0.167	0.535
y_2	0.957	0.749	-1.071	0.005	1.003	0.970	1.342	-0.433	-0.934
y_3	-0.505	-0.498	0.720	0.379	-0.704	-0.943	-0.538	0.040	0.085
y_4	-0.496	-0.498	0.699	0.377	-0.686	-0.925	-0.531	0.035	0.076
y_5	-0.477	-0.029	0.699	0.263	-0.725	-0.826	-0.606	0.094	0.038
y_6	1.758	0.996	-1.494	0.248	1.494	1.558	3.584	-0.993	-0.995
y_7	-0.739	-0.685	0.915	0.297	-0.882	-1.122	-1.066	0.205	-0.044

4.3.2 RGA Analysis

The RGA is a measure of the main effect of u_1 on y_1 compared to the total effect including the effect it provokes from the other controller, since it cannot control y_1 without upsetting of the other of the controlled variables. Thus RGA provides a measure of the extent of interaction in using u_1 to control y_1 while the other controlled variables be controlled by each manipulated variables.

$$\lambda = \frac{\text{main effect}}{\text{main effect + interaction effect}} = \frac{\text{main effect}}{\text{total effect}}$$

If RGA closes to 1, it indicates that loop i will *not* be subject to interaction effect from other control loops when they are closed, therefore u_j can control y_i without interference from the other control loops.

If RGA exceeds 1, it indicates that the interaction effects from the other loops acts in *opposition* to the main effect of u_j on y_i , but the main effect is still dominant. For large values, it indicates that the total effect is so low values, because the main effect close to the interaction effect. So that makes the closed-loop control of y_1 by u_1 will be very difficult to achieve.

If RGA is lower than 0, it indicates that the interaction effects are not only opposite in sign to the main effect, but are larger in the main effect. So the pairing in this case is not very desirable because the interaction effects of the other loop have effect to the controlled variable more than the main effect.

Table 4.9 to Table 4.11 present the RGA number of the reference control structure, the control structure1 and the control structure2, respectively.

Table 4.9 Steady-state RGA for reference control structure.

	u_1	u_2	u_3	u_4	u_5	u_6	u_7
	FFH_2	**Ftot-tol**	Q_{fuel}	F_{quench}	$Q_{cooling}$	$F_{stabilizer\text{-}feed}$	F_{purge}
Sep. Pressure	**2.348**	-0.227	4.599	-10.064	-7.252	14.629	-3.033
Tol-Total flow rate	0.663	**0.414**	-4.386	5.996	5.902	-10.232	2.642
Reactor Inlet Temp	-10.197	-2.248	**105.610**	-64.824	-78.278	57.579	-6.636
Hot-in Temp.	10.264	3.667	-133.840	**78.415**	108.240	-74.630	8.884
Sep. Temp.	-0.287	0.264	-1.712	4.901	**2.287**	-5.916	1.463
Separator level	0.057	0.133	-2.776	-0.088	2.731	**-0.447**	1.390
Methane in purge	-1.849	-1.001	33.513	-13.335	-32.633	20.017	**-3.711**

For the reference control structure, there are two loops in high RGA, which are Reactor Inlet Temp.-Q_{fuel} and Hot-in Temp.- F_{quench} . Because the temperature control has more effect to system. When these loops are closed, they will effect to the other control loops . Then the manipulated variable of the other loop will change each controlled variable to setpoint. So the interaction effect from the other loop will be back to both of temperature control loops. But the interaction effects are lower than the main effect so close-loop can be control. For two loops in negative RGA of the reference control structure, which are Separator level - $F_{stabilizer\text{-}feed}$ and Methane in purge - F_{purge}. Because these loops are long loop, the manipulated variable is far away the controlled variable. So when these loops are closed, the interaction effects from the other loop will be back to these control loops, which the interaction effects are more than the main effect.

Table 4.10 Steady-state RGA for alternative control structure1.

	u_1 FFH$_2$	u_2 **FFTol**	u_3 Q_{fuel}	u_4 F_{quench}	u_5 $Q_{cooling}$	u_6 $F_{stabilizer\text{-}feed}$	u_7 F_{purge}
Sep. Pressure	**2.421**	-8.414	27.555	6.085	-15.897	-11.849	1.100
Tol-Total flow rate	-1.409	**0.138**	8.074	1.267	-3.570	-4.295	0.794
Reactor Inlet Temp	2.832	29.532	**133.780**	-44.293	74.893	81.692	-9.879
Hot-in Temp.	-8.521	-52.042	254.400	**55.133**	-140.690	-126.870	19.582
Sep. Temp.	2.368	18.672	-101.870	-7.760	**65.081**	30.150	-5.639
Separator level	-0.582	-1.357	3.545	-0.211	-1.584	**-0.539**	1.727
Methane in purge	3.892	14.469	-56.929	-9.222	22.766	32.709	**-6.685**

For RGA of the control structure1, is showed by Table 4.10. The result of the control structure1 is similar to the result of the reference control structure. there are two loops in high RGA, which are Reactor Inlet Temp.-Q_{fuel} and Hot-in Temp.-F_{quench}. And two loops in negative RGA , which are Separator level - $F_{stabilizer\text{-}feed}$ and Methane in purge - F_{purge}.

Table 4.11 Steady-state RGA for alternative control structure2.

	u_1 FFH$_2$	u_2 **FFTol**	u_3 Q_{fuel}	u_4 $\mathbf{Q_{cooling2}}$	u_5 $Q_{cooling}$	u_6 $F_{stabilizer\text{-}feed}$	u_7 F_{purge}
Sep. Pressure	**2.85**	0.14	-21.32	-4.08	9.95	18.89	-5.42
Tol-Total flow rate	-2.04	**0.68**	12.78	-0.06	0.46	-15.42	4.60
Reactor Iinlet Temp	191.59	-60.60	**246.88**	-20.86	-508.18	200.96	-48.80
FEHE Hot-in Temp.	-139.96	48.44	-194.20	**28.49**	400.79	-182.14	39.58
Sep. Temp.	-11.63	0.10	3.27	4.64	**18.81**	-20.32	6.13
Separator level	29.32	-4.47	13.63	-0.20	-35.53	**8.66**	-10.40
Methane in purge	-69.13	16.72	-60.04	-6.92	114.70	-9.63	**15.31**

For RGA of the control structure2, is showed by Table 4.11. There is a loop in high RGA, which is Reactor Inlet Temp.-Q_{fuel}. The result of loop of Hot-in Temp.-F_{quench} isn't high RGA, because there is the added utility, which is Cooling2 in this control structure. So that eliminate propagation of heat to the others loop. And there isn't the nagative RGA. So the use of control structure2 seems to give the better alternative control structure from a steady-state point of view. However, a dynamic controllability analysis is needed.

4.4 Dynamic Simulation

Prior to constructing a dynamic flowsheet, model decisions have to be made regarding the flowsheet elements whose dynamics have to be taken into account Table 4.2. Dynamic simulations with step perturbations on the manipulated variables and disturbances show interesting response. All controlled variables will finally reach steady state values, but at different time.

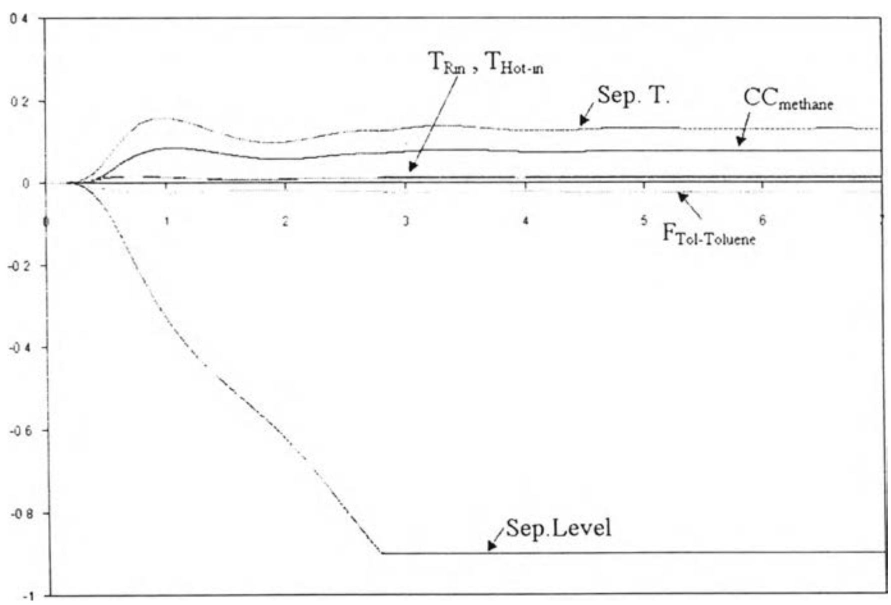

Figure 4.8 a) Dynamic response of the controlled variables after a step change in flow of FF_{H2}. for reference control structure.

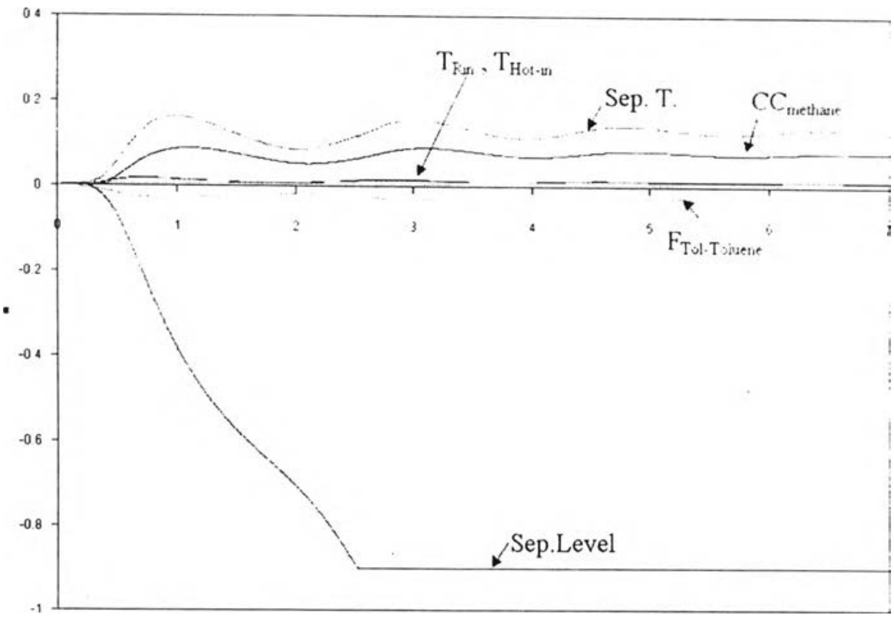

Figure 4.8 b) Dynamic response of the controlled variables after a step change in flow of FF_{H2}. for alternative control structure 1,

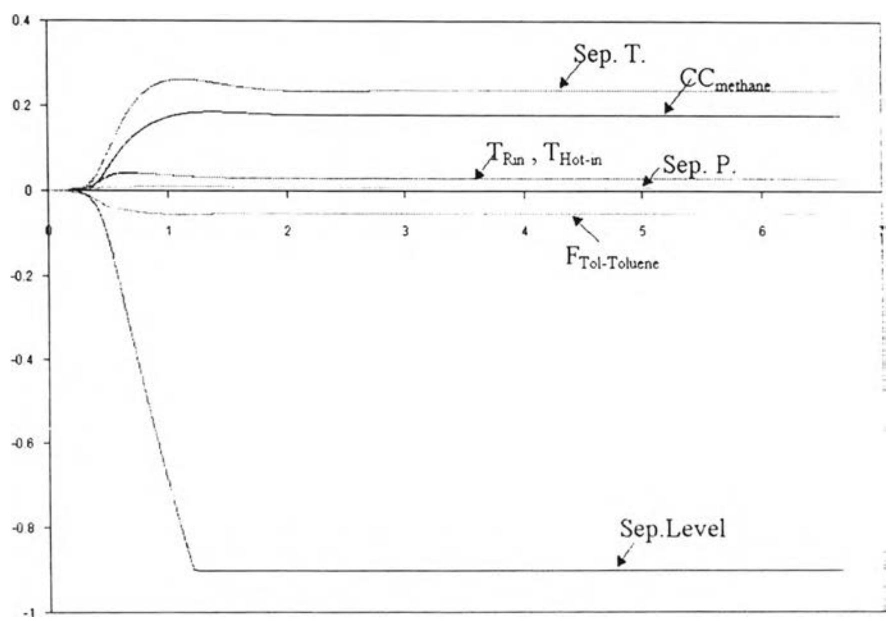

Figure 4.8 c) Dynamic response of the controlled variables after a step change in flow of FF_{H2} for alternative control structure 2.

For step increasing the FF_{H2} flow rate, (Fig 4.8 a, b and c) the effect of interactions on this loop is temperature of cold-in stream increasing. Since the increase in temperature increases reaction rates and diminishes toluene remaining while on the other hand methane concentration is being built up. So there is gas recycled into the system more than a nominal value. When flow rate of FFH2 is increased as well as pressure of the system increase. As a result of the response of three control structures, the alternative control structure 1 has response most oscillate and takes a long time into a new steady-state than the reference structure and the alternative control structure 2.

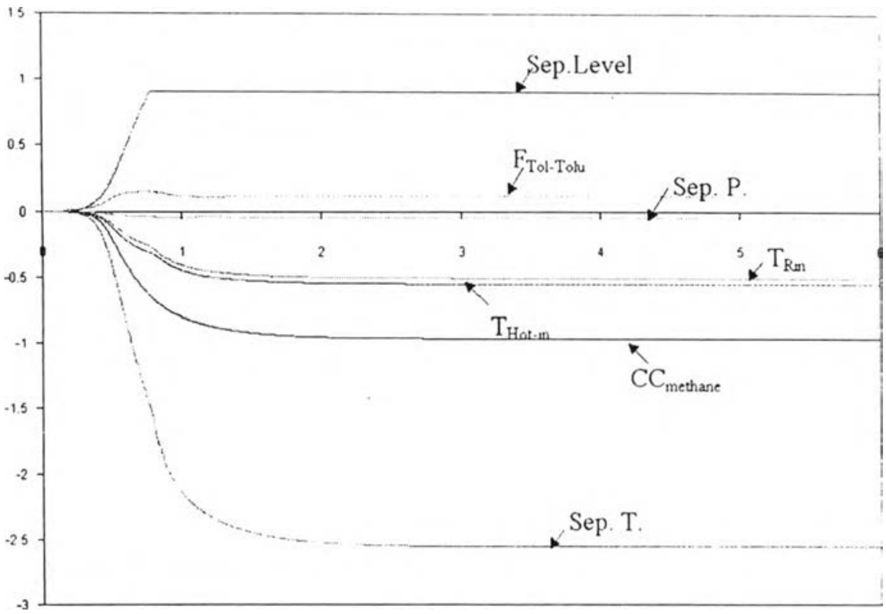

Figure 4.9 a) Dynamic response of the controlled variables after a step change in flow of FF_{tol}. for reference control structure.

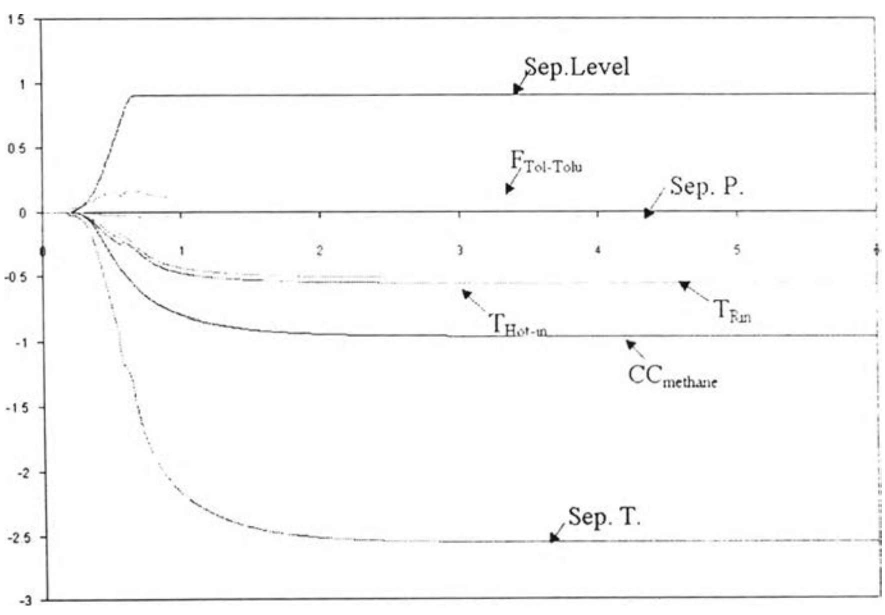

Figure 4.9 b) Dynamic response of the controlled variables after a step change in flow of FF_{tol}. for alternative control structure 1

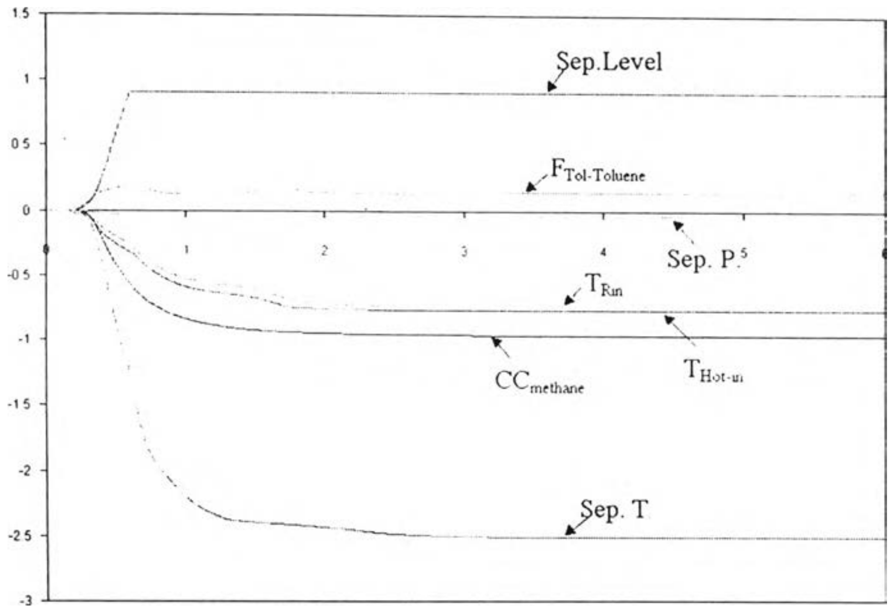

Figure 4.9 c) Dynamic response of the controlled variables after a step change in flow of FF_{tol}. for alternative control structure 2

Fig 4.9 a), b) and c) show the result of step flow rate of FFtol stream which effect on the total flow of toluene increased. The temperature of stream after mixed with other reactants is reduced. However, there is an increase of reaction rate. Because toluene is limiting reactant that make benzene increase The level of liquid in separator go up because of liquid increased into the system, but concentration of methane go down. From the comparison between the three control structures, each pairing responses are happened in the same direction and become to new steady state within the same time.

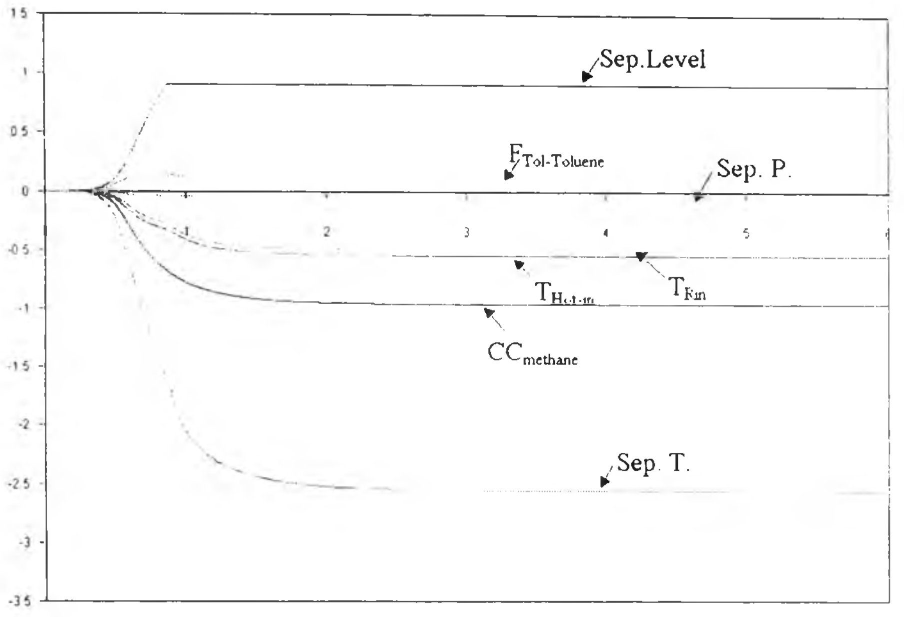

Figure 4.10 a) Dynamic response of the controlled variables after a step change in flow of Fquench. for reference control structure.

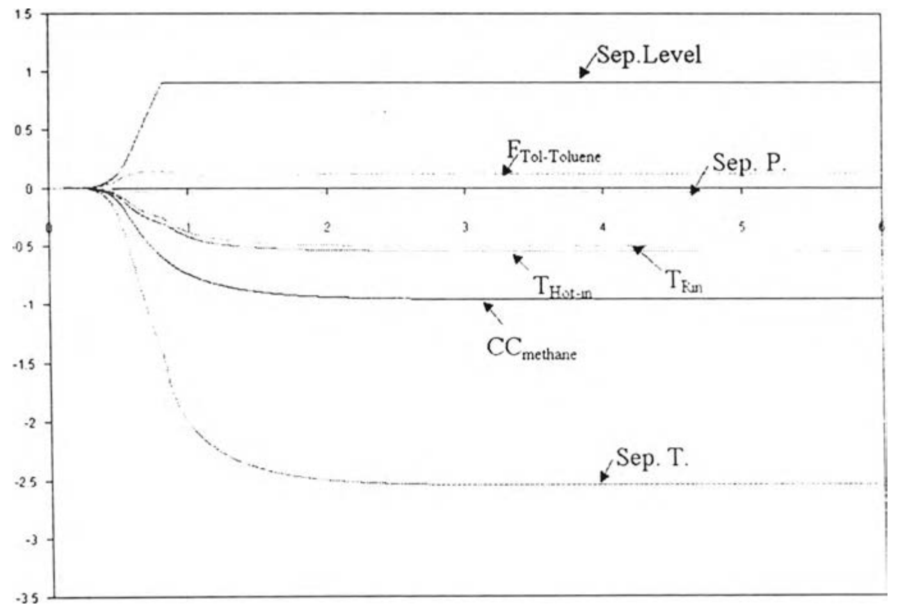

Figure 4.10 b) Dynamic response of the controlled variables after a step change in flow of Fquench. for alternative control structure 1,

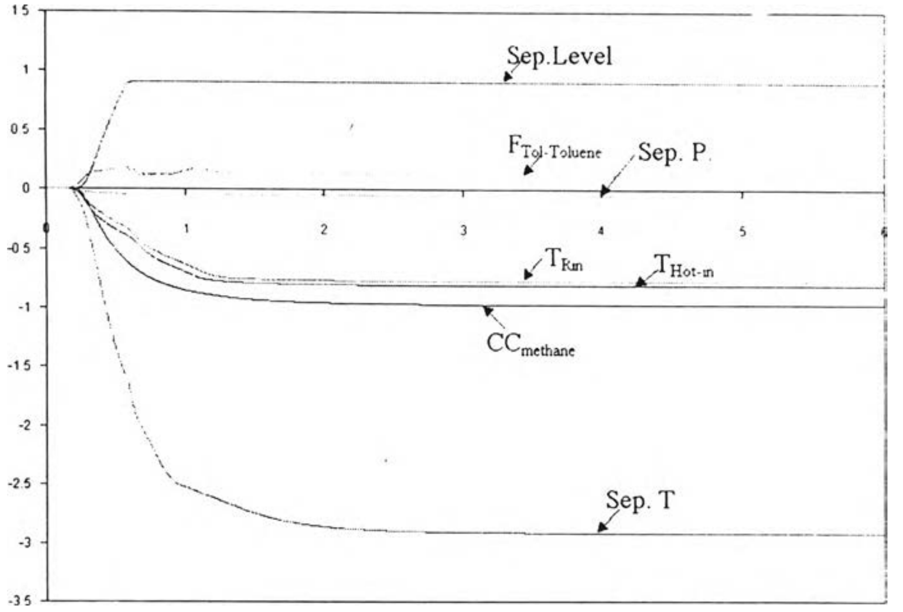

Figure 4.10 c) Dynamic response of the controlled variables after a step change in duty of cooling2 for alternative control structure 2.

For the reference structure and the control structure1, when flow rate of quench stream is changed step increase, the liquid that mix with stream will increase to come into heat exchanger. That has effect on stream's temperature was reduced and Reactor inlet stream's temperature was reduced as well. The reaction rate is reduced that make the concentration of methane reduced as Fig 4.10 a) and b) The result of control structure 2 happen like the first control structure except the change of duty of cooling 2 which make the response of other controlled variable is faster and stronger than the first one as Figure 10 c).

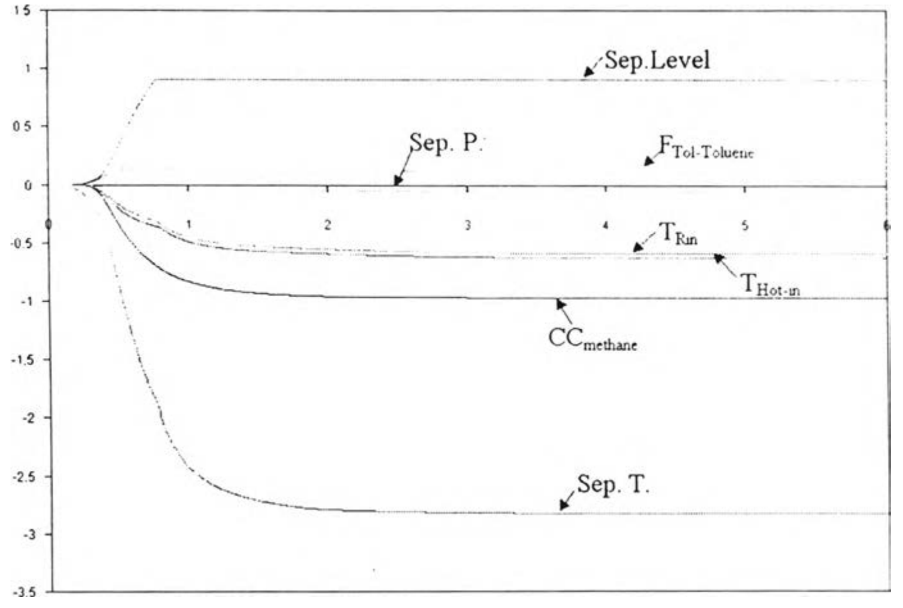

Figure 4.11 a) Dynamic response of the controlled variables after a step change in duty of cooling1 for reference control structure 1,

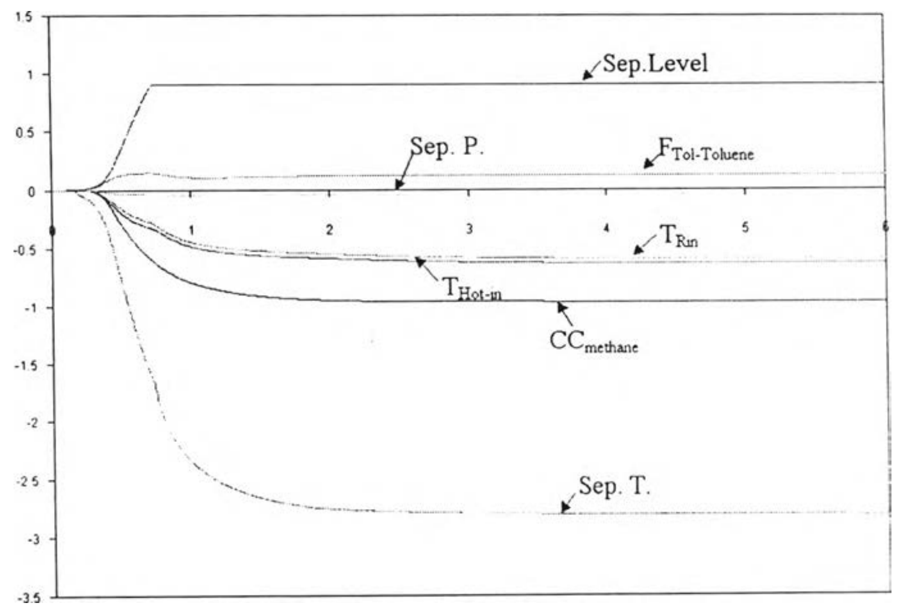

Figure 4.11 b) Dynamic response of the controlled variables after a step change in duty of cooling1 for alternative control structure 1,

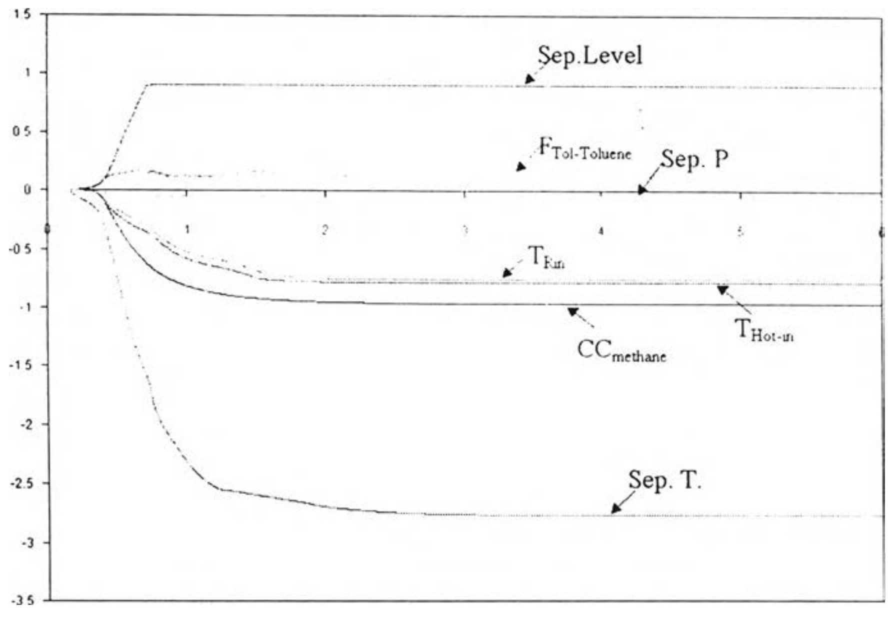

Figure 4.11 c) Dynamic response of the controlled variables after a step change in duty of cooling1 for alternative control structure 2.

While manipulated the duty of cooling1 increases, it effect on the separator temperature decreased. Therefore the streams which leave the separator have a decrease in temperature. The streams are the gas recycle stream and the sep. liq. outlet stream. So that while temperature of the gas recycle stream decreases, and it was brought to mix with FF_{H2} and Total-toluene stream. The temperature of stream after mixed with other streams is reduced .The reaction rate go down that make the concentration of methane decrease too. In the reference structure and the alternative control structure1, some of the liquid stream which leave the separator is mixed with the Hot-in stream. That is the quench stream which effect on temperature of reactor-inlet stream and temperature of hot-in stream. They are adjusted into the new steady-state slower than in alternative control structure2. Because T_{Rin} and $T_{hot\text{-}in}$ are influenced from the gas recycle stream and the sep. liq. outlet stream in control structure1. Figure 4.11 a), b) and c) show that.

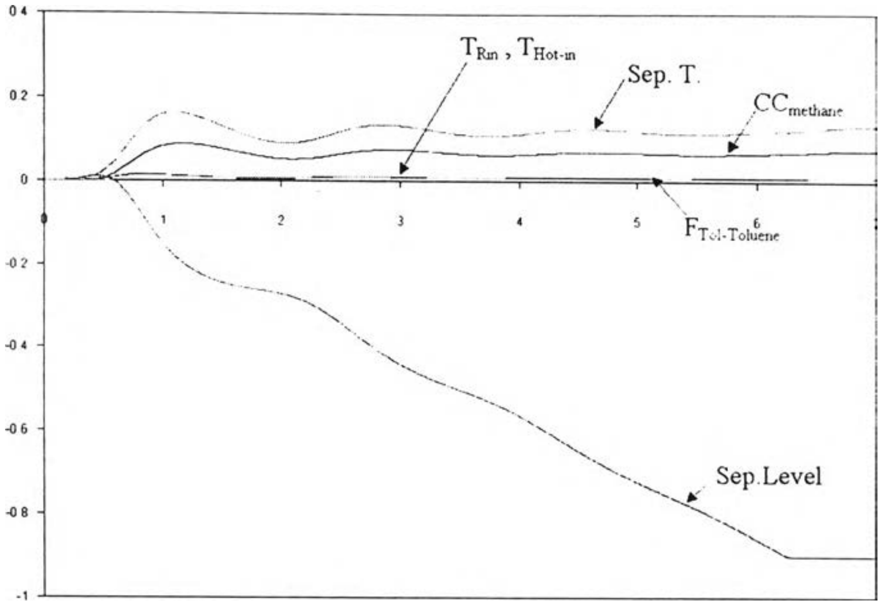

Figure 4.12 a) Dynamic response of the controlled variables after a step change in flow of purge stream for reference control structure.

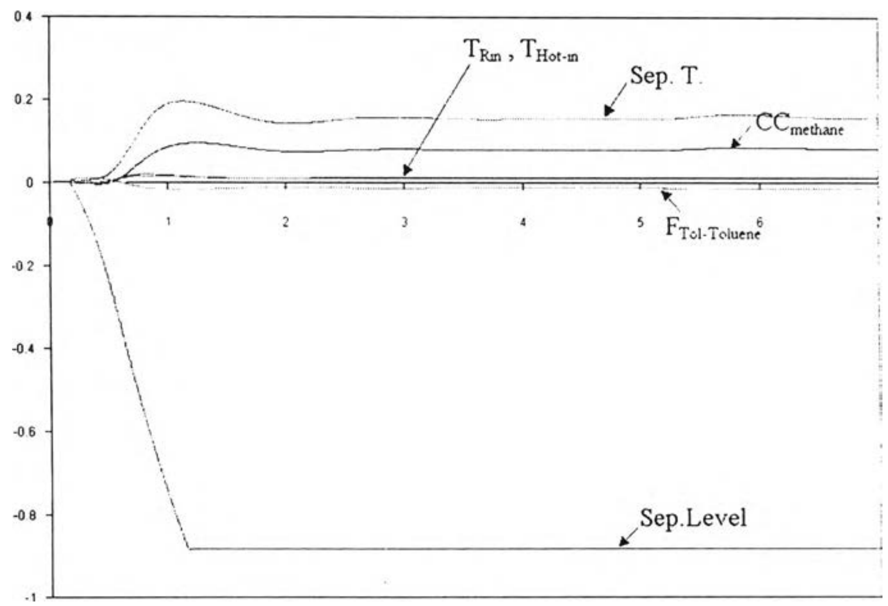

Figure 4.12 b) Dynamic response of the controlled variables after a step change in flow of purge stream for alternative control structure 1,

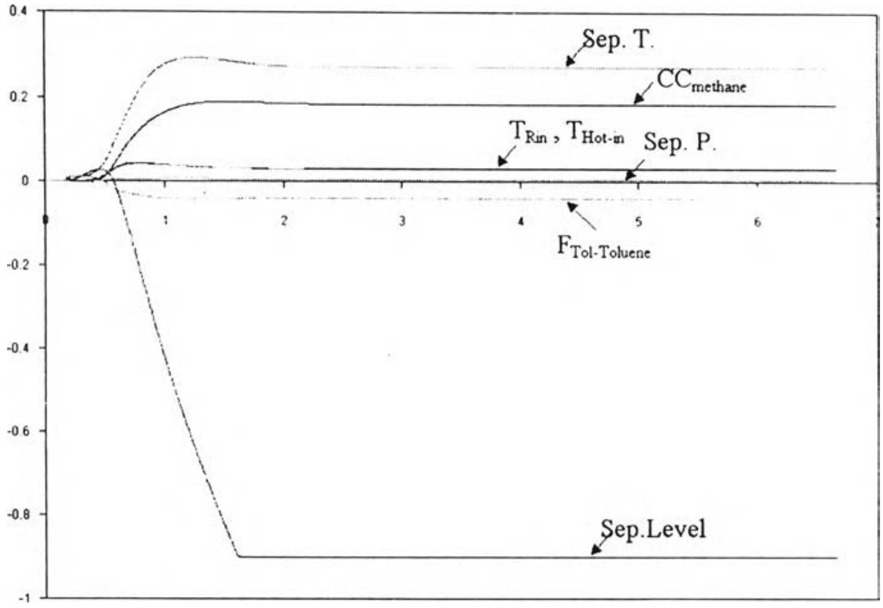

Figure 4.12 c) Dynamic response of the controlled variables after a step change in flow of purge stream for alternative control structure 2

Figure 4.12 a), b) and c) show the responses of increasing step change of purge flow rate. If the flow rate of purge increases, the gas recycle flow rate decreases. Which a decrease in flow rate effects on T_{Rin} and $T_{hot\text{-}in}$ increased. Because the temperature of gas recycle is more than the temperature of stream after mixed with others reactants. When temperature of reactor-inlet stream is increased that it make the reaction rate raised. Therefore toluene are used an increase. the volume of toluene remaining in the system goes down. The level of liquid in separator fall. In the reference structure and the alternative control structure1, a decrease in the liquid in separator that effect on the flow rate of quench stream decreased. The recycle make the response of alternative control structure2 became into the new steady-state fastest.

From the result can conclude that if there is a increased manipulated variable that makes temperature of reactor feed stream increase, the response of reference control structure and control structure1 have more oscillate and become into the new steady-state slower than the control structure2. However ,if a increased manipulated variable that makes temperature of reactor feed stream increase, the responses of three control structures are similar and become into the new steady-state in the same time.

4.5 Dynamic Controllability Analysis

A controllability analysis as a function of frequency was performed. In dynamic mode the transfer function could be identified through an open loop test by changed step input. First order plus dead time transfer function is used to model this response. Alternatively, transfer functions were generated. The results are similar.

The steady-state analysis indicates good sensitivity of the controlled variables to inputs. Although there are some differences in open-loop behavior of the alternatives, these differences do not justify a net preference. The steady-state RGA analysis predicts that a alternative control structure1 should be more affected by interactions resulting from the manipulation of alternative2, but it cannot be evaluated only by the inspection of numerical values. Because a steady-state analysis cannot predict how the real disturbances would be handled by the control system, a deeper controllability analysis is necessary in the frequency domain. Consequently, graphical representations versus frequency enable the robustness of control in the face of a certain frequency range of disturbances to be evaluated. So the range of frequency [0.01,10] in this study follows Groenendijk et al[1,2]. Here, we give only representative results.

4.5.1 RGA number

The RGA number provides a quantitative measure of the interactions in a diagonal decentralized control structure. The lower the RGA number, the more preferred the control structure. A value close to 0 means quasi-independent SISO controllers. Note that good controllability can be obtained up the frequency where the RGA number does not exceed 1.

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[1] Groenendijk, A. J.; Dimain, A. C.; and Iedema, P. Systems approach for evaluating dynamics and plantwide control of complex plants. AIChE 46 (2000):133-145.

[2] Dimian, A. C. ; Groenendijk, A. J.; and Iedema, P. D. Recycle interaction effects on the control of impurities in a complex plant. Ind. Eng. Chem. Res. 40 (2001): 5784-5794.

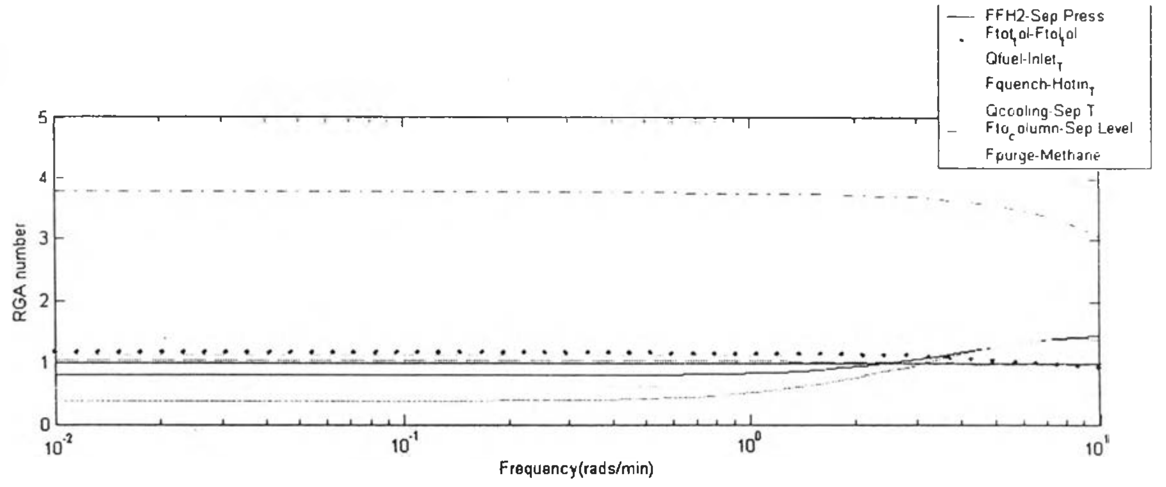

Figure 4.13 RGA number versus frequency for reference control structure

The RGA number of the reference control structure shows as figure 4.13. The loop of $F_{to\text{-}column}$-Sep.Level will be exceed 1, but it can keep stability at low frequencies. Figure 4.14 shows the evaluation of all pairing of alternative control structure1. All show quasi-constant low values at lower frequencies, up to 2 rad/min. There are four loops that have the RGA number exceed 1; FF_{tol}-$F_{tot\text{-}toluene}$, Q_{fuel}-$T_{reactor\text{-}inlet}$, F_{quench}-$T_{hot\text{-}in}$ and $F_{to\text{-}column}$-Sep.Level., but the value can be accepted. A increasing RGA number at higher frequencies indicates the degradation of controllability.

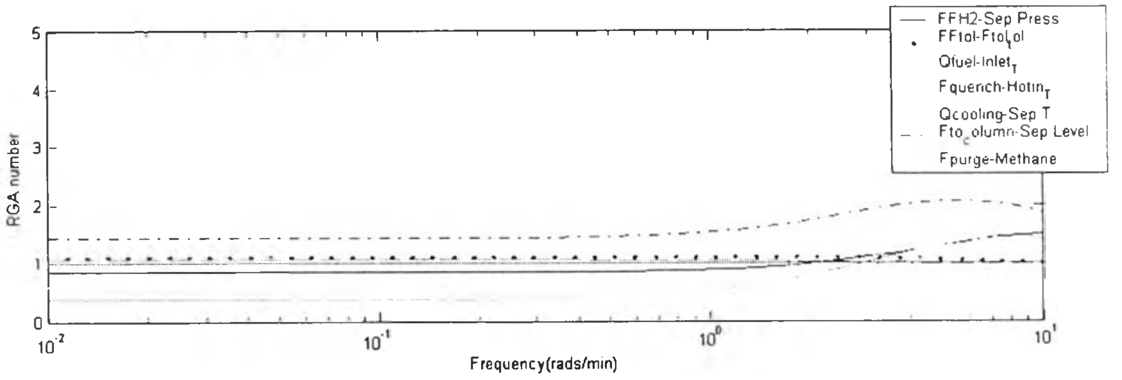

Figure 4.14 RGA number versus frequency for alternative control structure1.

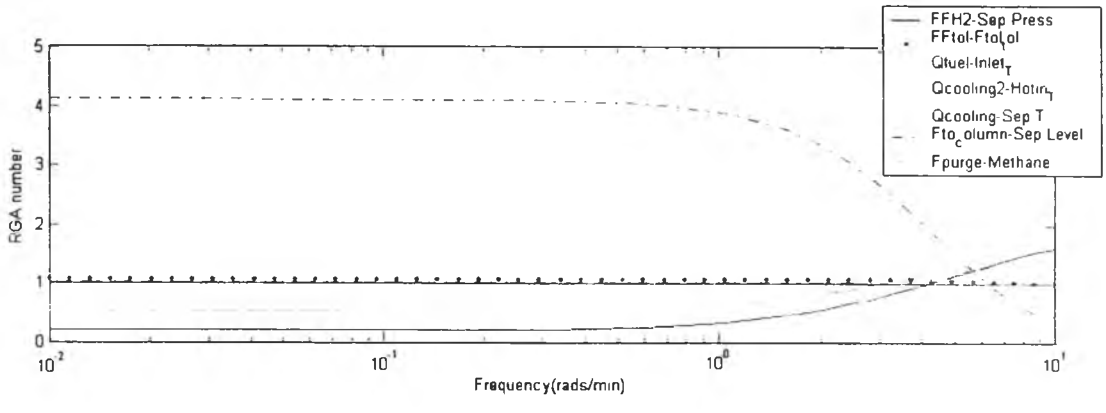

Figure 4.15 RGA number versus frequency for alternative control structure2.

If the loop of temperature of Hot-in stream is controlled by duty of cooling2, for alternative control structure2. Figure 4.15 presented the RGA number for all pairing of alternative control structure2. In the first place, the plot indicates that the alternative control structure2 is practically unaffected by interactions at low frequencies. Although the loop of $F_{to\text{-}column}$-Sep.Level will be exceed 1, but it can keep stability at low frequencies. And at higher frequencies, the RGA number of $F_{to\text{-}column}$-Sep.Level loop decrease, while The RGA number of the others loop will increase at 3 rad/min.

The loop of Sep.Level. has interaction between the different control loops for three control structures, in agreement with the steady-state analysis. So the dualistic RGA number of each pairing loop of three control structures are compared.

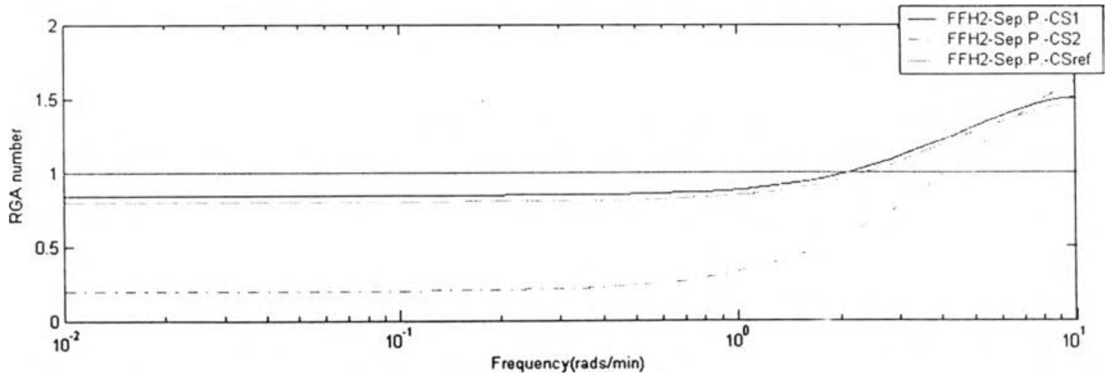

Figure 4.16 RGA number of FF_{H2}-Sep.Press. loop of three control structures.

For the Sep.Pressure loop (Figure 4.16), at low frequencies the RGA number for three control structures are lower the bound, the reference structure and the first alternative has the RGA number higher than the one. However at high frequencies three of them are increased which have a little difference.

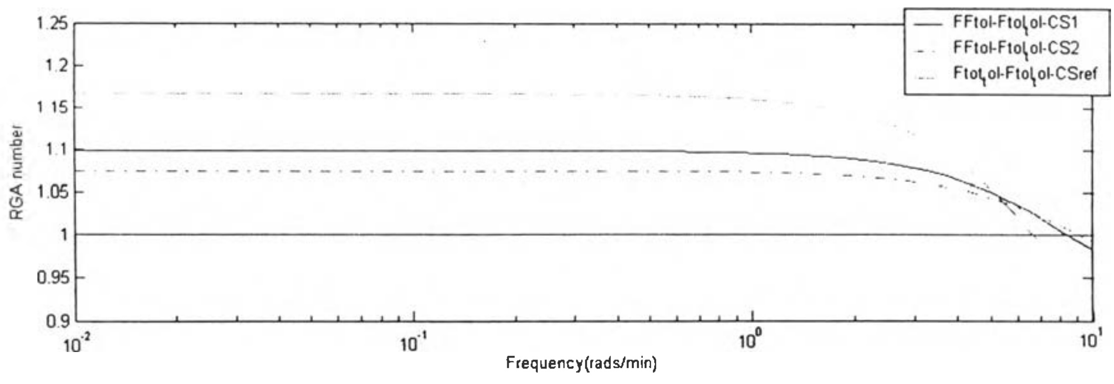

Figure 4.17 RGA number of $F_{tot-tol}$-$F_{tot-tol}$ for reference control structures and FF_{tol}-$F_{tot-tol}$. loop of two alternative control structures.

For the loop of flow of total toluene, they have RGA number higher than bound. By the reference control structure can be controlled more difficult than the both of alternative control structures. And the control structure2 has the lowest RGA number. Figure 4.17 shows this result.

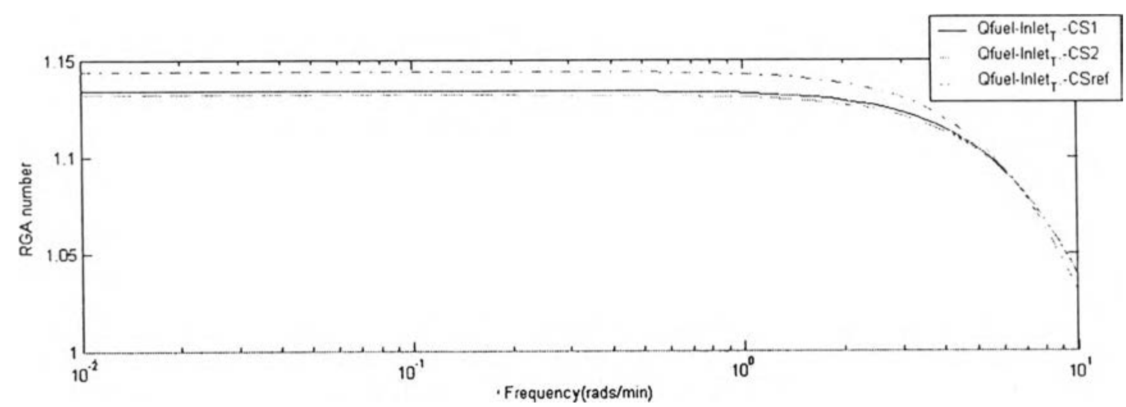

Figure 4.18 RGA number of Q_{fuel}-$T_{reactor-inlet}$ loop of three control structures.

Figure 4.18 shows the result of temperature loop of Reactor-inlet stream. Three of the results are similar. They have RGA number exceeding 1 a little bit at low frequencies. So the value can be accepted.

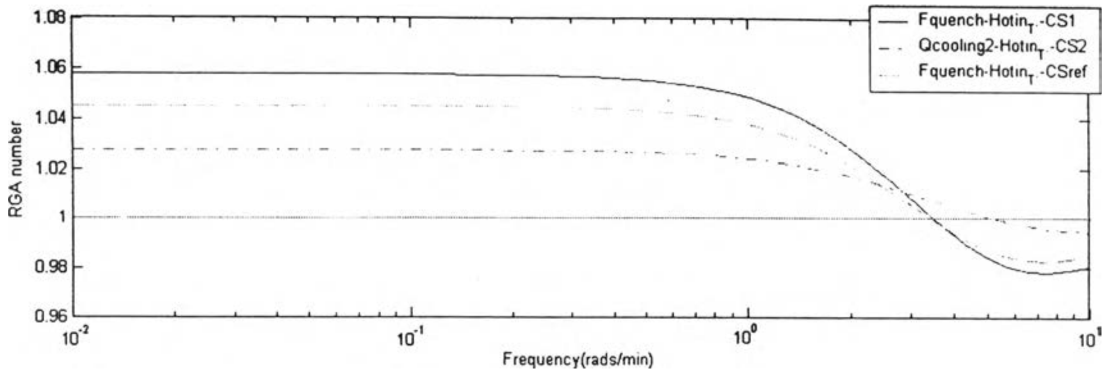

Figure 4.19 RGA number of F_{quench}-$T_{hot\text{-}in}$. loop for reference control structures and alternative control structures1, $Q_{cooling2}$-$T_{hot\text{-}in}$ loop for alternative control structure2

For the F_{quench}-$T_{hot\text{-}in}$. loop for the reference structure and the alternative control structures1 and $Q_{cooling2}$-$T_{hot\text{-}in}$ loop for alternative control structure2, the RGA number are presented by Figure 4.19. At low frequencies, the RGA number of the alternative control structure1 is the highest and the alternative control structure2 is the lowest. And they decrease lower than bound when frequency increase. Hence the control structure1 might be more difficult than the others.

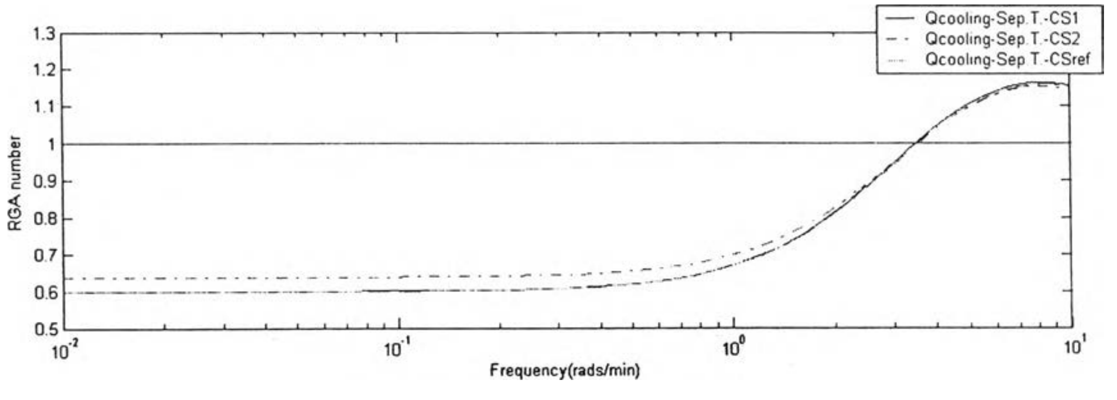

Figure 4.20 RGA number of Qcooling-Sep.Temp. loop of three control structures.

The results of RGA number for the Sep. Temp. loop are lower than 1 at low frequencies and increase at high frequencies. Three of the results are similar. They are presented by Figure 4.20.

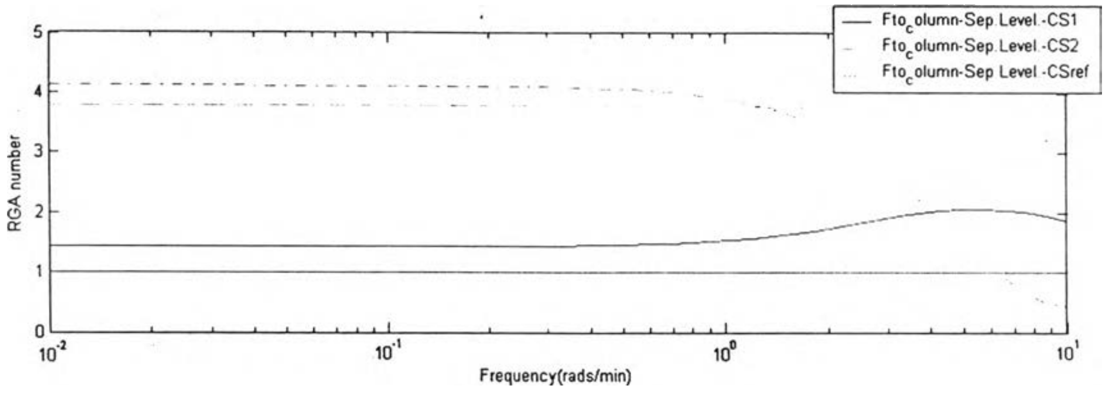

Figure 4.21 RGA number of $F_{Hto\text{-}column}$-Sep.Level. loop of three alternative control structures.

Figure 4.21 present the RGA number of $F_{Hto\text{-}column}$-Sep.Level. loop. The RGA number of this loop for three of the control structures have value exceed 1, but the value of the second control structure is the most at low frequencies and then it will decrease until lower than 1 at high frequencies. Therefore at low frequencies, this loop of the alternative control structure2 can be controlled most difficult but it can be controlled more easy than the others at high frequency.

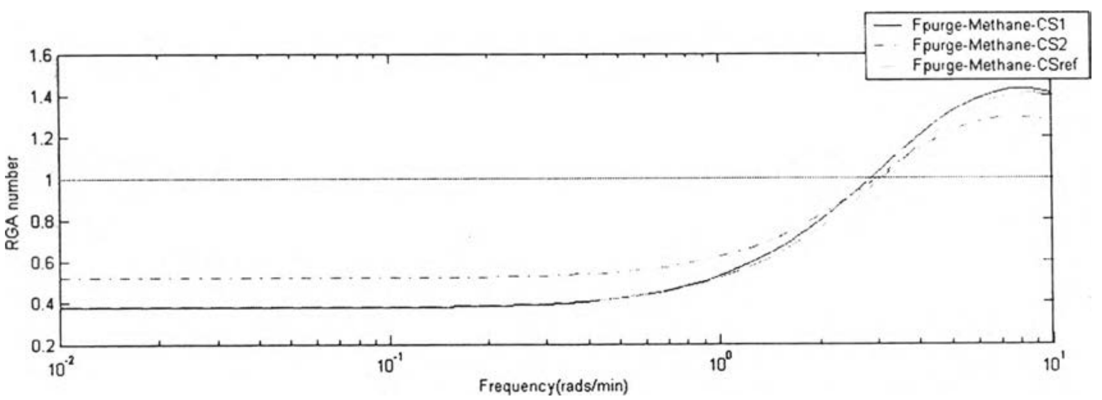

Figure 4.22 Dualistic RGA number of Fpurge-Methane in recycle gas. loop of two alternative control structures.

For the loop of methane concentration (Figure 4.22), at low frequencies the RGA number for three alternative control structures are lower the bound, the RGA number of the first alternative is similar to the reference structure which they are lower than the second alternative. However at high frequencies, three of them are increased which the reference structure and the first one increase more than the second one. So this loop of control structure2 might be controlled easier than the first one at high frequency.

4.5.2 Diagonal Controller Performance

Steady-state and dynamic RGA analyses have been used to study the interactions between control loops and to select the preferred input-output pairings. In this way two different control structures have been selected for the HDA process. Now the performance of these structures will be studied in terms of the controller errors. These should be kept between the scaled bounds [-1,1] under disturbances and reference changes.

An approximation of the controller errors *e* in terms of the disturbances *d* and the reference values *r* is given by

$$e = SG_d d - Sr \approx \bar{S}\,\bar{G}_d\, d - \bar{S}\,\Gamma r$$

where the sensitivity matrix S is decoupled and approximated by a product of two terms, $S \approx \bar{S}\Gamma$. The diagonal sensitivity matrix $\bar{S} = diag\{1/(1+k_i g_{ii})\}$, g_{ii} being the open-loop gain and k_i the controller gain, has only diagonal elements. This allows evaluation of the individual controllers independent from each other, which is convenient for tuning. The PRGA ($\Gamma = \bar{G}G^{-1}$, where $\bar{G}$ contains only the main diagonal of G) and CLDG ($\bar{G}_d = \Gamma G_d$) are counting for the interactions between the control loops, without actually closing them. Note that when all PRGA and CLDG elements for a certain control loop are below 1, no control is actually needed since then the error will never exceed its bounds.

These tools have been applied to the selected control structures for the HDA process.

4.5.2.1 Performance Relative Gain Array, PRGA

The PRGA has the same diagonal elememts as the RGA, but different off-diagonal elements. The PRGA gives the effect of interactions on closed-loop performance with decentralized control. PRGA is independent of *input* scaling, but it depends on output scaling. This is reasonable since performance is defined in terms of the magnitude of the outputs. We usually prefer to have γ_{ii} close to 1

Figure 4.23 to Figure 4.25 show the effect of a setpoint change between the bound [-1,1] as a function of frequency, respectively. For the reference control structure, there are the two loop which exceed their bound at low frequencies, so feedback control is no longer effective. These loops are Sep.Pressure and Concentration of methane.

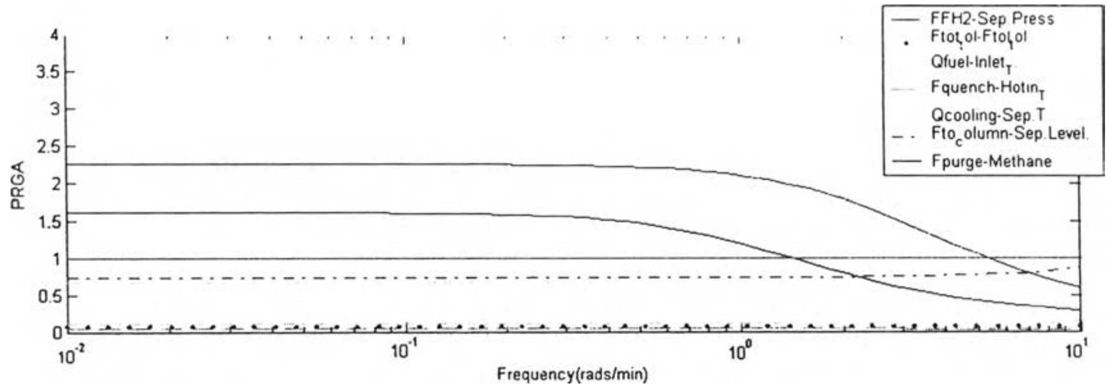

Figure 4.23 Performance relative gain array elements for the effect of a reference change on the outputs for reference control structure.

For the first alternative control structure, the interactions between the control loop become significant, there are the three loop which exceed their bound at low frequencies, so feedback control is no longer effective. These loops are Sep.Pressure, Sep. Level and Concentration of methane (as Figure 4.24)

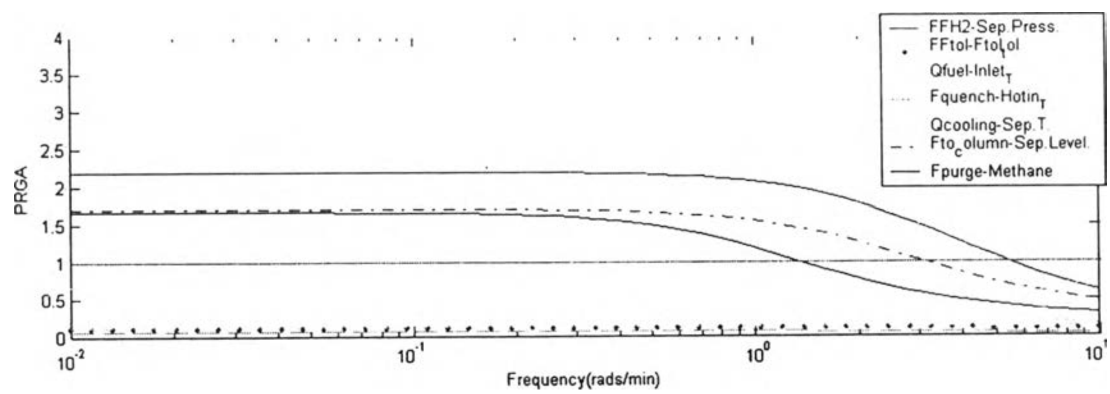

Figure 4.24 Performance relative gain array elements for the effect of a reference change on the outputs for alternative control structure1.

When the alternative control structure2 is used (Figure 4.25), the Sep. Pressure is only slightly affected, while all of controlled loop are controlled effectively at low frequencies. Note that although the structure shows violation at high frequencies, this is not expected to be a problem during operation.

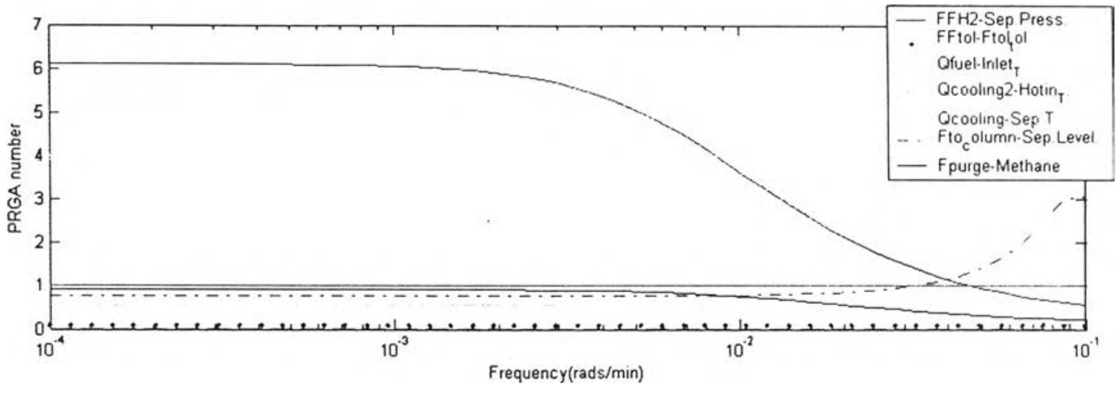

Figure 4.25 Performance relative gain array elements for the effect of a reference change on the outputs for alternative control structure2.

In conclusion, the PRGA analysis shows that the second control structure perform better than the reference structure and the first one. Because if setpoint is changed, the other outputs are automatically kept within their bounds, except the only Sep. Pressure loop.

4.5.2.2 Close Loop Disturbance Gain ,CLDG

After evaluating feasible pairings, we can estimate their performance by using the closed-loop disturbance gain (CLDG) index. To consider a single disturbance where feedback is effective so $\tilde{S}\Gamma$ is small. To keep the control error between acceptable bounds, ($|e_i| < 1$), the closed-loop disturbance gain should be smaller than 1,for each disturbance.

The CLDG analysis has been applied in the HDA process example for two disturbances: the pressure of FFH2, P_{FFH2} and the temperature of FFtoluene, $T_{FFtoluene}$, under the two diagonal control structure mentioned earlier. For the reference structure and both flowsheet alternatives; the results are shown in Figure 4.26 to Figure 4.31.

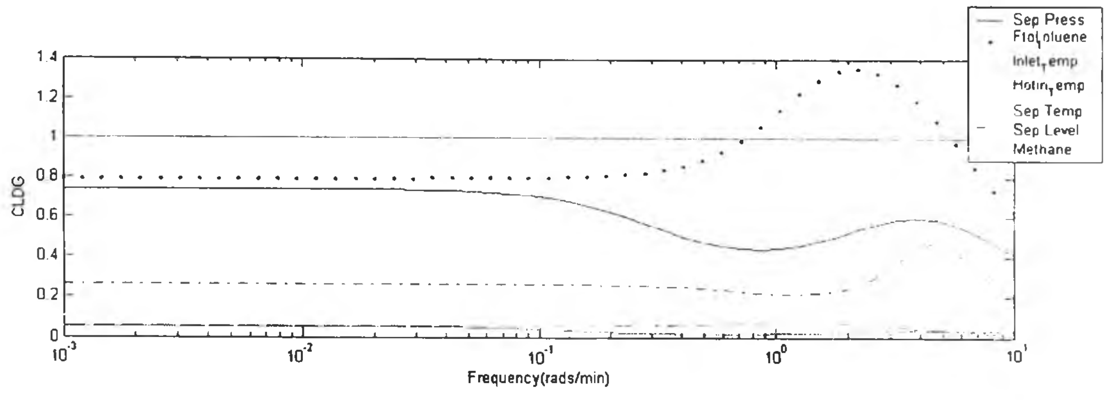

Figure 4.26 Close-loop disturbance gains for the pressure disturbance P_{FFH2} on output of reference control structure.

Figure 4.26 to Figure 4.28 show the behavior on disturbance P_{FFH2} of the reference control structure, the alternative control structure1 and the control structure 2, respectively. For the reference structure (as Figure 4.26), which shows the CLDG elements to be above one, indicates that extra control action is necessary to reject disturbances of the temperature $T_{Fftoluene}$. There is a only one loop, FFtol-Ftot-toluene, that should be controlled when it has the disturbances of the temperature $T_{Fftoluene}$. Which the result of CLDG of reference structure is similar to the control structure1.

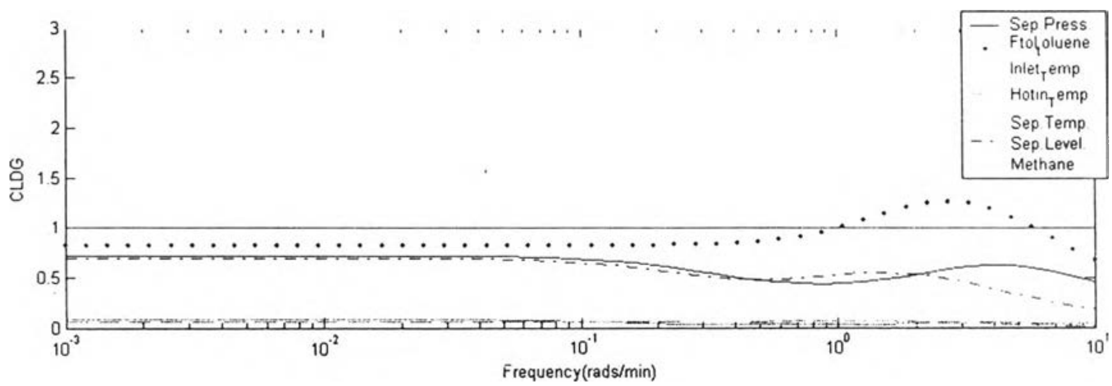

Figure 4.27 Close-loop disturbance gains for the pressure disturbance P_{FFH2} on output of alternative control stucture1.

Figure 4.28 shows the result for the alternative control structure2. The three loops of Sep.Pressure, Ftot-toluene and Sep. Level need control. Because the CLDG element of them are higher than 1, while the others loop do not require control. For the disturbance P_{FFH2} , hence, the reference structure and the alternative control structure1 performs better than the second one, since it has a only loop required control.

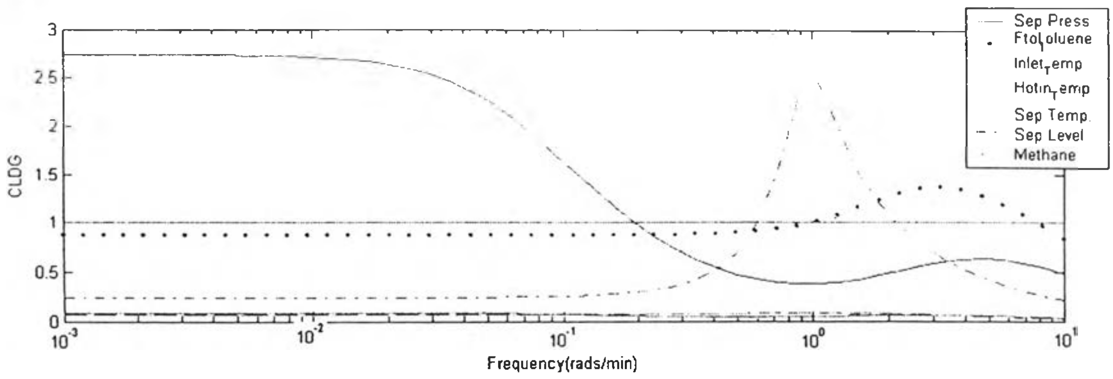

Figure 4.28 Close-loop disturbance gains for the pressure disturbance P_{FFH2} on output of alternative control stucture2.

For the other disturbance $T_{FFtoluene}$,the behavior of the reference structure , the alternative control structure1 and the control structure 2 are shown by Figure4.29 and Figure 4.31 , respectively.

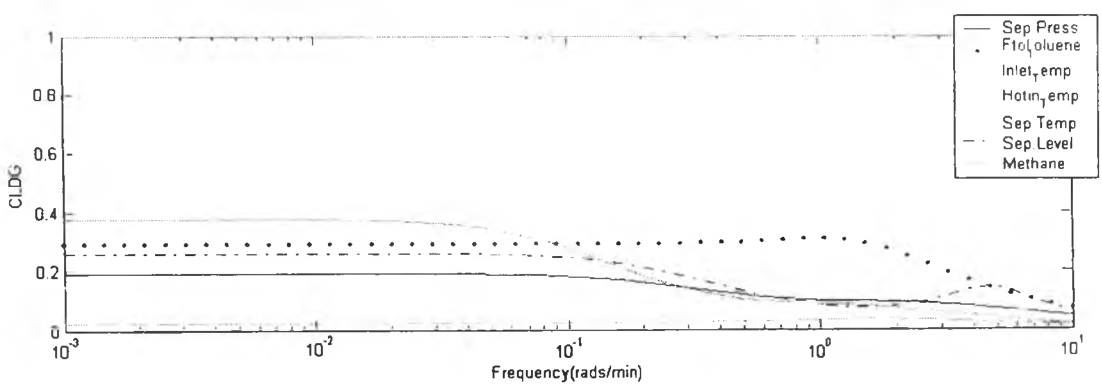

Figure 4.29 Close-loop disturbance gains for the temperature disturbance $T_{FFtoluene}$ on output of reference control structure.

The result of the reference structure is similar to the result of the control structure1 (as Figure 4.29 and Figure 4.30). Which that indicates the all of loop controller automatically stay with acceptable bounds. .

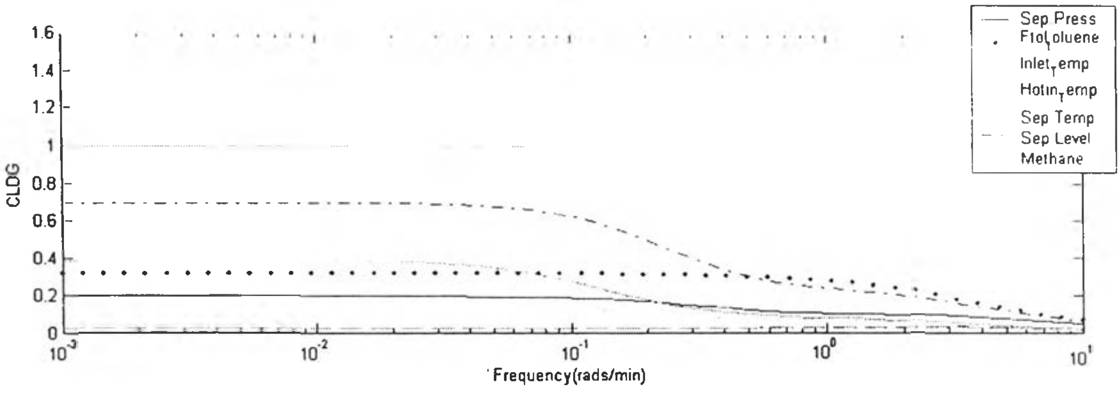

Figure 4.30 Close-loop disturbance gains for the temperature disturbance $T_{FFtoluene}$ on output of alternative control stucture1.

While Figure 4.31 shows the result for the alternative control structure2. It has a only loop, Sep. Level, that needs control and the other loops have CLDG element lower than bound

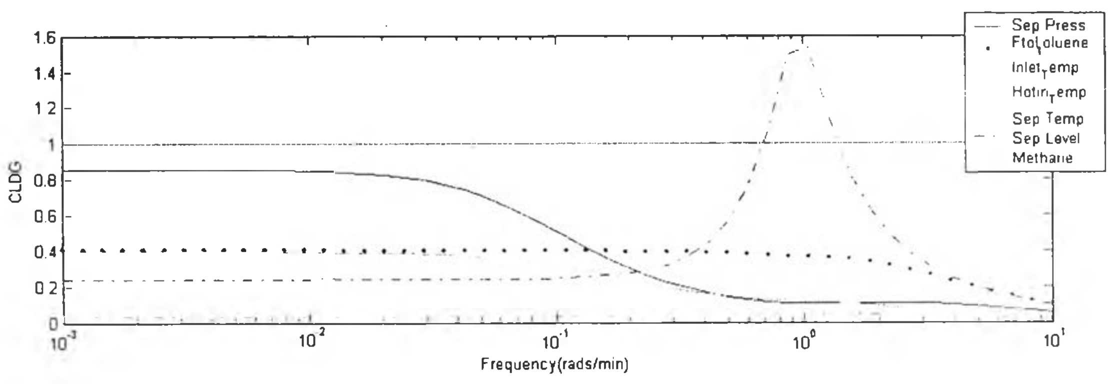

Figure 4.31 Close-loop disturbance gains for the temperature disturbance $T_{FFtoluene}$ on output of alternative control stucture2.

Hence for the disturbance $T_{FFtoluene}$, the reference structure and the alternative control structure1 performs better than the second one, since it has a only loop required control.