CHAPTER 5

RESULTS AND DISCUSSION

The modelling of the catalytic reforming of C_6 and C_7 hydrocarbons in a fixed-bed reactor is carried out using operation condition (temperature , pressure and hydrogen/hydrocarbon ratio) and feed line from experiments of the catalytic reforming on the Pt-Re/ Al_2O_3 catalyst. The results are compared with the experimental data under isothermal operation.

(1) The feed components of C_6 hydrocarbons. Input data from experiment for case 1 of Shum et al.(1985) and from experiment for case 2 and case 3 of Parera et al. (1986) are shown in Table E-1(Appendix E).

(2) The feed components of C_7 hydrocarbons. Input data from experiment for case 4 of Bickle et al.(1990), case 5 of Van Trimpont et al.(1986), case 6 of Shum et al. (1985), case 6 , 7, 8, 9, 10, 11, 12, 13, 14, 15 and 16 of Jothimurugesan et al. (1985), case 17 , 18 , 19 of Van Trimpont et al.(1986).

(3) The feed components are n-hexane, 2MP, 3MP, MCP, n-heptane, SBP_7, MBP_7, 5N7, MCH, benzene and toluene.

Input data from experiment for case 20 of Javier M.G. et al.(1988) are shown in Table E-2(Appendix E).

(4) The feed components are n-hexane, n-heptane, MCP, MCH, benzene and toluene. Input data for case 21 of Shantanu D. et al.(1988) are shown in Table E-3 (Appendix E).

Comparison of Modelling and Experimental Results

The results of computed concentration profiles against W/F_{HC}^{o}(kg catalyst.hr/kmol feed) which the results are compared with experimental data under isothermal operation.

Figure 5-1 shows the concentration profiles of isoheptane, benzene and cracked product against W/F_{HC}^{o} for case 1. The catalysts used in this case are 0.3 wt% Pt-0.3 wt% Re on alumina. From the modelling, it shows good agreement but the results of benzene and cracked product correspond more closely to isohexane when compared to experimental data of Shum et al.(1985).

Figure 5-2 and 5-3 show the concentration profiles of isohexane, benzene and cracked product against W/F_{HC}^{o} for case 2 and case 3. The catalyst used in these cases are 0.3 wt% Pt, 0.3 wt% Re, and 0.92 wt% Cl on alumina. From the modelling results for case 2 found that the results of isohexane and benzene correspond more closely to cracked product when compared to experimental data from Parera et al.(1986) and the result from case 2 (pressure 5 bar) is better than case 3 (pressure 15 bar).

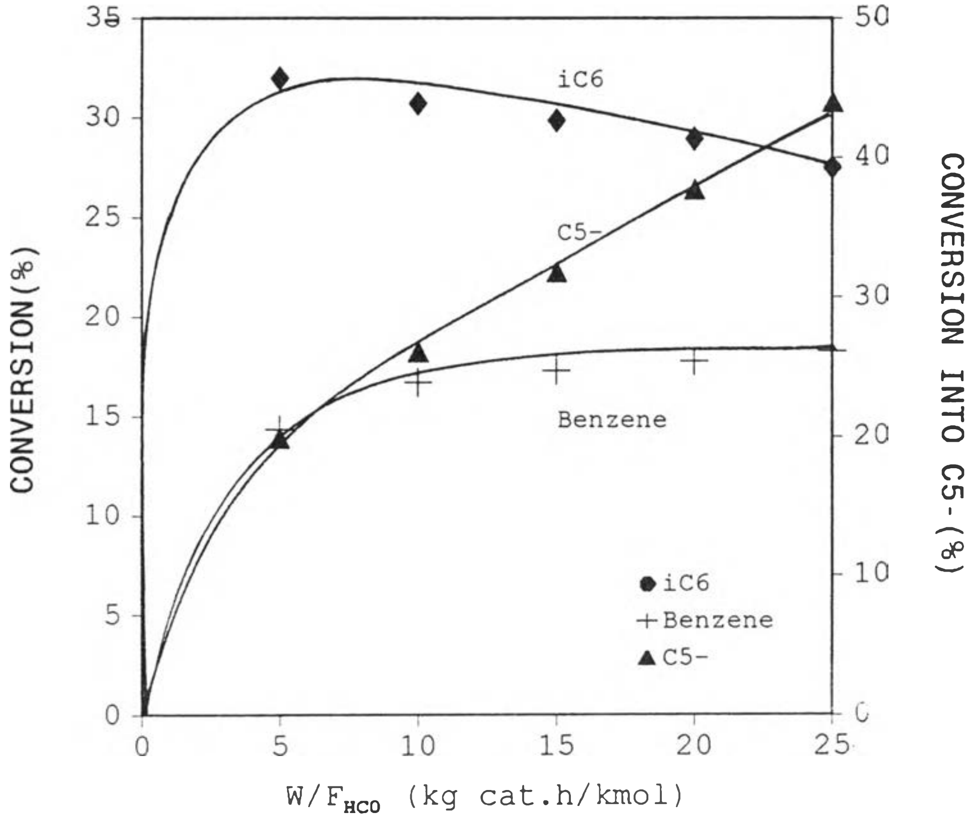

Figure 5-1 Conversion at 500 °C, 1 bar H_2/hydrocarbon ratio = 11, n-hexane feed. Computed:line. Experimental (Shum et al.(1985)):point.

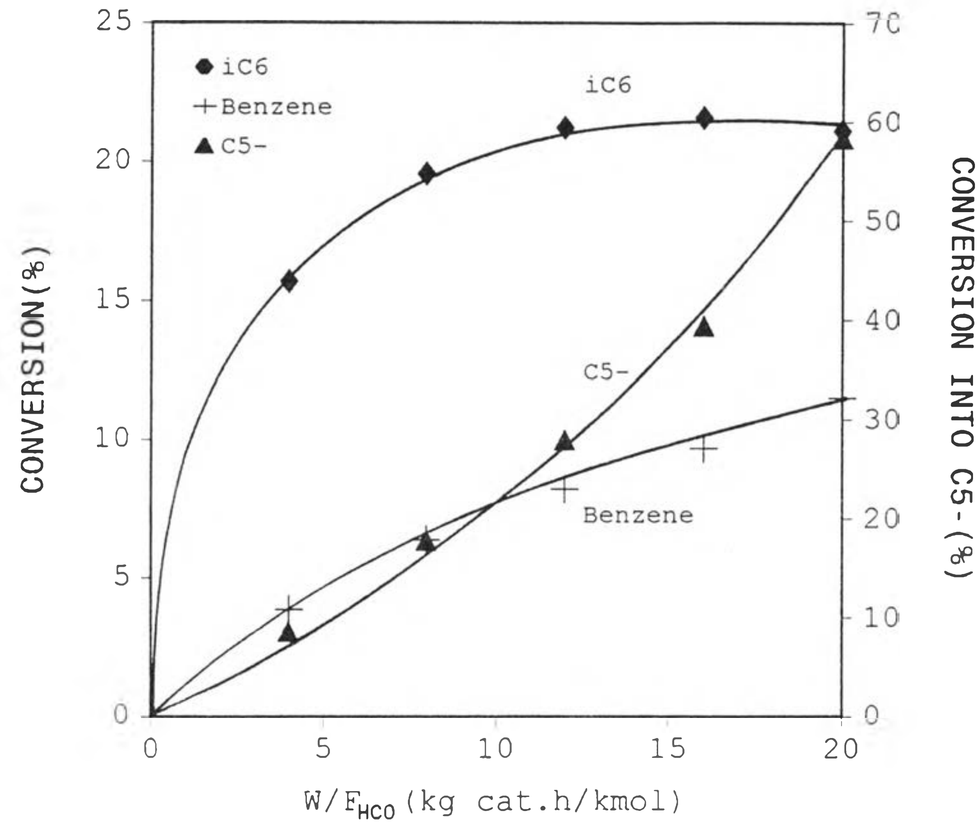

Figure 5-2 Conversion at 505 °C, 5 bar H_2/hydrocarbon ratio = 4, n-hexane feed. Computed:line. Experimental (Parera et al.(1986)):point.

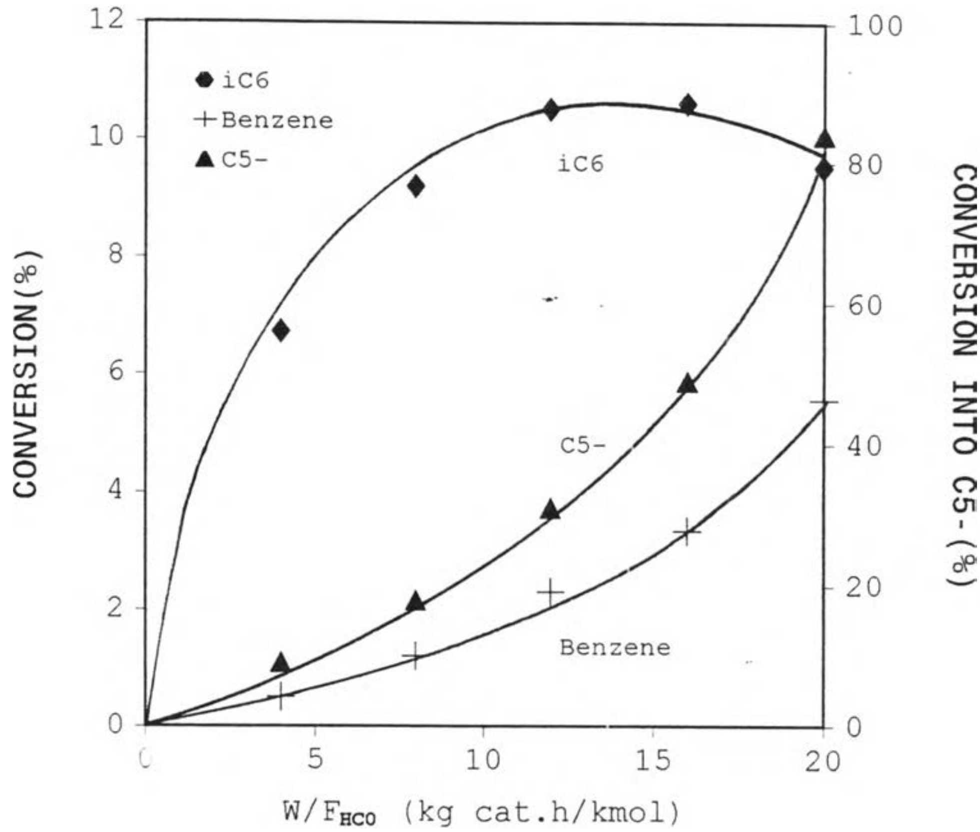

Figure 5-3 Conversion at 505 °C, 15 bar H_2/hydrocarbon ratio = 4, n-hexane feed. Computed:line. Experimental (Parera et al.(1986)):point.

Figure 5-4 shows the concentration profiles of isoheptane, toluene and cracked product againt W/F_{HC}° for case 4. Experimental data of Bickle et al.(1990) used 0.3-0.3 wt% Pt-Re on alumina-0.95 wt% Cl catalyst. The comparison between modelling and experimental data shows good agreement.

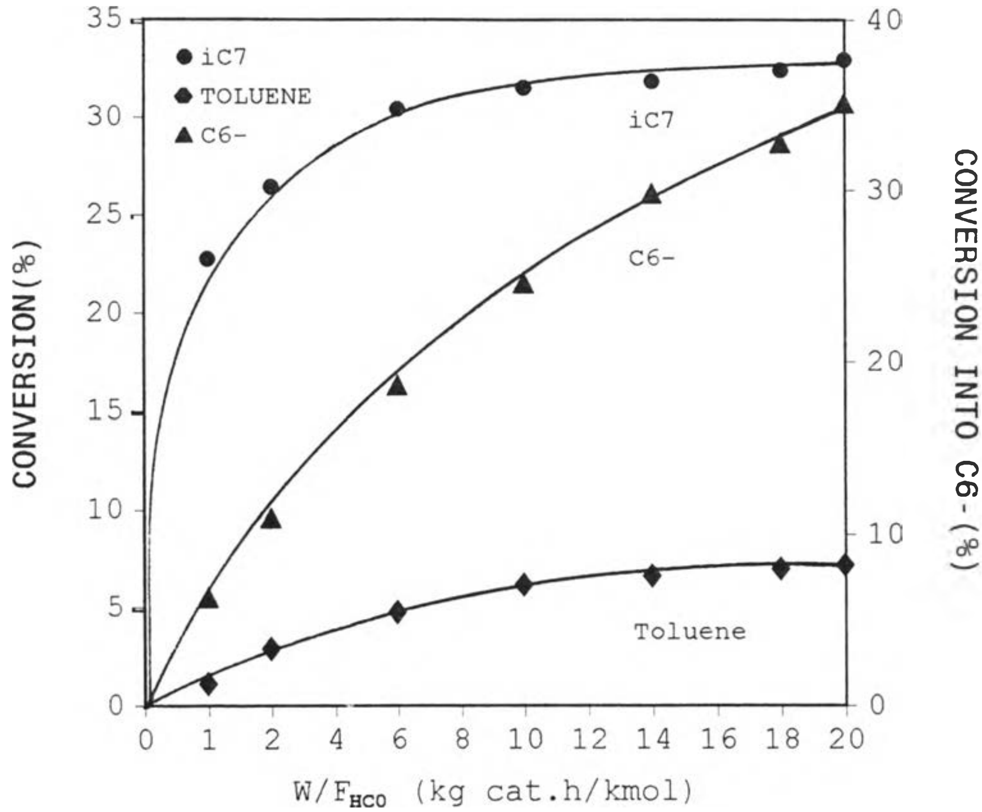

Figure 5-4 Conversion at 480 °C, 10 bar H_2/hydrocarbon ratio = 10, n-heptane feed. Computed:line. Experimental (Bickle et al.(1985)):point.

Figure 5-5 shows the concentration profiles of iso-heptane, five-ring naphthenes, methylcyclohexane, toluene and cracked product against $W/F_{HC^{\circ}}$ for case 5. Experimental data of Van Trimpont et al.(1986) are compared with the calculated results in this case. The catalyst is 0.296 wt% Pt, 0.311 wt% Re and 0.95 wt% Cl on alumina support. The results of isoheptane, five-ring naphthenes, methyl-cyclohexane are better than the results from toluene and cracked product.

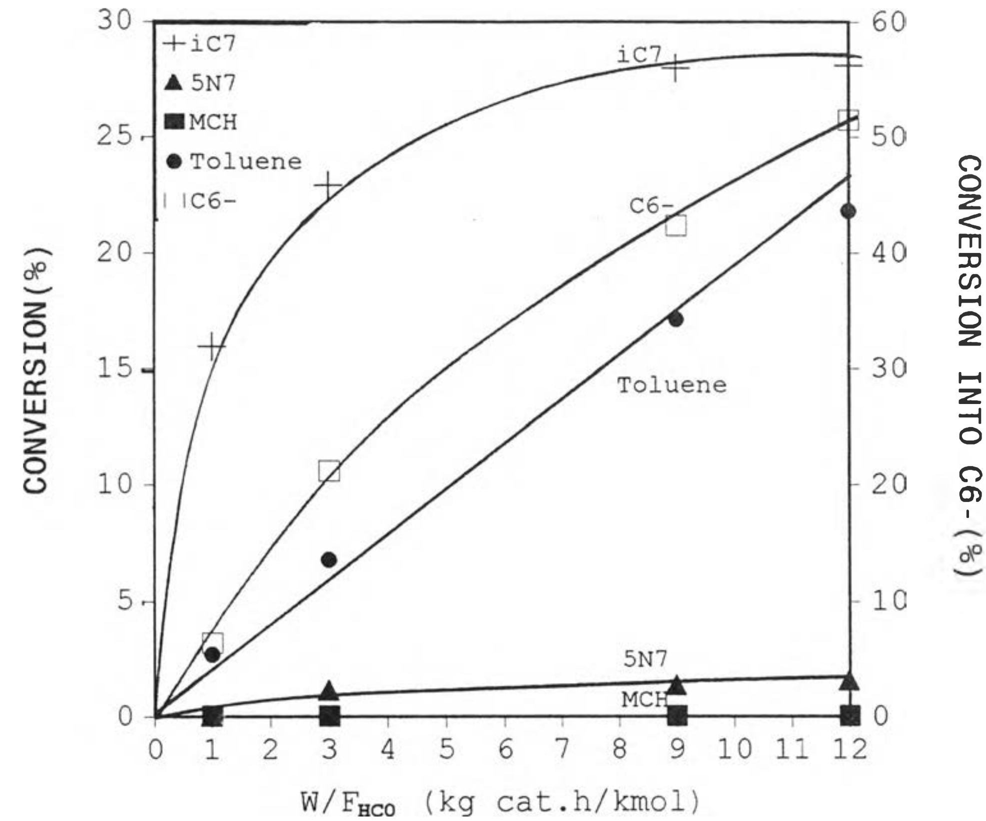

Figure 5-5 Conversion at 490 °C, 10.5 bar H_2/hydrocarbon ratio = 20, n-heptane feed. Computed:line. Experimental (Van Trimpont et al.(1986)):point.

Figure 5-6 shows the concentration profiles of isoheptane, toluene and cracked product against W/F_{HC}° for case 6 with the same catalyst as in case 1. From the modelling of this case found that isoheptane and cracked product correspond more closely to toluene when compared with experimental data of Shum et al.(1985).

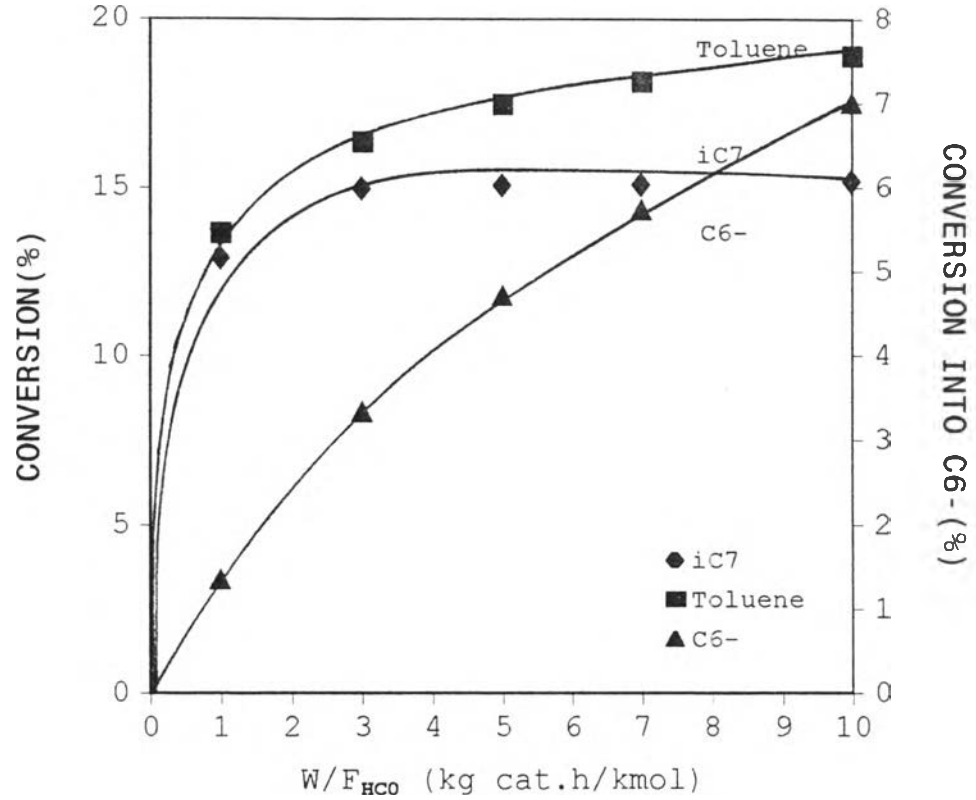

Figure 5-6 Conversion at 500 °C, 1 bar H_2/hydrocarbon ratio = 8, n-heptane feed. Computed:line. Experimental (Shum et al.(1985)):point.

Figure 5-7, 5-8 and 5-9 show the concentration profiles of toluene against W/F_{HC}° for case 7, 8, 9, 10, 11, 12, 13, 14, 15 and 16. The catalysts contain 0.3 wt% Pt-0.3 wt% Re on alumina. Experimental data of Jothimurugesan et al.(1985) are compared with the computed results of these cases. Figure 5-7 shows the pure methylcyclohexane feed for case 7, 8, 9 and 10 at 325, 350, 375, and 425 °C, respectively. At high temperature, the results gave higher toluene due to higher rate coefficent and also gave a good agreement when compared to experimental data. Case 11, 12, 13, and 14 are for methylcyclohexane mixed with toluene in the proportion of 14%:16%. The comparison between modelling result and experimental data show better results from 325, 350 and 375 than 425 °C. Figure 5-9 shows the effect of feed composition for case 8, 12, 15 and 16. It is found that the higher toluene component inhibit the production of toluene and therefore pure methylcyclohexane feed convert to higher toluene and also gave a good agreement when compared to experimental data.

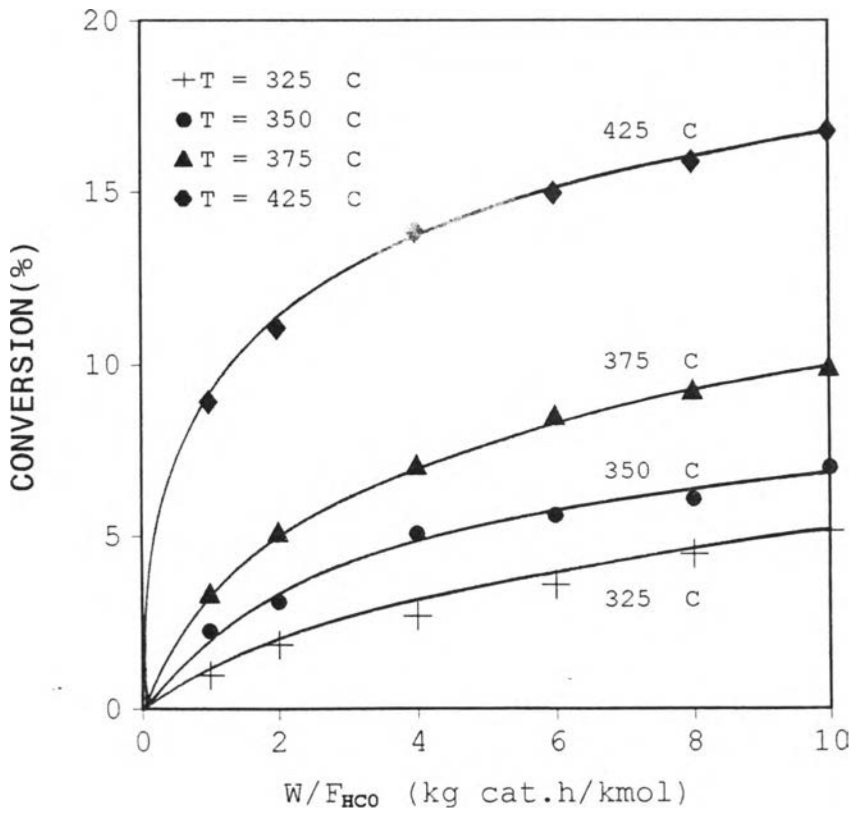

Figure 5-7 Dehydrogenation of methylcyclohexane at 1 bar, H_2/hydrocarbon ratio = 5. Effect of temperature on yield of toluene. Computed:line. Experimental (Jothimurugesan et al.(1985)):point.

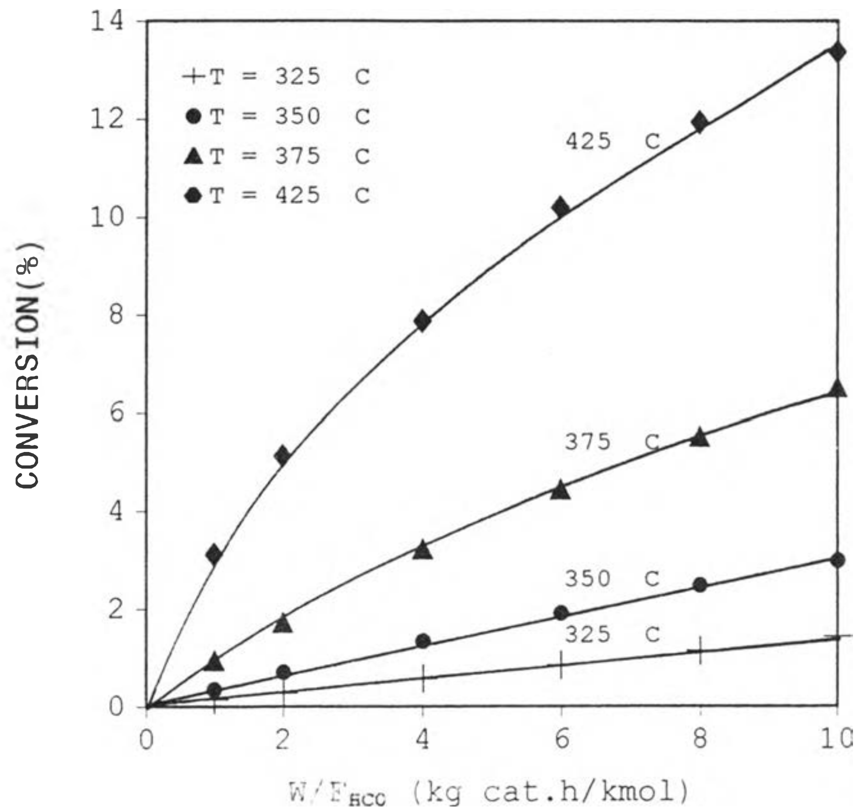

Figure 5-8 Dehydrogenation of methylcyclohexane at 1 bar, H_2/hydrocarbon ratio = 5 and MCH:Toluene (0.14:0.16) feed. Effect of temperature on yield of toluene. Computed:line. Experimental (Jothimurugesan et al.(1985)):point.

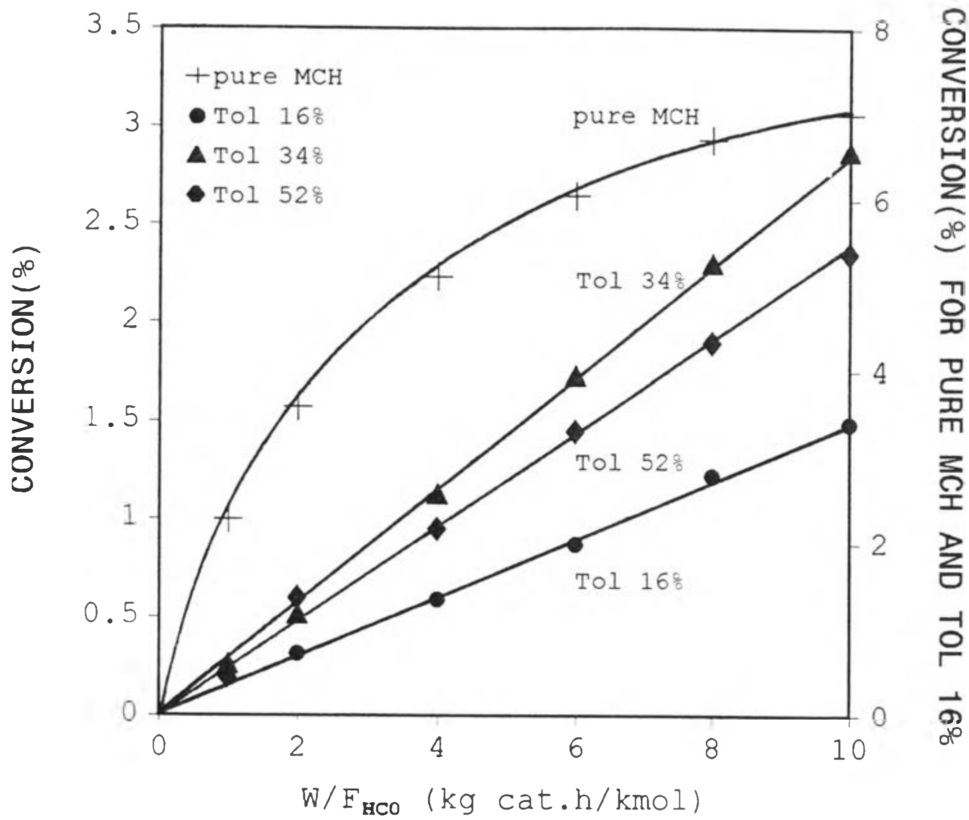

Figure 5-9 Dehydrogenation of methylcyclohexane at 350 °C, 1 bar, H_2/hydrocarbon ratio = 5. Effect of feed composition on yield of toluene. Computed :line. Experimental (Jothimurugesan et al. (1985)):point.

Figure 5-10 shows the concentration profiles of toluene against $W/F_{HC}{}^{o}$ for case 17, 18, 19. Experimental data from Van Trimpont et al. (1986) using 0.3 wt% Pt -0.3 wt% Re on alumina catalyst are compared with calculated results in this case. The result from modelling indicated that higher H_2/Hydrocarbon ratio gave low concentration of toluene than lower H_2/Hydrocarbon ratio and agreed with experimental data.

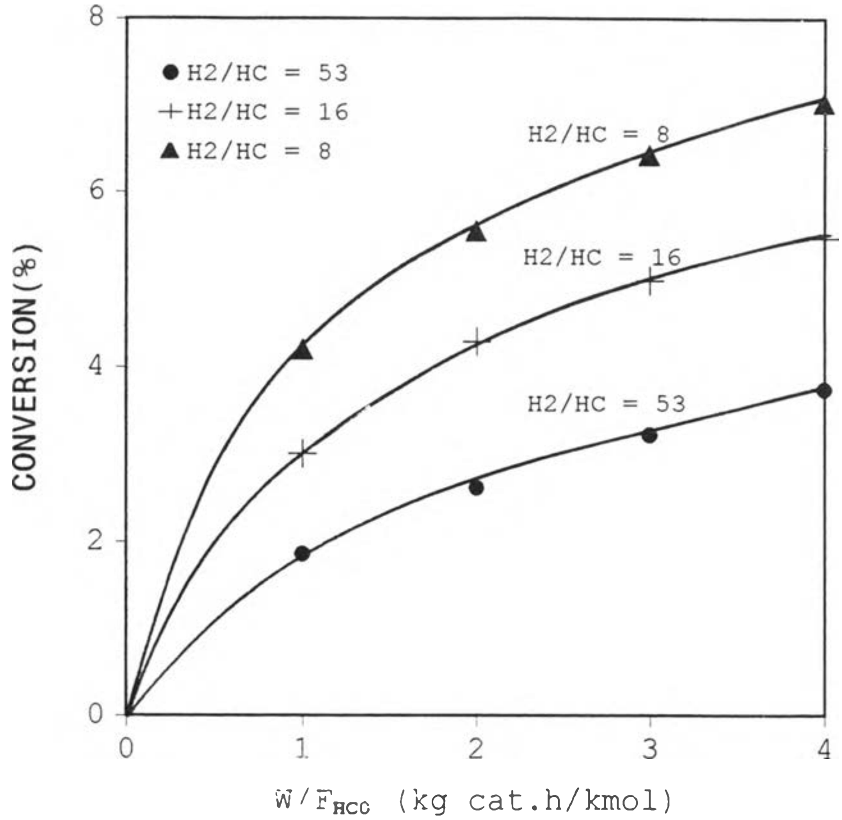

Figure 5-10 Dehydrogenation of methylcyclohexane at 400 °C. Effect of pressure and H_2/hydrocarbon ratio on yield of toluene. Computed:line. Experimental (Van Trimpont et al.(1986)):point.

Figure 5-11 shows the concentration profiles of benzene and toluene against W/F_{HC}° for case 20. The catalysts contain 0.3 wt% Pt, 0.3 wt% Re, 0.96 wt% Cl on alumina. The comparison between results and experimental data show good agreement.

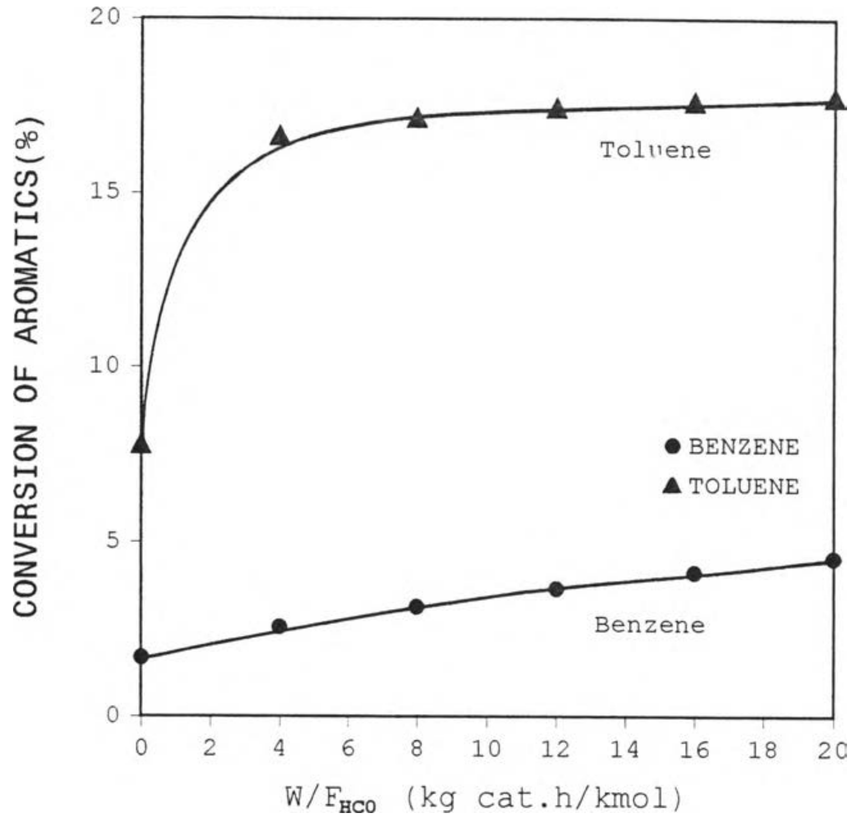

Figure 5-11 Comparison of conversion of aromatics between computed:line and experimental data:point(Javier et al.(1988)). Feed and operating condition are case 20

Figure 5-12 shows the concentration profiles of benzene and toluene against W/F_{HC}° for case 21. The catalysts used in this case are 0.3 wt% Pt-0.3 wt% Re on alumina. From the modelling, it shows good agreement.

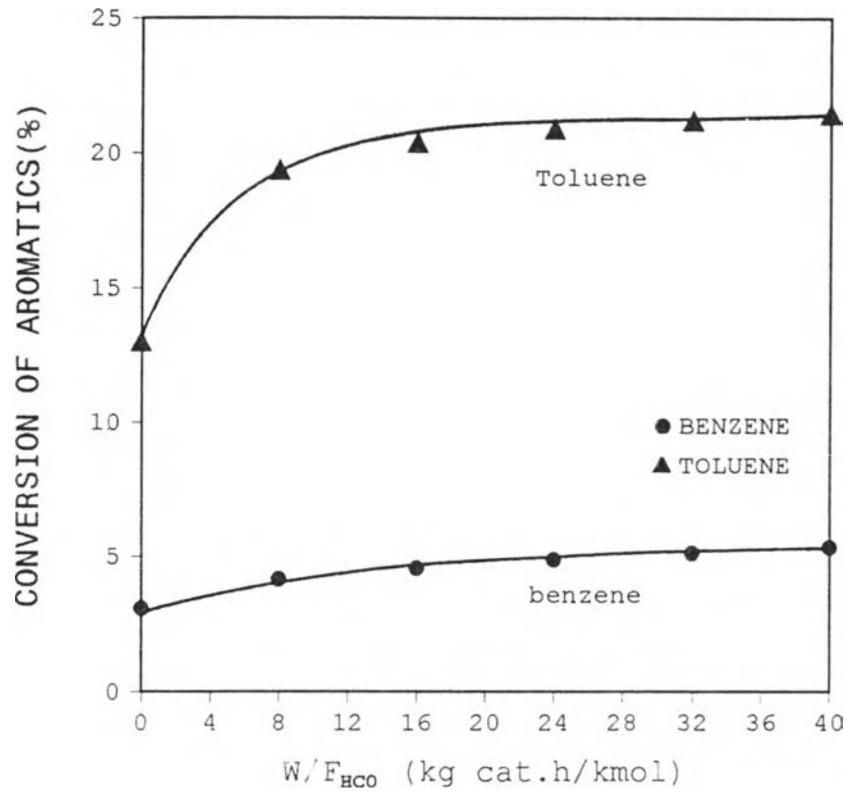

Figure 5-12 Comparison of conversion of aromatics between computed:line and experimental data : point (Shantanu et al.(1988)). Feed and operation condition are case 21.