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APPENDICES

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APPENDIX A

DETAILS OF SOME EXPERIMENTAL RESULTS

A-1:

PRESSURE	5 bars
TEMPERATURE	240 °C
LIQUID HOURLY SPACE VELOCITY	2.7 h ⁻¹
CATALYST TYPE	0.5 wt% Pt/USY

Component	Selectivity (%)	Product Distribution (wt%)	STY (g/cm ³ cat-h)
C ₃ H ₈	1.27	1.31	1.01x10 ⁻²
i-C ₄ H ₁₀	1.32	1.34	1.04x10 ⁻²
2,2-DMP	3.08	3.08	2.43x10 ⁻²
2,4-DMP	4.70	4.70	3.72x10 ⁻²
3,3-DMP	1.70	1.70	1.35x10 ⁻²
2-MH	45.81	45.79	0.36
3-MH	38.90	38.88	0.31
3-EP	3.20	3.20	2.53x10 ⁻²
n-Heptane conversion (%)			42.80
Selectivity of C ₇ isomers (%)			97.40
Selectivity of cracked products (%)			2.60
STY of C ₇ isomers (g/cm ³ -h)			0.77
STY of cracked products (g/cm ³ -h)			0.02

A-2:

PRESSURE	5 bars
TEMPERATURE	260 °C
LIQUID HOURLY SPACE VELOCITY	2.7 h ⁻¹
CATALYST TYPE	0.5 wt% Pt/USY

Component	Selectivity (%)	Product Distribution (wt%)	STY (g/cm ³ cat-h)
C ₃ H ₈	8.36	8.56	0.12
i-C ₄ H ₁₀	8.43	8.52	0.12
2,2-DMP	6.24	6.22	9.14x10 ⁻²
2,4-DMP	6.69	6.66	9.80x10 ⁻²
2,2,3-TMB	0.79	0.79	1.16x10 ⁻²
3,3-DMP	4.01	4.00	5.88x10 ⁻²
2-MH	32.69	32.58	0.48
2,3-DMP	3.02	3.00	4.42x10 ⁻²
3-MH	27.42	27.32	0.40
3-EP	2.35	2.34	3.45x10 ⁻²
n-Heptane conversion (%)			79.34
Selectivity of C ₇ isomers (%)			83.21
Selectivity of cracked products (%)			16.79
STY of C ₇ isomers (g/cm ³ -h)			1.22
STY of cracked products (g/cm ³ -h)			0.25

A-3:

PRESSURE	5 bars
TEMPERATURE	280 °C
LIQUID HOURLY SPACE VELOCITY	2.7 h ⁻¹
CATALYST TYPE	0.5 wt% Pt/USY

Component	Selectivity (%)	Product Distribution (wt%)	STY (g/cm ³ cat-h)
C ₃ H ₈	25.63	26.04	0.44
i-C ₄ H ₁₀	23.93	24.03	0.41
N-C ₄ H ₁₀	0.68	0.69	1.18x10 ⁻²
i-C ₅ H ₁₂	0.21	0.21	3.68x10 ⁻³
2,2-DMP	4.84	4.79	8.33x10 ⁻²
2,4-DMP	4.12	4.08	7.09x10 ⁻²
2,2,3-TMB	1.10	1.09	1.90x10 ⁻²
3,3-DMP	3.53	3.50	6.08x10 ⁻²
2-MH	16.63	16.45	0.29
2,3-DMP	3.48	3.44	5.99x10 ⁻²
3-MH	14.61	14.46	0.25
3-EP	1.23	1.22	2.11x10 ⁻²
n-Heptane conversion (%)			93.19
Selectivity of C ₇ isomers (%)			49.54
Selectivity of cracked products (%)			50.46
STY of C ₇ isomers (g/cm ³ -h)			0.85
STY of cracked products (g/cm ³ -h)			0.87

A-4:

PRESSURE	5 bars
TEMPERATURE	300 °C
LIQUID HOURLY SPACE VELOCITY	2.7 h ⁻¹
CATALYST TYPE	0.5 wt% Pt/USY

Component	Selectivity (%)	Product Distribution (wt%)	STY (g/cm ³ cat-h)
C ₃ H ₈	43.86	44.23	0.80
i-C ₄ H ₁₀	41.41	41.28	0.75
N-C ₄ H ₁₀	1.83	1.82	3.33x10 ⁻²
i-C ₅ H ₁₂	0.36	0.36	6.61x10 ⁻³
2,2-DMP	1.12	1.10	2.04x10 ⁻²
2,4-DMP	0.93	0.91	1.69x10 ⁻²
2,2,3-TMB	0.37	0.36	6.75x10 ⁻³
3,3-DMP	0.85	0.84	1.55x10 ⁻²
2-MH	3.96	3.88	7.20x10 ⁻²
2,3-DMP	1.39	1.36	2.52x10 ⁻²
3-MH	3.63	3.57	6.61x10 ⁻²
3-EP	0.29	0.28	5.23x10 ⁻³
n-Heptane conversion (%)			98.52
Selectivity of C ₇ isomers (%)			12.54
Selectivity of cracked products (%)			87.46
STY of C ₇ isomers (g/cm ³ -h)			0.23
STY of cracked products (g/cm ³ -h)			1.59

A-5:

PRESSURE	5 bars
TEMPERATURE	320 °C
LIQUID HOURLY SPACE VELOCITY	2.7 h ⁻¹
CATALYST TYPE	0.5 wt% Pt/USY

Component	Selectivity (%)	Product Distribution (wt%)	STY (g/cm ³ cat-h)
C ₃ H ₈	50.59	50.87	0.93
i-C ₄ H ₁₀	46.08	45.81	0.85
N-C ₄ H ₁₀	2.94	2.93	5.44x10 ⁻²
i-C ₅ H ₁₂	0.39	0.39	7.26x10 ⁻³
n-Heptane conversion (%)			100
Selectivity of C ₇ isomers (%)			0
Selectivity of cracked products (%)			100
STY of C ₇ isomers (g/cm ³ -h)			0
STY of cracked products (g/cm ³ -h)			1.85

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APPENDIX B

EXAMPLE OF CALCULATION

PRESSURE	5 bars
TEMPERATURE	240 °C
LIQUID HOURLY SPACE VELOCITY	2.7 h ⁻¹
CATALYST TYPE	0.5 wt% Pt/USY
SIZE RANGE OF CATALYST	20-30 mesh
AMOUNT OF CATALYST	1.3447 g
VOLUME OF CATALYST	1.5 cm ³
RATIO OF H ₂ /N-HEPTANE	10 mol/mol
N-HEPTANE FEED RATE	2.77 g/h

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MATERIAL BALANCEBasis : 1 hour operationInput

Component	G-mol	Grams
1. H ₂	0.3499	0.6998
2. n-Heptane	<u>0.0277</u>	<u>2.7731</u>
Total	<u>0.3776</u>	<u>3.4729</u>

Output

Component	G-mol	Grams
1. H ₂	0.3496	0.6992
2. C ₃ H ₈	5.54x10 ⁻⁴	1.56x10 ⁻²
3. i-C ₄ H ₁₀	2.74x10 ⁻⁴	1.59x10 ⁻²
4. 2,2-DMP	3.66x10 ⁻⁴	3.66x10 ⁻²
5. 2,4-DMP	5.58x10 ⁻⁴	5.58x10 ⁻²
6. 3,3-DMP	2.02x10 ⁻⁴	2.02x10 ⁻²
7. 2-MH	5.44x10 ⁻³	0.544
8. 3-MH	4.62x10 ⁻³	0.462
9. 3-EP	3.80x10 ⁻⁴	3.80x10 ⁻²
10. n-Heptane	<u>1.59x10⁻²</u>	<u>1.586</u>
Total	<u>0.3779</u>	<u>3.4733</u>

CONVERSION OF N-HEPTANE

$$\begin{aligned}
 \text{N-HEPTANE} &= \frac{\text{GRAM MOLES OF N-HEPTANE CONVERTED}}{\text{GRAM MOLES OF N-HEPTANE FED}} \times 100 \\
 \text{CONVERSION} &= \frac{(2.77 \times 10^{-2}) - (1.59 \times 10^{-2})}{2.77 \times 10^{-2}} \times 100 \\
 &= 42.80 \%
 \end{aligned}$$

ISO-HEPTANE SELECTIVITY

$$\begin{aligned}
 \text{ISO-HEPTANE} &= \frac{\text{GRAM ATOMS OF CARBON IN ALL } i\text{-C}_7 \text{ PRODUCTS}}{\text{GRAM ATOMS OF CARBON IN CONVERTED N-C}_7\text{H}_{16}} \times 100 \\
 \text{SELECTIVITY} &= \frac{\{(3.66+5.58+2.02+54.4+46.2+3.8) \times 10^{-4}\} \times 7}{\{(2.77 \times 10^{-2} - 1.59 \times 10^{-2}) \times 7\}} \times 100 \\
 &= 97.40 \%
 \end{aligned}$$

SPACE TIME YIELD (STY)

$$\begin{aligned}
 \text{STY OF } i\text{-C}_7\text{H}_{16} &= \frac{\% \text{CONV} \times \% \text{SEL} \times \text{N-HEPTANE FEED RATE (mol h}^{-1}\text{)}}{100 \times 100 \times \text{CATALYST VOLUME (cm}^3\text{)}} \\
 [\text{g/cm}^3\text{-h}] &= \frac{42.80 \times 97.40 \times 0.028}{100 \times 100 \times 1.5} \\
 &= 7.70 \times 10^{-3} \text{ mol/cm}^3\text{-h} \quad (0.77 \text{ g/cm}^3\text{-h})
 \end{aligned}$$

PRODUCT DISTRIBUTION

COMPONENT	PRODUCT DISTRIBUTION (wt%)
C ₃ H ₈	1.31
i-C ₄ H ₁₀	1.34
2,2-DMP	3.08
2,4-DMP	4.70
3,3-DMP	1.70
2-MH	45.79
3-MH	38.88
3-EP	3.20
TOTAL	100.00

Note : % PRODUCT DISTRIBUTION OF EACH COMPONENT
 = $\frac{\text{GRAM(S) OF EACH COMPONENT IN PRODUCT} \times 100}{\text{TOTAL GRAMS OF ALL COMPONENT}}$

VITA

Mr. Mana Amornkitbamrung was born on March 30, 1965, in Nongkhai, Thailand. He graduated from Chulalongkorn University, with a Bachelor of Science in Chemical Engineering in 1987. Prior to study in Master's program he worked at Lever Brothers (Thailand) Ltd. as production supervisor in 1987-1988.



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