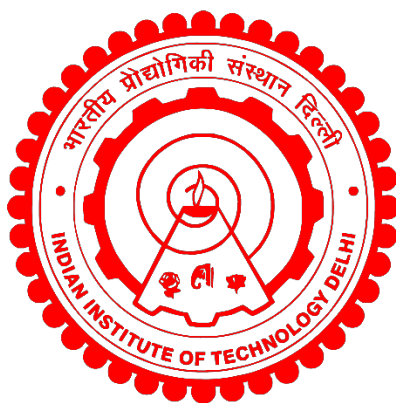


CONVERSION OF DI-AROMATICS TO MONO- AROMATICS OVER Y-ZEOLITE AT FCC CONDITIONS

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JULY 2024

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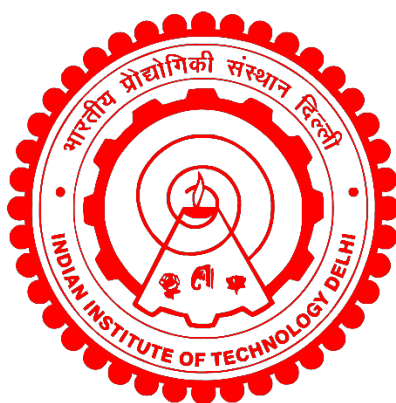
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Department of Chemical Engineering

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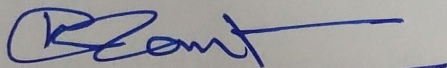
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Dedicated to my family
for the endless love, support, and encouragement

CERTIFICATE

This is to certify that the thesis entitled "Conversion of di-aromatics to mono-aromatics over Y-zeolite at FCC conditions", being submitted by Satheesh V K to the Indian Institute of Technology, Delhi, is worthy of consideration for the award of the degree of Doctor of Philosophy and is a record of the original bonafide research work carried out by him under our guidance and supervision. The results contained in the thesis have not been submitted in part or full, to any other University or Institute for the award of any degree or diploma. We certify that he has pursued the prescribed course of research.

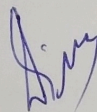
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Satheesh V K

ABSTRACT

Due to the increasing demand of chemicals/petrochemicals and global plans on reduction of fossil fuels in view of reduction of CO₂ emissions, there is a thrust in refining sector to convert the various hydrocarbon streams into value-added chemicals/petrochemicals for improving the refining margin. Light Cycle Oil (LCO) from Fluid Catalytic Cracking (FCC) unit is normally blended in diesel pool after improving its cetane number in the hydrotreating unit. Therefore, opportunity exists for the conversion of LCO to predominantly chemicals/petrochemicals feedstock in FCC unit itself through the selection of proper Y zeolite catalyst. Upon detailed characterization of LCO used in the current study, it was found that LCO consists of more than 60% di-aromatic molecules.

In the current research work, experimental cracking was carried out in fixed and fluidized bed micro reactors using a two-ring naphthenic compound (Decalin), di-aromatic compound [2-methyl naphthalene (2MN)], and Y zeolite based catalyst to assess the formation of mono-aromatics. The gas and liquid products were analysed in Refinery Gas Analyser and Mass Spectroscopy equipped with Gas Chromatography to identify the individual molecules formed during cracking. For ease of analysis, the product molecules were lumped together based on the type of molecules as Gas, paraffin + naphthene (PN), mono-aromatics (MA), naphtheno-aromatics (NA), di-aromatics(DA), tri-aromatics (TA), and Coke.

The cracking pathways were studied using Decalin and 2MN separately over Y zeolite. It was noted that Coke and Gas was found increased with increase in conversion while all other products were decreased. While analysing the products formed based on various classes of reactions such as cracking, alkylation, hydrogen transfer, ring opening and ring contraction, it was found that cracking and hydrogen transfer reactions predominates over others at higher

conversion. This can be explained based on higher acidity of Y zeolite. The extent of such reaction was much lower in case of 2MN due to its higher stability as compared to Decalin.

Cracking study was further extended for 2MN using a catalyst derived from Y zeolite. Experiments were conducted at various reaction temperatures and catalyst-to-oil ratios pertaining to FCC unit operation. Based on the analysis of products, it was found that the alkylation and cracking reactions were predominant in this case. The reaction pathways indicate that the coke was predominantly formed through poly-aromatics by disproportionation reactions. Hydrogen was also formed during this reaction, which will be consumed in the hydrogen transfer and ring opening/cracking reactions. The major pathway for the mono-aromatics formation was the hydrogen transfer followed by cracking and ring opening reactions. Estimation of kinetic parameters was also carried out for the reaction network considered. Model prediction showed a good match with the experimental data.

The effect of hydrogen donor (Decalin) concentration and rare earth content of catalyst on improving the yield of mono-aromatics was also studied. It was found that both hydrogen donor and high rare earth content catalyst were increasing the conversion of 2MN to mono-aromatics. Finally, LCO was also cracked over the catalyst to identify the feasibility of increasing the mono-aromatics yield in FCC unit. Overall, the current research will provide a systematic insight that will help in designing the optimized catalyst and the hydrogen rich stream to be used for maximizing the conversion of LCO to mono-aromatics in FCC unit.

सार

रसायनों/पेट्रोकेमिकल्स की बढ़ती मांग और CO₂ उत्सर्जन में कमी के मद्देनजर जीवाश्म ईंधन में कमी की वैश्विक योजनाओं के कारण, रिफाइनिंग मार्जिन में सुधार के लिए विभिन्न हाइड्रोकार्बन धाराओं को मूल्य वर्धित रसायनों/पेट्रोकेमिकल्स में परिवर्तित करने के लिए रिफाइनिंग क्षेत्र में जोर दिया जा रहा है। एफसीसी यूनिट से लाइट साइकिल ऑयल (एलसीओ) को हाइड्रोट्रीटिंग यूनिट में सीटेन संख्या में सुधार के बाद आम तौर पर डीजल पूल में मिश्रित किया जाता है। इसलिए, उचित वाई जिओलाइट उत्प्रेरक के चयन के माध्यम से एफसीसी इकाई में ही एलसीओ को मुख्य रूप से रसायनों/पेट्रोकेमिकल्स फीडस्टॉक में बदलने का अवसर मौजूद है। एलसीओ के विस्तृत लक्षण वर्णन पर, यह पाया गया कि एलसीओ में 60% से अधिक डाय-एरोमैटिक अणु होते हैं।

वर्तमान शोध कार्य में, मूल्यांकन के लिए दो-रिंग नैफ्थेनिक यौगिक (डेकालिन), डाय-एरोमैटिक यौगिक (2-मिथाइल नैफ्थलीन (2MN)) और वाई जिओलाइट आधारित उत्प्रेरक का उपयोग करके स्थिर और द्रवीकृत बिस्तर माइक्रो रिएक्टरों में प्रायोगिक क्रैकिंग अध्ययन आयोजित किया गया था। मोनो-एरोमैटिक्स का निर्माण. क्रैकिंग अध्ययन में गठित व्यक्तिगत अणुओं की पहचान करने के लिए गैस और तरल उत्पादों का क्रमशः गैस क्रोमैटोग्राफी से सुसज्जित रिफाइनरी गैस विश्लेषक और मास स्पेक्ट्रोस्कोपी में विश्लेषण किया गया था। विश्लेषण में आसानी के लिए, उत्पाद अणुओं को गैस, पैराफिन + नैफ्थीन (पीएन), मोनो-एरोमैटिक्स (एमए), नैफ्थेनो-एरोमैटिक्स (एनए), डी-एरोमैटिक्स (डीए), ट्राई- जैसे अणुओं के प्रकार के आधार पर एक साथ जोड़ा गया था। एरोमेटिक्स (टीए) और कोक।

क्रैकिंग पथों का अध्ययन वाई जिओलाइट पर अलग-अलग डेकालिन और 2 एमएन का उपयोग करके किया गया था। यह देखा गया है कि रूपांतरण में वृद्धि के साथ कोक और गैस में वृद्धि देखी गई जबकि अन्य सभी उत्पाद घट रहे हैं। क्रैकिंग, एल्किलेशन, हाइड्रोजन ट्रांसफर, रिंग ओपनिंग और रिंग संकुचन जैसी प्रतिक्रियाओं के विभिन्न वर्गों के आधार पर गठित उत्पादों का विश्लेषण करते समय, यह पाया गया कि क्रैकिंग और हाइड्रोजन ट्रांसफर प्रतिक्रियाएं उच्च रूपांतरण पर दूसरों पर हावी होती हैं। इसे वाई जिओलाइट की उच्च अम्लता के आधार पर समझाया जा सकता है। डेकालिन की तुलना में इसकी उच्च स्थिरता के कारण 2MN के मामले में ऐसी प्रतिक्रिया की सीमा बहुत कम है।

वाई जिओलाइट से प्राप्त उत्प्रेरक का उपयोग करके क्रैकिंग अध्ययन को 2MN के लिए आगे बढ़ाया गया था। एफसीसी इकाई संचालन से संबंधित विभिन्न प्रतिक्रिया तापमान और तेल उत्प्रेरक अनुपात पर प्रयोग किए गए। उत्पादों के विश्लेषण के आधार पर, यह पाया गया है कि इस मामले में एल्किलेशन और क्रैकिंग प्रतिक्रियाएं प्रमुख हैं। प्रतिक्रिया पथ से संकेत मिलता है कि कोक मुख्य रूप से पॉली-एरोमैटिक्स के माध्यम से असंगत प्रतिक्रियाओं द्वारा बनता है। इस प्रतिक्रिया के दौरान हाइड्रोजन भी बनता है, जो हाइड्रोजन स्थानांतरण और रिंग ओपनिंग/क्रैकिंग प्रतिक्रियाओं में खर्च हो जाएगा। मोनो-एरोमैटिक्स के गठन का प्रमुख मार्ग हाइड्रोजन स्थानांतरण है जिसके बाद क्रैकिंग और रिंग ओपनिंग प्रतिक्रियाएं होती हैं। काइनेटिक मॉडलिंग भी किया गया और प्रतिक्रिया नेटवर्क के लिए गतिज मापदंडों का अनुमान लगाया गया। मॉडल पूर्वानुमान ने प्रयोगात्मक डेटा के साथ अच्छा मेल दिखाया।

मोनो-एरोमैटिक्स की उपज में सुधार पर हाइड्रोजन दाता (डेकालिन) सांद्रता और उत्प्रेरक की दुर्लभ पृथ्वी सामग्री के प्रभाव का भी अध्ययन किया गया। यह पाया गया कि हाइड्रोजन दाता और उच्च दुर्लभ

पृथ्वी सामग्री उत्प्रेरक दोनों 2MN के मोनो-एरोमैटिक्स में रूपांतरण बढ़ा रहे थे। अंत में, एफसीसी इकाई में मोनो-एरोमैटिक्स उपज बढ़ाने की व्यवहार्यता की पहचान करने के लिए उत्प्रेरक पर एलसीओ को भी क्रैक किया गया। कुल मिलाकर, वर्तमान शोध एक व्यवस्थित अंतर्दृष्टि प्रदान करेगा जो एफसीसी इकाई में एलसीओ के मोनो-एरोमैटिक्स में रूपांतरण को अधिकतम करने के लिए उपयोग किए जाने वाले अनुकूलित उत्प्रेरक और हाइड्रोजन समृद्ध धारा को डिजाइन करने में मदद करेगा।

Contents

CERTIFICATE.....	i
ACKNOWLEDGMENTS	ii
ABSTRACT	iv
LIST OF FIGURES	xiii
LIST OF TABLES	xvii
NOMENCLATURE	xix
CHAPTER 1 : INTRODUCTION.....	1
1.1 Petroleum refining	1
1.2 Refinery configuration evolution.....	2
1.3 Importance of Catalytic Cracking in the COTC configuration.....	4
1.3.1 Fluidized Catalytic Cracking process	5
1.3.2 Zeolite as the cracking catalyst.....	9
1.4 Genesis of current research.....	13
CHAPTER 2: LITERATURE REVIEW	14
2.1 Upgradation of LCO & poly aromatic hydrocarbons	16
2.2 Catalytic Cracking of naphthene & naphthenic aromatics	20
2.3 Hydrogen transfer reactions.....	29
2.4 Coke formation	31
2.5 Zeolite catalyst used in catalytic conversion of aromatics.....	36
2.6 Effect of rare earth content of catalyst in Catalytic Cracking.....	43
2.7 Reactions of model compounds over zeolite catalyst.....	47
2.8 Kinetic modelling.....	47

2.9	Identified gaps in literature	53
2.10	Research objectives.....	54
CHAPTER 3 : MATERIALS AND METHODS		55
3.1	Introduction.....	55
3.2	Materials	55
3.2.1.	Feedstock	55
3.2.2.	Catalyst	58
3.3	Catalyst characterization studies.....	59
3.3.1.	X-ray Diffraction	59
3.3.2.	X-ray Fluorescence	60
3.3.3.	Temperature Programmed Desorption.....	60
3.3.4.	Brunauer–Emmett–Teller method	61
3.3.5.	Apparent Bulk Density	63
3.4	Analysis of feedstock and products	63
3.4.1.	Two Dimensional Gas Chromatography	63
3.4.2.	Gas Chromatography - Mass Spectrometry	64
3.4.3.	Gas Chromatography for composition of gas	64
3.4.4.	Gas Chromatography for Simulated Distillation of liquid product	66
3.5	Catalytic reaction studies	67
3.5.1.	Hydrothermal deactivation of catalyst	67
3.5.2.	Micro reactor unit	68
3.5.3.	Conversion & Product yields	70
3.6	Estimation of kinetic parameters	71

CHAPTER 4 : REACTION STUDIES ON CRACKING OF MODEL COMPOUNDS

OVER Y-ZEOLITE 73

4.1	Introduction.....	73
4.2	Results & discussion	74
4.2.1	Catalyst characterization studies.....	74
4.2.2	Analysis of feedstocks	76
4.2.3	Cracking studies using Y zeolite.....	79
4.2.3.1	Cracking of decalin	82
4.2.3.2	Cracking of 2-methyl naphthalene.....	95
4.3	Conclusion	101

CHAPTER 5 : REACTION STUDIES ON CRACKING OVER FCC CATALYST .. 102

5.1	Introduction.....	102
5.2	Results & discussion	102
5.2.1	Cracking studies of 2-methyl naphthalene using FCC catalyst A	102
5.2.1.1	Effect of WHSV on cracking of 2MN	105
5.2.1.2	Effect of Reaction Temperature.....	115
5.2.1.3	Trends in reaction types against conversion	117
5.2.2	Mechanism of catalytic cracking of 2MN	118
5.2.3	Cracking studies of 2-methyl naphthalene with hydrogen donor	127
5.2.4	Effect of rare earth content of catalyst on cracking of 2MN	131
5.2.5	Cracking studies of LCO using Catalyst A.....	132
5.3	Conclusion	133

CHAPTER 6 : ESTIMATION OF KINETIC PARAMETERS 135

6.1	Reaction scheme	135
-----	-----------------------	-----

6.2	Mathematical model.....	136
6.3	Validation of estimated kinetic parameters.....	141
6.4	Conclusion	143
CHAPTER 7 : CONCLUSIONS & FUTURE WORK		145
7.1	Summary and conclusion of current research.....	145
Annexure-I		148
Bibliography		153

LIST OF FIGURES

Figure 1.1 : Petroleum product demand in India during 2022-23.....	3
Figure 1.2 : Production of Petrochemical and capacity in India.....	4
Figure 1.3 : Production of Aromatics and capacity in India	4
Figure 1.4 : Schematic of Fluidized Catalytic Cracking Unit.....	7
Figure 1.5 : Unit cell of Y-zeolite	12
Figure 2.1: Reaction network of multi-ring aromatics as explained by Zhang et al.....	17
Figure 2.2 : Reaction mechanism proposed by Shimada et al. for cracking of the 3-ring PAHs	19
Figure 2.3 : Proposed reaction pathways in the conversion of tetralin	22
Figure 2.4 : Proposed reaction pathways in the conversion of naphthalene	23
Figure 2.5 : Formation of coke from hydrocarbons over acid and bifunctional metal-acid catalysts	32
Figure 2.6 : Probable structures of coke samples derived from spent & regenerated catalysts	35
Figure 2.7 : Proposed sequence of cracking and hydrogenation of anthracene over $ZnCl_2$ or $AlCl_3$	42
Figure 2.8 : Proposed kinetic scheme.	53
Figure 3.1 : Molecular composition of LCO	56
Figure 3.2 : Distribution of di-aromatics in LCO	56
Figure 3.3 : Schematic of experimental set up.....	68

Figure 4.1 : XRD plot of Y zeolite	74
Figure 4.2 : Acid strength distribution of Y zeolite	75
Figure 4.3 : GC-MS chromatogram of decalin	77
Figure 4.4 : GC-MS chromatogram of 2MN	77
Figure 4.5 : Optimized geometry of 2MN molecule (length shown in Å)	78
Figure 4.6 : Conversion of decalin with WHSV at 500°C.....	87
Figure 4.7 : Yield of Gas from catalytic cracking of decalin at 500°C	87
Figure 4.8 : Yield of components of Gas from cracking of decalin at 500°C.	88
Figure 4.9 : Yield of MA from catalytic cracking of decalin at 500°C	88
Figure 4.10 : Yield of PN from catalytic cracking of decalin at 500°C.....	88
Figure 4.11 : Yield of NA from catalytic cracking of decalin at 500°C.....	89
Figure 4.12 : Yield of DA from catalytic cracking of decalin at 500°C.....	89
Figure 4.13 : Yield of Coke from catalytic cracking of decalin at 500°C	89
Figure 4.14 : Yield of mono-aromatics from catalytic cracking of decalin at 500°C.....	90
Figure 4.15 : Various class of reactions - decalin as feed.....	93
Figure 4.16 : Conversion of 2MN at 500°C.....	98
Figure 4.17 : Yield of various products from catalytic cracking of 2MN at 500°C.	98
Figure 4.18 : Yield of components of Gas product of 2MN at 500°C.....	99
Figure 4.19 : Yield of mono-aromatics components from catalytic cracking of 2MN at 500°C	100
Figure 4.20 : Various class of reactions from catalytic cracking of 2MN at 500°C.....	100

Figure 5.1 : Conversion of 2MN with WHSV at different reactions temperatures	110
Figure 5.2 : Yield of components of Gas from cracking of decalin at 500°C, 530°C and 550°C.....	110
Figure 5.3 : Yields of Gas and Paraffin + Naphthene from cracking of 2MN at 500°C	112
Figure 5.4 : Yields of mono & tri-aromatics and coke from cracking of 2MN at 500°C.....	112
Figure 5.5 : Yield of di-aromatics from cracking of 2MN at 500°C	112
Figure 5.6 : Yields of Gas and Paraffin + Naphthene from cracking of 2MN at 530°C	113
Figure 5.7 : Yields of mono & tri-aromatics and coke from cracking of 2MN at 530°C.....	113
Figure 5.8 : Yield of di-aromatics from cracking of 2MN at 530°C	113
Figure 5.9 : Yields of Gas and Paraffin + Naphthene from cracking of 2MN at 550°C	114
Figure 5.10 : Yields of mono & tri-aromatics and coke from cracking of 2MN at 550°C....	114
Figure 5.11 : Yield of di-aromatics from cracking of 2MN at 550°C	114
Figure 5.12 : Effect of reaction temperature on products yield at WHSV of 15.7 h ⁻¹	116
Figure 5.13 : Effect of reaction temperature on products yield at WHSV of 17.5 h ⁻¹	116
Figure 5.14 : Effect of reaction temperature on products yield at WHSV of 19.6 h ⁻¹	116
Figure 5.15 : Yield of components of mono-aromatics from cracking of 2MN at various temperatures.....	117
Figure 5.16 : Various reactions happening during cracking of 2MN	118
Figure 5.17 : Formation of probable carbocations from 2MN	126
Figure 5.18 : Protonation of C atom at 2 nd position of 2MN as an example	126
Figure 5.19 : Effect of hydrogen donor in the conversion of 2MN	130
Figure 5.20 : Effect of hydrogen donor on product yields.....	131
Figure 5.21 : Effect of rare earth content of catalyst on product yields.....	131
Figure 5.22 : Cracking of LCO over Catalyst-A.....	133

Figure 6.1 : Reaction network.....	135
Figure 6.2 : Representation of differential volume of catalyst bed in the plug flow reactor .	137
Figure 6.3 : Algorithm used for solving the governing equations	139
Figure 6.4 : Comparison of experimental data with model predicted data	141
Figure 6.5 : Prediction of product yields using kinetic model at 500°C.....	142
Figure 6.6 : Prediction of product yields using kinetic model at 530°C.....	142
Figure 6.7 : Prediction of product yields using kinetic model at 550°C.....	143

LIST OF TABLES

Table 1.1 : Typical product yields in low and high severity FCC units	6
Table 1.2 : Properties of liquid product from low severity FCC unit	8
Table 1.3 : Properties of liquid product from high severity FCC unit	8
Table 1.4 : Various zeolites and their properties	11
Table 2.1 : Reaction yields at ~10 % conversion of naphthalene and tetralin	21
Table 2.2 : Average structural parameters obtained from NMR analysis.....	34
Table 2.3 : Stretched reaction times.....	49
Table 3.1 : Properties of 2-methyl naphthalene	57
Table 3.2 : Properties of decalin	57
Table 4.1 : Properties of Y zeolite and FCC catalyst.....	76
Table 4.2 : Properties of LCO.....	79
Table 4.3 : Typical product molecules identified based on the analysis of products	80
Table 4.4 : Yield of products from cracking of decalin over Y zeolite at 500°C	83
Table 4.5 : Classification of products based on the molecular species.....	85
Table 4.6 : Yields of molecular species at reaction temperature of 500°C.....	85
Table 4.7 : Yield of products from cracking of 2MN over Y zeolite at 500°C	95
Table 4.8 : Yields of molecular species from cracking of 2MN at 500°C.....	97

Table 5.1 : Product molecules identified based on the analysis of products	103
Table 5.2 : Experimental data of cracking of 2MN at various reaction temperatures at varying WHSV	106
Table 5.3 : Compound classes on cracking of 2MN at various reaction temperatures and WHSV	109
Table 5.4 : Length of bonds in 2MN after optimization of geometry in Dmol3	124
Table 5.5 : Yields of products from cracking of 2MN along with decalin at 550°C.....	128
Table 5.6 : Experimental data of cracking of LCO at 550°C.....	132
Table 6.1 : Kinetic parameters	139

NOMENCLATURE

A	Cross-sectional area of catalyst bed (m^2)
C^{exp}	Experimental value of molar concentration
C^{cal}	Calculated value of molar concentration
d	Diameter of reactor (m)
dz	Differential length of catalyst bed in the reactor(m)
E_i	Activation energy as per Arrhenius equation (kJ/mole)
$F_{i(feed)}$	Weight of i^{th} component of feed (g)
$F_{i(product)}$	Weight of i^{th} component of unconverted feed in product (g)
Gas	H_2 and C_1 to C_4 hydrocarbons
h	Height of the catalyst bed (m)
k_{0i}	Frequency factor as per Arrhenius equation (1/s)
N_{exp}	number of experiments
$P_{i(product)}$	Weight of i^{th} component of product (g)
r_i	Rate of reaction of i molecule
t	Time of injection of feed (s)
W_F	Weight of feed injected (g)
W_C	Weight of catalyst loaded into the reactor (g)
2D GC	2 dimensional Gas Chromatography
2MN	2-methyl naphthalene
ABD	Apparent Bulk Density
BDE	Bond Dissociation Energy
BET	Brunauer–Emmett–Teller

BYLP	Becke's three-parameter exchange functional combined with the Lee-Yang-Parr correlation functional
CLO	Clarified Oil
C/O	Catalyst to oil ratio
COTC	Crude to chemicals
DA	Di-aromatics (two ring aromatics including any side chain),
FCC	Fluid Catalytic Cracking
FCCG	FCC Gasoline
GC-MS	Gas Chromatograph with mass spectrometer
GGA	Generalized Gradient Approximation
HCN	Heavy Cracked Naphtha
LCO	Light Cycle Oil
LCN	Light Cracked Naphtha
MA	Mono-aromatics (Benzene & its derivatives)
NA	Naphtheno-aromatics (all aromatics with naphthenic ring)
OF	Objective function
PBU	Primary Building Units
PN	All paraffin products having C no > 4 and all Naphthenes
PONA	Paraffins, Olefins, Naphthenes & Aromatics
RGA	Refinery Gas Analyzer
SBU	Secondary Building Units
TA	Tri-aromatics (all aromatics having three rings or more)
TPD	Temperature-Programmed Desorption
USY	Ultra Stable zeolite Y
UCS	Unit Cell Size

WHSV Weight Hourly Space Velocity

XRD X-ray Diffraction

XRF X-ray Fluorescence

Subscripts

i Index used for referring components

j Index used for referring experiments

Greek letters

τ Residence time, s

ϵ Porosity of catalyst bed

ϑ_T Volumetric flow rate at reaction conditions (m^3/s)