DEVELOPMENT OF ZINC-BASED/ZSM-5 CATALYST FOR PROPANE AROMATIZATION

BY

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A THESIS SUBMITTED TO THE SCHOOL OF POSTGRADUATE STUDIES AHMADUBELLO UNIVERSITY IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE AWARD OF DOCTOR OF PHILOSOPHY IN CHEMICAL ENGINEERING

DEPARTMENT OF CHEMICAL ENGINEERING,

FACULTY OF ENGINEERING,

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APRIL, 2021

DECLARATION

I declare that the work in this thesisentitled '**DEVELOPMENT OF ZINC-BASED/ZSM-5 CATALYST FOR PROPANE AROMATIZATION'**has been performed by me in the Department of Chemical Engineering, Ahmadu Bello University, Zaria.The information derived from the literature has been duly acknowledged in the text and a list of references provided. No part of this thesis was previously presented for another degree or diploma at this or any other Institution.

Godwin Gbenga OSEKE_____ _____
Name of Student Signature Date

CERTIFICATION

This thesis entitled**DEVELOPMENT OF ZINC-BASED/ZSM-5 CATALYST FOR PROPANE AROMATIZATION**by Godwin Gbenga OSEKE meets the regulations governing the award of the degree of Doctor of Philosophy of Ahmadu Bello University, and is approved for its contribution to knowledge and literary presentation.

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DEDICATION

This thesis is dedicated to Jesus; the author, perfecter and finisher of my faith.

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Now unto God thathas the ability to do exceeding abundantly above all that we ask or think according to His divine power that is at work in us be all glory honour and praise for ever more. For the abundant supply of supernatural and extraordinary wisdom and intelligence, knowledge and understanding, sound health, overflow of inexhaustible resources, strength and courage, to Him be the glory.

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TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF PLATES

ABBREVIATION

BET	Brunauer-Emmett-Teller
BTEX	Benzene Toluene Ethylbenzene Xylene
FTIR	Fourier Transform Infra-Red
GC	Gas Chromatography
GHSV	Gas Hourly Space Velocity
H_2-TPR	Hydrogen-Temperature Programming Reduction
SEM	Scanning Electron Microscopy
TEM	Transmission Electron Microscopy
TOS	Time of Stream
XPS	X-Ray Photoelectron Spectroscopy
XRD	X-Ray Diffraction
XRF	X-Ray Fluorescence

ABSTRACT

Aromatization is an important process for catalytic conversion of light alkanes to aromatics which are essential feedstocks to petrochemical industries. A number of catalysts have been used for this transformation among which Zn/ZSM-5 emerged so far best owing to its good dehydrogenating activity, lower cost and environmental friendliness. Compared with similar metals used in aromatization reaction, zinc is known to be unstable at reaction conditionsdue to its low melting point and density, hence declines in alkane conversion and aromatic selectivity. Therefore, in this research,four different metals Me (where Me is iron, cobalt, nickel or copper of 1-3 wt. %) were co-impregnated with 2 wt. % zinc to formbimetallic catalysts Zn-Me/ZSM-5 in mitigating this stability challenge at reaction condition. The role of the second metal is to improve catalyst activity, stability and selectivity towards aromatics. The prepared catalystsphysicochemical properties were analyzed with XRD, BET, N_2-adsorption, FTIR, FTIR-Pyridine, SEM, TEM, H_2-TPR and XPS. The XRD and FTIRshowed that the bimetallic catalysts were crystalline and possessed basic features of HZSM-5. XPS analysis confirmed the metal species had oxidation states of +2. The XPS and H_2-TPRalso showed that there is synergistic metal-metal interaction between the co-impregnated metals with zinc through changes in binding energies of metals on HZSM-5 and reduction temperatures, which is believed to have strengthened and stabilized the zinc metal species at the reaction temperature. Incorporation of the selected metals with the zinc on HZSM-5 showed reductions in Bronsted acidity from the FTIR-Pyridine. N_2-adsorption isotherms confirmed that the metal modified catalysts were all microporous (90 % microporosity in surface area) as the parent HZSM-5. Performance test was conducted in a fixed bed reactor using gas hourly space velocity of 1,200 ml/hr. at 540 ^oC and atmospheric pressure. Zn-Fe/ZSM-5 showed improved propane conversion and selectivity

towards aromatic products for all metal compositions except for 1 wt. % Fe, when compared with Zn/ZSM-5 and HZSM-5. Zn-Co/ZSM-5 catalysts of 1 and 3 wt. % cobalt have improved and sustained propane conversion.Zn-Ni/ZSM-5 and Zn-Cu/ZSM-5 (1-3 wt. % of Ni and Cu) also showed sustained and improved propane conversion and selectivity better than Zn/ZSM-5 and HZSM-5 catalyst. This is because the metals have the same oxidation states with zinc.Co-impregnation of Zinc with selected metal improved the catalytic activity with sustained aromatic selectivity at an average 12 hours' time on stream as compared to parent HZSM-5 (10%) and Zn/ZSM-5 (50%). The products distribution for modified bimetallic catalysts showed reduced light hydrocarbon formation but enhanced aromatics production.All metal impregnated catalysts had improved selectivity for toluene with Zn-Co/ZSM-5 (2 wt. % each) toluene selectivity between 40 to 45% of the total aromatic products. Zn-Cu/ZSM-5 was highly selective towards m and o-xylene. Zn-1Fe/ZSM-5, Zn-1Cu/ZSM-5 and Zn-3Ni/ZSM-5 catalysts were highly selective towards ethylbenzene of about 10 to 15 %. 2 and 3 wt. % loading of impregnated metals with zinc had good selectivity for benzene of about 10 to 15 % of the total aromatic products. Equal 2 wt. % of Zinc with other metalperformed better among other catalysts for aromatic selectivity and stability out of whichZn-Ni/ZSM-5gave thebest in propane conversion (55 %), aromatic selectivity (85 %), and stability for twelve hours'time on stream. The effect of temperature variation on the best catalyst showed that temperature increase haspropane conversion and aromatic selectivity. Effect of flow rate increase on Zn-Ni/ZSM-5 (2 wt. % each) catalyst showed reduced conversion from80 to 38 %andincreased selectivity from 54 to 80 %. In general, aromatic yield for the bimetallic catalysts were improved and sustained by 2 wt. % equal metal dosage with Zn over Zn/ZSM-5 and HZSM-5 catalysts. Thus, more stable bimetallic bifunctional Zn-Metal based catalysts for propane aromatization were developed.

CHAPTER ONE

INTRODUCTION

1.1 Preamble

The catalytic conversion of light alkanes (hydrocarbons) to aromatic compounds is of research importanceto industrialists and academia alike. Aromatics produced (mainly, benzene, toluene, ethylbenzene and xylene) are used as feedstocks for the manufacture of valuable petrochemical building blocks in the manufacture of chemicals,polymers,detergents, pharmaceuticals, agricultural inputs and explosives (Choudhary *et al.*,2000;Bhan and Nicholas, 2008).

Aromatization of light alkanes is a relatively new attractive and economical route for the production of aromatics. Aromatization reaction is a very complex reaction involving a large number of complex chemical reactionsteps generally grouped into three stages:

I. Unsaturation or alkane activation reaction: Alkane transformation to alkene, that is the alkane C-H bond activation by protonation and carbonium ion dehydrogenation to carbenium ion and finally to yield alkene.
II. Oligomerization and cracking: Alkene (unsaturated hydrocarbon) inter-conversion to build-up higher alkenes by quick isomerization, β-scission and hydrogen removal from higher alkenes to form dienes (dehydrogenation).
III. Cyclization and aromatization: Cyclic chain development from dienes to cycloalkane and resonation of the double bond to C_6-C_{10}aromatic hydrocarbons (Meriaudeau *et al.,* 1999; Ha *et al*., 2002; Lukyanov *et al*., 1995; Guisnet *et al.*, 1992).

Aromatization is highly endothermic, therefore catalytic routes have been employed over the years to save energy and reduce cost. A number of catalysts have been used among which are Metal/Alumina, Zeolites Y, ZSM-5, Modernite and Zeolite beta.ZSM-5 catalyst has been reported to have the greatest application becauseof its unique two-dimensional pore system, relative slow deactivation ability, ability to withstand high temperatures, high activity and resistance to coke formation in many catalytic conversions. Light alkanes conversion (C_2– C_7) and alkenes (C_2=- C_4=) into useful aromatic compounds which are feedstocks to chemical and petrochemical industriesis one of the catalytic processes in which the metal modified ZSM-5 catalysts have proved their superiority. Light alkanes are majorly found innatural gas wells, associated gas and liquefied petroleum gas (LPG). There are several existing industrially commercialized processeswith use of ZSM-5 based catalysts for transforming light alkanes into aromatic compounds among which are: HZSM-5 (M2 Forming Process – Mobil Oil (Mnqanqeni, 2009, and Chen and Yan1986) and M- Forming Process – Mobil (Ga/HZSM-5 (Cyclar-BP/UOP (UOP, 2001) and Z-Forming (Mitsubishi Oil and Chiyoda) (Saito *et al.,* 1994); Zn/HZSM-5 (Alpha process of Asahi Chemical and Petrochemical) (Nagamori and Kawase 1998); Pt/K(Ba)L (AromaxTM process –Chevron – Phillips Chemical Co. (Asaftei *et al*, 2016); RZ- Platforming process – UOP [Tamm *et al*., 1998; UOP, 1999]; Aroforming from IFP; Salutec based on metal oxides-HZSM-5 (Asafteie*t al.,* 2016).

Parent HZSM-5exhibitsfavourable high cracking, isomerization and β-scission reactivity that lead to loss of carbon atoms to undesirable lighter hydrocarbon caused by rejection of hydrogen from surface throughhydrogen transfer to alkanes whichlimitsthe yield of obtainable aromatics yield (Bhan and Nicholas, 2008).

Modification of this parent HZSM-5 with activating metals which are largely in transition seriessuch as iron, manganese, molybdenum, nickel, platinum, vanadium, chromium, copper, zincand gallium helps to minimise cracking. These metals in the form of extra-framework species principally help in recombination of surface hydrogen (Xu and Lin, 1999; Shu and Ichikawa, 2001; Xu *et al.,* 2007; Xu *et al*., 2008). Zinc, gallium and platinum metals had shown highactivity and selectivity towards aromatics.

Despite the attention given to the utilization of platinum, gallium and zincas dehydrogenating metals on ZSM-5for light alkane aromatization, they have their shortcomings which limit their use.On one hand, platinumshowsgood dehydrogenationcharacteristics but deactivates easily, prone to hydrogenolysis of oligomers and cyclic compounds and it is expensive. Galliummodified ZSM-5 has the benefit of withstanding high temperature and not volatile under reduced atmosphere. It has drawn significant consideration because of its good dehydrogenation leading to high aromatic selectivityof about 60%and marginal leaching of metal species but highly expensive and hazardous to human health (Bhan and Delgass, 2008; Choudhary *et al.,* 2006). The health concern issuesin terms of its hazardous nature and the high price of gallium salt has limited its use. On the other hand, Zinc ion(Zn^{2+}), with complete d_{10} electronic configuration displays a good dehydrogenation, hence higher selectivity towards aromatic compound. However, it is unstable at aromatization process condition ($\geq$ 450 ^{o}C)because of its low melting point(Tshabalala and Scurrell, 2015: Sarath, 2015).

There are studies to stabilize zinc on HZSM-5.Lubango and Scurrell(2002) studied propane conversion to aromatics over bimetallic Zn-Fe/ZSM-5 at 490 ^{o}C and 4 atm at shorter time on stream. In the same vein, Zn-Cu/ZSM-5 was used for the aromatization of butane-butene to achieve aromatic selectivity of 68 %;the presence of butene was reported to be responsible for

the enhanced activation of butane (Asaftei *et al*, 2016). Zn-Ni/ZSM-5 bimetallic catalyst had been used for methanol aromatization. The presence of nickelminimized loss of zinc species by converting zinc oxide to Zn^{2+} to $ZnOH^{+}$species with aromatic yield of 56% (Jia*et al*., 2017).

1.2 Problem Statement

Zn/ZSM-5 catalyst has been reported to show loss of activity due to its instability for light alkane aromatization at reaction conditions and time on stream. This therefore reduces conversion, aromatic selectivity and formation of undesired alkanes.

1.3 Aim and Objectives

The aim of this research is to developZn-Me/ZSM-5 bimetallic catalysts for propane aromatization.

The objectives of this research work were to:

i. Synthesize of Zn-based ZSM-5 catalyst using wetincipient co-impregnation method (Zn, Zn-Fe, Zn-Co, Zn-Ni and Zn-Cu/ZSM-5).
ii. Characterize the synthesized catalysts using FTIR, Pyridine FTIR, XRD, XRF, BET, H_2-TPD, TEM, SEM and XPS.
iii. Comparepropane aromatization performance test of the prepared catalysts for activity, selectivity and stability in a fixed bed reactor of 9 mm internal diameter and 0.64 m height.
iv. Analyze obtained productsfrompropane aromatization using the prepared catalysts.
v. Determine of selectivities of eachcatalyst towards specific aromatic compound.

vi. Determine effect of temperature and feed flow rate study on conversion, selectivity and yield using the best catalyst.

1.4 Scope

This research work is limited tosourcing ammonium-ZSM-5 from Zeolyst International, and modified by metal impregnation to 2 wt. % Zn/ZSM-5 and the Zn-Me (where Me is the 1-3 wt. % of Fe, Co, Ni and Cu as bimetallic catalyst with fixed 2 wt. % of Zn). Propane aromatization was conducted in a fixed bed reactor of 9 mm internal diameter and 0.64 m height.

1.5 Justification

i. Production of stable, environmentally friendly and economically viable industrial catalyst for productionof aromatics for laboratory and industrial application from available light hydrocarbon.
ii. Selective production of catalyst tuned towards desired aromatic compound for targeted use from available local resources.
iii. Determination of optimum metal loading for improved aromatic production.
iv. Effective utilization and transformation of liquefiedrefinery gases to usable aromatic products for petrochemical use.
v. Production of aromatic compounds via this technology will improve Nigerian economy in petrochemical industries and minimize importation of expensive catalyst.

CHAPTER TWO

LITERATURE SURVEY

2.1 Hydrocarbon and Chemistry of Alkanes

The word ‘hydrocarbon’ means compounds containing carbon and hydrogen. Theyplay important roles in humanliving as energy supply sources. The major sources include coal, biomass and crude oil. Gaseous hydrocarbon includes liquefied petroleum gas (LPG),compressed natural gas (CNG) and liquefied natural gas (LNG) while liquid phase hydrocarbons are petrol, diesel and kerosene obtained from crude oil fractional distillation. Coal is a solid hydrocarbon which when passed through destructive distillation yield coal gas, coal tar, coke and ammoniacal liquor which are all hydrocarbon sources. Theyare used for production of polymers (polyethene, poly-propene, polystyrene etc.), solvents for paints, dyes and drugs. Hence, hydrocarbons are important in our daily life especially in the energy sector.Alkanes popularly known as paraffins (meaning lacking affinity) are examples of hydrocarbon,(Geetu, 2006).

There are three major classes of hydrocarbon, namely:

1. Saturated hydrocarbon having single bond i.e.straight or branched alkanes, cycloalkanes etc.
2. Unsaturated hydrocarbon: they are alkenes and alkynes-with double and triple carbon-carbon bond respectively.
3. Aromatic hydrocarbon.

Alkane is a major group member of aliphatic hydrocarbons consisting of only hydrogen and carbon atoms with all bonds as single bonds. They have a general molecular

formula C_nH_{2n+2}. Alkanes can be linear, branched and/or cyclic (cycloalkanes). Alkane are non-polar in nature and hence the reason for their poor reactivity with ionic compounds. The first member in alkane series is methane (CH_4) which is the most abundant in nature called natural gas. Ethane (C_2H_6) and propane (C_3H_8) follow down the homologous seriesof alkanes (Geetu, 2006). Ethane is the alkane next to methane in structural simplicity, followed by propane. Table 2.1 shows some physical characteristics of some alkanes.

Table 2.1: Some of the physical properties of alkanes (Morrison and Boyd, 1992)

Alkane	Formula	Boiling point [°C]	Melting point [°C]	Density [g·cm^{-3}]	Physical state [20 °C, 1 atm]
Methane	CH_4	−162	−182	0.668	gas
Ethane	C_2H_6	−89	−183	1.265	gas
Propane	C_3H_8	−42	−188	1.867	gas
Butane	C_4H_{10}	-1	−138	2.493	gas
Pentane	C_5H_{12}	36	−130	0.626	liquid
Hexane	C_6H_{14}	69	−95	0.659	liquid
Octane	C_8H_{18}	125	–57	0.703	liquid
Decane	$C_{10}H_{22}$	174	–30	0.730	liquid

2.2 Aromatics

Aromatic compounds are important petrochemical industries building blocks for global level of use and consumption. They are used for the production of intermediates for polymers. They include benzene, toluene, ethylbenzene and xylenes which are largely produced industrially with

global report of approximately forty million metric tons per annum for benzene and xylene each while the remaining goes for toluene and other aromatics as at 2012 (Figure 2.1 a and b). As at 2017, the global production declined a bit with Asia-Pacific still the largest region in the aromatics market, accounting for $75.0 billion or 40.3% share in the market. This was due to high consumption of aromatics in crude oil refining, automotive and pharmaceutical industries. North America was the second largest region in the aromatics market of 19.7% share in the market while Middle East was the smallest region in the aromatics market in 2017, accounting for 4.0% share in the market as shown in Figure 2.1 (c and d).

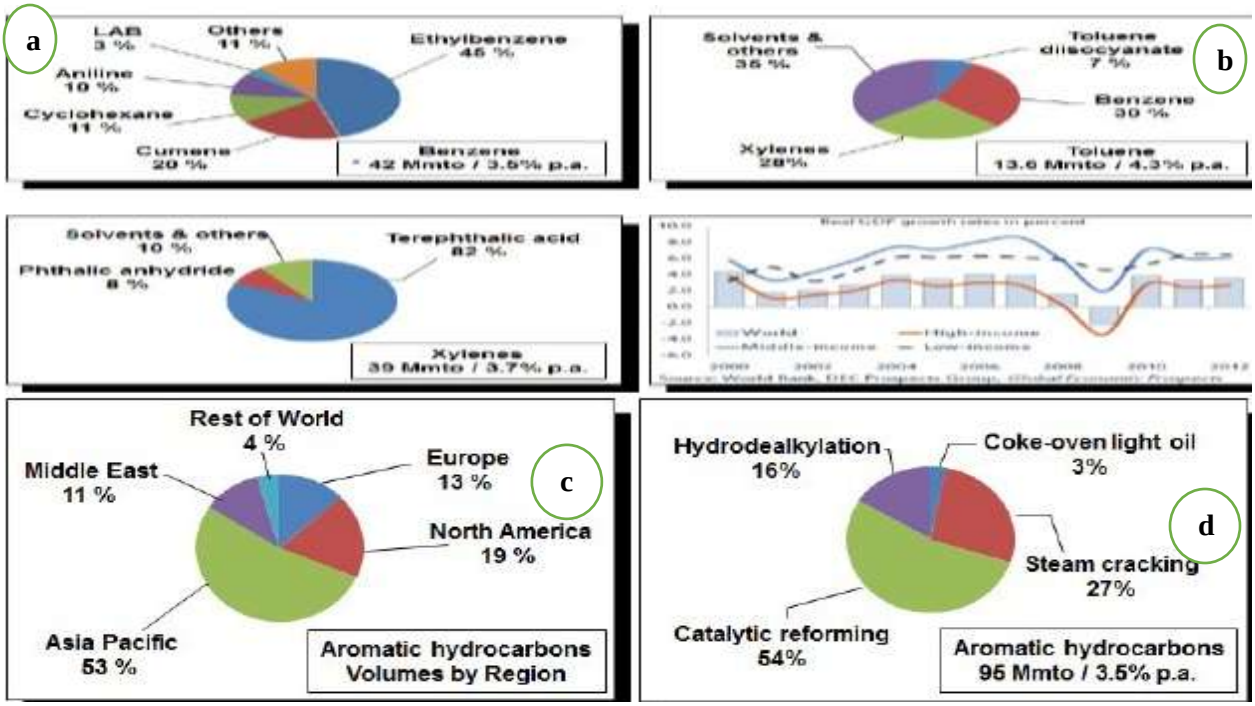


Figure 2.1: Global industrial production and consumption of aromatics (Bender, 2013)

2.3Zeolite Chemistry

The history of zeolites as a catalyst began around1756 with the finding of stilbite mineral in Sweden byCronsted (Coombs *et al.*,1959). Zeolite name emanated from zeo which means to boil and lithos meaning stones. When heated, it loses water as it seems to boil, hence the name

boiling stone (Barrer ,1982). The channels of naturalzeolite are aluminosilicateframework structure containing channels water and exchangeable cations which are mobile at 100^{o}C.

Zeolites arepermeable materialwith unique arrays ofpores and channels (3-15 Å)which are the most distinctiveproperties that are peculiar with molecular sieves.Apical oxygen present in the structure helped Al and Si linkage thereby enabling channels and cavities formation of unique molecular dimension which permits ease of diffusion of molecules of appropriate size to intracrystalline pores. Available zeolites that are commonly used are shown in Figure 2.2.

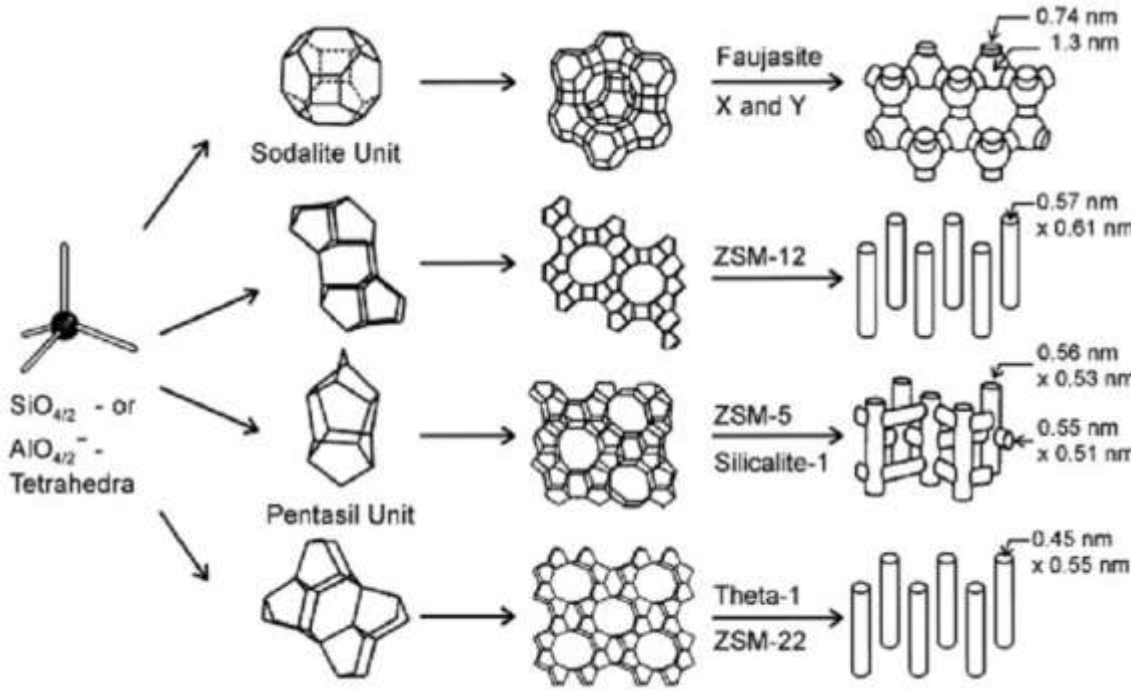


Figure 2.2: Zeolitestructures with micropore systems and dimensions (Weitkamp, 2000).

Pentasil units are the building basis for ZSM-5 and other silicates analogue. They are made up of interconnecting systems of ten-membered–ring pores (straight one and the other sinusoidal). Their microporous nomenclature from IUPAC stems from thepossessionequal diameters and pore width in the order of molecule dimensions (Weitkamp, 2000).

2.3.1 Zeolite acidity

Zeolites acidity is caused by isomorphous replacement of lattice Si^{4+} cations by trivalent cations such as Al^{3+}, Fe^{3+}or Ga^{3+}leaving it to be negatively charged which must be balanced by cation from an alkali. Bronsted acidity is always introduced by using protons as compensating ion. Ammonia ions have been used over time subsequently to exchange these original compensating cations and decomposed at high temperature to generate this acidity. Production of zeolites as catalysts depend on the generation of Bronsted sites (active sites) by using ammonium hydroxide for ion exchange and then calcining to have it in acidic form (Holmes*et al.*, 2011). High charge excess of+3/4 leads to strong acidity from generated proton from the linking oxygen atom to which it is attached (Sandoval-Diaz *et al.*, 2015). According to the use to which the catalyst may be subjected to, doping of aiding metals leads to formation of Lewis acid sites(Chezeau *et al.*, 1991). The total acidity of ZSM-5 catalysts is due to the amount of acid sites (proportional to the Al content of framework) and to the strength of acid sites (determined by the number of Al atoms that are adjacent to a proton as second- nearest neighbours). The activity of zeolite is dependent on the acid sites total number, Bronsted to Lewis sites ratio and the acid strength distribution.

2.3.2 Industrial zeolite catalystselectivity features

Some important properties like size and shape of zeolite makes it a widely used industrial catalyst especially the nature of its pore size and cavities as molecular sieves. The following are considered taking place in catalysis mechanism in and outside zeolite pores during reaction:

Reactant Selectivity: For molecular sieve application, this helps in reactions when one reactant is small enough for ease of diffusion through the micropores while others are excluded from diffusing through intra-crystalline pores.

Product Selectivity: Here, the steric effect of the newly formed product and the zeolite crystal size are taken into consideration for ease of diffusion out of the zeolite micropores.Small sized products diffuse easily through the micropores to the surface of the framework of zeolites to leave the larger ones to stay longer in the framework. This is highly considered to minimize further formation of undesired products and catalyst deactivation.

Restricted Transition-State Selectivity: This property accounts for reactions involving formation ofbulky intermediates in the pores which may not be sterically favoured to be converted to desired products because of lattice shape, micropore size andintermediate access to active sites.

Zeolite has applications in the following industrial processes:

i. Petroleum fractions conversion into gasoline in FCC unit.
ii. Methanol to gasoline conversion.
iii. Methanetransformation to liquid fuels over ZSM-5 zeolite.

2.4 Mechanism of Propane (C_3H_8) Aromatization

Light alkanes transformation to aromatics results increation of useful intermediates in the chemical and petrochemical industries such as higher value aromatic compounds which are benzene, toluene ethylbenzene and xylene (BTEX). Aromatization reaction as transformation of several hydrocarbons to aromatic compounds isvery complex, thus it involves different reaction steps. Lukyanov *et al.*(1995), Guisnet and Gnep (1996) and Biscardi *et al.* (1999) highlighted three major steps as follows:

i. Alkanes into alkenes transformation.
ii. Alkenes interconversions into higher alkenes

iii. Alkenes aromatization.

Further studies on aromatization of alkanes according to Meriaudeau and Naccache (1997), Guisnet *et al*. (1992) and Lukyanov *et al.* (1995) revealed series of reactions which include:

i. Alkane protonation (activation of C-H) through a pentavalent carbonium ion and of alkene C-H through a trivalent carbenium ion (through protonation).
ii. Carbonium to carbenium ion dehydrogenation tolower alkenes, $C_2 = C_4=$
iii. Oligomerization of small alkenes to higher alkenes, C_6- C_{10}.
iv. Rapid isomerization.
v. Beta (β)- scission.
vi. Alkylation/Dealkylation.
vii. Higher alkenes dehydrogenation to dienes.
viii. Dienes cyclization to cyclic alkenes.
ix. Cyclic alkenes dehydrogenation to cyclic di-alkenes
x. Aromatics formation, C_6- C_{10}.

The chemical species such as hydrogen H_2, light alkanes CH_4–C_8H_{18}, Olefins C_2H_4 – C_8H_{16}, and aromatics (BTEX) were found in several reactive steps as illustrated by the reaction pathway in Figure 2.3 (Michele *et al*., 2014).

2.4.1 Propane activation

The preliminaryinitiation of propane to aromatics as described by Derouane *et al*. (1994) involved the following major reactions steps:

I. Propane protolytic dehydrogenation: $C_3H_8 \rightarrow C_3H_6 + H_2$
II. Propane protolytic cracking: $C_3H_8 \rightarrow C_2H_4 + CH_4$

III. Hydride transfer to propane: $C_3H_8 + C_n^+ \rightarrow C_3H_7^+ + C_nH$

IV. Alkylation of propane: $C_3H_8 + C_n^+ \rightarrow C_{3+n}$ Alkanes $+ H^+$

V. Cyclization and aromatization: $2C_3H_8 \rightarrow C_6H_6 + 5H_2$

The first reaction route as shown in Figure 2.3 is rapid propaneactivation on acid sites by protolytic cracking or dehydrogenation (Michele *et al.*, 2014).

These reactions visibly revealed that together with protolytic cracking, hydride abstraction from propane yield carbenium ions aided with presence of sufficient strong Lewis acid sites. The formation of olefins (C_2H_4–C_8H_{16}) is followed by rapid oligomerizationto yield heavier olefins (dienes), which further activate propane (CH_4 – C_8H_{18}) with H-transfer reactions giving the equivalent alkane.

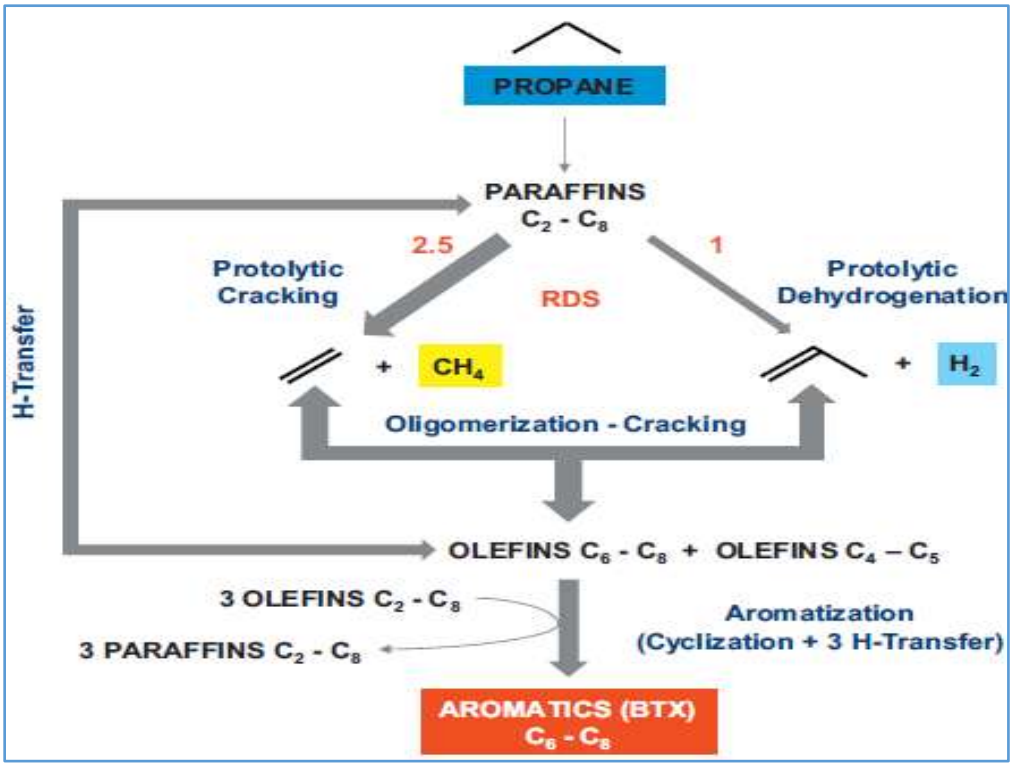
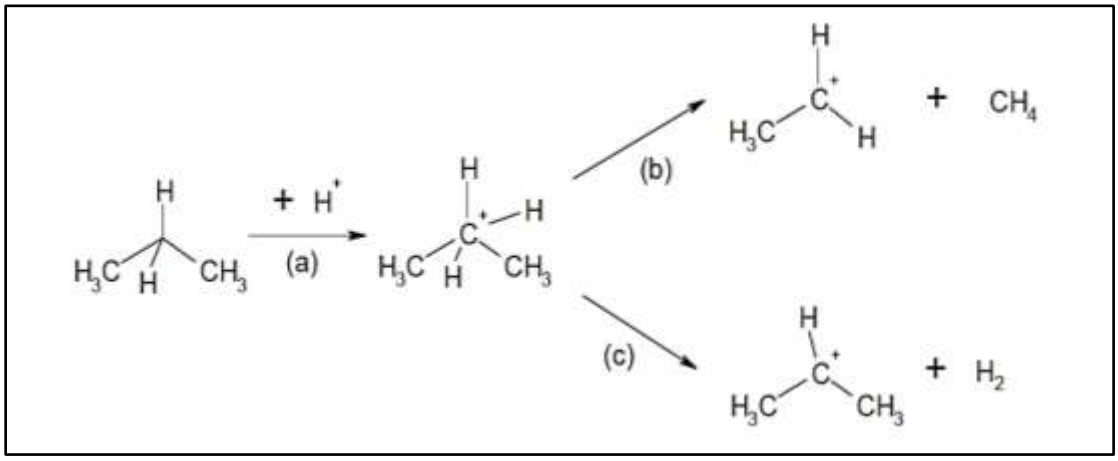


Figure 2.3: Reaction pathway for aromatization of propane (Michele*et al,* 2014)

Derouane *et al.* (1994) assessed the thermodynamic viability of the three reactions (aromatization, dehydrogenation, and cracking) at temperature range between 400 to 550^{o}C. The outcomespointed out that propane dehydrogenation is the least thermodynamically supported reaction at all temperatures. Propane cracking is the most thermodynamically preferred reaction over aromatization for temperatures below 502^{o}C.

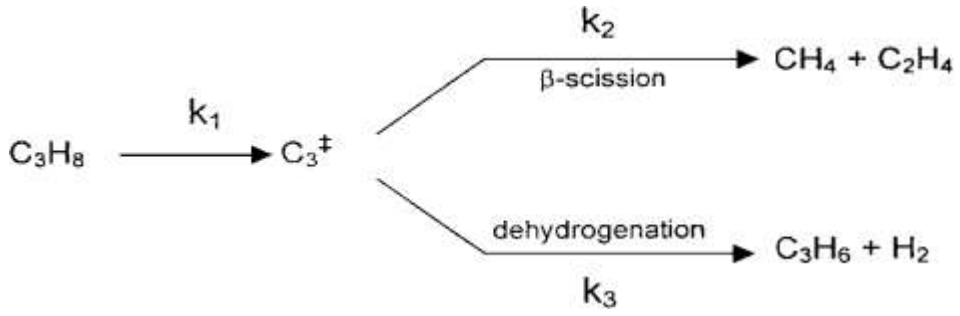
The similar mechanism was presented by Haag *et al.* (1984) for the monomolecular conversion of alkanes. It was shown that at temperatureof eight hundred (800) K, zeolites can protonate alkanes to form highly unstable pentavalent carbonium ions as shown in Scheme 2.1a. This carbonium ion formed quicklydeterioratefurther to form carbenium ion and an alkane as shown in Scheme 2.1b or a carbenium ion and hydrogen gas shown in Scheme 2.1c.



Scheme 2.1: Propane protolytic activation: (a) Alkane protonation to form carbonium ion (b) protolytic cracking, (c) protolytic dehydrogenation (Haag *et al.*, 1984)

The presence of zinc or othermetal cations increases dehydrogenation rate by lessening the concentration of intermediate alkenes during conversion of propane and also aids in recombining surface hydrogen thereby minimise cracking. Biscardi and Iglesia (1999) reported that when Zn

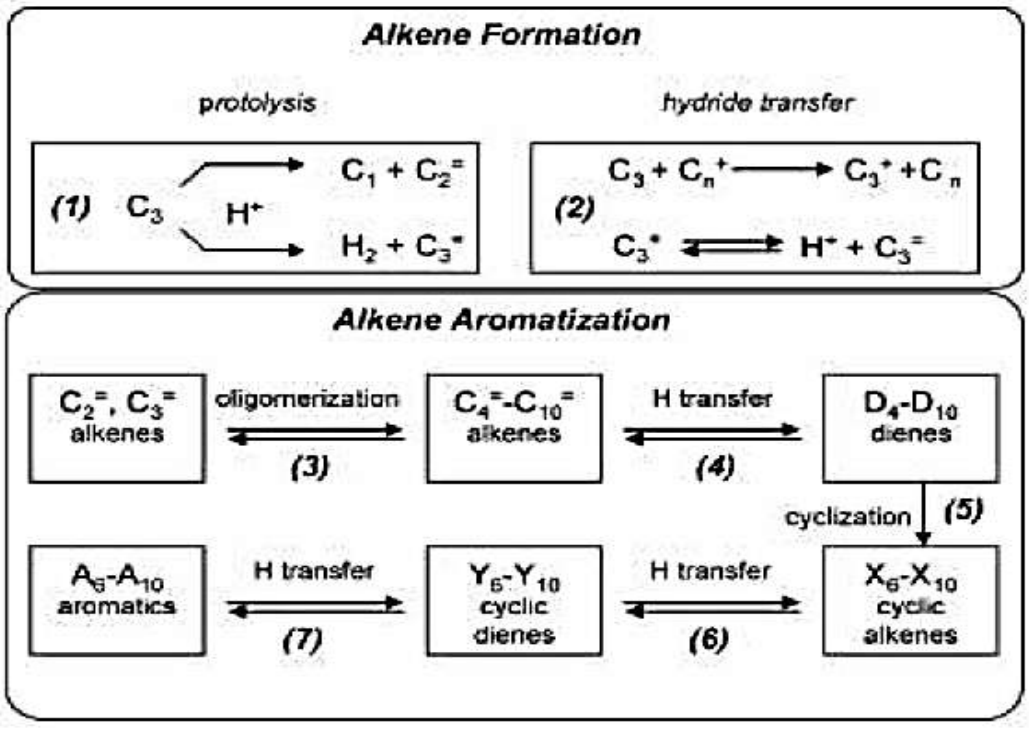
is added during activation, k_3 controls and β-scission rates reduces. Further increase in Zn content increases$k_1$uniformly more than k_3, hence $k_1$controls.



Scheme 2.2. Reaction mechanism for propane.

2.4.2 Propane conversion over gallium modified-HZSM-5

Propane conversion to aromatic compounds over Ga/ZSM-5 catalysts has been greatly employed in the industries. This reaction requires several chain growth and building up (oligomerization) and cracking events before aromatization (Biscardi and Iglesia, 1996). H-ZSM-5 zeolites without dehydrogenating metal takes the reaction through the route shown in Scheme 2.3.

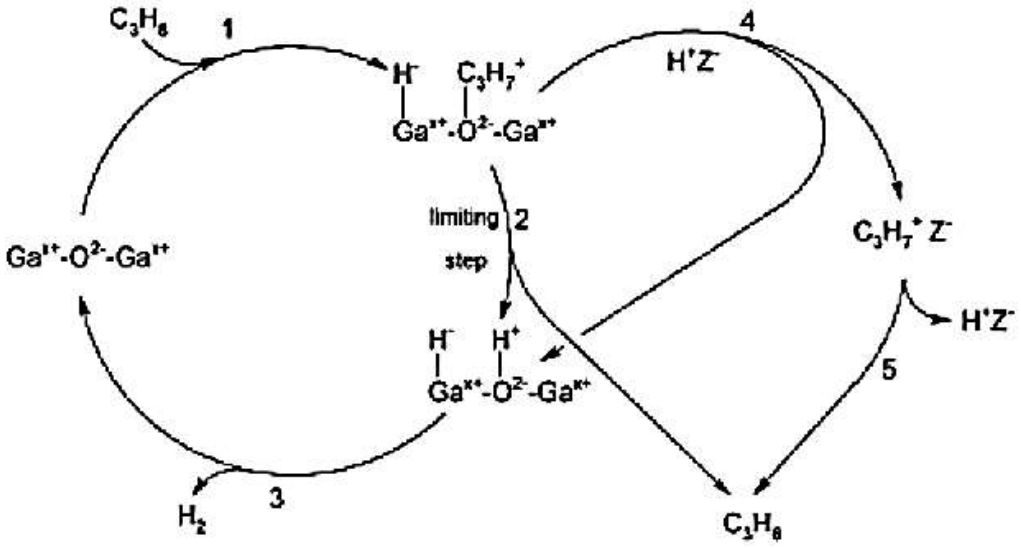


Scheme 2.3:Propane aromatization reaction route onparent HZSM-5 catalysts (Caeiro *et al.*, 2006).

Reaction 1 involves propane activation resulting inhydrogen removaland propane cracking. However, as shown by reaction 2, propane through hydride transfer can be dehydrogenated to form carbonium ions resulting from the adsorption of alkene product to further produce propene. The resulting product from reactions 1 and 2 (propene and ethylene) go throughquickcontinuous reactions: oligomerization, dehydrogenations, cyclization, dehydrocyclization, hydrogen transfers, dehydrogenation and finallyaromatization to C_6-C_{10}. Reactions 4, 6 and 7 are all hydrogen transfer reactions leading to formation of undesired short chain alkanes (from olefins) whose conversion is in similitude of slow reactions 1 and 2. This studies concluded that transformation of alkanes occur by the protolytic cracking and hydride transfer reaction pathways.

From the reaction Scheme 2.3shown for propane aromatization, gallium species as dehydrogenating metal work in hand with the Bronsted sites are responsible for the dehydrogenation of propane (reaction 1), oligomers formation (reaction 4) and cyclic olefins and diolefins formation (reactions 6 and 7) (Caeiro *et al.,* 2006; Nguyen *et al.,* 2006). During the aromatization of propane with gallium as dehydrogenation metal, the chemical state of gallium is yet to be properly ascertained.

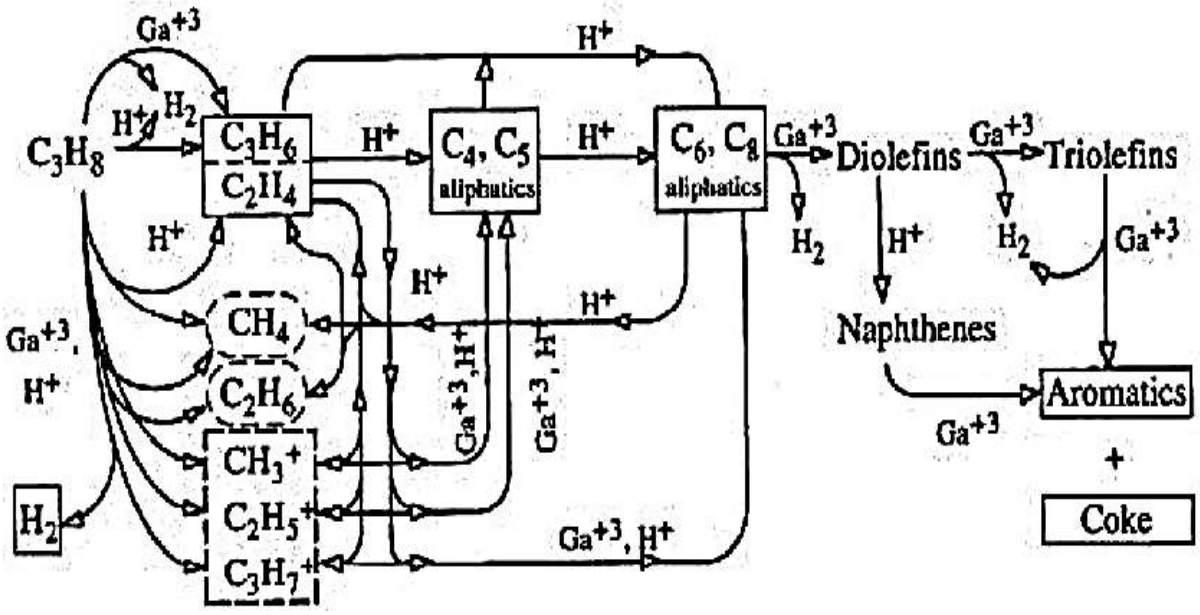
Propane is activated over Ga/ZSM-5 through a bifunctional mechanism in a similar way with the activation of propane over Ga_2O_3 as shown in Scheme 2.4 (Meriaudeau and Naccache, 1996)



Scheme 2.4. Propane dehydrogenation bifunctional mechanism of over Gallium modified HZSM-5 (Caeiro *et al.*, 2006).

The first stage shows theextraction of the hydride from propane by Ga^{x+} ions to form $C_3H_7^+$ adsorbed on the oxygen of Ga_2O_3 or the zeolite. The $C_3H_7^+$species further decomposed into H^+ and C_3H_6 on the zeolite with discharge of hydrogen H_2 through recombinative desorption reaction.

Scheme 2.5shows complete propane aromatization reaction mechanisms on gallium modified-ZSM-5.



Scheme 2.5: Propane aromatization reaction mechanism over Gallium modified-ZSM-5 (Derouane *et al.,* 1994; Caeiro *et al.,* 2006)

Zinc or gallium species on ZSM-5 perform the major role of speeding up the recombination of surface hydrogen, produced through dehydrogenation and dehydrocyclization steps in converting alkanes to aromatics (Nicolaides *et al.,* 2001; Biscardi and Inglesia, 1999).Dehydrogenation is essential to avoid further cracking of oligomerized alkene to alkane thereby limiting BTEX selectivity. This is why low aromatic selectivity has been reported and recorded for use of parent HZSM-5 in light alkane aromatization.

2.4.3 Mechanism of propane aromatization over zinc modified-ZSM-5

The dehydrogenation equation of zinc in aromatization is given by $[ZnH]^+ + H^+ \rightarrow Zn^{2+} + H_2$ where the protonic sites are principally accountable forZnH^+ species sift caused by propane dissociation. Light alkanes and alkenes transformation to aromatic compoundsinvolves lengthening carbon atom chain from six upward. Series of consecutive and parallel reactions occur which include alkanes to alkenes dehydrogenation, alkene oligomerization to dienes and trienes, resulted dienes and trienescyclization to naphthenes and dehydrocyclization of

naphthenes into corresponding aromatic hydrocarbons. Alkane dehydrogenation occurs because of carbon-hydrogen bond cleavage alongsidecorresponding alkenes and of hydrogen atom formed. The carbon-carbon bonds in alkane possessing lower bond energy than carbon-hydrogen bond has the likelihood to been cracked with formation of lower alkanes (C_1, C_2) and alkenes. This cracking reaction is responsible for the reduction in selectivity to aromatics hence the need for dehydrogenating metals (Tian *et al*., 2014).

The alkenes from cracking and dehydrogenating reactions proceeds further to isomerization, oligomerization to higher alkenes and dienes, cracking (β- scission) and cyclization reactions with particularly formation of naphthenes. The resulted naphthenes are further dehydrogenated into respective aromatics and alkanes as a result of hydrogen transfer.

Zn/HZSM-5 catalysts contain average acidity which reduces cracking. Well dispersed zinc inZSM-5 has cationic stability in form of Zn^{2+} while $ZnOH^{+}$will require two Al tetrahedra (-O-Zn^{2+} -O charge compensation because of its lowthermal stability. Zn^{2+} is the Lewis acid sites responsible for alkanes to alkenes and oligomers dehydrogenation to oligomers to dienes, suppression of β-scission rates and enhances removal of surface hydrogen atom thereby preventing hydrogenation backward reaction of alkenes needed for cyclization and finally aromatization. In co-catalyst containing zinc cations Zn^{2+},the zinc oxide serves as hydro-dehydrogenating component while ZSM-5 in hydrogen form serves as acidic component. Dispersion of zinc oxide on HZSM-5 is carried out by mechanical mixing and heating the mixture at 500^{o}C or wet impregnation.

Zinc oxide alone is not active to directly dehydrogenate propane but it is a strong hydrogen adsorbent which prevents hydrogenation of alkenes(backward reaction). The behaviour of ZnO/HZSM-5 co-catalyst obtained by physical mixture is different from ZnO/HZSM-5 obtained

by wet impregnation. During the heating of physically mixed zinc oxide and HZSM-5(strong ≡Si–OH–Al≡ and low silanol a ≡Si–OH), zinc cations (Zn^{2+}, ZnO^{+}) are produced which are active for aromatization of alkanes and alkenes as given in equation (i) (Meriaudeau and Naccache, 1997).

$$ZnO + 2H+ -OZ \rightarrow Zn^{2+} (- OZ)_2 + H_2O \qquad [2.1]$$

Only a small amount of zinc oxide migrates into the zeolite pores and reacts with the hydroxyl bridging groups. (Asaftei *et al.*,2009, Asaftei *et al.,* 2016). Zinc oxide in the combined catalyst may promote the activation of alkane's molecules by a polarization effect of carbon-hydrogen bondsand lead to molecular hydrogen formation via recombinative desorption of hydrogen atoms in dehydrogenation reactions.

2.5 Transition Metals Chemistry

Transition elements are elements with partially or completely filled d and f-orbitalsas atoms or ions.In the periodic table, they occupy four series in the middle part of the table (group 3-12) between s and p-block elements in the following order: scandium-zinc (Atomic number 21-30),Yttrium-Cadmium (Atomic number 39-48), Lanthanum-Mercury (Atomic number 57-80) and finally Actinium-Copernicium(Atomic number 89-112) respectively(Sarath, 2015). Zinc, cadmium and mercury do not have partially filled d subshell either in the elemental state. They exhibit metallic properties through transits between s and p-block properties s-block elements. They also displayelectropositivity from s-block end to the smallest electropositivity p-block elements hence the nametransition elements(Sarath, 2015).

2.6 Formation of Alloy and Solid Solution in Bimetallic Catalysts

Alloy is the combination of metals in homogeneous solid solutions. One active metal is evenly distributedover atoms of the others. This help in properties compensation between metals to form a desired material for a particular use. Examples of industrial alloys include: steels andstainless steel (made up of Mn, Cr, V, Mo and Fe), brass (Cu-Zn) and bronze (Cu-Sn)(Sarath, 2015).

The following are the conditions; which metals must satisfy to form solid bimetallic solutions (Smith *et al*., 2006; Hume-Rothery, 2002):

i. ***Atomic size:***Stable bimetallic alloy can be formed with metals of atomicradii difference not more than 15% to avoid creation of substantial lattice distortions that will lead to formation of newphase.
ii. ***Similarity in crystal structure***.
iii. ***Similarity in electronegativity:*** This helps in formation of substitutional solid solution instead of compound.
iv. ***Oxidation states similarity.***With other conditions fulfilled, equal valency whether at stable state of transitory state of metals enhances intra and inter orbital mixing.

Presented in Table 2.2 are the physical properties of the first transition series taking into consideration the condition for bimetallic solutions.

Table 2.2 gives the summary of the properties of first transition series which form the basis for decision in formation of bi or tri-metallic solid solutions:

Table 2.2: Some important properties of the first d-block series (Sarath, 2015)

A	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Co	Zn
No	21	22	23	24	25	26	27	28	29	30
1	$3d^14s^2$	$3d^24s^2$	$3d^34s^2$	$3d^44s^2$	$3d^54s^2$	$3d^64s^2$	$3d^74s^2$	$3d^84s^2$	$3d^44s^2$	$3d^{10}4s^2$
2	160	146	131	125	139	126	125	124	128	133
3	--	90	88	84	80	76	74	72	69	79
4	81	76	74	69	66	64	63	63	--	--
5	fcc	hcp	bcc	bcc	bcc	bcc fcc	hcp fcc	fcc	fcc	hcp
6	3.1	4.5	6.1	7.2	7.6	7.9	8.7	8.9	8.9	7.1
7	1817	1998	2173	2148	1518	1809	1768	1726	1356	693
8	3003	3533	3723	2138	2423	3723	3173	3003	2868	1179
9	+3	+4	+3,4,5	+2,3,6	+2,3,4,7	+2,3	+2,3	+1,2	+1,2	+2
10	632	659	650	652	717	762	758	736	745	906
11	1.3	1.5	1.05	1.6	1.05	1.8	1.8	1.8	1.8	1.6
12	15.9	15.5	17.6	13.8	14.6	15.3	15.2	17.6	13.0	7.4
13	338.9	445.6	443.6	305.4	224.7	353.9	389.1	380.7	338.9	114.6

A= Properties

1*=Outer electronic configuration 2*=Atomic radius (pm) 3*=Ionic r M^{2+}(pm)

4*=Ionic radius M^{3+}(pm) 5*=Crystal structure 6*=Density (g/m3) 7*=Melting Point (K)

8*=Boiling Point (K) 9*=Stable Oxidation states 10*=1st Ionization energy (kJ/mol)

11*=Electronegativity 12*=Heat of fusion (kJ/mol) 13*=Heat of vap.(kJ/mol)

The chemical properties oftransition metals are based on the electron mobility in the partially filled d-orbital which include the following:

i. Catalytic properties
ii. Formation of alloys
iii. Show variable oxidation states
iv. Formation of coloured compound
v. Form paramagnetic species because ofpartially filed shells
vi. Form coordination compounds (complexes)and organometallic compounds(Sarath, 2015).

2.7 Chemistry and Properties of Zinc Metal

Zinc is the last metal of the first transition series with completely filled d-orbital like Cadmium and Mercury in second and third transition series respectively.Zinc metal possess some unique properties when compared with other d-block elements. These are given in the sections below.

2.7.1 Melting and boiling points

The d-block elements generally possess higher melting and boiling points greater than s-block elements due to higher electron density. Zinc has the lowest melting and boiling points when compared with other elements in the 3d-block. At higher temperature, it melts and vaporises reducing its concentration in any system of application.This is responsible for its instability when impregnated on HZSM-5 for light alkane aromatization. Figure 2.4 shows the melting point and boiling point fall as compared to other metals in the series. These inform the selection of other stabilizing metals like iron, cobalt, nickel and copper of higher densities, melting and boiling points than zinc, nearly equal electronegativities and oxidation states. These are clearly shown in section 2.6, Table 2.2 and Figures 2.4 and 2.5.

2.7.2Density and electronegativity

Though d-block metals exhibit higher densities when compared to s- and p-block elements, they are less electropositive in comparison with alkali metals. The density and electronegativity increase from scandium to copper but falls when it gets to zinc. Figure 2.5 a and b shows the changes in densities and electronegativities respectively.

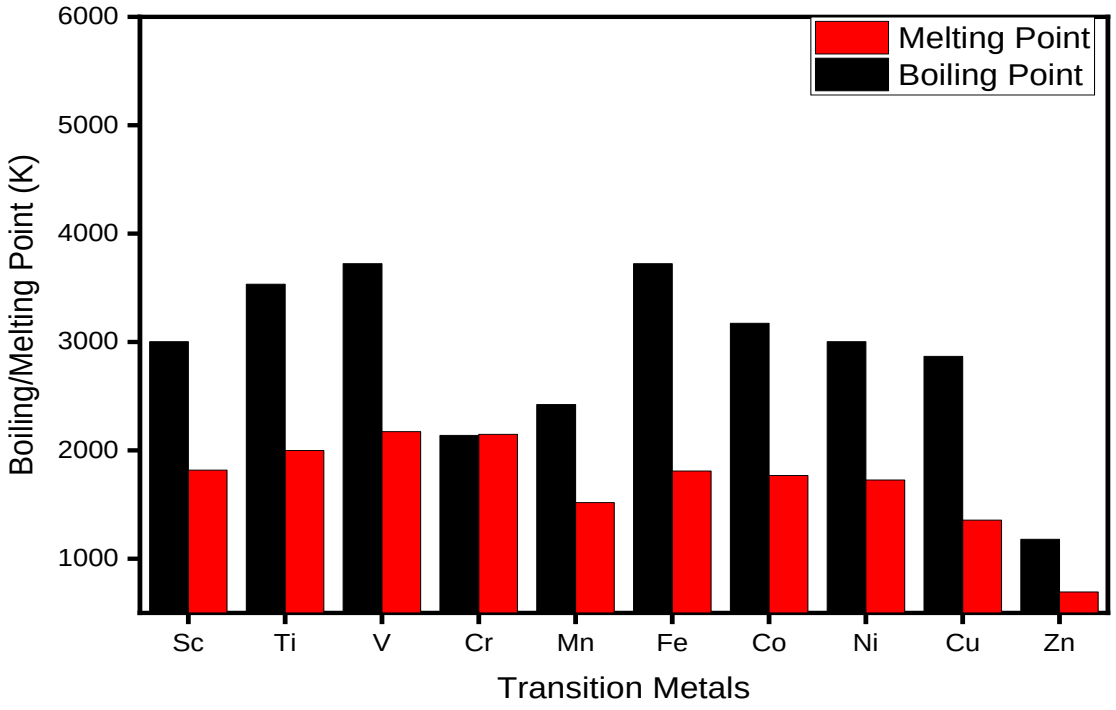


Figure 2.4: Melting and boiling point of 3d-series(Sarath, 2015)

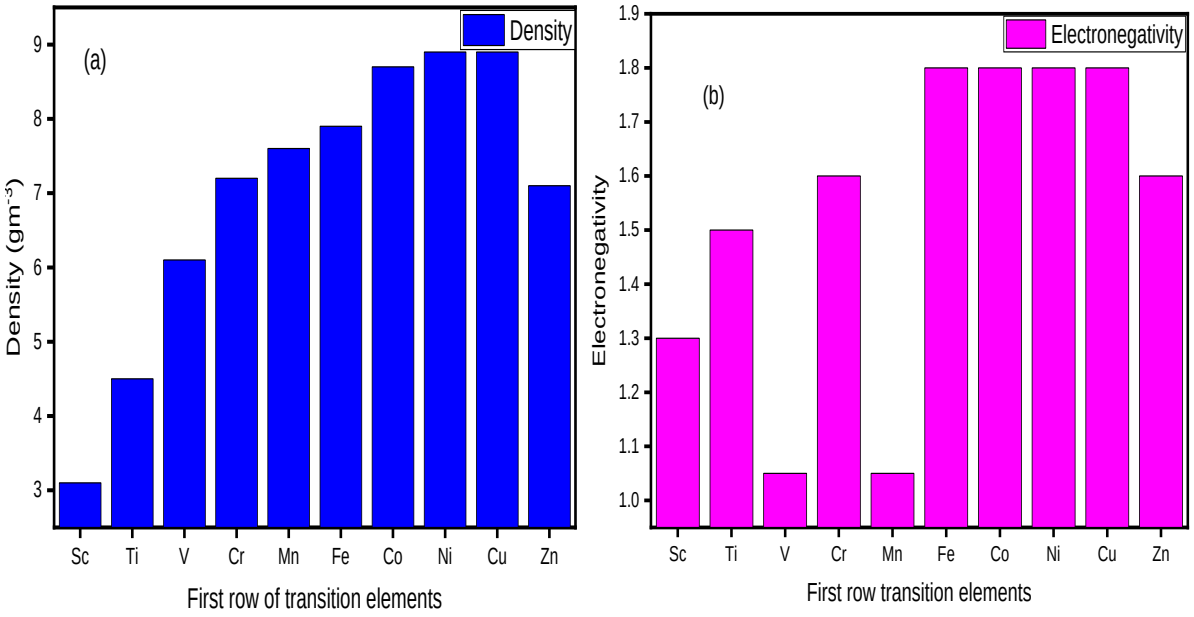


Figure 2.5: Variation in densities (a) and electronegativities (b) of 3d-series.(Sarath, 2015)

Iron, cobalt, nickel and copper appear to have nearly similar properties worthy of co-impregnation with zinc as the last metal on the series in strengthening its stability when impregnated on HZSM-5 for aromatization.

2.7.3 Zinc oxide

Pure crystalline zinc oxide is a white powder that is thermochromic (changes colour) in nature, with reversible white to yellow transition. Oxygen loss from the surface due to instability is responsible for the colour change (Wiberg *et al.*,2001). Zinc oxide is amphoteric in nature, does not dissolve in water but soluble in inorganic acids. Zinc oxidevaporizes around 1975 ℃ with a standard oxygen pressure. In a reaction with carbon when heated, it vaporizes at 950 ℃ (Greenwood and Earnshaw, 1997). The decomposition equation is given in equation (ii).

$$ZnO + C \rightarrow Zn(Vapour) + CO \qquad [2.2]$$

2.8 Related Aromatization Past Researches on Modified ZSM-5 Catalysts.

Use of ZSM-5 as an efficient catalyst for light alkane aromatization had been reported to be as a result of its linear alternating and interconnected unique properties thus giving it a three dimensional in nature. This favours dispersion of anchored metals on its pores, aromatic products shape selectivity, its acidity andhydrothermal stability thus making it highly preferred among other zeolites. This sinusoidal channel uniqueness of its structure suppresses formation of longer chain hydrocarbon (coke precursors and naphthenes) which are larger than its micro-channels size hence its coke resistant ability (Mroczek *et al*., 1991; Corma, 2003; Bellussi and Pollesel, 2005; Kim *et al.*, 2012; Momayez *et al*., 2015).

The need to improve the selectivity of HZSM-5 towards aromatics had led to screening of several metals anchored on the zeolite for dehydrogenation purpose. Platinum, Gallium and Zinc were

the most outstanding dehydrogenating metals base on catalytic performance test as they were incorporated on ZSM-5. However, despite their high dehydrogenating effect, they have their flaws.

Platinum is of high cost and has hydrogenolysis limitation (Maggiore *et al.,* 1992). Gallium similarly is very expensive alongside with associated health hazard concern of handling (Ogunronbi *et al.,* 2015; Xiao *et al.,* 2015). Zinc is cheap and highly dehydrogenating but unstable at operating temperature (Asaftei *et al.,*2016; Dauda *et al.,* 2020). Hence the need to stabilize the zinc at reaction condition arise. Some of the approaches to mitigate this challenge include incorporating Zn into the zeolite intra-framework or create hierarchical structure in the zeolite; while others are focusing on introducing a second metal to producebimetallic catalysts of high improved activity and selectivity towards aromatic compounds (Guisnet *et al.,* 1991; Mroczek *et al.,*1991; Lubango and Scurrell, 2002; Caeiro *et al.,* 2006; Penner andArmbrüster, 2015; Dauda *et al*., 2020).

Design of bimetallic catalysts for aromatization of light alkanes are aimed at new prospect for new catalyst synthesis geared towards improving catalyst stability, activity and selectivity towards desired product. This creates new electronic and chemical properties that are quite different from those individual materials.

New mixed orbitals, inter-atomic bonds and intra-metallic bond length and interaction changes are formed leading to ligands and strain effects (Jarvis *et al.,* 2018). A good number of bimetallic

catalysts have been used for hydrocarbon conversions and other reactions. The second metal were added to help enhance and promote metal dispersion, stability and activity of active dehydrogenating metal on ZSM-5 which will in turn improve selectivity towards desired products. Examples of bimetallic catalytic reactions in which the effect of the second metal added improved catalyst stability, activity and aromatic selectivity includes: Propane and cyclohexane conversions over Pt-Cr/ZSM-5 (de Araujo and Schmal, 2002), Pt-Zn/ZSM-5 for propane dehydrogenation (AlZahrani, 2004), methanol conversion over La-Zn/ZSM-5 (Youming *et al*., 2011), Zn-Mo and Fe-Mo on ZSM-5 for methane dehydroaromatization (Abdelsayed *et al.,* 2015; Al-Fatesh, 2015), methane-carbon(iv)oxide reforming over bimetallic Ni–Co/Al_2O_3(Al-Fatesh, 2015), methane and heptane aromatization over Ga–Zn/ZSM-5 (Li *et al.*, 2018), deactivation mechanism and regeneration study of Ga–Pt/HZSM-5 catalyst in ethane dehydroaromatization (Bai *et al*., 2018), aromatization of naphtha and methane over Pt-Zn/HZSM-5 (Jarvis *et al.,* 2018; Jarvis *et al.,* 2019) and methanol aromatization over Zn-Ni/ZSM-5 (Jia *et al.*, 2017).

2.8.1 Research gap

All past works in propane conversion to aromatic compounds over metallic/ZSM-5 has not recorded appreciable selectivity because of its short carbon length. The use of Zn on HZSM-5 as a highly dehydrogenating metal is posed with instability challenge. Co-impregnation of metals of nearly equal properties as given in section 2.5 would enhance its stability thus increasing activity and selectivity towards aromatic compounds.

2.9Adsorption Isotherm for Catalyst Surface Properties Determination

Porous nature of heterogeneous catalysts stems out from the methods of preparation which may include.

i. Precursor precipitation from solution to form porous catalyst
ii. Hydrothermal crystallization to yield uniquely arranged microporous intra-crystalline molecular sieves
iii. Thermal removal of volatile materials during thermal treatments (calcination) as we have in wet incipient impregnation
iv. Components selective suspension
v. Employing different shaping procedures for special use in industrial set ups which include tableting, extrusion, spray drying.

The pore sizes are grouped into three major classes which include:

i. Microporosity (size less than 2.7 nm)
ii. Mesoporosity(2 nm less than size less than 50 nm),
iii. Macroporosity (size greater than 50 nm).

Adsorption isotherm using nitrogen gas atboilingtemperature(77K) is generally employed in the determination of pore texture and surface area of catalysts.

There are four commonly used IUPAC classification. They are:

i. ***Type II (Macroporous solids)***: It's formed monolayer of molecules adsorbed that is dominant at a relatively low pressure formation while multilayer occur at high relativepressure: the thickness of adsorbate graduallyrisesto reach the pressure of condensation pressure.

ii. ***Type IV (mesoporous solids)***: It's the same process at low pressure with microporous solids but at high pressure,mesopores adsorption tilts toward formation of multilayer formation till condensation is reached,creating a sharp increase in adsorption volume. Immediately the mesopores are occupied, adsorption continues but on the low external surface. Carrier oxides used as carriers and most catalysts are typical examples.

iii. ***Type I (microporous solids)***: Because of strong interface between pore walls and adsorbate in microporous solid, adsorption happens at a relatively low pressure. Filling up the pores often require higher pressure which is enhanced by intermolecular interactions. Adsorption proceeds outside the surface of the micropores ones they are filled. Zeolitic catalysts fall in this category.

iv. ***Type VI (uniform ultra-microporous solids)***: Here, adsorbate surface interaction is a key factor upon which adsorption pressure is dependent on (Leofanti *et al.,* 1998).

CHAPTER THREE

MATERIALS AND METHODOLOGY

This section presents the list of chemical compounds, analytical equipment, laboratory tools and methodology employed in this research.

3.1 Materials

The list of chemicals in this researchwork are given in Table 3.1

Table 3.1: List of chemicals in this research

S/N	Materials	Grade/Percentage purity	Manufacturer
1	Commercial NH_4-ZSM-5 (Si/Al = 50)	Laboratory grade	Zeolyst International, USA
2	Zinc nitrate	99.5 %, analytical grade	Sigma Aldrich, Kaduna
3	Copper nitrate	99.5 %, analytical grade	Sigma Aldrich, Kaduna
4	Cobalt nitrate	99.5 %, analytical grade	Sigma Aldrich, Kaduna
5	Iron nitrate	99.5 %, analytical grade	Sigma Aldrich, Kaduna
6	Nickel nitrate	99.5 %, analytical grade	Sigma Aldrich, Kaduna
7	Nitrogen gas	99.99 %, laboratory grade	BOC Gas Company, Kaduna

8	Propane	99.99 %, laboratory grade	BOC Gas Company, Kaduna
9	Helium	99.99 %	BOC Gas Company, Kaduna
10	De-ionized water		Chemical Engg. Dept. A.B.U, Zaria

3.2 Equipment

The equipment used in this research are listedin Table 3.2:

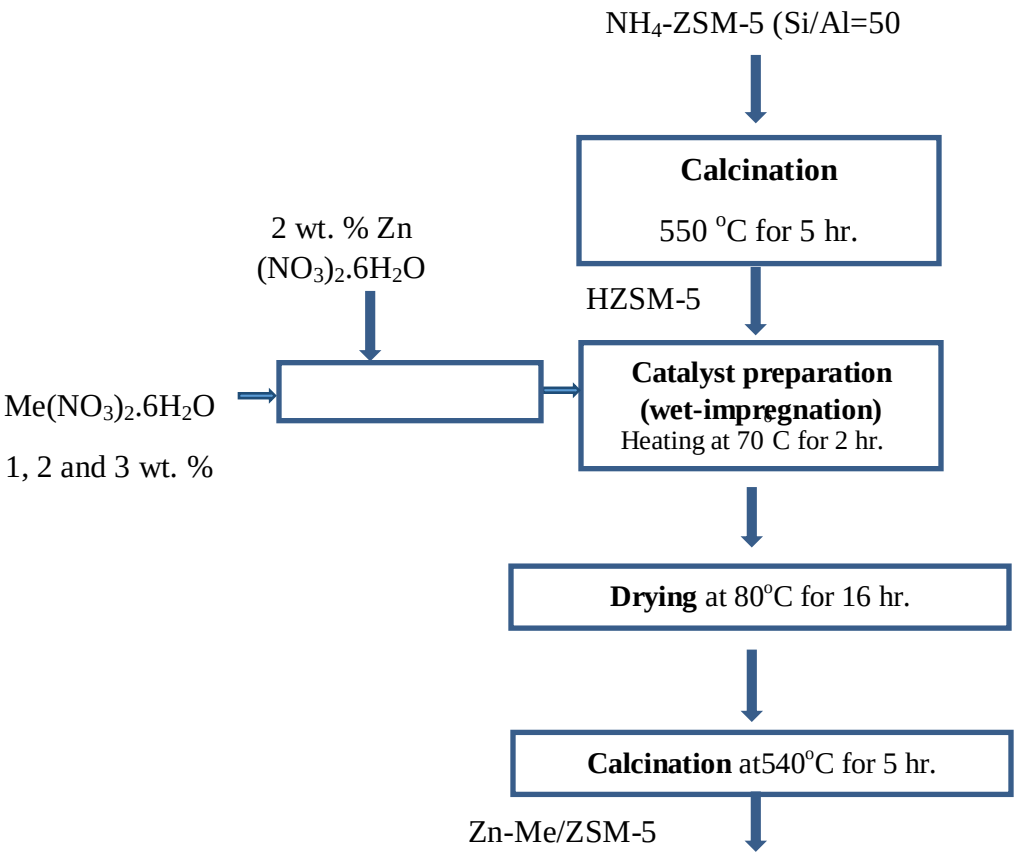
Table 3.2: List of equipment

S/N	Name	Model	Manufacturer	Availability
1	Thermometer	Pyrex	Pyrex	NARICT
2	Furnace,	LH 120/14 Nabertherm ,	Nabertherm , Bremen, Germany	Chem. Engg. A.B.U.
3	Fixed-bed reactor	Fine Reactor®-4100	Fine Reactor	NARICT
4	Hydrogen generator			NARICT
5	Weighing balance	Adventurer ModelAV264	Pro X Phe Netherland	NARICT
6	Heating mantle	AD574DT, Faiotech	Faiotech Sci. Instrument, Germany	Chem. Engg. A.B.U.
7	Online GCMS,	Buck Scientific GC 910	Buck Scientific GC 910	National Research Institute of Chemical Tech. Zaria, Kaduna.
8	FTIR Machine	FTIR – 8400S.	Shimadzu, Japan.	
9	XRF-Machine	NITON XL3t XRF	Thermofisher Scientific Waltham, Massachusetts, USA	KADPOLY
10	XRD Machine	Empyrean Panalytical BV	PANanalytical, Netherland	Umar-Musa Yaradua University,

				Katsina
11	SEM	Pro X Phenom model, Netherland	Pro X Phenom Netherland	Research Institute for
12	TEM	Hitachi S-4800		Chemical Industry,
13	XPS	Axis Ultra DLD	Kratos Analytical ltd. Manchester.	Beijing, China
14	TPR	Micrometrics Auto Chem 2920	Micrometrics	
15	BET	Micromeritics ASAP-2020	Micromeritics	University of Nottingham

3.3 Methodology

The methodology employed for this research is presented in the flow chartin Figure 3.1.



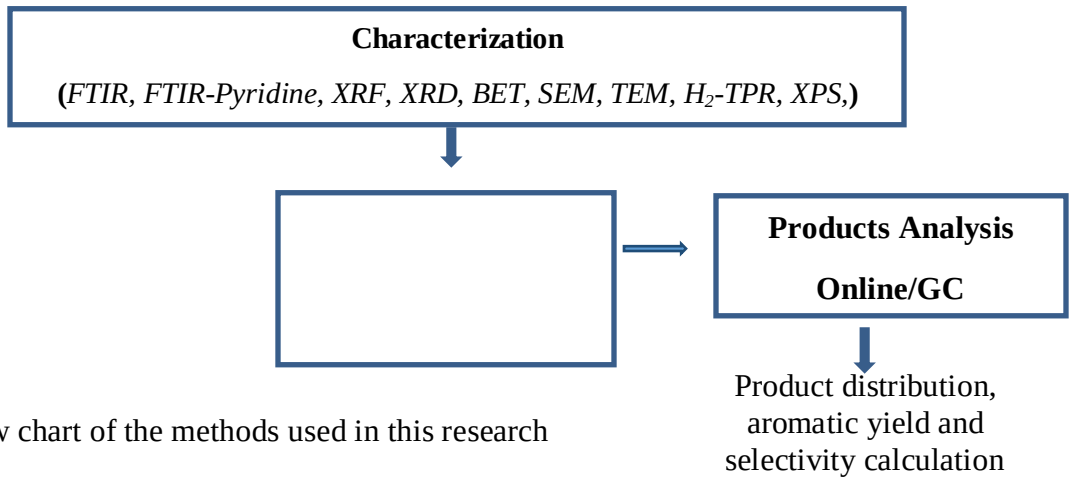


Figure 3.1: Flow chart of the methods used in this research

3.3.1 Catalyst experimentalpreparation

NH_4ZSM-5 (Si/Al = 50) sample used in this experiment was commercially sourced from Zeolyst International. The ammonia present wasremoved by calcinationin furnace for five hours at 550 ^oC to have it inacidic form (HZSM-5).

3.3.2 Preparation of Zn-Metal modified/HZSM-5

Acidic ZSM-5 sample was impregnated with $Zn(NO_3)_2$,to obtain 2 wt. % Zn/ZSM-5. $Zn(NO_3)_2$ was co-impregnated with respective dosage of $Fe(NO_3)_2$, $Co(NO_3)_2$, $Ni(NO_3)_2$and $Cu(NO_3)_2$, heated to dryness in heating mantle for two hours at 70^oC to obtain 1-3 wt. % of the metals on ZSM-5. The samples were then oven dried to remove moisture present at 80^oC for 16 hoursbefore calcination in a temperatureprogrammed furnace at 550^oC for 5 hours. During calcination, the impregnated metal nitrates precursors were converted by the giving off nitrogen (iv) oxide totheir respective oxides. The samples were denoted as Zn-Me/HZSM-5.

3.3.3 Catalyst characterization

Modified catalysts were characterized by the following analytical methods.

3.3.3.1 X-Ray Diffraction

Catalyst crystallinity was determined using the XRD patterns obtained from Rigaku MiniFlex II X-ray diffractometer using Cu Kα radiation (operated at 40 kilovolts and 40 mill ampere, K_{alpha1}=1.540598, K_{alpha2}=1.544426 and K_{beta}=1.392218, 2θ from 3^o-70^o at scanning speed of 12° per minutes.XRD analysis was used to determine the sample crystallinity.

3.3.3.2 X-RayFluorescence (XRF)

Elemental composition of the metal oxide added to modify the HZSM-5 catalyst were determined suing the XRF equipment at atmospheric condition.A handheld Thermofisher Scientific NITON XL3t (Waltham, Massachusetts USA) XRF machine was used to analyse the

chemical composition of HZSM-5. After bringing out the analyzer from its carrying case and inserting the rechargeable battery into the battery holder, “Mining Cu/Zn” testing mode was selected on the machine. Samples were placed in the XRF sample cup provided with the machine. The cup then was placed on the stand then the machine was placed directly on the sample. It was ensured that the machine’s measurement window flushes with the sample; then the trigger was pulled to start measurement. The machine’s trigger was held for a testing time of 180 s. Readings were taken from the computer for ease; although they are available from the machine’s flip-up, touch-screen display.

3.3.3.3 Fourier transform infra-red (FTIR)

IR-spectra measurements were performed using Shimadzu FTIR-8400s spectrophotometerinstrument (64 scans, 4 cm^{-1}). Background spectrum of air at ambient condition was conducted before sample analysis. 20 mg wafer of the catalyst sample consisting of 1% of the sample and 99% KBr window was used. The mixture was pressed under pressure to produce a thin film wafer. The wafer was further inserted in the sample holder of the FTIR equipment, then, FTIR spectra of the sample was recorded from 400 to 4000 cm^{-1}.

3.3.3.4 Pyridine-fourier transform infra-red

Pyridine-IRanalysis was conducted to determinepresence and strengthBronsted and Lewis acid sites presence in Shimadzu FTIR-8400s Spectrophotometer equipment. 20 mg of each catalyst sample was degassed at 200^{o}C in an oven. Samples were removed and kept in a desiccator for pyridineadsorption at atmospheric condition. Adsorption was allowed for about thirty minutes after which the catalyst sample was re-weighed to measure the increment in mass due to pyridine adsorption. Catalyst samples were subsequentlyinserted into the IR-system for adsorbed spectrumbackground analysis for the pyridine.

3.3.3.5 Surface area and micropore analysis

Adsorption using nitrogen gas was conducted at 77 K using Micrometrics ASAP-2020 model. Catalyst vacuum-degassing was conducted at 573 K for ten hours. Catalysts specific surface werecalculated with use of nitrogen adsorption isotherm data using BET model. Analysis from t-plot were used to measure the micropore volumes and areas (Brunauer*et al.,* 1938; Lippens*et al.,* 1964); Choudhary *et al.,* 2006; Thommes*et al.,* 2015).

3.3.3.6 Scanning electron microscopy (SEM)

SEM micrograph of catalysts samples were taken to study surface morphology using SEM Hitachi S-4800 model (15 kV).The sample was prepared by picking amount of the catalyst sample with a tweezer and placed on the sample stab. It was then treated with acetone to wash off impurity and ensure particles dispersion. The stab set up was placed in the sputter coater to polish the surface gold film. After the sample preparation and sputtering the sample stab was placed in the SEM analysis chamber with the vacuum on. Required magnification with operating voltage were set and the focus of the microscope was manipulated with the equipment software until a sharp clear image was obtained and picture captured and recorded.

3.3.3.7 Transmission electron microscopy (TEM)

Transmission electron microscopy images of the catalyst samples were obtained on a FEI Tecnai G2 Spirit STEM microscope operated at 740 kilovolts using a carbon coated holey film on catalysts.Sonication of samples were conducted in acetone medium for fifteenminutes for particle suspension.Small droplet of the solution was introduced ontoa 400-mesh copper-grids coated with carbon coated and then introduced into TEM system. Focuses electron beam throughhigh voltage set is made to pass through 150 nm thick catalyst samples placed in high

vacuum compartment. Electrons were diffracted from lattice planes in the crystalline phase of materials, to giveidentify the material phase. Generated distinguishing x-rays were observed in a detached detector for qualitative elemental analysis.A charged coupled device was used to generate micrograph.

3.3.3.8 Hydrogen-temperature programming reduction (H_2-TPR)

Catalysts hydrogen reducibility were investigated using hydrogen-TPRchemisorption Micrometrics Auto Chem 2920 machine to detect reducibility of catalysts. The catalyst (70 mg) was pretreated with argon (32 mL per minute) for an hour at 500^{o}C and made to cool atmospherically to 100^{o}C. Gasflow was changed to a 10%hydrogen-argon50.0 cm^3 STP per minutemixture The TPR was done between 100-800^{o}C at 10^{o}C per minute ramping. Hydrogen consumed during TPR run was monitored by a thermal conductivity detector

3.3.3.9 X-ray photoelectron spectroscopy (XPS)

XPS were conducted with an Axis Ultra Dld photoelectric spectrometer by working with AlKα radiation (Source: Mg Kalpha-radiation, 15 kV, 30mA (450W) at a pressure ranging from 1 to 7 × 10− 9 mbar). The charge neutraliser was adjusted at 10 eV. Catalyst samples were preheated three times for 15 minutes before analysis under vacuum in the pre-treatment chamber and then degassed overnight before being introduced in the analysis chamber. The binding energies were calculated according to C-(CH) component of the C1s adventitious carbon(at 284.8 eV). The spectra were deconvoluted with the least squares fitting routine provided by the manufacturer with a Gaussian method and several photoelectron lines were obtained with respect to the metals.

3.4 Catalyst Performance Tests

Performance testwas conducted in a stainless-steelmadecontinuous flowfixed bed reactor 9mminternal diameter and 0.64 mheight. Catalyst weight of0.5 g and silica of 0.5g(catalyst

support) were mixed and packed into the reactor.Degassing under inert nitrogen flow environment at 540^{o}C for 2 hr.before the reaction was carried out. Propane was introduced to flow through the reactor for thirty minutes for aromatization reaction before sampling through the online GC at 540℃, gas hourly space velocityof 1200, propane and nitrogen of ratio 1:2at one atmosphere from previous work (Dauda., 2020).Buck Scientific GC 910 fitted with thermal conductivity detector connected to a Molsieve 13X packed column and Restek MTX1 and HAYESEP D oven packed column flame ionization detector was used to analyze the gaseous products. Figure 3.2 shows the diagrammatic flow set-up of the fixed

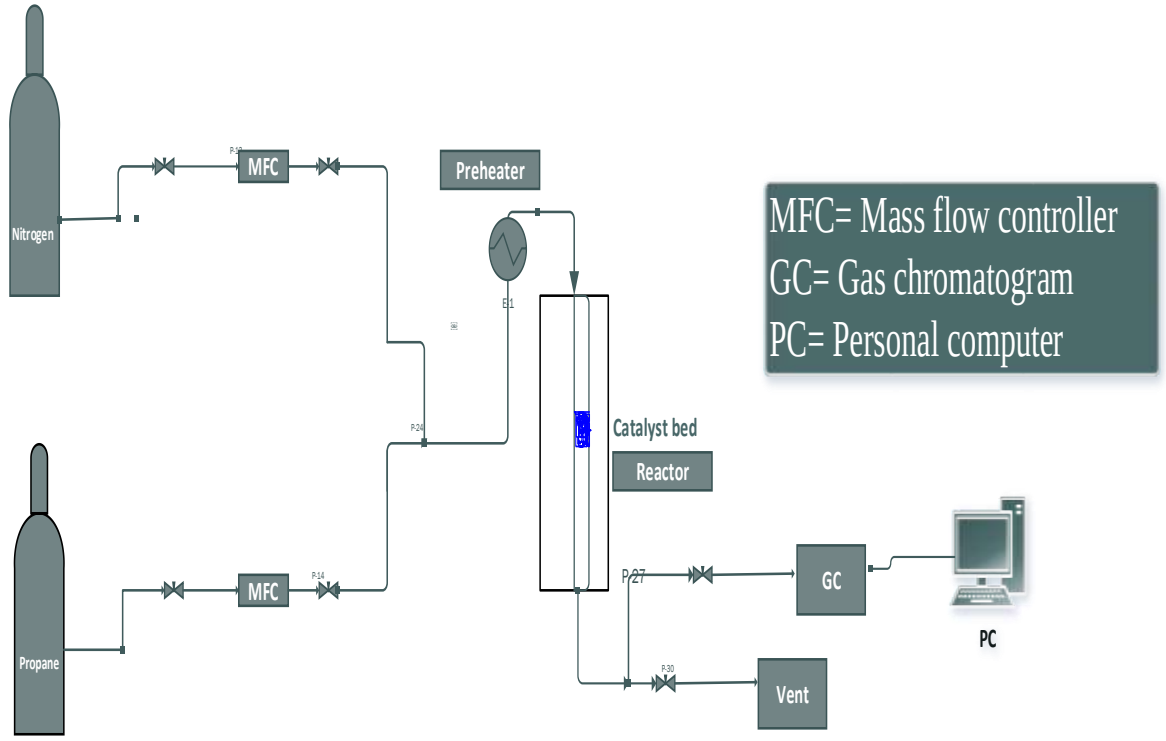


Figure 3.2 Schematic Flow diagram and set-up of the fixed bed reactor

Products peak positions were detected on the on-stream gas chromatograph and matched with that of all the products from the fixed bed reactor into the GC detected during calibration

experiment. Peak areas for each product from the reactor were measuredand calculated with the concentration of each product with respect to the calibrated standard.Propane conversion, aromatic selectivity and yield were calculated suing the set of equations listed below.

$$Propane\ conversion = \frac{Mole\ of\ propane\ consumed}{Mole\ of\ a\ given\ propane\ started\ with} * 100\%$$

$$= \frac{N_{propane}(in) - N_{propane}(out)}{C_{propane}(in)} * 100\ \% \quad (3.1)$$

Selectivity is the ratio of desired product to the total products.

$$Selectivty_{BTEX} = \frac{Mole\ of\ BTEX}{Mole\ of\ total\ products} * 100\ \% = \frac{xiC_{xi}H_{yi}}{\sum xiC_{xi}H_{yi}} \quad (3.2)$$

Yield: is the quantity of the given product (wanted or unwanted) to the quantity consumed.

$$Yield\ \% = \frac{xiC_{xi}H_{yi}}{3C_3H_8} \quad (3.3)$$

Reactant and products weight were measured carbon balance using the component weight calculated from the calibrated standards of each component and are given in Appendix B.

$$mole = \frac{Component\ weight(g)}{Component\ molar\ weight\ (\frac{g}{mol})} \quad (3.4)$$

CHAPTER FOUR

RESULTS AND DISCUSSION

Presented in this chapter are the detailed results and discussion of analysis carried out on the synthesized catalysts and the reaction tests.

4.1 Catalyst Characterization

The modified catalyst samples were characterized using the XRF, XRD, FTIR, Pyridine-FTIR, BET, SEM, TEM, Hydrogen-TPR and XPS analytical tools. The results are given in this section.

4.1.1 X-Ray fluorescenceelemental composition of catalysts

The elemental composition of fourteen catalyst samples prepared is shown in Table 4.1.Zinc composition for all the fourteen catalysts aside from HZSM-5 was fixed to be 2 wt. % within Zn-Fe, Zn-Co, Zn-Ni and Zn-Cu composition. The percentage loading for zinc did not measure up to 2 wt. %. The measurements were in percentage error of +3 to +5% which within experimental allowable limit.

The stabilizing metal loadings were varied from 1, 2 and 3 wt. % for iron, cobalt, nickel and copper with 2 wt. % zinc on ZSM-5. The percentage error of real from actual measurements were from +4 to +6 %. Cobalt 3 wt. % and all copper loadings were on percentage error of -0.2 to -0.1 %. The bold figures in Table 4.1 is the measure concentration of the loaded metal on HZSM-5.

4.1.2 X-ray diffraction analysis of the catalyst samples

XRD diffractograms of sample catalysts are presented in Figure 4.1 to Figure 4.4 showing variation of metal loadings. It could be observed that metal loading effect is insignificant in

comparison with parentHZSM-5 structure except for suppressed peak observed due to metal impregnated on the zeolite (Jia*et al.,* 2017). Modification by metal impregnation on HZSM-5 surface made catalysts still crystalline as the parent HZSM-5 because there is no collapse of structure. The bimetallic catalysts showed a distinguished reduction in peak intensities compared to parent HZSM-5.

Table 4.1: XRF elemental composition of HZSM-5 and metal modified catalyst

Elem	Zn-Co (1%)	Zn-Co (2%)	Zn-Co (3%)	Zn-Cu (1%)	Zn-Cu (2%)	Zn-Cu (3%)	Zn-Fe (1%)	Zn-Fe (2%)	Zn-Fe (3%)	Zn (2%)	HZSM5	Zn-Ni (1%)	Zn-Ni (2%)	Zn-Ni (3%)
Mg	0.877	0.714	0.724	1.251	< LOD	< LOD	0.863	< LOD	0.906	0.771	1.248	1.003	0.655	1.136
Al	1.131	0.623	0.716	1.221	1.15	0.493	0.843	2.659	0.796	0.763	1.023	0.942	0.693	0.802
Bal	47.712	53.676	46.826	42.082	54.087	50.381	46.407	48.289	45.607	48.741	46.142	46.131	47.846	44.296
Si	47.357	41.119	47.415	52.26	40.912	44.346	48.895	42.867	47.897	47.737	51.459	48.739	46.78	48.679
P	< LOD	< LOD	< LOD	< LOD	0.078	< LOD	< LOD	2.159	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
S	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	0.038	< LOD	< LOD
Cl	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	0.023	< LOD	< LOD
K	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Ca	0.039	0.022	0.055	0.034	0.058	0.386	0.101	0.101	0.05	0.085	0.071	0.118	0.064	0.066
Ti	0.004	0.004	0.006	0.007	0.006	0.01	0.005	0.01	0.007	0.005	0.008	0.007	0.006	0.009
V	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Cr	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	0.004	< LOD	< LOD	< LOD	< LOD	< LOD
Mn	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Fe	0.02	0.006	0.025	0.017	0.023	0.026	**0.937**	**1.943**	**2.861**	0.037	0.03	0.025	0.024	0.039
Co	**0.982**	**1.898**	**3.003**	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Ni	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	**0.966**	**1.95**	**2.962**
Cu	< LOD	< LOD	< LOD	**1.018**	**2.007**	**3.086**	0.004	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
Zn	**1.866**	**1.924**	**2.034**	**1.928**	**1.963**	**1.949**	**1.831**	**1.959**	**1.792**	**1.842**	**0.002**	**1.991**	**1.942**	**1.988**
Total	99.988	99.359	100.804	99.818	99.984	100.677	99.886	99.987	99.92	99.981	99.983	99.983	99.96	99.977

**LOD= Low on Detection

It can be attributed to a high impregnated metal absorption coefficient and increased thickness of the ZSM-5.There were no observable distinctive peaks of impregnated metals because of low concentration but the XRF results had already indicated the presence of the metals on the ZSM-5 structure (Van der*et al.*, 2015; Wannapakdee*et al*., 2019). The observed typical peaks of HZSM-5 appearedfor all modified catalysts at 2θ angle= 7.89°, 8.73°, 14.82°, 23.04°, 23.86°, and 24.26°.Figure 4.1 to Figure 4.4 show the XRD of impregnated metals (Zn, Fe, Co, Ni and Cu) loadings in comparison with HZSM-5.

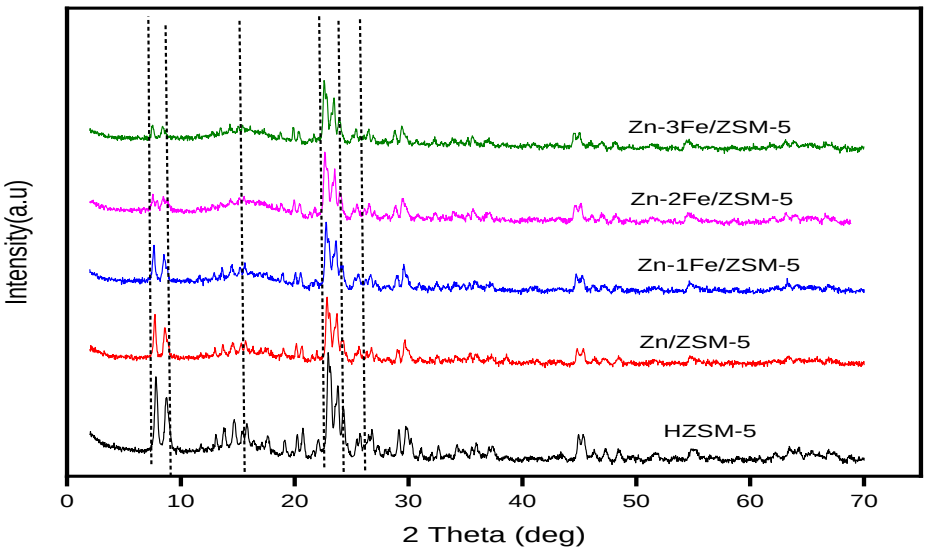


Figure 4.1: X-ray diffractogram of Zn-Fe/ZSM-5 catalyst samples

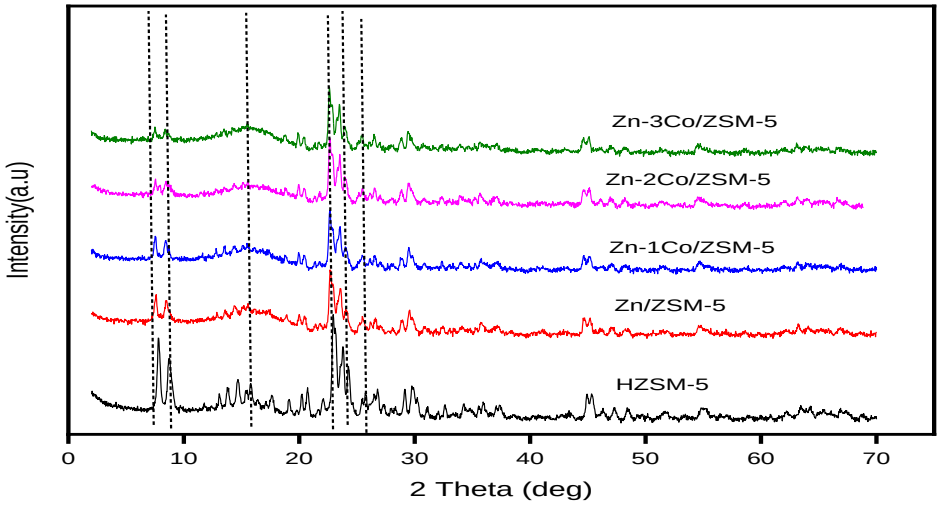


Figure 4.2: X-ray diffractogram of Zn-Co/ZSM-5 catalyst samples.

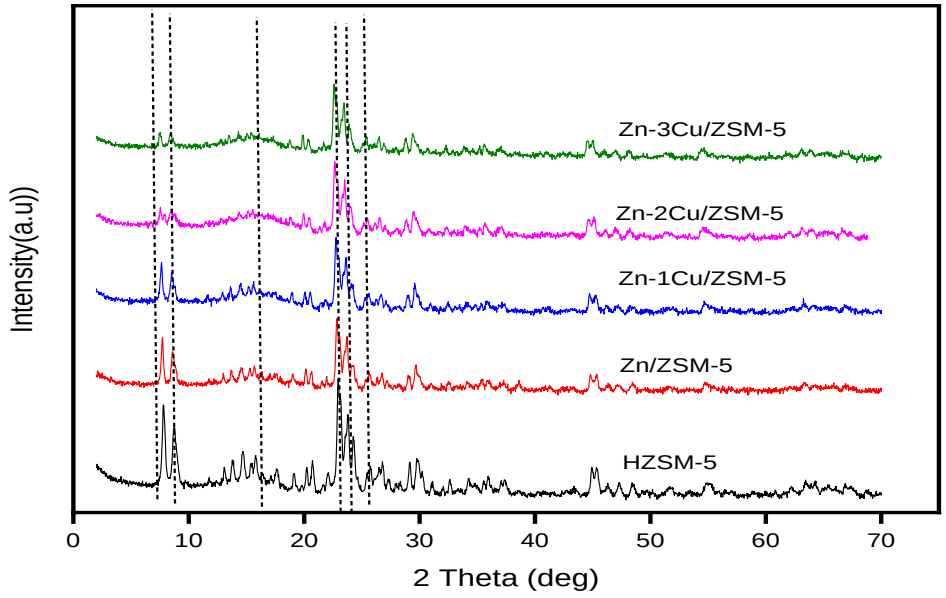


Figure 4.3: X-ray diffractogram of Zn-Cu/ZSM-5 catalyst samples.

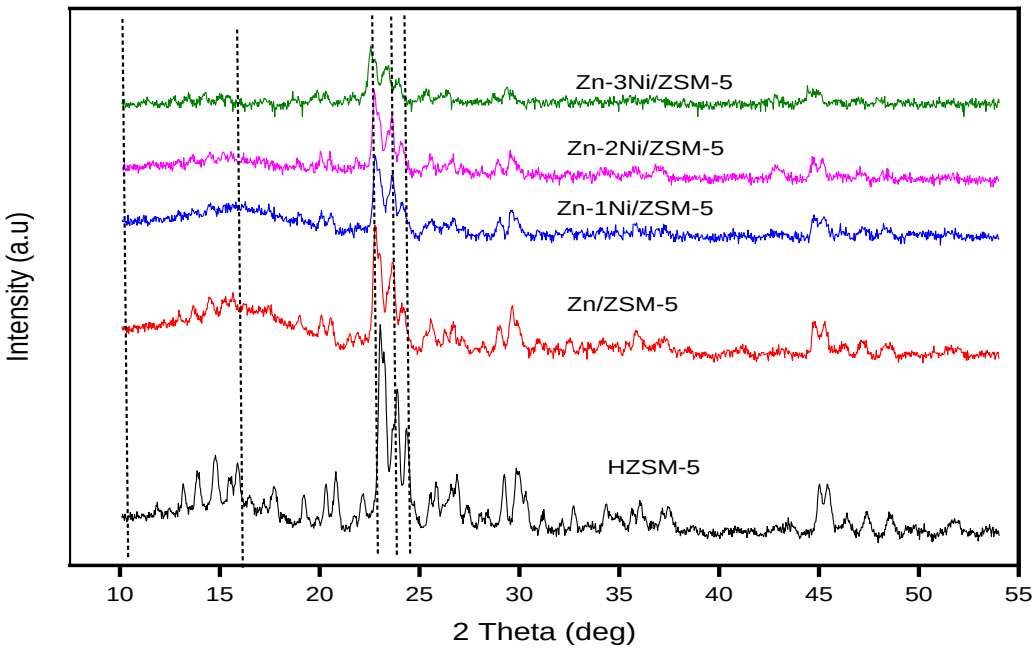


Figure 4.4: X-ray diffractogram of Zn-Ni/ZSM-5 catalyst samples.

4.1.3 Fourier transform infrared analysis of catalysts

Figure 4.5 to Figure 4.8 show the FTIR spectra of catalyst samples. Characteristic peaks corresponding to parent HZSM-5 were present on the metal modified bimetallic catalysts irrespective of loading only that they were widened because of the effects of metal stretching when compared with HZSM-5. Peak intensities at 450cm^{-1} and 550 cm^{-1} depicts T-O bend

and double-5 ring of crystalline of ZSM-5 while 1100cm^{-1} and 1225 cm^{-1} correspond to internal and external asymmetric stretch respectively. Peak at 3400cm^{-1} and 1700 cm^{-1} corresponds to stretching and vibrational bending of hydroxyl (OH^{-}) group of water absorbed HZSM-5 surface which also were been stretched and widened because of metal impregnated on the surface of HZSM-5. Peak at 3610 cm^{-1}is OH stretching region of Bronsted acid groups with the structuralaluminum [Si(OH)Al], 3740 cm^{-1} is the secluded external silanol groups, mobile internal silanol groups present at 3730 cm^{-1} and delocalized hydrogen-bonded groups located on 3500 cm^{-1}. The Bronsted acid peak region (3610-3630 cm^{-1})were also observed showingsome adjustment in the peak regions as a result of H-protons replacement by the anchored Zn and other metals. (Sabarish and Unnikrishnan, 2019; Chu*et al*., 2009;Liu *et al.*, 2014).

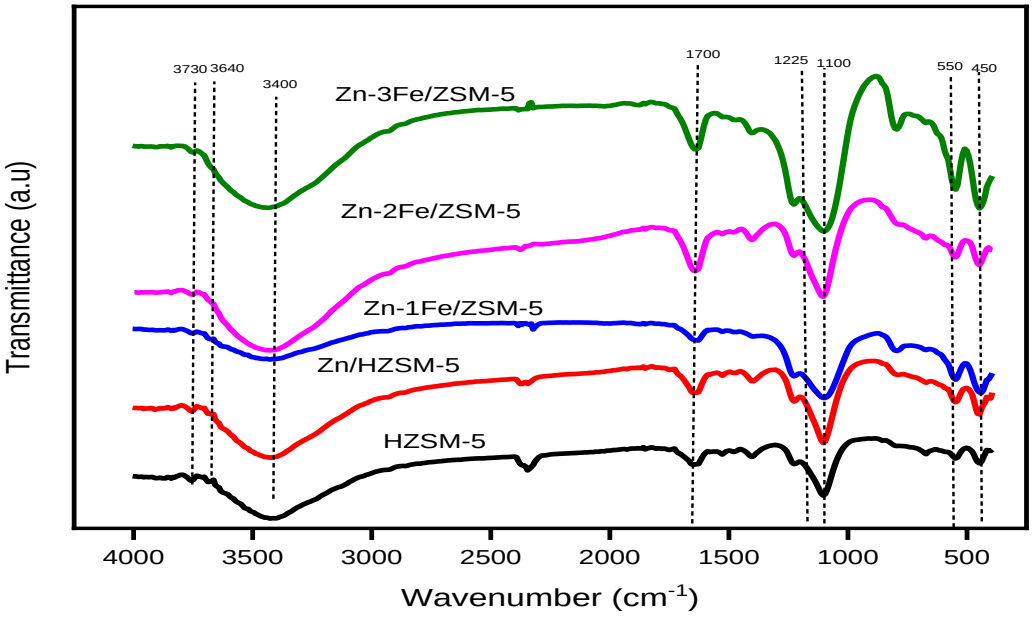


Figure 4.5: FTIR spectra of Zn-Fe/ZSM-5 catalyst samples

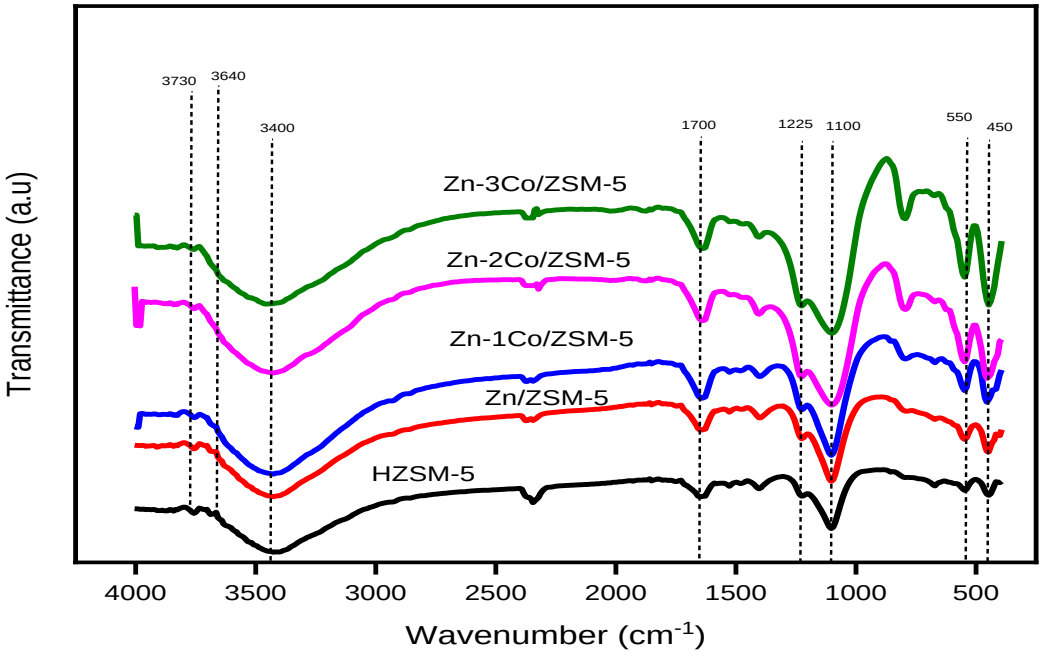


Figure 4.6: FTIR spectra of Zn-Co/ZSM-5 catalyst samples.

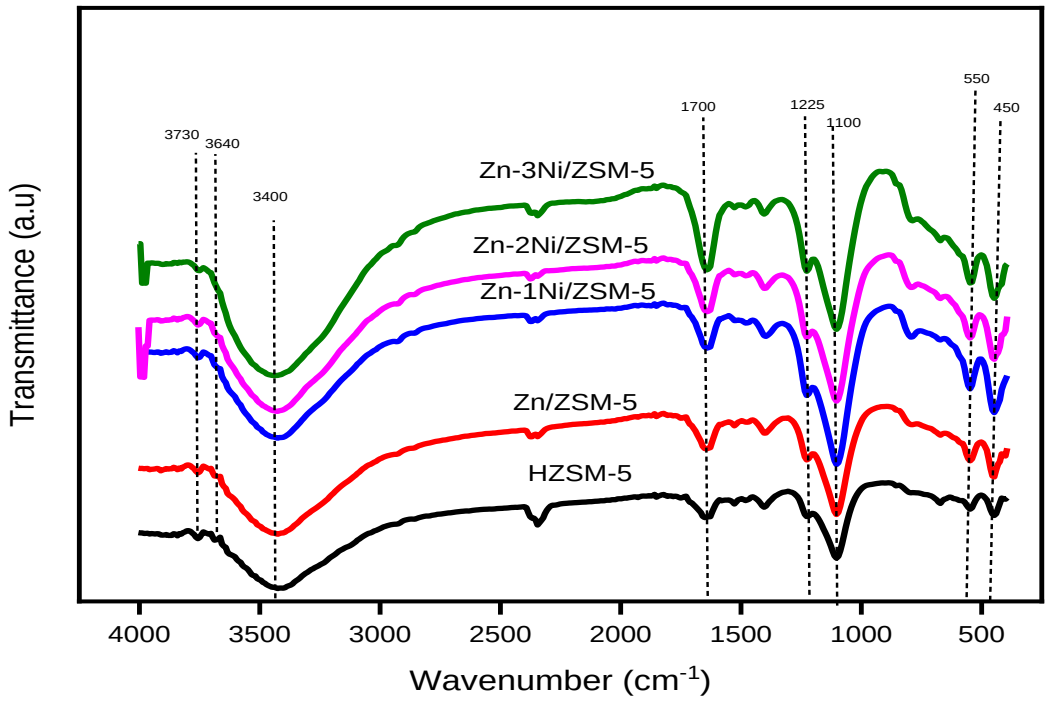


Figure 4.7: FTIR spectra of Zn-Ni/ZSM-5 catalyst samples.

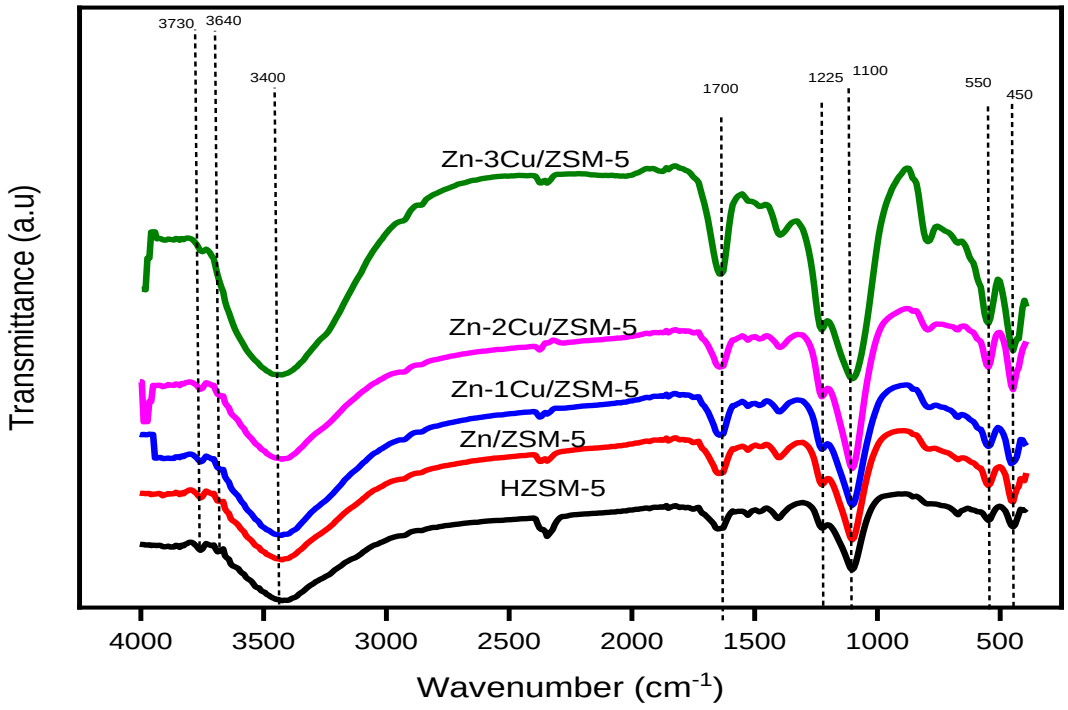


Figure 4.8: FTIR spectra of Zn-Cu/ZSM-5 catalyst samples.

4.1.4 FTIR-pyridine analysis of the catalystsamples

FTIR-Pyridine indicating the strength of the catalyst acidity with increase metal loadings are as presented in Figure 4.9 to Figure 4.12.Peaks around1450 cm^{-1}, 1490 cm^{-1} and 1540 $cm^{-1}$are the general observed peaks with respect to pyridine adsorption to characterize Lewis acid sites, Lewis acid sites and Bronsted acid sites combination and Bronsted acid sites respectively with little shifts from ideal. They were observed around vibration bands of 1400~1600 cm^{-1} region (Xiao*et al.*, 2015).1440 cm^{-1} and 1540 cm^{-1}were attributed to the Lewis sites pyridine vibration C-C stretching and pyridinium ion complex on Bronsted sitesrespectively (Parry, 1963; Hughesand White, 1967).The Lewis acid wave number peak was not observable as expected when metal loading increases from literature. It was generally observed that the Bronsted acidity decreased as metal loading increased on parent ZSM-5 as identified by XRF analysis. This is due to replacement of Bronsted sites by the impregnated metals on the catalystsurface (Wang*et al.*, 2015). Same effects were observed for all the four bimetallic catalysts.

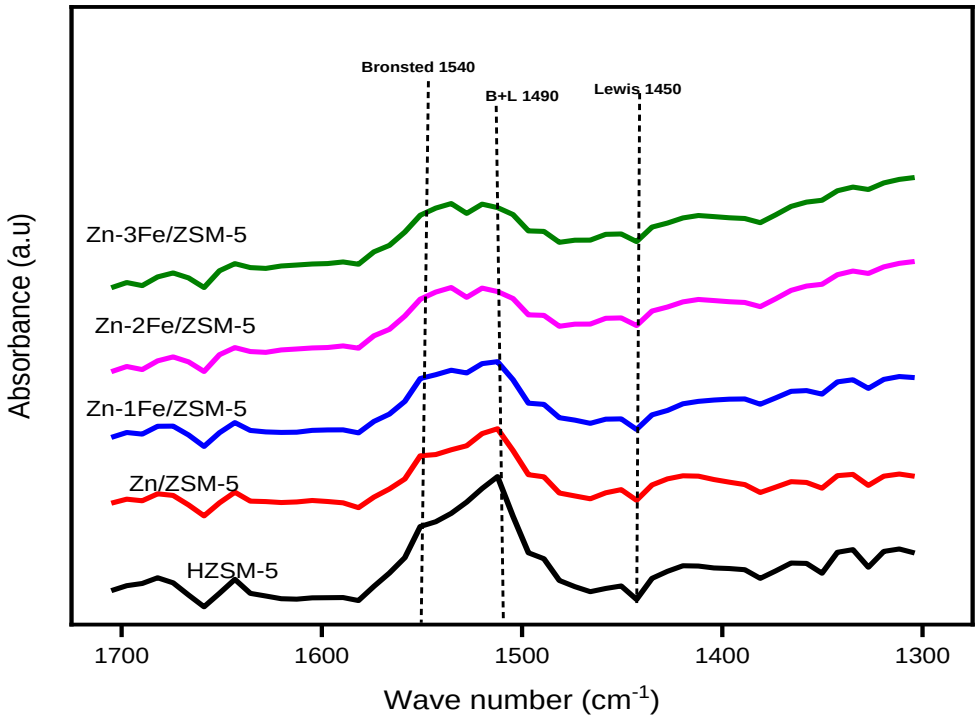


Figure 4.9: FTIR-pyridine absorption spectra of Zn-Fe/ZSM-5 of catalyst samples

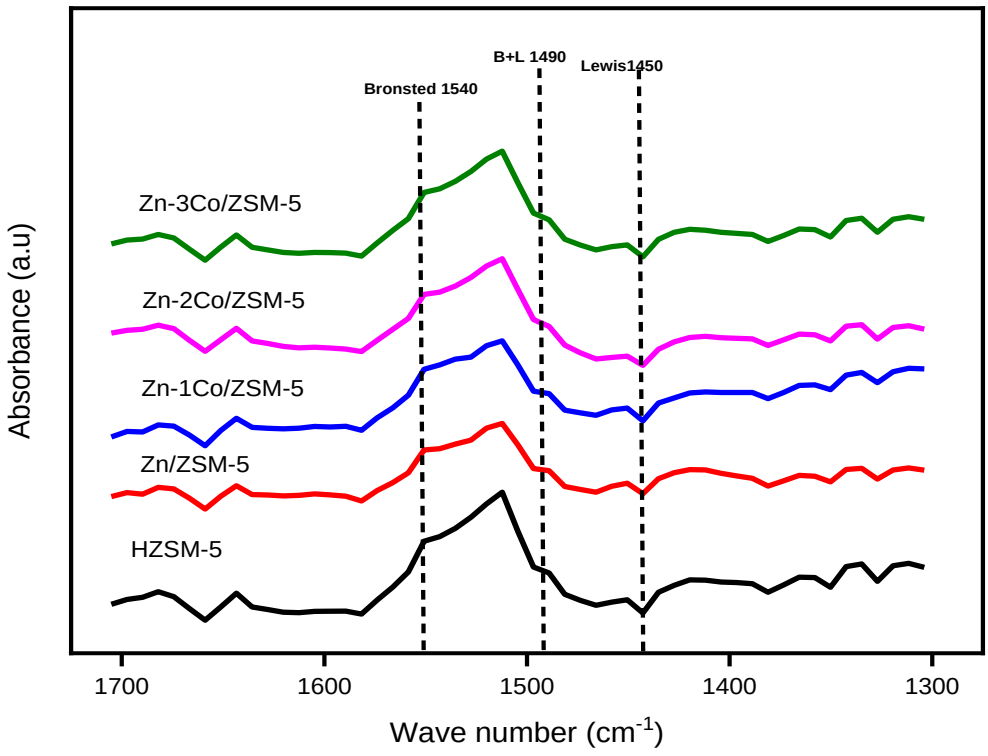


Figure 4.10: FTIR-pyridine absorption spectra of Zn-Co/ZSM-5 of catalyst samples.

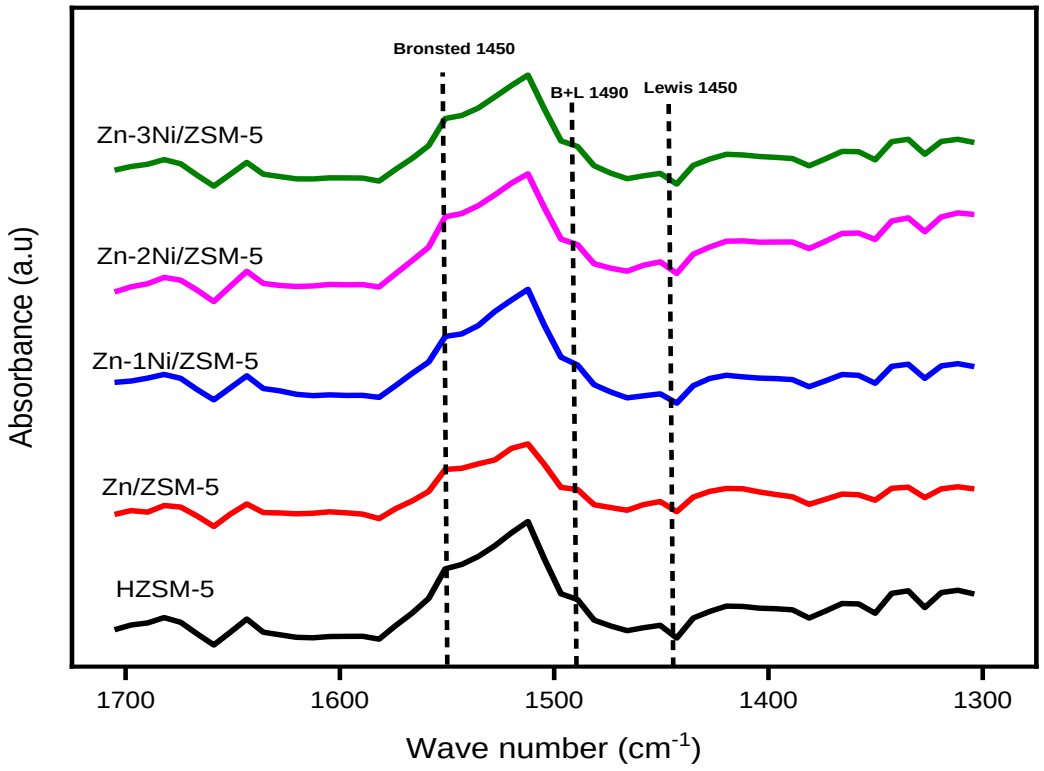


Figure 4.11: FTIR-pyridine absorption spectra of Zn-Ni/ZSM-5 of catalyst samples.

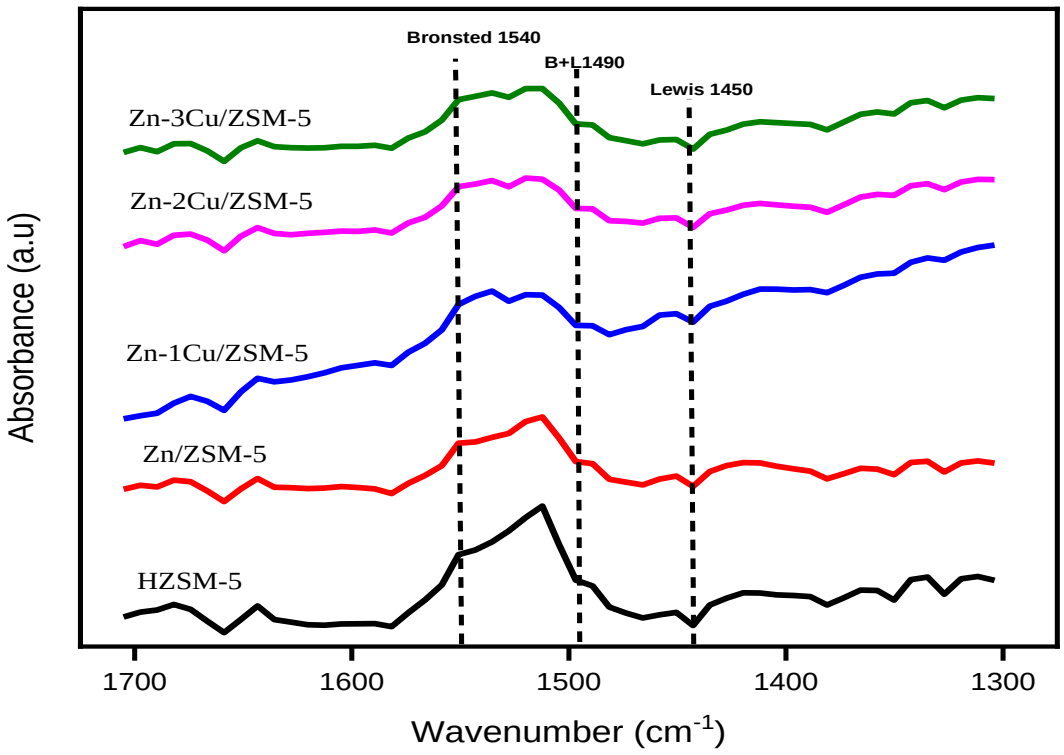


Figure 4.12: FTIR-pyridine absorption spectra of Zn-Cu/ZSM-5 of catalyst samples.

4.1.5Scanning electron microscopyanalysis of the catalyst samples

The scanning electron microscopy (SEM) image are presented in Plate 1 for six catalyst samples. Surface morphology and shape of the metal modified catalysts were not significantly changed. This implies that impregnation of metals did not present any substantial changes in the catalyst shape and structure. There are however darker spots on the metal modified catalysts when compared with parent HZSM-5indicating the presence of metals on HZSM-5 (Ahmad*et al*., 2016; Kosinov*et al*., 2018).

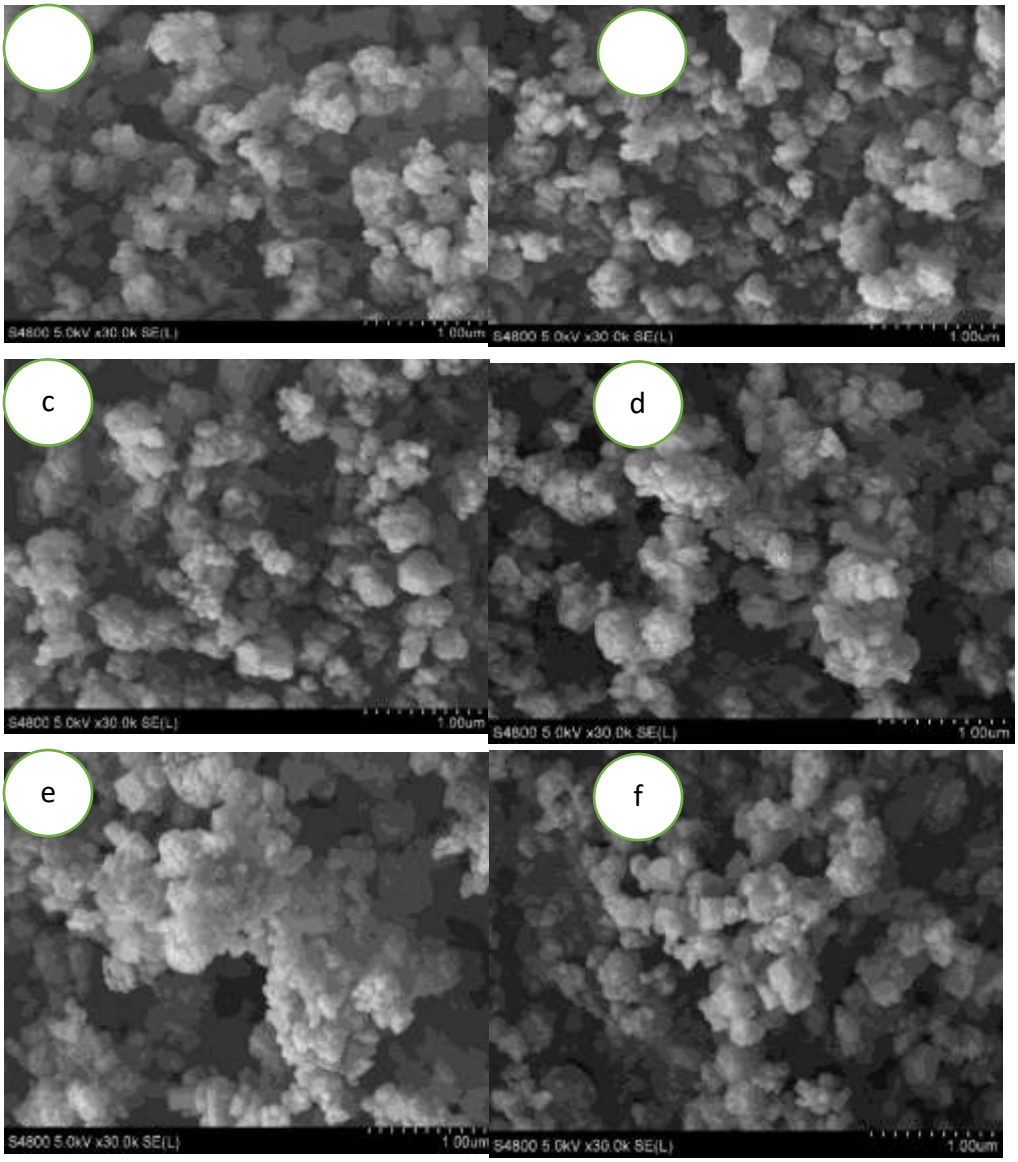


Plate I: SEM microgram of the prepared catalysts (**a**-HZSM-5, **b**-Zn/ZSM-5, **c**-Zn-Fe/ZSM-5,**d**- Zn-Co/ZSM-5, **e**-Zn-Ni/ZSM-5 and **f**-Zn-Cu/ZSM-5 respectively X=30,000).

4.1.6Transmission electron microscopy analysis of the catalystsamples

The transmission electron microscopy (TEM) microgram are presented in Plate II for the six catalyst samples. The voids were occupied on addition of zinc as shown in Plate II (h). Plate

4.2(i-l) are the bimetallic catalysts. Though each metal could not be identified due to the magnification, enhanced dispersion of impregnated metals on HZSM-5 were observed when compared with parent HZSM-5 and Zn/ZSM-5catalyst. This would also imply aided dispersion of zinc on ZSM-5 by the second metalsto make more active sites of zinc species available for reaction.

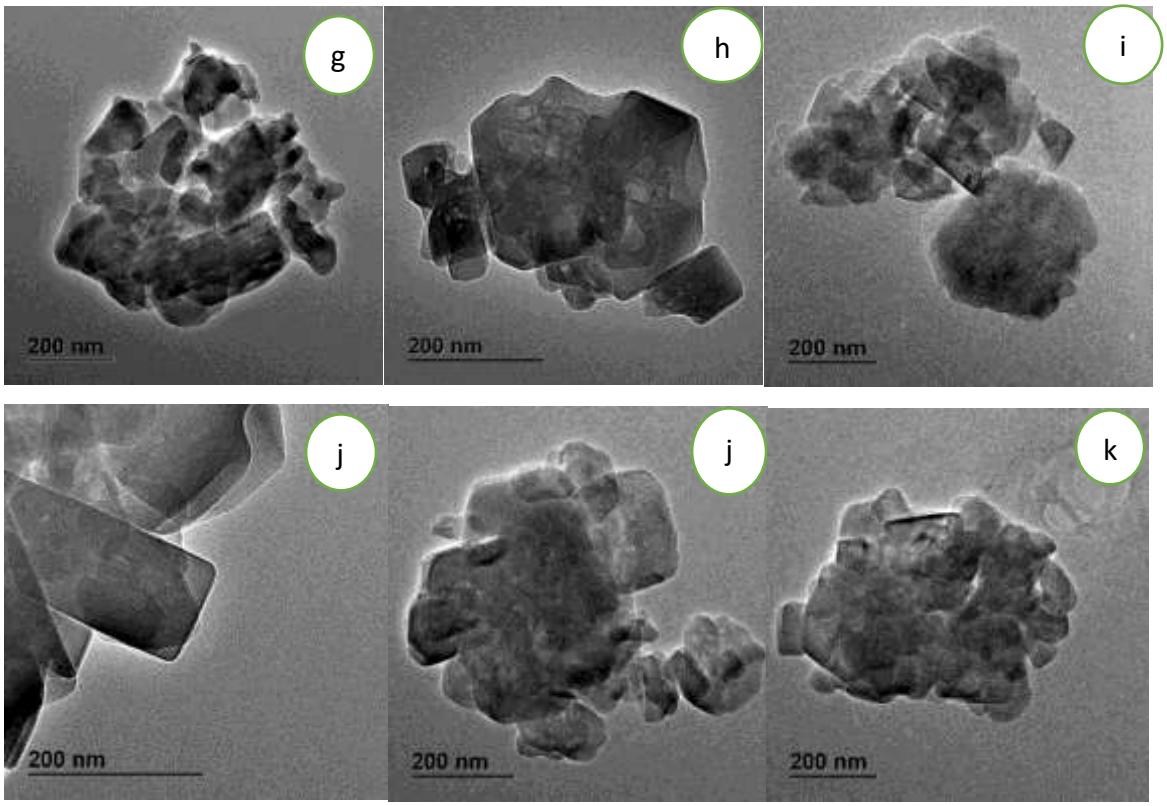


Plate II: TEM microgram of the preparedcatalysts (**g**-HZSM-5, **h**-Zn/ZSM-5, **i**-Zn-Fe/ZSM-5,**j**- Zn-Co/ZSM-5, **k**-Zn-Ni/ZSM-5 and **l**-Zn-Cu/ZSM-5 respectively).

4.1.7Textural properties and nitrogen adsorption analysis of catalyst samples

Presented in Table 4.2 are the catalysts textural properties. Type I nitrogen-adsorption-desorption isotherms were exhibited by catalyst samples with absence ofseparate hysteresis loops. The retention of catalysts microporosity is also shown in the BET surface area in Table 2 (Brunauer*et al.,* 1938).Specific surface area and total pore volume reduced as the metal loading increased on ZSM-5. Surface impregnation of zinc and metal on HZSM-5 reduced the total surface area (meso and micropores) as compared to the parent HZSM-5 except for

Zn-Fe/ZSM-5 and Zn-3Co/ZSM-5. This showed that addition of a promoter metal had significance on the dispersion of Zn species to some level as the surface areas. 2 and 3 wt. % Cu bimetallic catalysts alongside Zn-Fe/ZSM-5 and Zn-3Co/ZSM-5 which were slightly higher than that ofHZSM-5 in mesopores. This observed scenario suggested that most of the co-impregnated Fe, Cu and Co resided on the external surfaces of zeolite crystallites which could probably had suppressed somewhat Zn species dispersion into the zeolite channels, and subsequently left more Zn-unoccupied Bronsted acid sites in the zeolite channels (Xu *et al*., 2013; Ramasubramanian *et al.,* 2019).Addition of metals to HZSM-5resulted in decrease in mesopore volume, pore size and increasemicroporous volume (Vmicro) signifying that the metals mostlydeposited on the external surfaces and had blocked the catalyst mesopores (Berndt, *et al.*, 1996; Mhamdi *et al.*, 2009; Chen *et al.*, 2015; Coqueblin *et al.*, 2017; Thommes et al., 2015). Addition of metals to HZSM-5. There were reductions in BET specific surface area and total pore volume as the total metal weight loading increased. This may be attributed to strong interactionsbetween metals and HZSM-5. The reduction in XRD peaks of the catalysts as metals were impregnated in Figure 4.1 to Figure 4.4 agreed with the surface properties. The introduction of zinc to HZSM-5 reduced the surface area and pore volume. However, some bimetallic like Zn-Fe/ZSM-5, Zn-3Co/ZSM-5 and Zn-Cu/ZSM-5 catalysts had increase in surface area, pore volume and width. This could be attributed to increase metal loading and sideway attachment of metal to the zeolite. Other catalysts on the general had decrease in micropore volume (V_{micro}) and surface area of the modified catalyst which might have been caused by diffusion of part of the metallic oxide phase into HZSM-5 micropores atwet impregnation and calcinationstages (Sapawe *et al*., 2013; Tempelman *et al.*, 2015).Higher surface area experienced will increase higher catalyst activity. Appendix B shows the calculations for the BJH adsorption-desorption process and surface area.

The summary of the specific surface area and micropore analysis is shown in Table 4.2.

Table 4.2: Textural properties of catalyst samples

Catalyst(s)	S_{BET}a (m^2/g)	S_{micro}[c] (m^2/g)	S_{mesoc} (m^2/g)	V_{total}b (cm^3/g)	V_{micro}c (cm^3/g)	Pore width(nm)
HZSM-5	373.22	333.36	39.87	0.260	0.151	2.793
Zn/ZSM-5	361.08	323.10	37.99	0.255	0.141	2.778
Zn-1Fe/ZSM-5	386.10	346.67	39.40	0.266	0.156	2.760
Zn-2FeZSM-5	386.64	345.01	41.63	0.272	0.113	2.617
Zn-3Fe/ZSM-5	379.93	336.85	43.08	0.276	0.153	2.610
Zn-1Co/ZSM-5	358.34	324.70	34.64	0.251	0.144	2.769
Zn-2Co/ZSM-5	359.19	324.45	34.73	0.246	0.145	2.735
Zn-3Co/ZSM-5	381.42	348.70	32.72	0.258	0.153	2.707
Zn-1Ni/ZSM-5	371.52	331.31	40.21	0.268	0.149	2.761
Zn-2Ni/ZSM-5	362.12	324.72	37.30	0.246	0.145	2.720
Zn-3Ni/ZSM-5	362.94	324.09	38.85	0.257	0.144	2.710
Zn-1Cu/ZSM-5	359.96	325.36	34.60	0.254	0.144	2.767
Zn-2Cu/ZSM-5	377.39	347.48	31.93	0.26	0.150	2.694
Zn-3Cu/ZSM-5	368.61	337.64	32.51	0.25	0.150	2.668

The nitrogen adsorption isotherm for the metal modified catalysts are shown in Figure 4.13 to Figure 4.16. N_2-adsorption–desorption isotherms of all catalysts with parentHZSM-5 are shown inFig. 5. All catalysts exhibited type I because of their uniform microporous structures from the figures. These are regularly connected with materials that have tremendously fine micropores and small fractions of mesopores, according to IUPAC grouping nomenclature and arrangement (Leofanti *et al.*, 1998; Condon, 2006; Thommes *et al.*, 2015; Dauda *et al.*, 2020). This has been appropriately discussed in the published works in Appendix C.

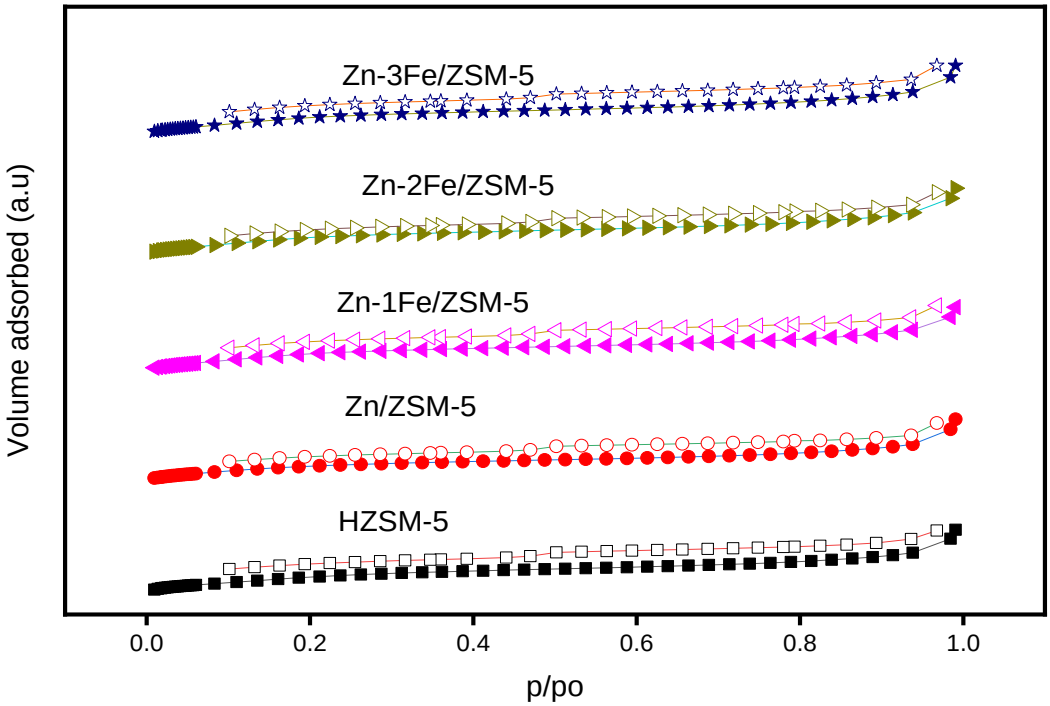


Figure 4.13: Nitrogen adsorption isotherm for Zn-Fe/ZSM-5

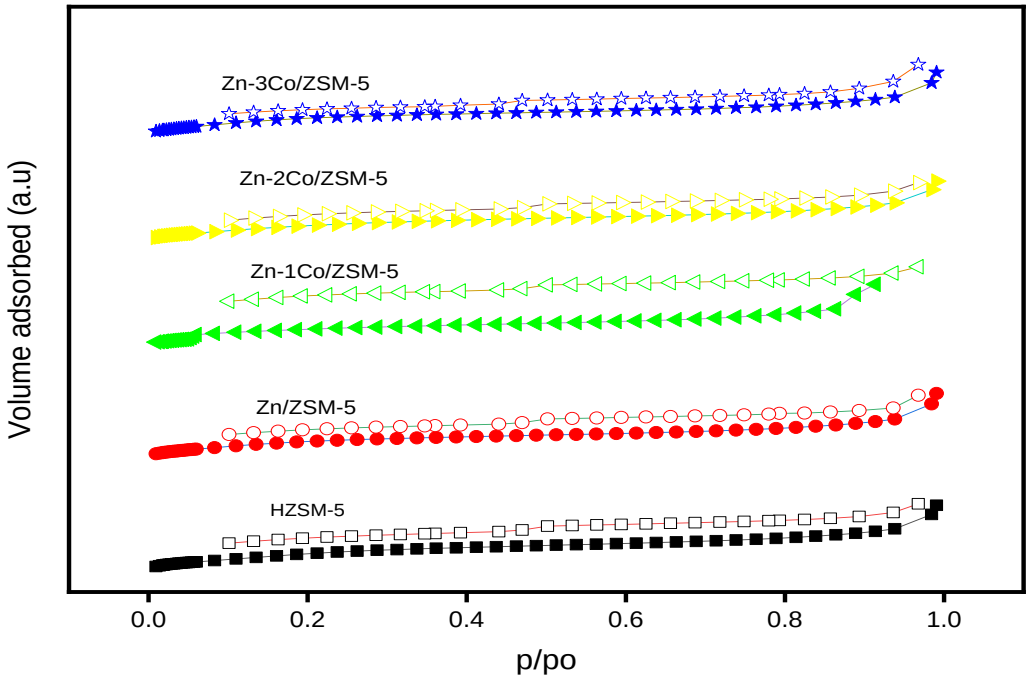


Figure 4.14: Nitrogen adsorption isotherm for Zn-Co/ZSM-5

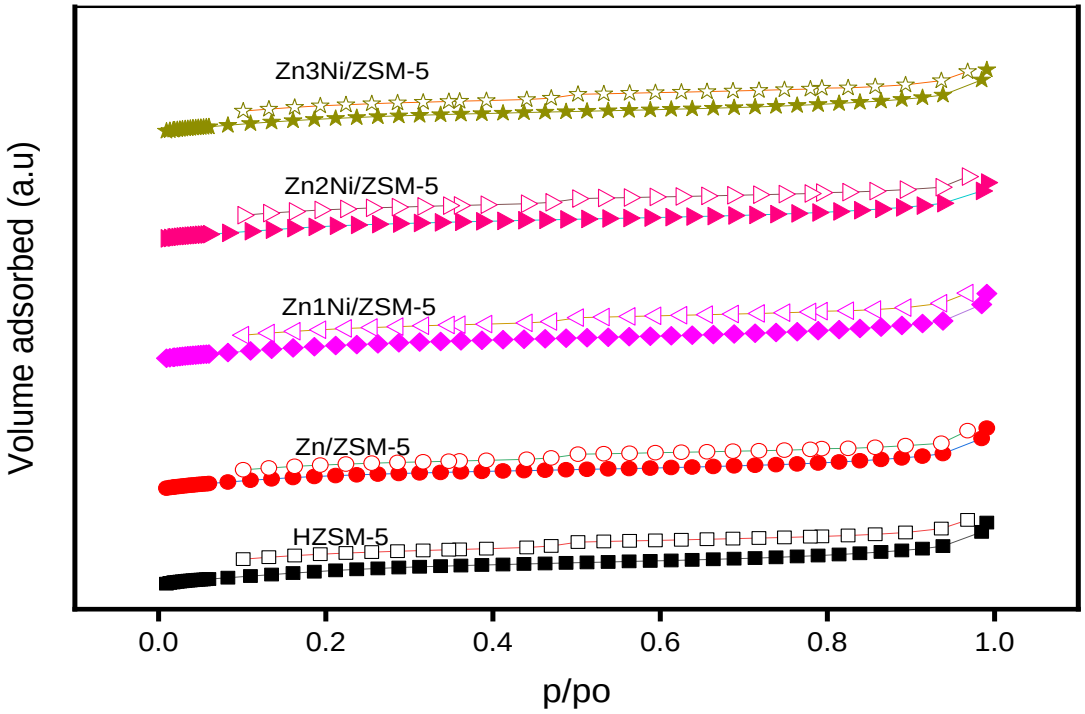


Figure 4.15: Nitrogen adsorption isotherm for Zn-Ni/ZSM-5

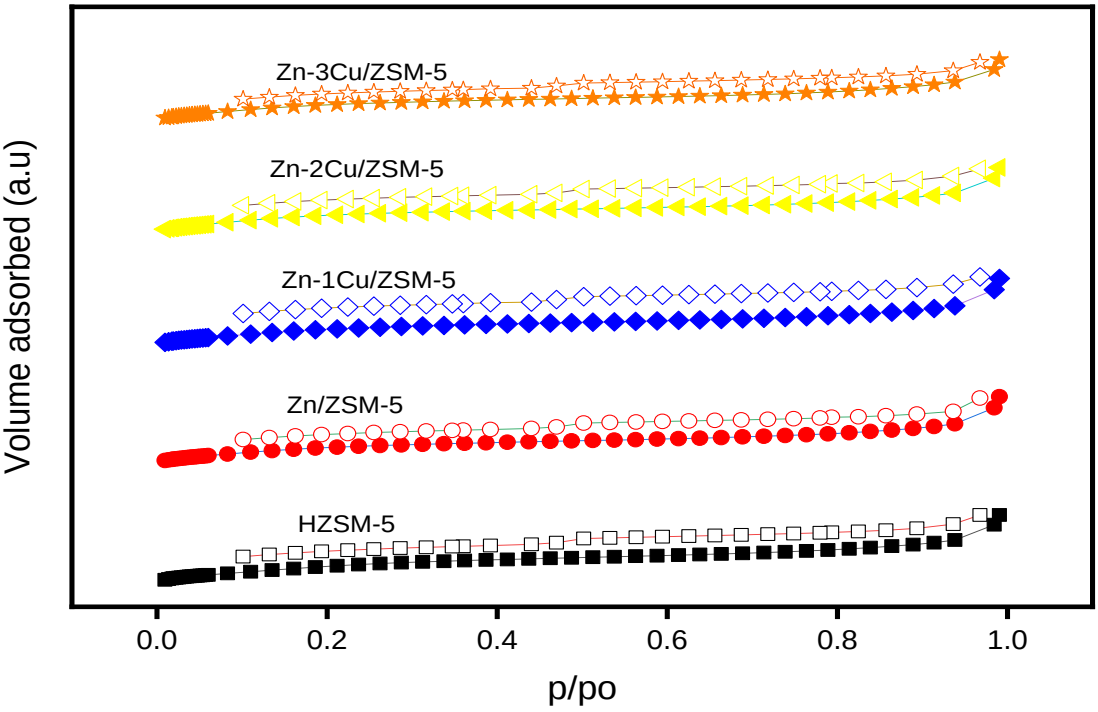


Figure 4.16: Nitrogen adsorption isotherm for Zn-Cu/ZSM-5

4.1.8 Hydrogen temperature programmingreduction of catalyst samples (TPR)

Hydrogen-TPR analyses were carried out to study how reducible metal modified HZSM-5 catalysts for 2 wt. % bimetallic loading each. These are shown in Figure 4.17. HZSM-5

andZn/ZSM-5 showed peaks that can be attributed to H_2-consumption for reduction at 430 and 620 ^oC as against literature reportnot showing reduction peaks (Lan *et al.,* 2017). This maybe as a result of proper mixing of zinc species with ZSM-5 structure at synthesis. Fe/HZSM-5 samples contained double peaks as reported by Dao *et al.,* 2015,with temperature of reduction at 350 ℃ and 580 ℃ indicating two-stage reduction profile.Zn-Fe/ZSM-5 had slight reduction around 390 and 560^oC (Yan*et al.,* 2015: Lumbago and Scurrell, 2002). Cu/ZSM-5 was reported to have hydrogen reduction peak at 445 ^oC fromCu^+ to Cu°(Dao and Luu, 2015). Zn-Cu/ZSM-5 catalyst containing the additional zinc reduced it to 150, 200 and 380 ^oC whose peaks are still attributable to the reduction of Cu cations. Zn-Ni/ZSM-5 showed reduction that can also be attributed to the presence of nickel at 540 ^oC as against the reported peak for Ni/ZSM-5 at 350 and 490 ^oC (Yung *et al.,* 2016; Dao and Luu., 2015).The reduction peak for cobalt on ZSM-5 as reported by Dao and Luu, 2015 is 335 ^oC. Zn-Co/ZSM-5showed a little shift hydrogen consumption at around 340, 400 and 600 ^oC. It was recommended that metal-metal interaction led to shift in peak either to left or right from the normal single metal hydrogen-TPR thus enhancing formation of stable metal-metal alloy on ZSM-5. This also enabled the reduction of hardly zinc oxide that is difficult to reduce. This occurrence could relate to the interactionselectronically between zinc and iron, cobalt, nickel, and copper. Ingeneral view, the strongest metal-metal interface is observed in catalyst systems with metal possessing almost or completely filled valence band and another with almost empty valence band. Thus, the rearrangement of charge moves theelectrons from zinc and added metals creating an interface (Yang and Weng, 2009).

4.1.9 X-ray photoelectron spectroscopy (XPS) analysis of catalyst samples

Figure 4.17 to Figure 4.22 show the XPS analysis of the catalyst samples. HZSM-5 and Zn/ZSM-5 zeolite catalyst samples were analysed using XPS as presented in Figure 4.17 and 4.18 respectively.The normal XPS binding energy of zinc oxide are $2p_{3/2}$ and Zn $2p_{1/2}$ are

1021 and 1045. With zinc on HZSM-5, it became 1025 and 1048 eV due to zinc bonding to ZSM-5 surface(Long *et al.*, 2014).

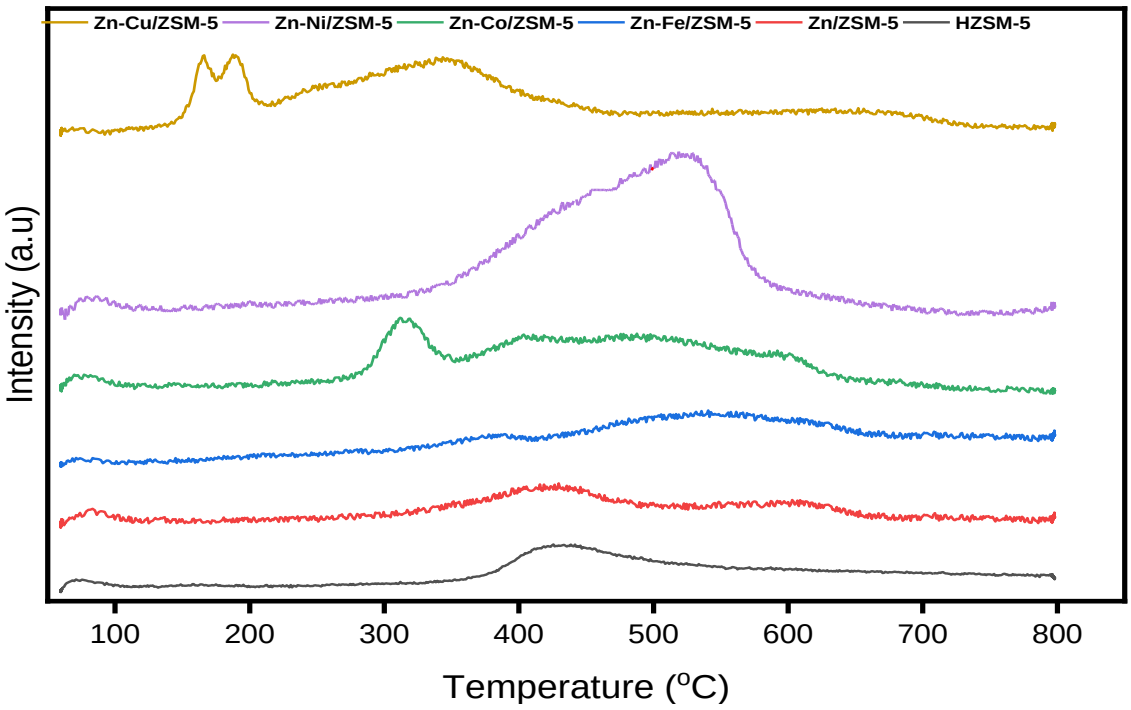


Figure 4.16: Hydrogen-temperature programing reduction of catalyst samples.

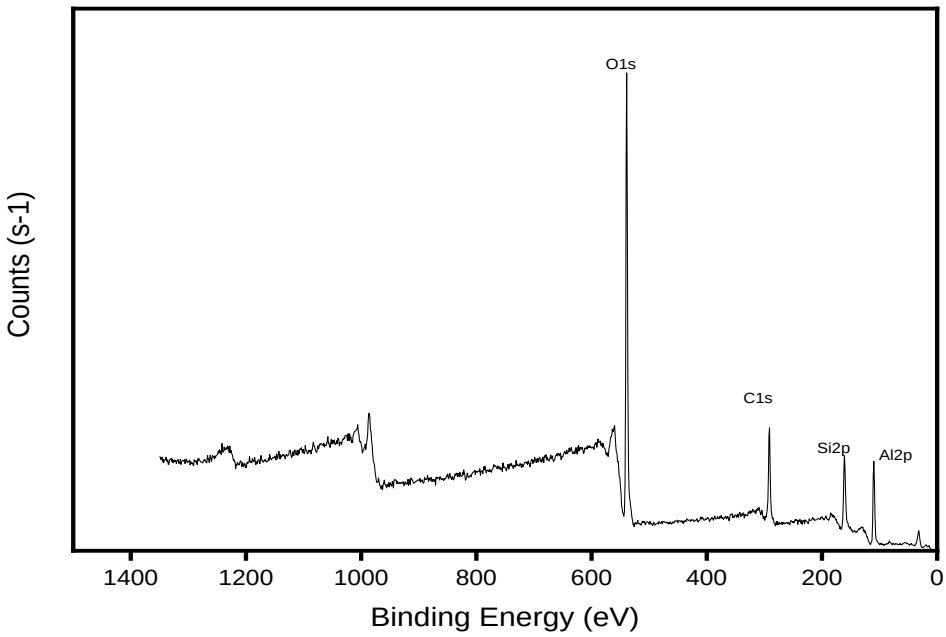


Figure 4.17: XPS spectra of parent HZSM-5 catalyst samples

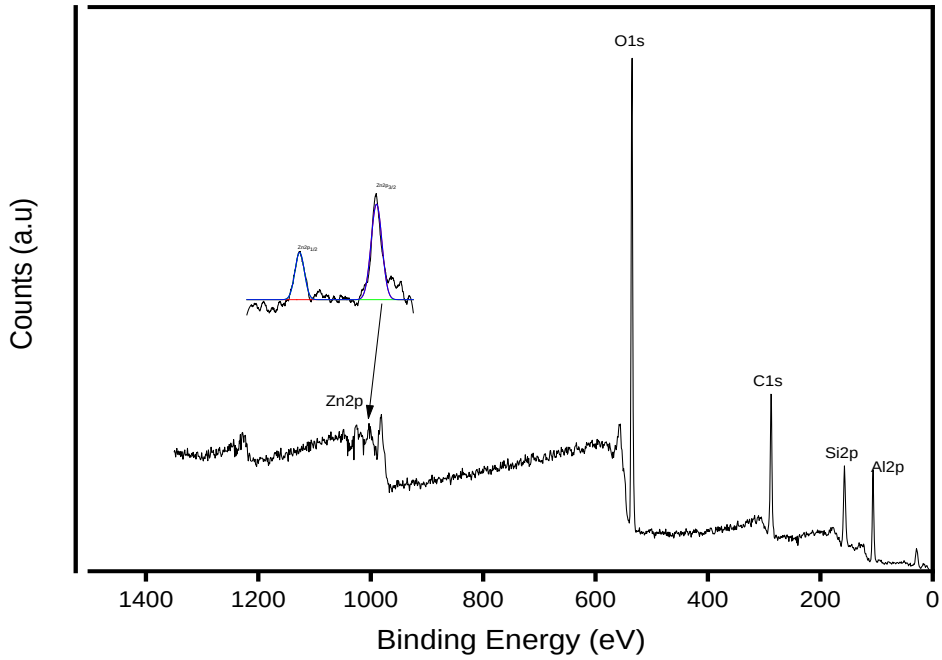


Figure 4.18: XPS spectra of Zn/ZSM-5 catalyst samples

The XPS spectra of Zn $2p_{3/2}$ and Zn $2p_{3/2}$ were observed at binding energy spectra of 1,029 and 1051 eV respectively in Figure 4.19 for Zn-Fe/ZSM-5. The lower binding energy of Zn $2p_{3/2}$ shows the zinc oxide dispersed on ZSM-5 surface and the higher Zn $2p_{1/2}$ binding energy corresponds to the presence of $ZnOH^+$ species (Wang *et al.*, 2016; Roy *et al.*, 2015). The Fe $2p_{3/2}$ and Fe $2p_{1/2}$ XPS binding energy at 717.2 and 730.1 eV respectively could be attributed to the Fe_2O_3 phase, which suggests that a portion of clusters loaded on the surface of Zn-Fe/ZSM-5 was Fe_2O_3 species. Iron loading enhanced the spreading of zinc oxide and increased the concentration of $ZnOH^+$ which was also confirmed by XPS spectra in Figure 4.19(Long *et al.*, 2014).The shift in the binding energy of Zn (1021.7 and 1045 eV) and Fe (710 and 725 eV) lower and higher energy level respectively from their basic oxides when compared are attributed to inter-metallic bonding and electron balancing on zeolite surface.

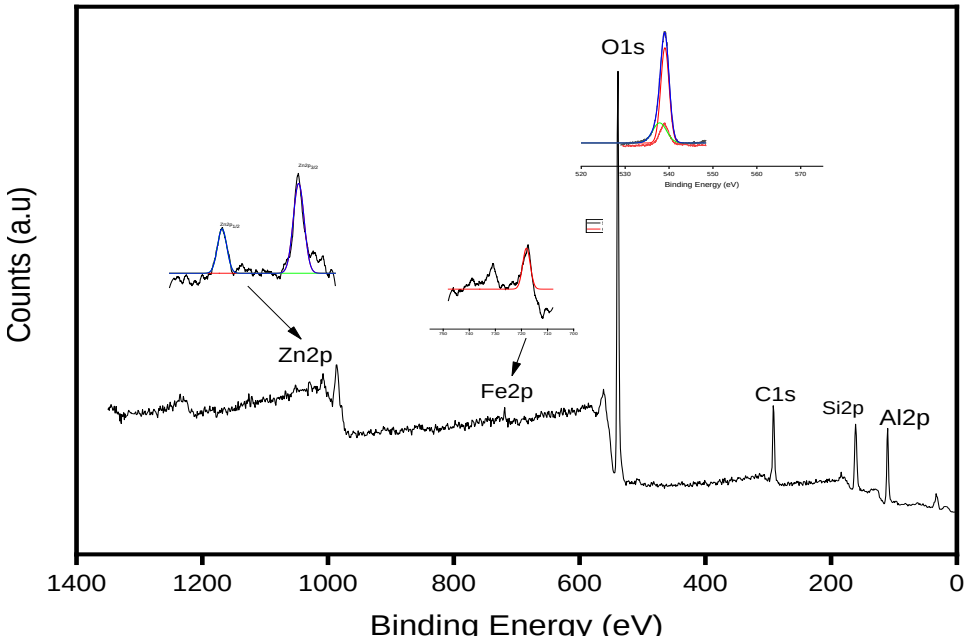


Figure 4.19: XPS Spectra of Zn-Fe/ZSM-5 catalyst samples

The observed binding energy spectra for cobalt in Zn-Co/ZSM-5 (Co3p/2788 eV) and zinc ($2p_{3/2}$ and Zn $2p_{3/2}$) 1,029 and 1051 eV respectively are shown in Figure 4.20.The presence of $ZnOH^+$ improved alkane aromatization and inhibitedlight olefins formation. The shift in the binding energy of Zn (1021.7 and 1045 eV) and Co(780 and 796 eV) lower and higher energy level respectively from their basic oxides on zeolite when compared are attributed to inter-metallic bonding and electron balancing on zeolite surface and enhanced dispersion of zinc on zeolite surface (; Durando *et al*., 2008; Sapawe *et al.*,2013; Wang *et al*., 2016; Roy *et al*., 2015; Jia *et al.*, 2015).

Zinc specie binding energy spectra changed as nickel was added to due to interaction between the metals to 1030 and 1054 eV which is believed to have aided in strengthening and improving zinc stability.The observed nickel binding energy on bimetallic catalyst in Figure 4.21 are 862 and 880 eV for $2p_{3/2}$and $2p_{1/2}$. As against the 853 and 872 eV for Nickel, this suggest presence of new link between the two metals on the catalyst surface via Zn-Ni interaction. The competition of Ni^{2+} and Zn^{2+} ions to compensate for charge on zeolite would

also allow enhanced dispersion of metals on catalyst surface, thus making more active sites available for propane contact.

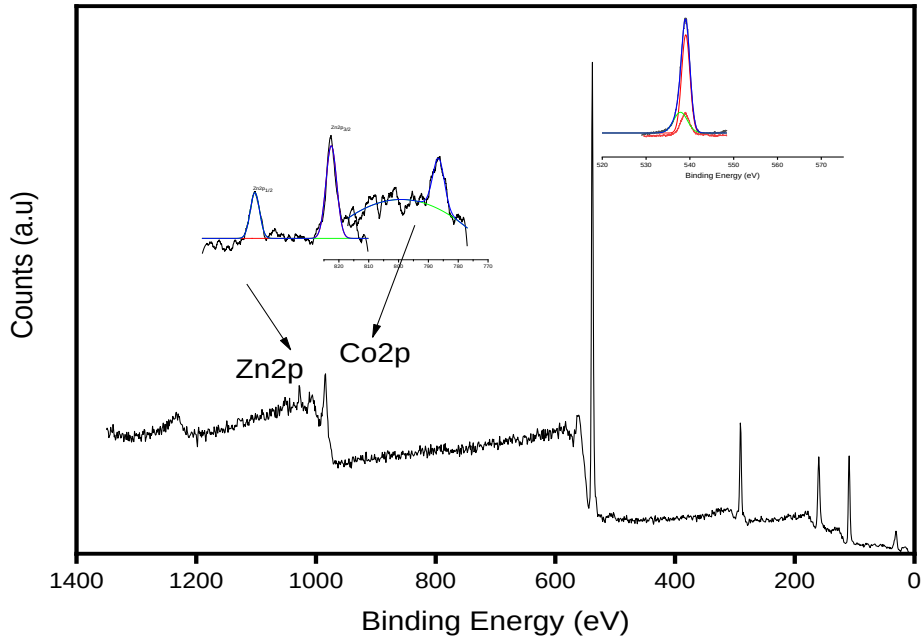


Figure 4.20: XPS spectra of Zn-Co/ZSM-5 catalyst samples

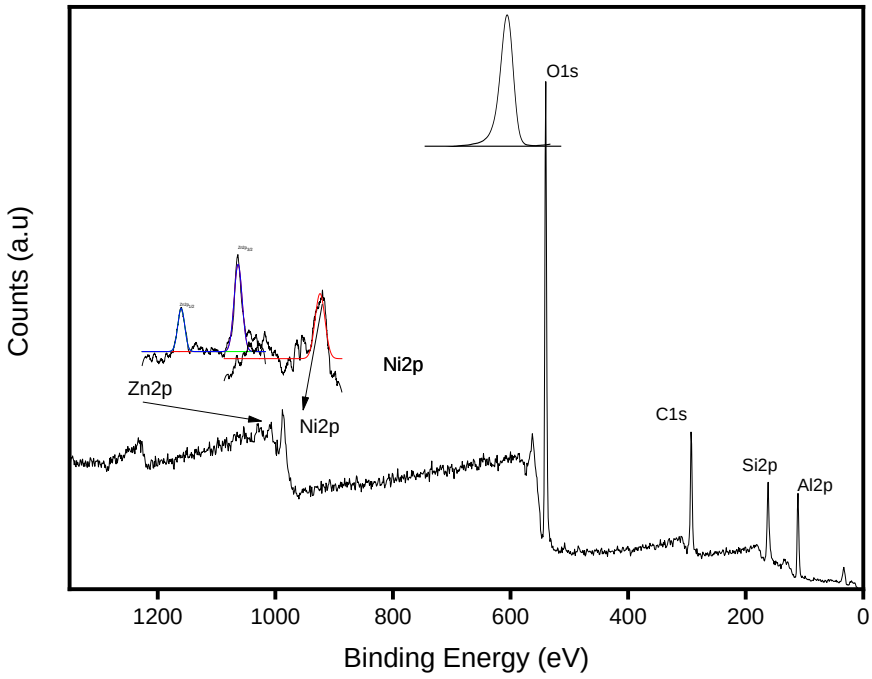


Figure 4.21: XPS Spectra of Zn-Ni/ZSM-5 catalyst samples

The observed XPS spectra of copper in Zn-Cu/ZSM-5as shown in Figure 4.22is 940 and 960 eV for $2p_{3/2}$ and $2p_{1/2}$. As against the normal 933 and 952 eV for copper, this suggest presence of new bond created on the catalyst surface (Jia *et al.*, 2015; Biesinger, 2017).

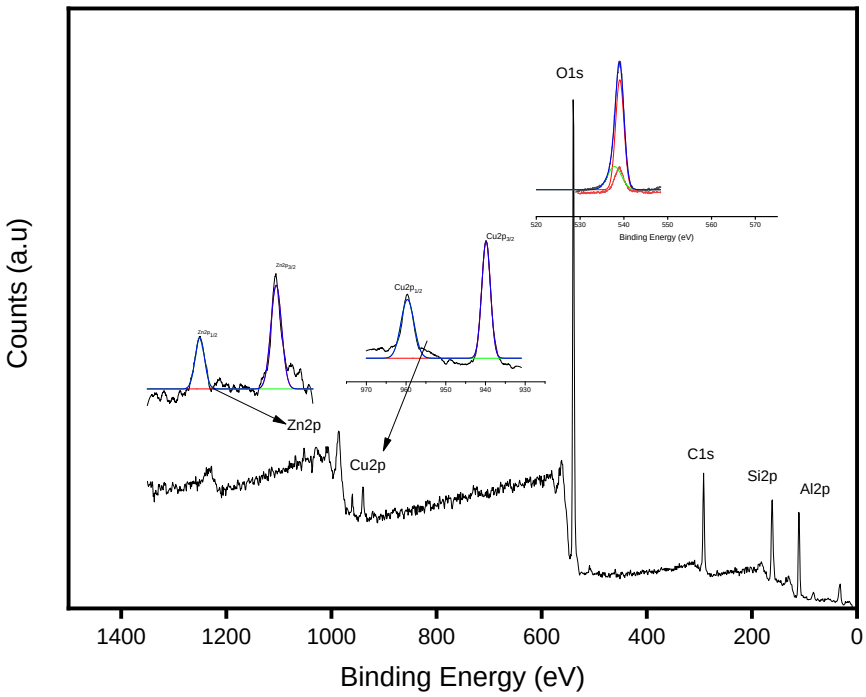


Figure 4.22: XPS Spectra of Zn-Cu/ZSM-5 catalyst samples

It has been shown from literatures that the presence of second metal helps to increase the concentration of $ZnOH^{+}$species which always improved alkane aromatization and suppressed the formation of light olefins(Niu *et al.*, 2014; Sapawe *et al.*, 2013), hence the reason for improved and sustained selectivity towards aromatics. O1s HZSM-5, Zn/ZSM-5 and Zn-Cu/ZSM-5 catalysts are similar which when deconvoluted still did not split at 538.5 eV corresponding to the surface lattice oxygen of the catalyst and ZSM-5 (Jia *et al.*, 2017).

Table 4.3 showed the transition in binding energies of metal in bimetallic catalyst synthesis.

Table 4.3: Catalyst samples binding energy summary

Metal	Free binding energy (eV)	Bimetallic binding energy (eV)
Zinc	1021, 1045	Zn (1025, 1048)
Iron	710, 725	Fe (717.2 ,730.1) Zn (1,029, 1051)
Cobalt	780	Co (788) Zn (1,029, 1051)
Nickel	853 and 872	Ni (862, 880) Zn(1030, 1054)
Copper	933 and 952	Cu (940, 960) Zn (1032, 1055)

4.2Catalytic Conversion of Propane

Conversion of propane over ZSM-5 based catalysts was carried out at a reaction temperature of 540^{o}C and atmospheric pressure. The results which include conversion, aromatic yield and selectivity are presented in Figure 4.23 to Figure 4.34.

4.2.1 Conversion of propane over HZSM-5 and Zn/ZSM-5

Catalytic conversionsof propane over HZSM-5 and Zn/ZSM-5 are presented in Figure 4.23. Propane reaction on ZSM-5 began with propane activation resulting in cracking and dehydrogenation. This occurs via hydride transfer from propane to carbonium ions following adsorption-desorption of propene. The resulting product from reactions went through quick continuous oligomerization, dehydrogenation, cyclisation, dehydrocyclization and finally C_6-C_{10} aromatic formation. All these reactions involve hydrogen transfer from HZSM-5 leading to formation of undesired short chain alkanes (from olefins) whose conversion is very slow which eventually resulted in low aromatic selectivity as presented in Figure 4.24.

Zinc species on ZSM-5 aided in speeding up the recombination of surface hydrogen, produced through dehydrogenation of propane and cyclized oligomers' dehydrocyclization as important reaction in alkanes transformation to aromatics (Nicolaides *et al.*, 2002; Biscardi

and Inglesia, 1999). Zn species helps in promoting the dehydrogenation of light alkanes, while Brønsted acid sites facilitate oligomerization and aromatization (Sattler et al., 2014; Wannapakdee *et al*., 2019; Lukyanov and Vazhnova, 2006; Migliori *et al*., 2017). This is clearly shown in rapid increase in aromatic selectivity from 10 % to 80 %. Recombination of surface hydrogen to avoid obvious propensity for it to take part in transfer of hydrogen causing cracking as observed in propane conversion over HZSM-5 leading to low aromatic selectivity. At 1-6 hours TOS, Zn/ZSM-5 had lower but rising propane conversion with corresponding declining aromatic selectivity until compared to parent HZSM-5 catalyst. The conversion was a bit stable at 7-9 TOS and later start declining till 12^{th} hours TOS. This can be attributed to zinc instability at reaction condition thus losing its activity. Furthermore, the transfer of hydrogen directly as a proton from alkenes intermediates at dehydrogenation of cyclized oligomers to other intermediates of alkene leads to undesired alkanes, lowering BTEX selectivity. This accounted for HZSM-5 low aromatic selectivity. However, zinc instability on ZSM-5 became obvious as aromatic selectivity kept reducing with time on stream up to 50 % at twelfth hour. Hence the need to enhance its stability for sustained aromatic production. Propane conversion, aromatic yield and selectivity were calculated using equations 3.1-3.4 in section 3.4. Appendix B1 and B2 detailed the carbon balance calculation processes for HZSM-5 and Zn/ZSM-5.

4.2.2 Effect of iron loading with zinc on ZSM-5

Effect of iron loading with zincon HZSM-5 in comparison with HZSM-5 and Zn/ZSM-5 for propane conversion is shown in Figure 4.23.Metallic ZSM-5 catalysts are bifuctional in role of alkane conversion. Zinc helps in alkane dehydrogenation while Bronsted sites enable oligomerization and aromatization (Sattler*et al.,* 2014; Wannapakdee*et al*., 2019; Lukyanov and Vazhnova, 2006;Miglior*iet al*., 2017).Propane conversion over twelve hours' time on stream was relatively stable and sustained but slightly increasing with increasing loading.

This was clearly shown as the presence of zinc on ZSM-5 cause initial decrease in propane conversion but eventually picked up as time on stream for the reaction (TOS) increased, probably due to slow activation of ZnO to $ZnOH^+$. Catalyst activitywas improved on addition of iron thereby increasing the conversion of propane (Figure 4.23). Propane conversion, aromatic yield and selectivity using Zn-Fe/ZSM-5 catalysts were calculated using equations 3.1-3.4 in section 3.4. Appendix B3 and B7 detailed the carbon balance calculation processes for catalytic performances over Zn-Fe/ZSM-5 bimetallic catalysts.

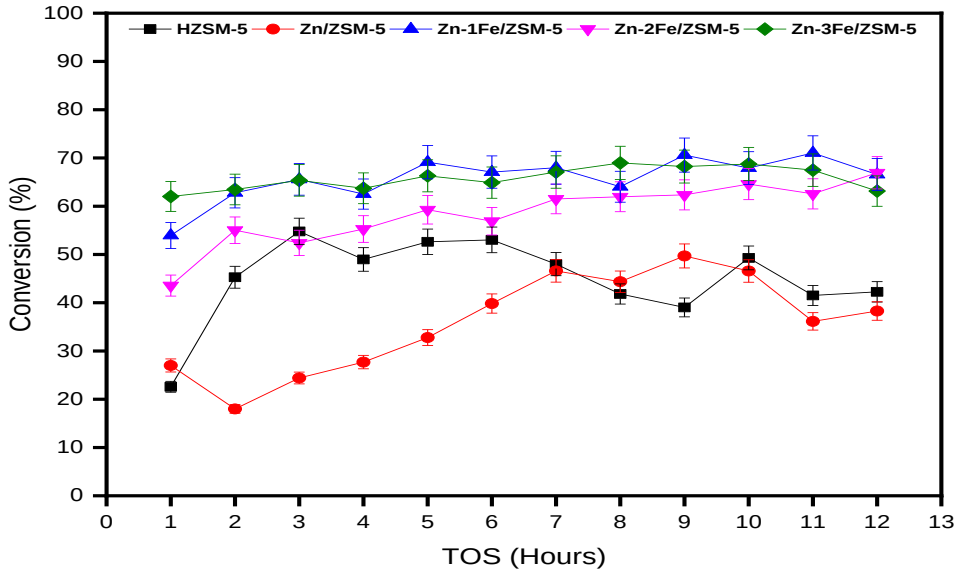


Figure 4.23: Propane conversion over HZSM-5, Zn/ZSM-5 and Zn-Fe/ZSM-5

Propaneimproved conversion on second metal co-impregnation with zinc can be accredited stable dehydrogenation due to the presence of Zn-Fespecies in the ZSM-5channels (Choudhary *et al.,* 2000).The XPS and hydrogen-TPR results had shown good metal-metal interaction to have enhanced zinc stability thus promoting its activity and selectivity towards aromatic. Good dehydrogenating ability of zinc species on ZSM-5 was clearly seen as aromatic selectivity on HZSM-5 increased from 10 % to 80 %from 2 -12 hour TOS but kept decreasing on account of zinc specie instability at reaction condition to 50 %. Co-impregnation of iron fairly stabilized and sustained selectivity from 2nd hr. TOS as seen in

Figure 4.24. The presence of zinc in the bimetallic catalyst improved selectivity towards aromatics though it gradually decreased with TOS. Zinc specie help in dehydrogenation by recombining hydrogen thus suppressing cracking (Beta-scission), minimizing hydrogenation of backward reaction and enhancing oligomerization, cyclization over twelve hours' time on stream.Iron also undergoing reduction process since they are in form of oxides, thus co-dehydrogenating together with zinc, thus increasing aromatization. Figure 4.25 clearly showed improved yield on addition of iron as the second metal.

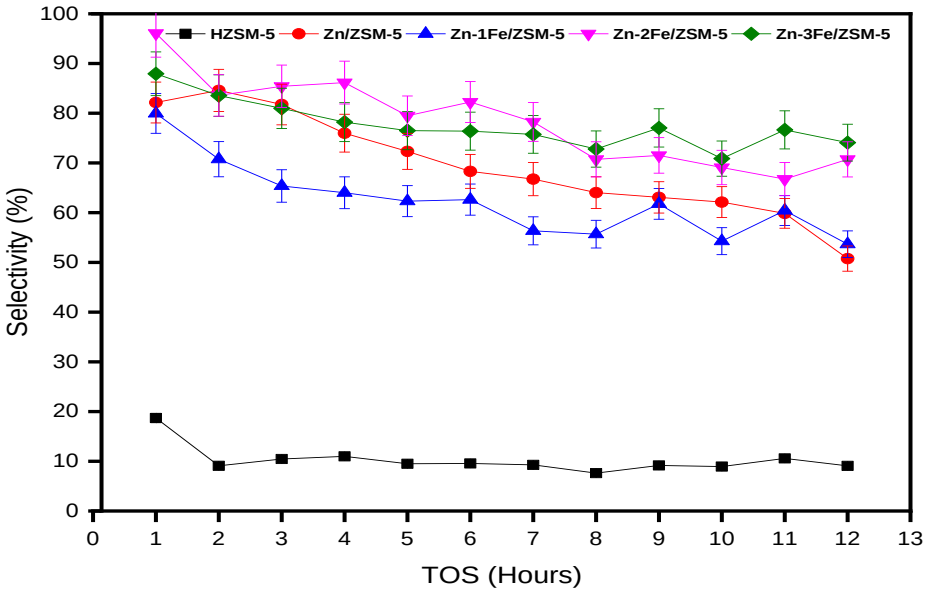


Figure 4.24: Aromatic selectivity on HZSM-5, Zn/ZSM-5 and Zn-Fe/ZSM-5

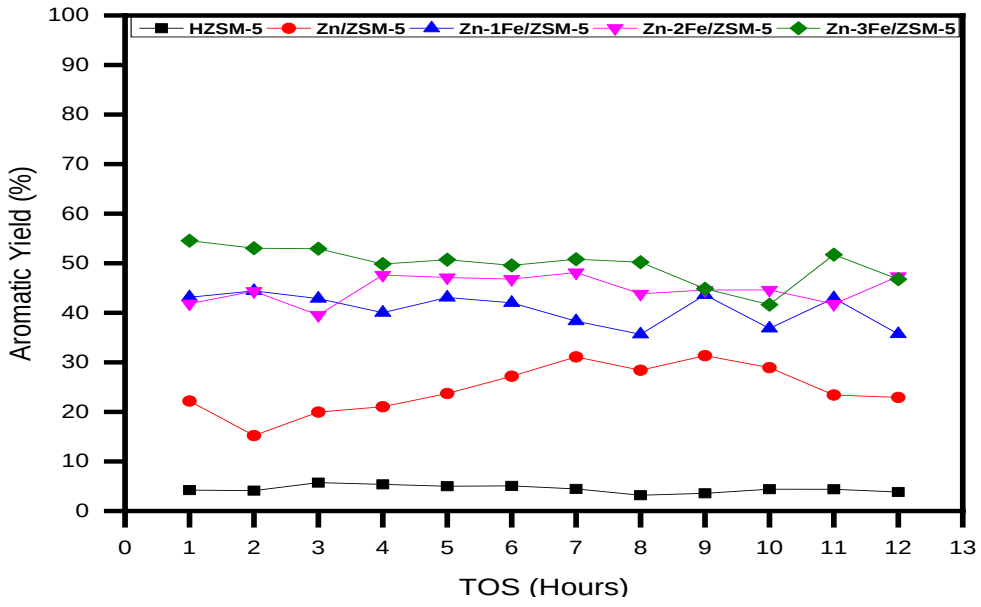


Figure 4.25: Aromatic yield on HZSM-5, Zn/ZSM-5 and Zn-Fe/ZSM-5

It was generally observed that bimetallic Zn-Fe/ZSM-5 has higher aromatic yield due to Iron strengthening effect on Zinc thus sustaining its activity and selectivity effect on propane aromatization.

4.2.3 Effect of cobalt (III)-zinc (II)co-impregnation loading on ZSM-5

Presented here are results of the effect of the co-impregnation of cobalt and zinc on parent ZSM-5 on propane conversion carried out at 540^{o}C and atmospheric pressure with corresponding aromatic selectivity and yield in comparison with parent ZSM-5 and Zn/ZSM-5. Catalytic activity and aromatic selectivity were improved to a reasonable extent thereby increasing the conversion of propane significantly as reported in section 4.2.2. Thus, the activity of the catalysts was sustained for twelve hours' time on stream because of the strengthening effect of cobalt on zinc at the reaction temperature which resulted to the enhanced recorded stability presented in Figure 4.26.Figure 4.27 shows lower but sustained selectivity for 1 and 3 wt. % loading of cobalt on Zn/ZSM-5. Above 2 wt. % of cobalt with zinc, the selectivity drops. 2 wt. % Cobalt with 2 wt. % Zn on ZSM-5 had the highest sustained selectivity of about 90% over twelve hours' time on stream which could have resulted from effective mixing of same loading. The yield and selectivity for aromatics increased for metal modified ZSM-5 from mono to bimetallic.

Aromatic yield of Zn-Co/ZSM-5 bimetallic catalysts were improved and sustained for the twelve hours' time on stream as presented in Figure 4.28. The effect of metal addition improved both yield and selectivity towards aromatic significantly. Propane conversion, aromatic yield and selectivity using Zn-Co/ZSM-5 catalysts were calculated using equations 3.1-3.4 in section 3.4. Appendix B4 and B7 detailed the carbon balance calculation processes for catalytic performances over Zn-Co/ZSM-5 bimetallic catalysts.

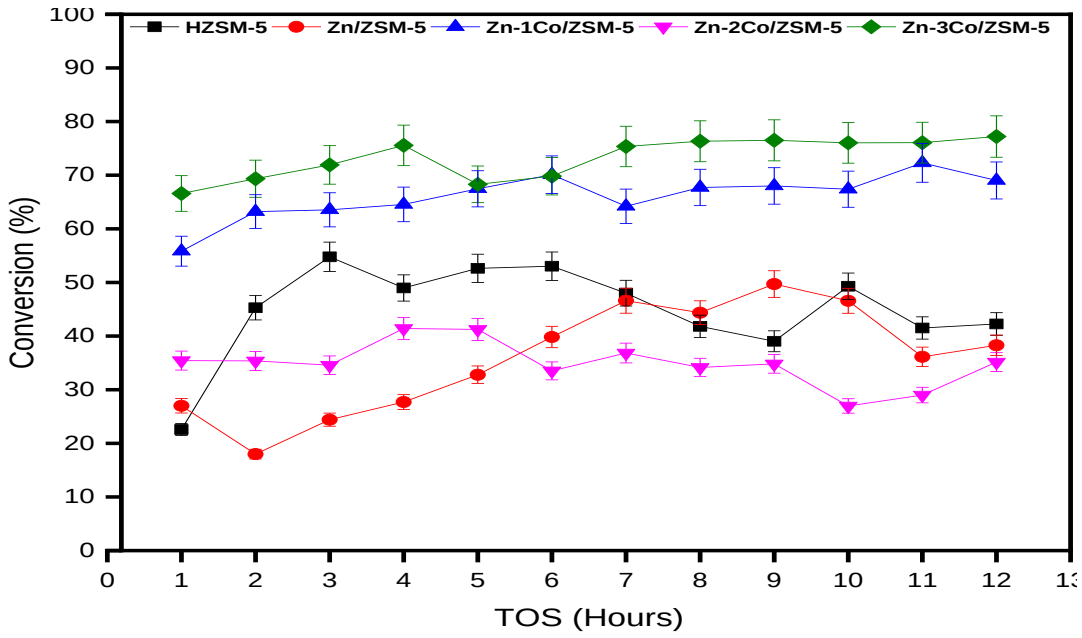


Figure 4.26: Propane conversion over HZSM-5, Zn/ZSM-5 and Zn-Co/ZSM-5

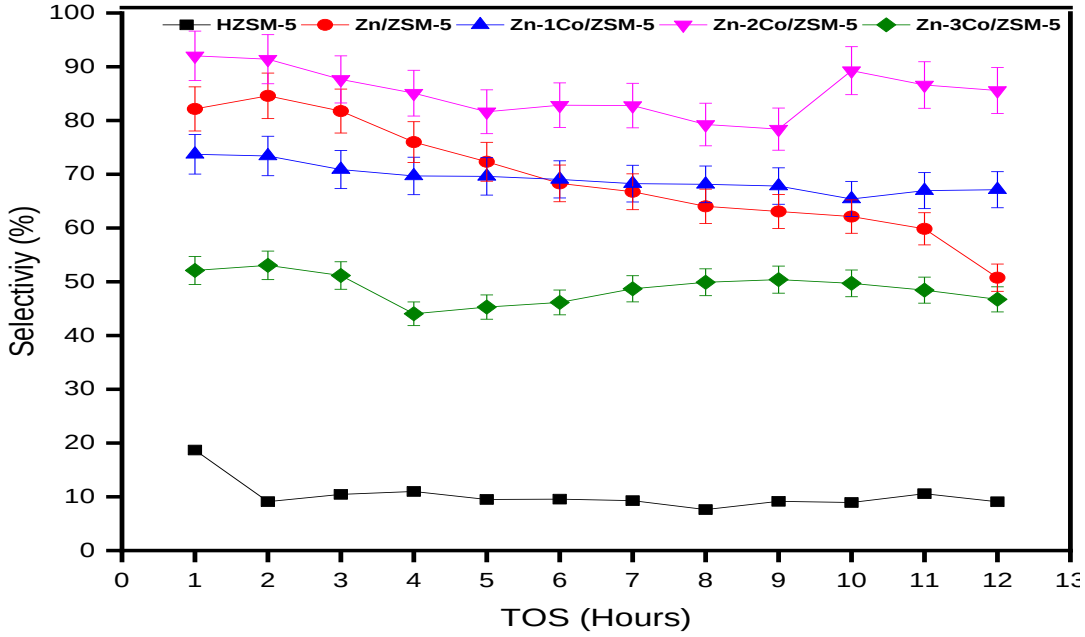


Figure 4.27: Aromatic selectivity on HZSM-5, Zn/ZSM-5 and Zn-Co/ZSM-5

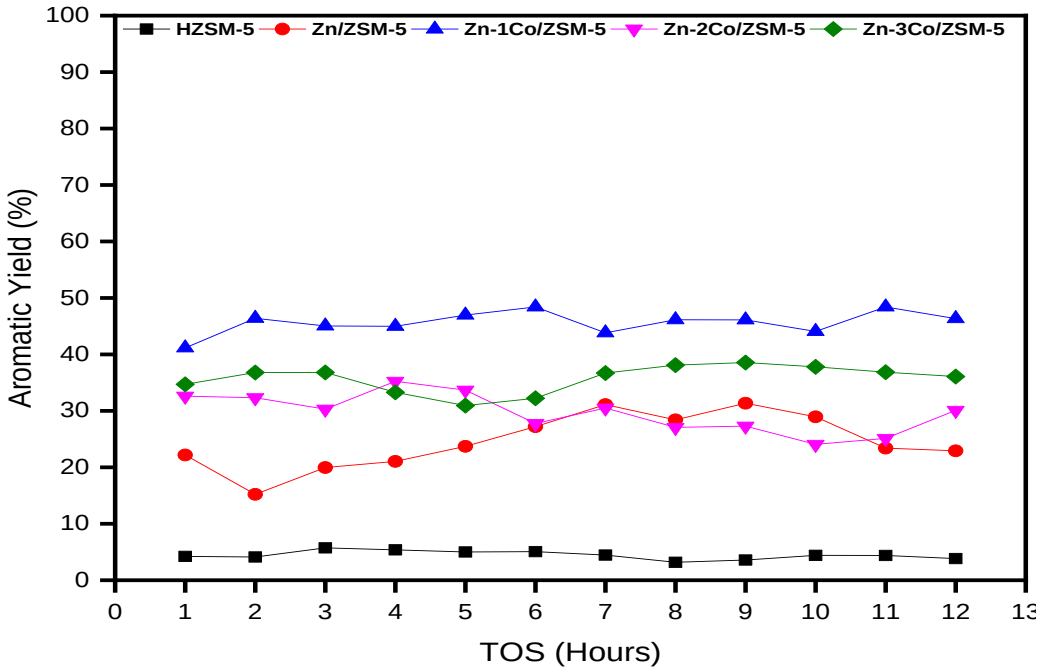


Figure 4.28: Aromatic yield on HZSM-5, Zn/ZSM-5 and Zn-Co/ZSM-5

4.2.4 Effect of nickel (II)-Zinc oxide co-impregnation loading on ZSM-5

This sub-section presents the effect of nickel and zinc on HZSM-5 in the catalytic conversion of propane at 540^{o}C and atmospheric temperature. Activity of the catalysts was improved through increased and sustained conversion of propane for twelve hours' time on stream as observed in Figure 4.29. Highcatalytic performance of Zn-Ni/ZSM-5 both for activity and aromatic selectivity is attributed to increased Lewis acid sites with increased metal loading as shown in FTIR-Pyridine and possession of same valency and oxidation state of both +1 and +2 of zinc and nickel as shown by the XPS results. Thus at any stage of species transition in oxidation, effective bonding is enhanced.Improved and sustained selectivity as presented in Figure 4.30was also achieved due to synergistic effect of Bronsted and Lewis acid sites as seen from FTIR-Pyridine. Transition in oxidation state during reaction favoured each metalspecie bonding in recombining hydrogen thus suppressing cracking (Beta-scission), minimizing hydrogenation backward reaction and enhancing oligomerization and cyclization compared to only Zinc oxide on ZSM-5.The 2 wt. % Zn-2 wt. % Ni//ZSM-5 possessed the

lowest conversion but highest selectivity. This may probably be due toequal wt. % loading of metal species, same oxidation state and co-dehydrogenation of nickel as shown from the Hydrogen-TPRand XPS thereby forming a stable Zn-Ni network on ZSM-5 network and further enhanced dehydrogenation without loss of active sites (Zhou *et al*., 2019).

Appendix B5, B9 and B11 detailed the carbon balance calculation processes for catalytic performances over Zn-Fe/ZSM-5 bimetallic catalysts.

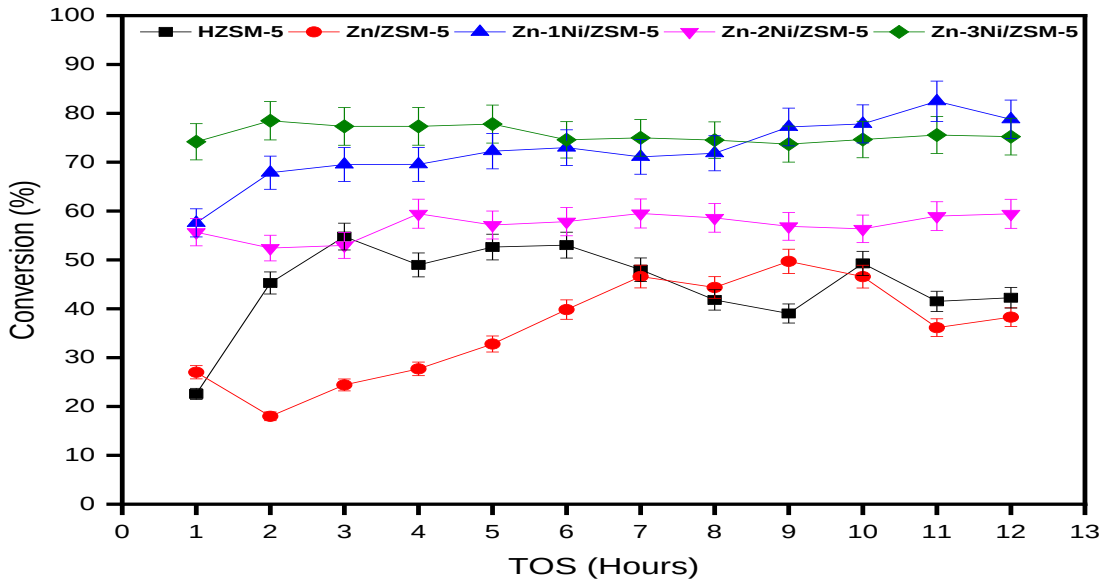


Figure 4.29: Propane conversion over HZSM-5, Zn/ZSM-5 and Zn-Ni/ZSM-5

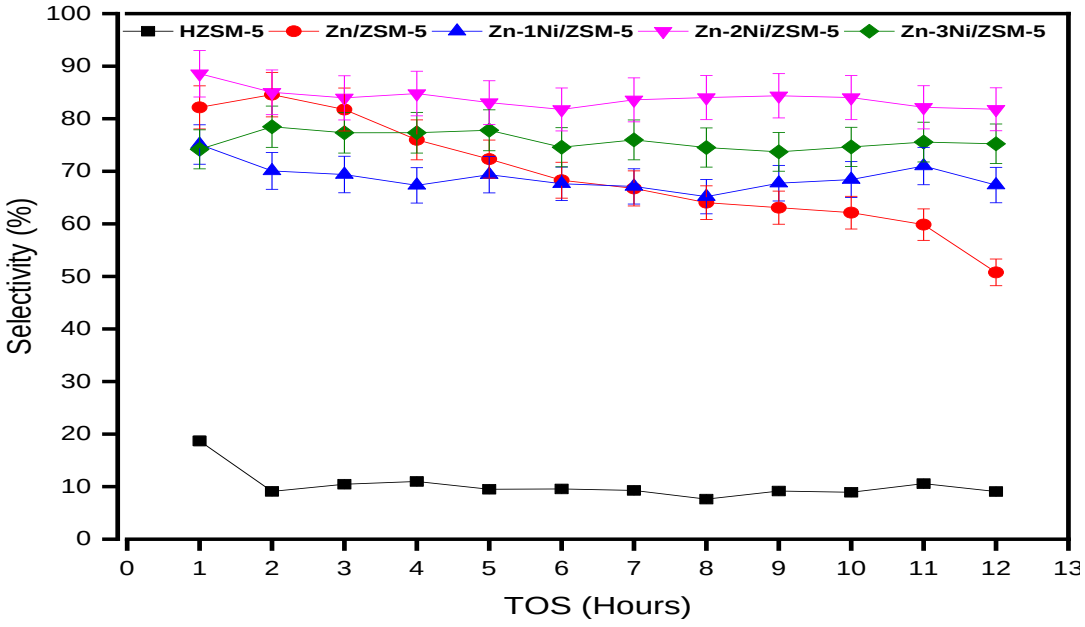


Figure 4.30: Aromatic selectivity on HZSM-5, Zn/ZSM-5 and Zn-Ni/ZSM-5

Figure 4.31 presents the improved aromatic on account of zinc and nickel co-impregnation as compared to parent HZSM-5 and Zn-ZSM-5 catalyst. It could be observed that both yield and selectivity increased bimetallic catalyst as compared to HZSM-5 and Zn/ZSM-5.

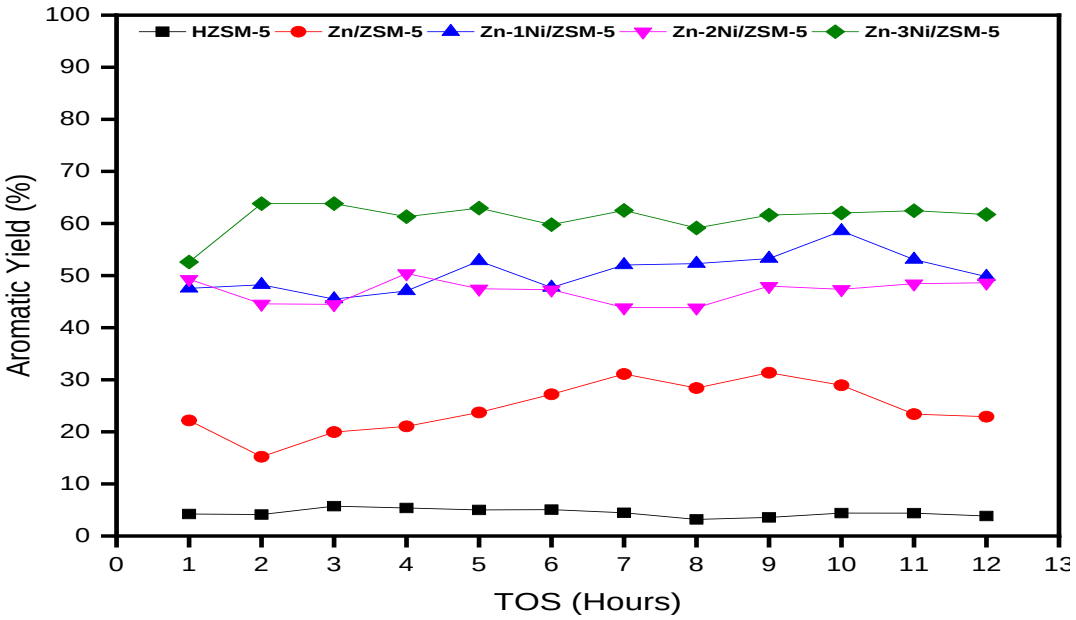


Figure 4.31: Aromatic yield on HZSM-5, Zn/ZSM-5 and Zn-Ni/ZSM-5

4.2.5 Effect of copper (II)-zinc oxide co-impregnation loading on ZSM-5

Presented here is the effect of the copper and zinc loading on parent ZSM-5 on propane conversion at 540^{o}C and atmospheric pressure. Improved activity of the catalysts as seen in other metals through increased and sustained propane conversionand aromatic selectivity for twelve hours' time on stream as presented in Figure 4.32 to Figure 4.33 were recorded. Also the dehydrogenating effect of Zn-Cu can also be attributed to possession of same valency and oxidation state of both +1 and +2 of zinc and copper which enhanced metal-metal interaction. Change in oxidation state during reactionmight have also favoured each metal specie interactionand recombining hydrogen, which suppressed cracking, minimized hydrogenation (backward reaction) and enhanced oligomerization and cyclization compared to only Zinc oxide on ZSM-5.Equal 2 wt. % of copper and zinc on ZSM-5 possessed the lowest conversion but highest selectivity as also observed in other metals. This may probably be due

toeffective and stable metal-metal interaction on ZSM-5 network because of equal wt. % loading, thus enhanced dehydrogenation without loss of active sites.

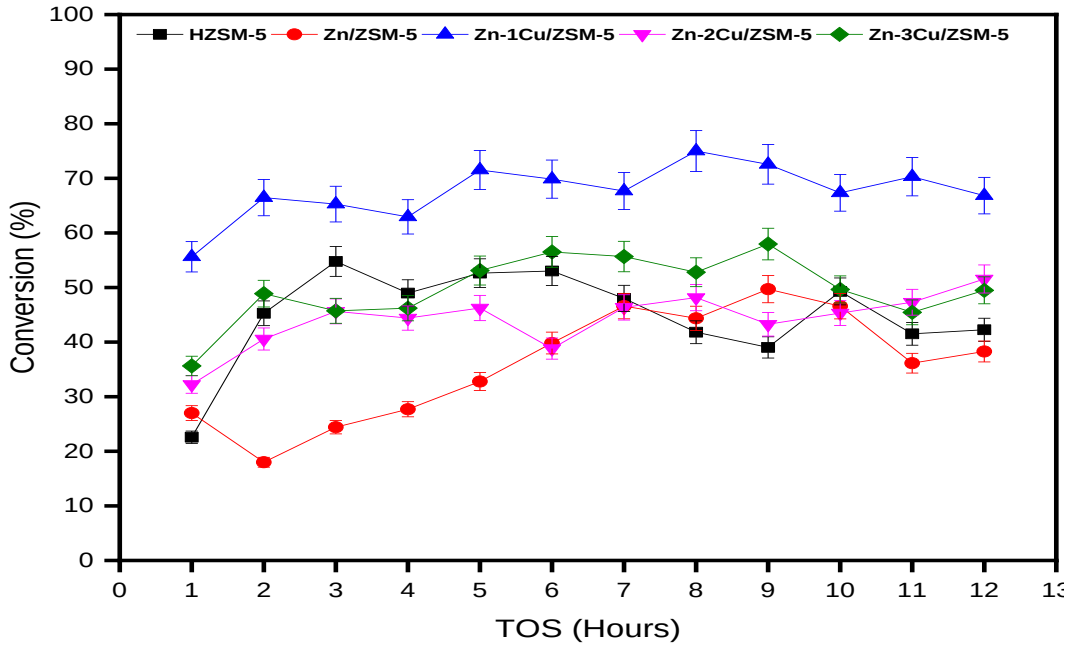


Figure 4.32: Propane conversion over HZSM-5, Zn/ZSM-5 and Zn-Cu/ZSM-5

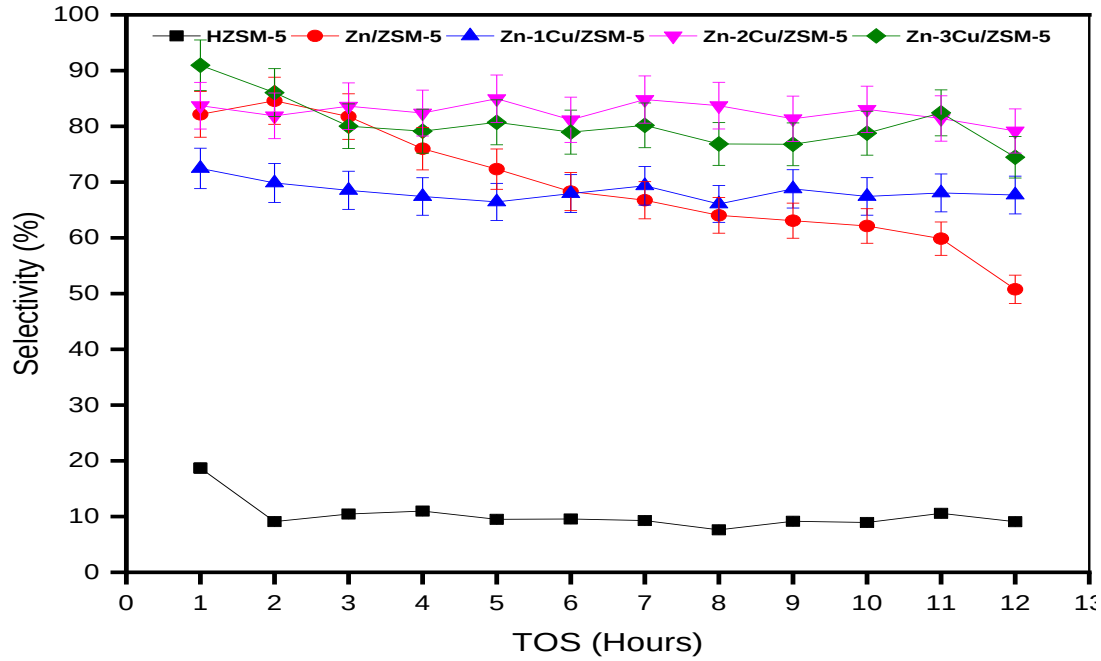


Figure 4.33: Aromatic selectivity on HZSM-5, Zn/ZSM-5 and Zn-Cu/ZSM-5

The yield of different metal loading also showed significant levels of sustained improvement higher than the parent zeolite and Zinc impregnated one as presented in Figure 4.34.

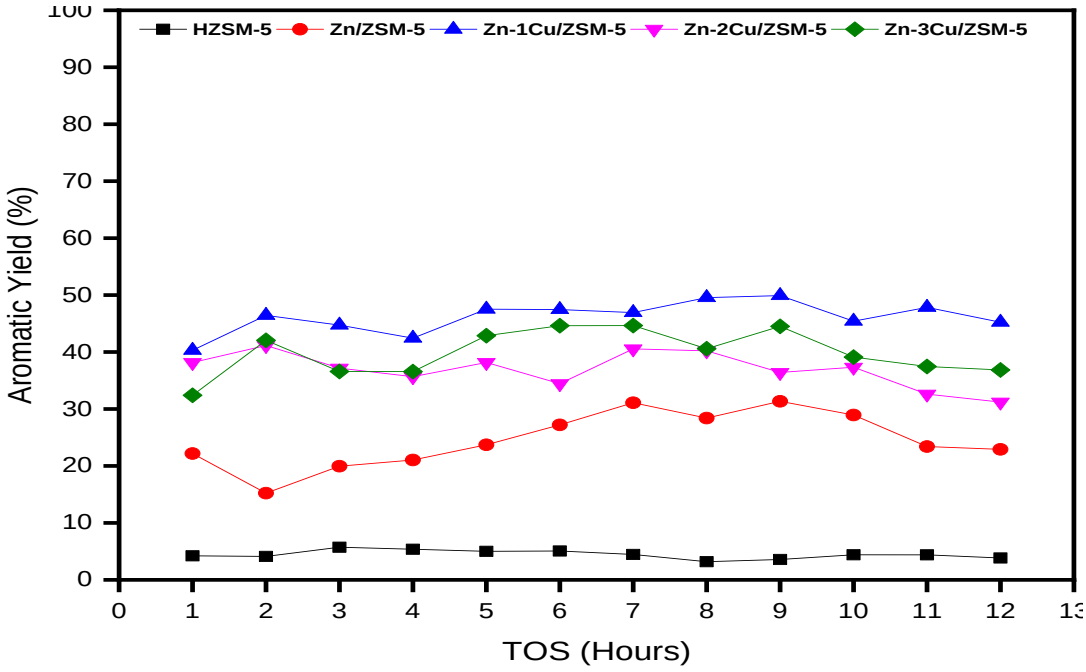


Figure 4.34: Aromatic yield on HZSM-5, Zn/ZSM-5 and Zn-Cu/ZSM-5

Table 4.4 shows the average conversion, selectivity and yield of the catalyst performances of propane aromatization for twelve hours' time on stream (TOS).

Appendix B6 and B10 detailed the carbon balance calculation processes for catalytic performances over Zn-Fe/ZSM-5 bimetallic catalysts.

4.3 Effect of Bimetallic ZSM-5 Catalyst on Product Distribution of Propane aromatization

This sections present the product distribution of each designed catalyst on propane aromatization. Figure 4.35 is the product distribution of the parent HZSM-5 catalyst with high percentage of light gases due to cracking and formation of cyclohexanes and heptanes (C_6-C_7). High Bronsted acidity of HZSM-5 catalyst is responsible for the high percentage of C_5-C_{10} aliphatic hydrocarbons.

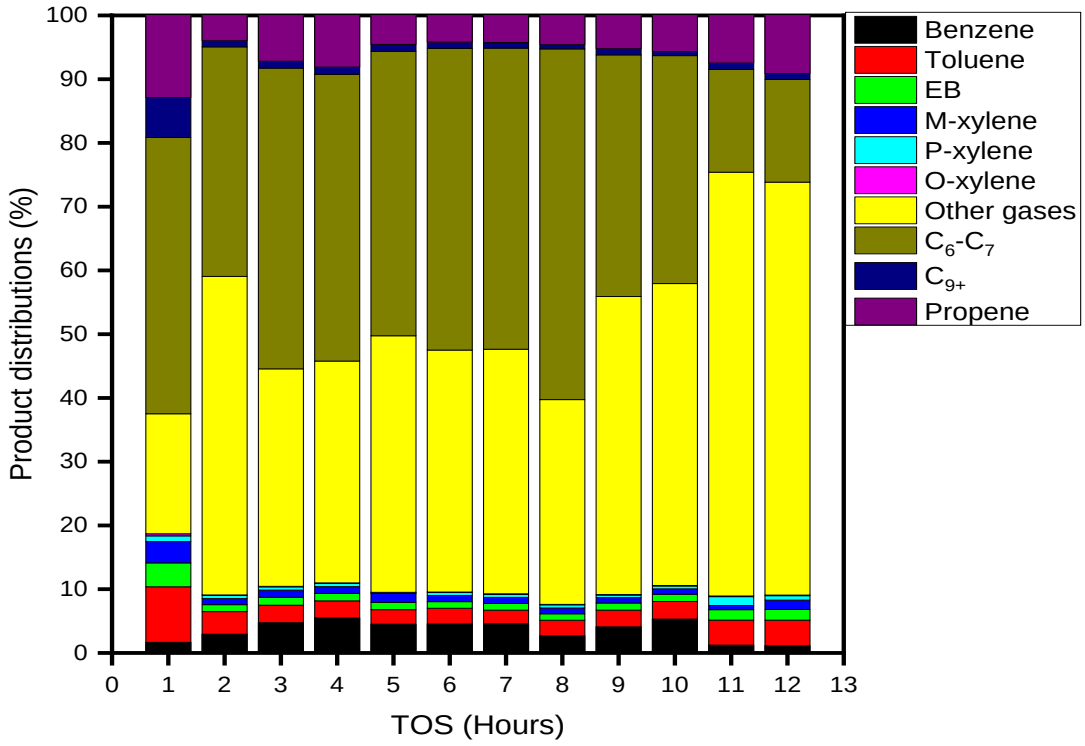


Figure 4.35: Products distribution on propane aromatization over HZSM-5 catalyst

The dehydrogenation capacity of zinc was clearly shown as there is a boost in the aromatic compound selectivity minimizing cracking and side reactions as shown in Figure 4.36. As the time on stream continues, the other gases (ethane, methane, ethane, butane, neo-pentane), propene and C_{9+} components increase showing loss of active site due to instability of zinc at reaction temperature.

The effect of 1 wt. % metal loadings was clearly shown in the sustained selectivity of each aromatic component with time on stream with toluene being the most stable of all. This is because of methyl group attached to it as electron donor to the benzene ring. The light gases, propene and C_{9+} production were reduced because of metal stabilizing on Zinc as active component in the synthesized catalysts. Figure 4.37 to Figure 4.40 show 1 wt. % iron Fe, cobalt Co, nickel Ni and copper Cu loadings with zinc on ZSM-5. It was also observed all through product distribution of competitive formation of toluene and m-xylene.

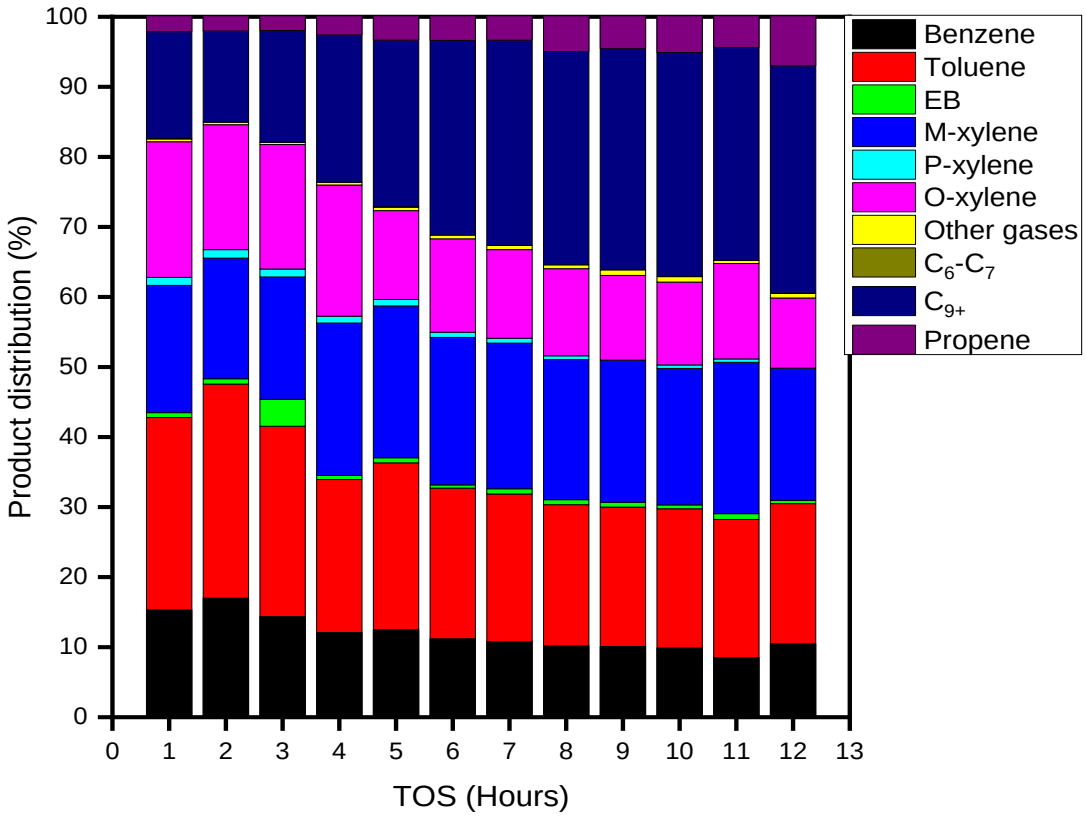


Figure 4.36: Products distribution of propane aromatization over Zn/ZSM-5 catalyst

This is ascribed to the geometry and orientation of the component in zeolite pore. In the process of products competitive diffusion out of the pore of the zeolite, demethylization will always occur on of one of the methyl group of m-xylene thereby favoring more toluene as clearly seen in 2 wt. % Co with Zn on ZSM-5 (Figure 4.42). Chances are also that C_{9+} formation is also favored by alkylation process of higher alkyl group like propyl, butyl and also coming together of other aromatics as clearly observed in Figure 4.37 and Figure 4.39.

2 wt. % metal oxide-2 wt. % ZnO/ZSM-5 catalysts product distribution shows higher selectivity towards each component of aromatics which were stable and sustained over twelve hours' time on stream than 1% metal loading as shown in Figure 4.41 to Figure 4.44. This is attributed to enhanced active sites performance thus improved and sustained its dehydrogenation.

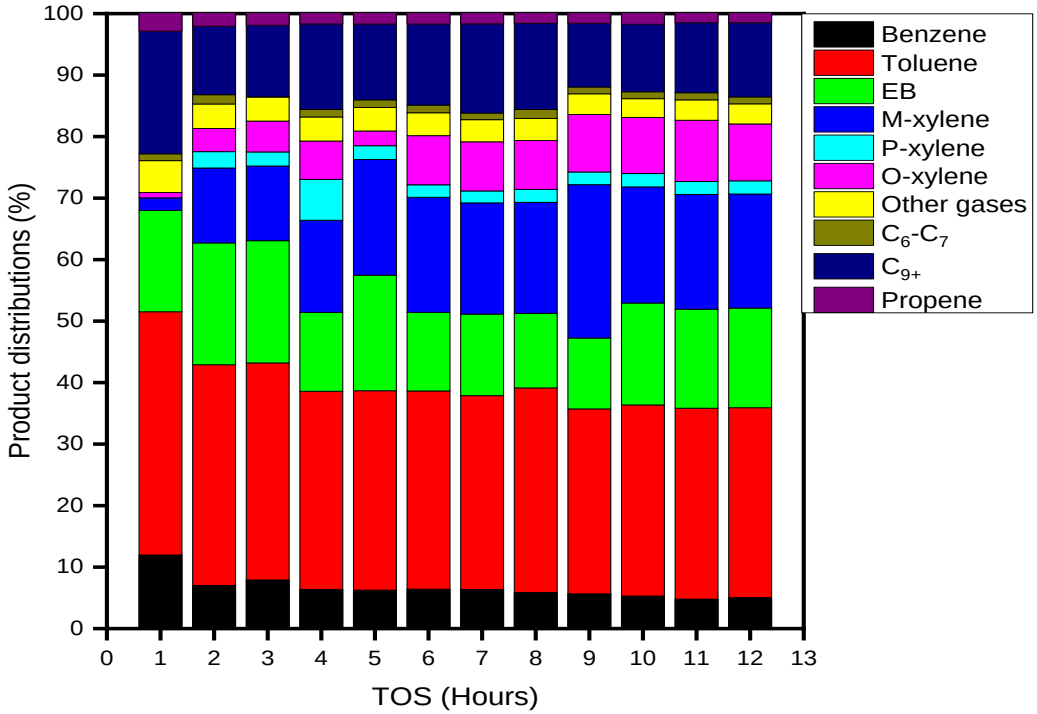


Figure 4.37: Products distribution of propane aromatization over Zn-1Fe/ZSM-5

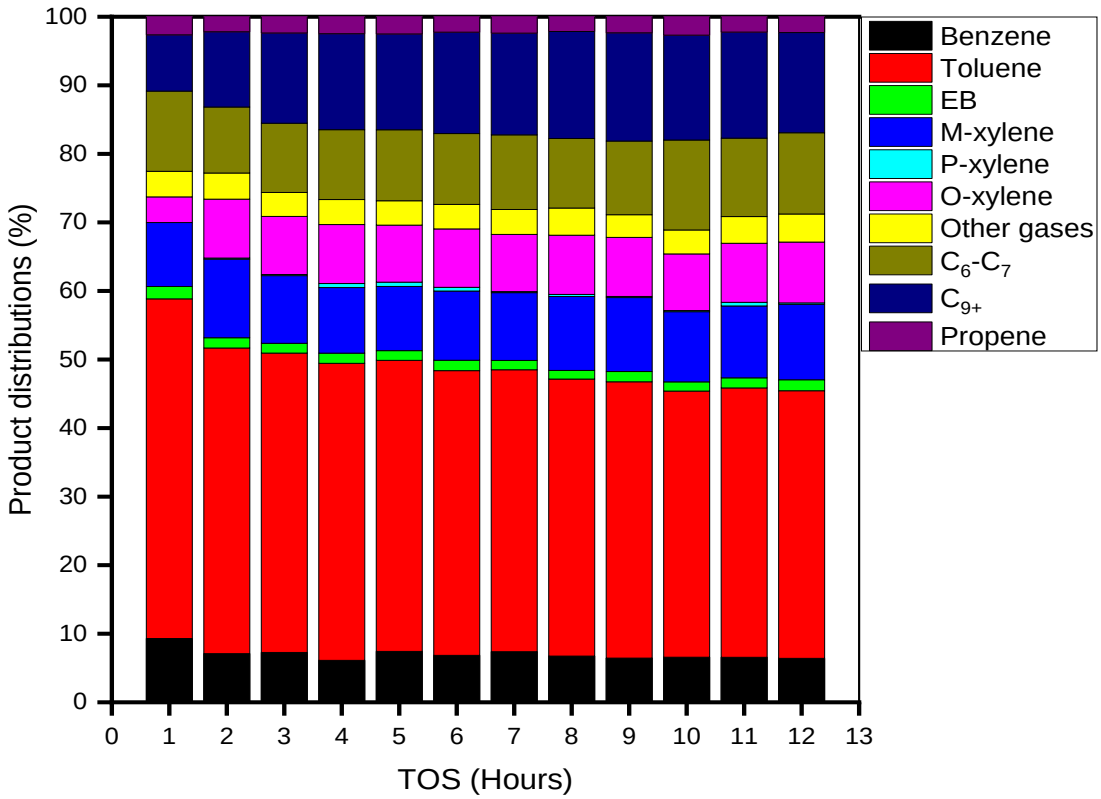


Figure 4.38: Products distribution of propane aromatization over Zn-1Co/ZSM-5

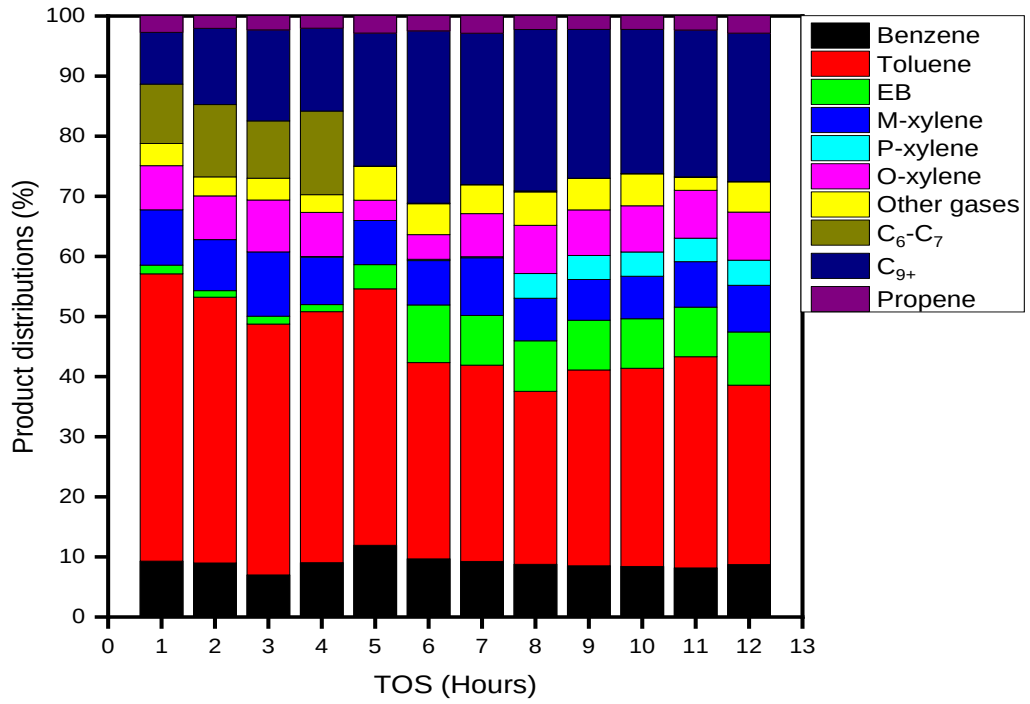


Figure 4.39: Products distribution of propane aromatization over Zn-1Ni/ZSM-5

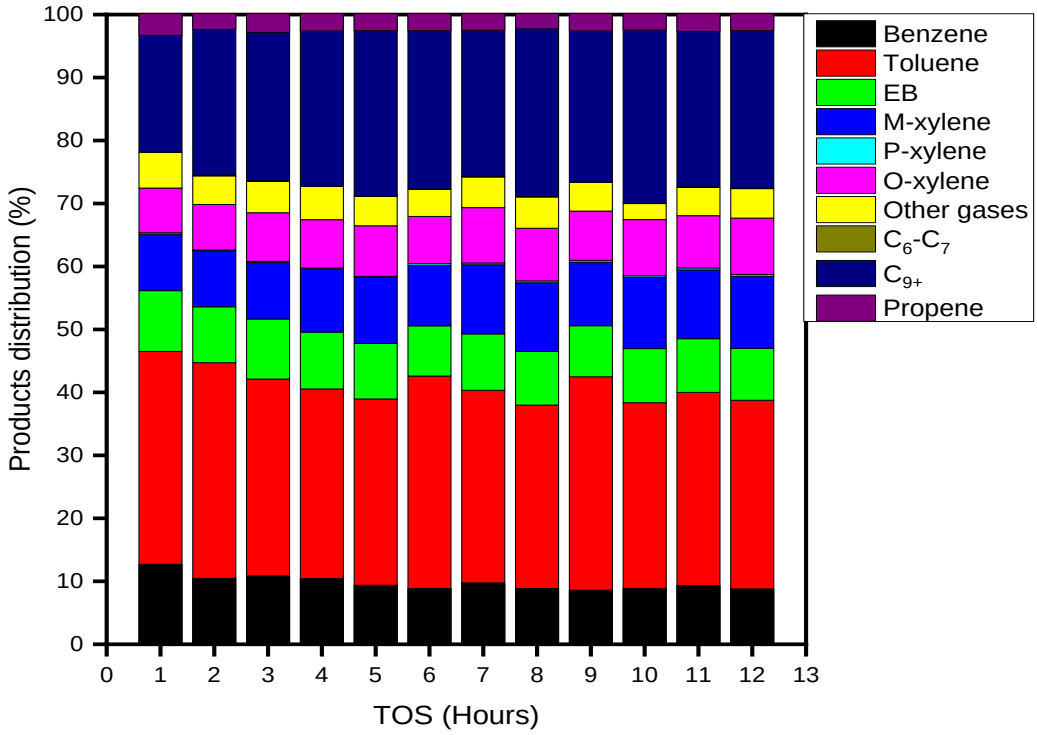


Figure 4.40: Products distribution of propane aromatization over Zn-1Cu/ZSM-5

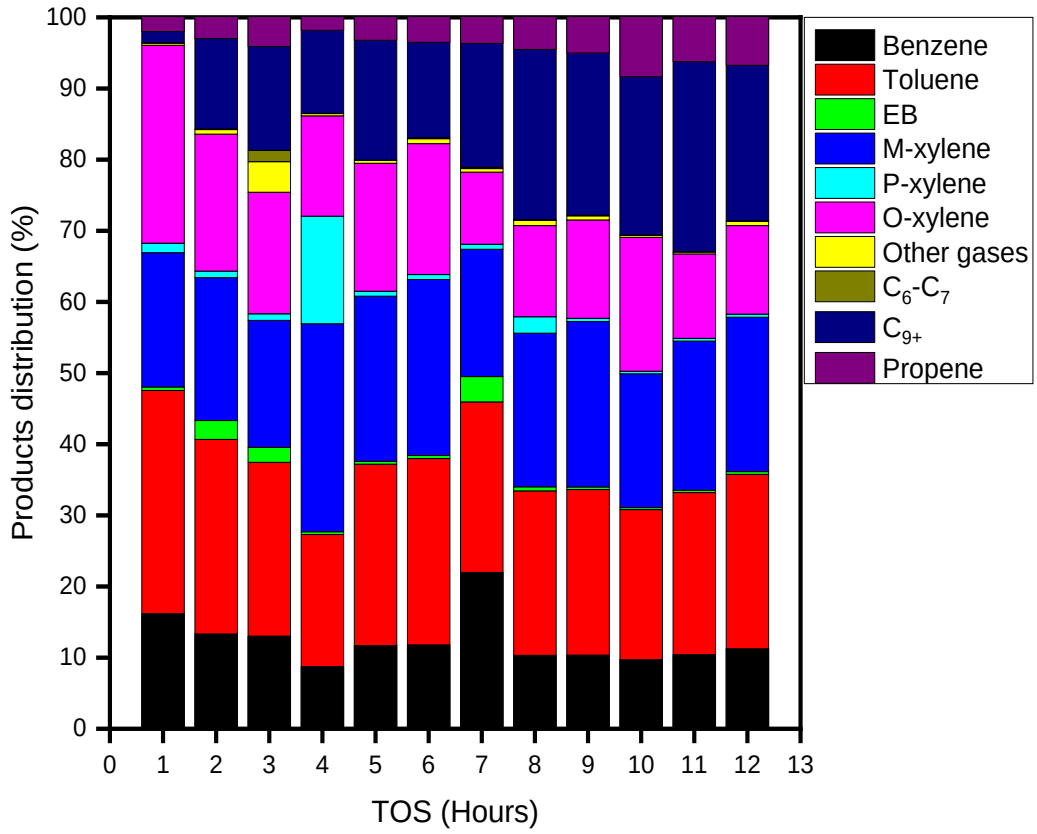


Figure 4.41: Products distribution of propane aromatization over Zn-2Fe/ZSM-5

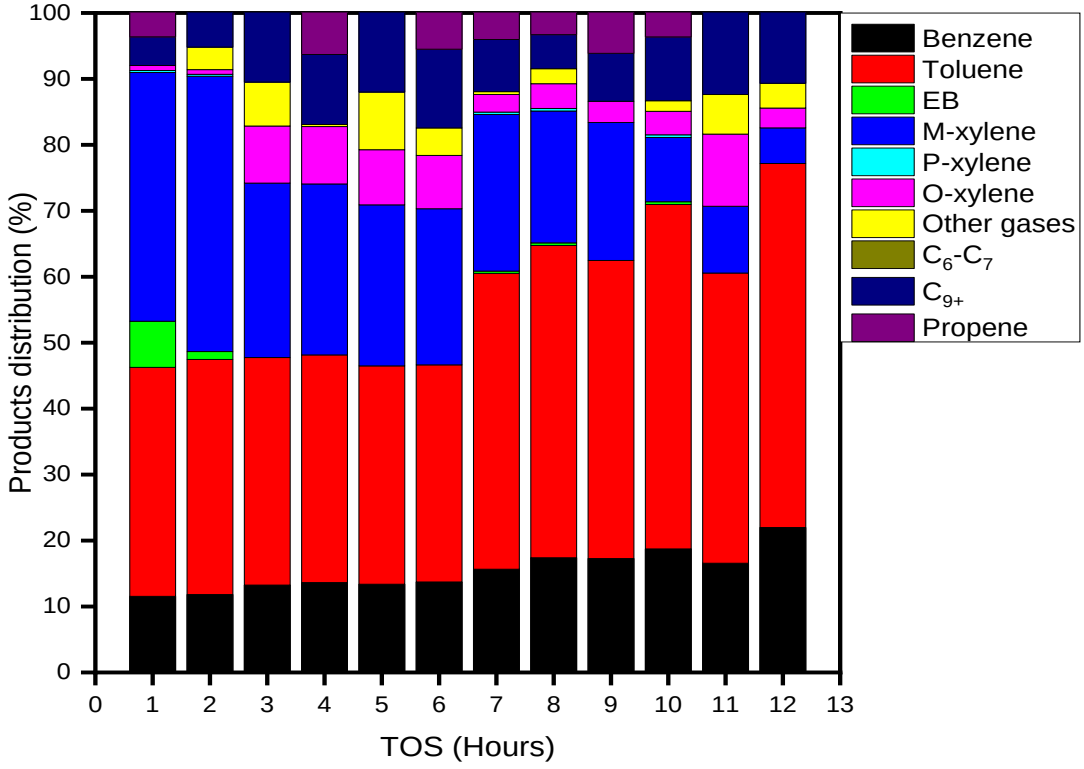


Figure 4.42: Products distribution of propane aromatization overZn-2Co/ZSM-5

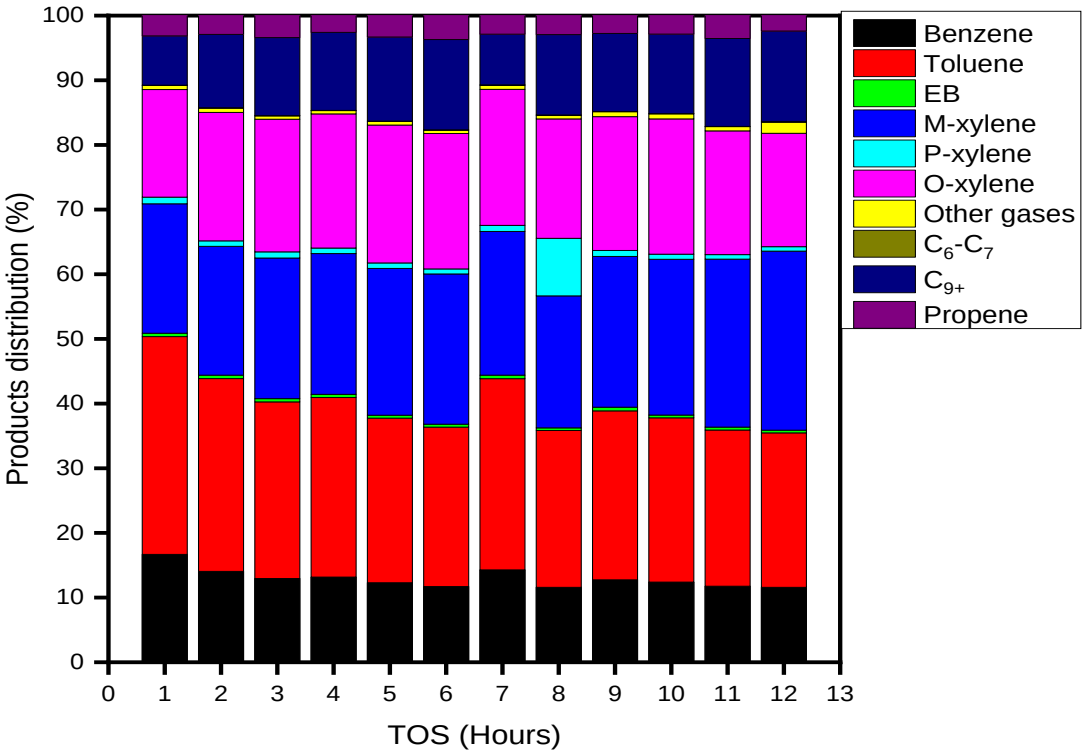


Figure 4.43: Products distribution of propane aromatization over Zn-2Ni/ZSM-5

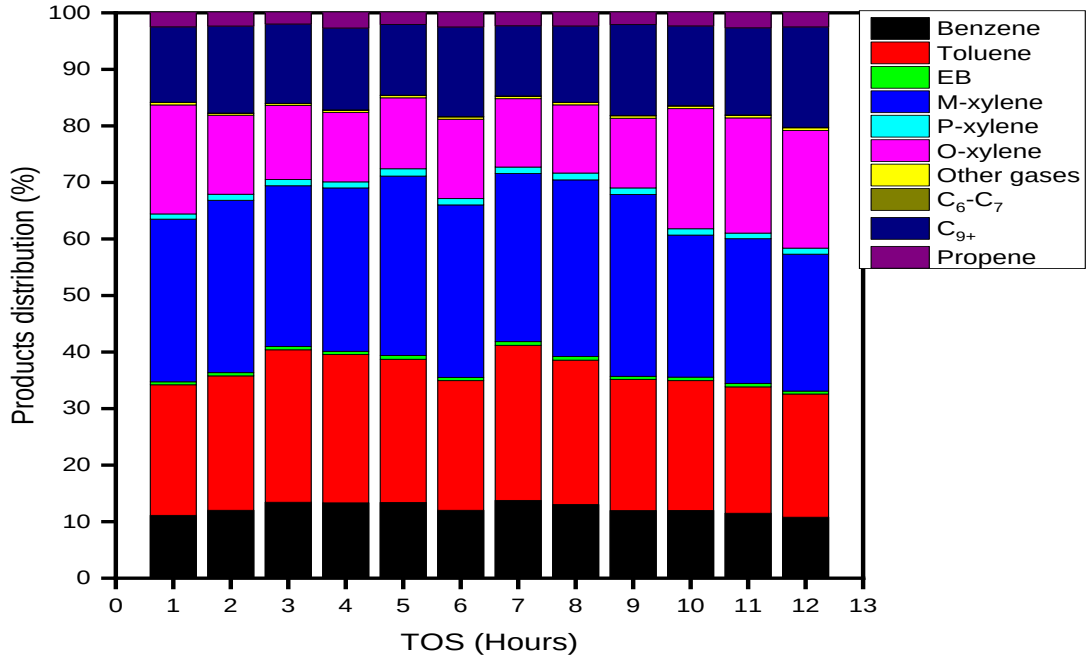


Figure 4.44: Products distribution of propane aromatization over Zn-2Cu/ZSM-5

The 3 wt. % metal co impregnated catalysts with 2 wt. % Zn on ZSM-5 catalyst showed sustained aromatic compounds formation though because of stability. The product distributions are all shown in Figure 4.43 to Figure 4.46.

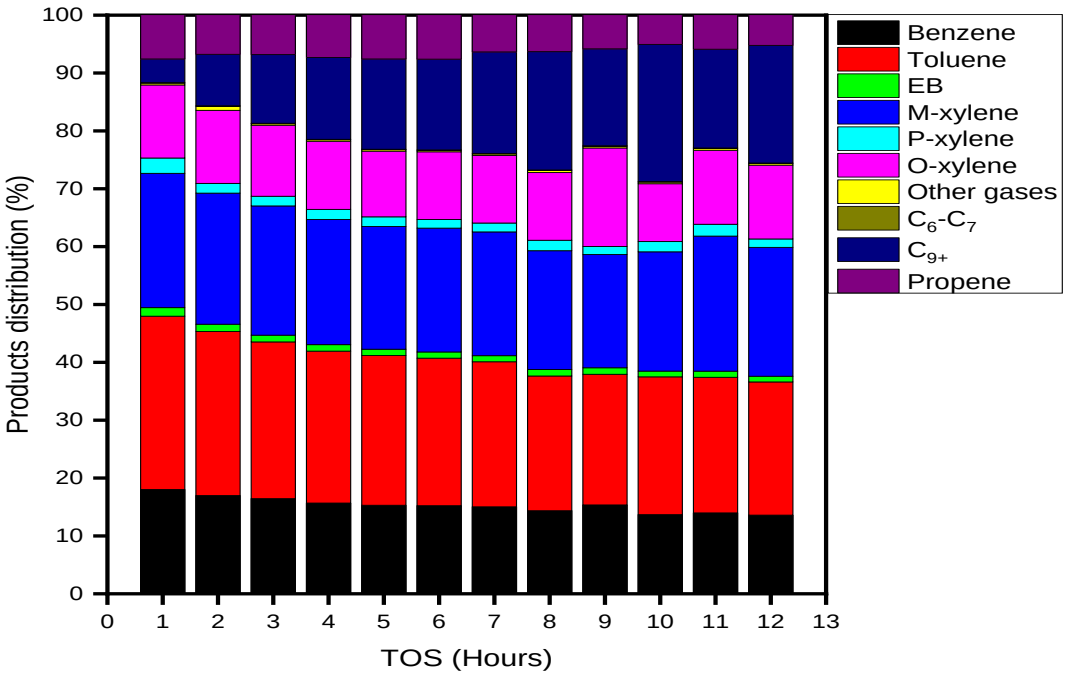


Figure 4.42: Products distribution of propane aromatization over Zn-3Fe/ZSM-5

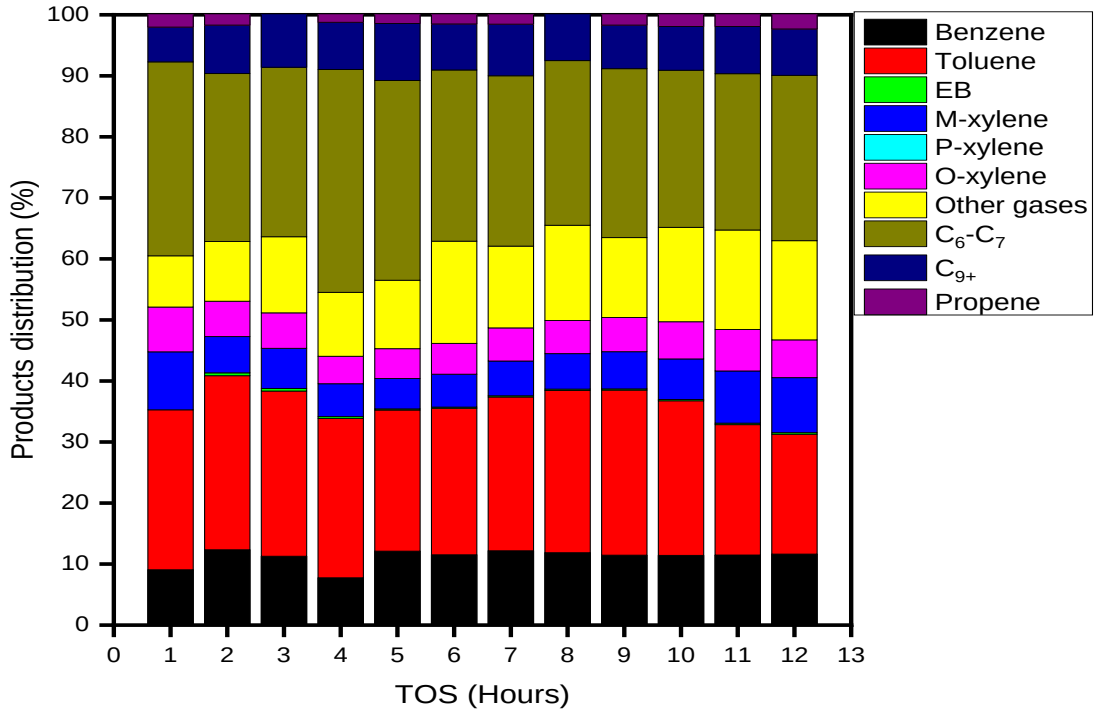


Figure 4.43: Products distribution of propane aromatization over Zn-3Co/ZSM-5

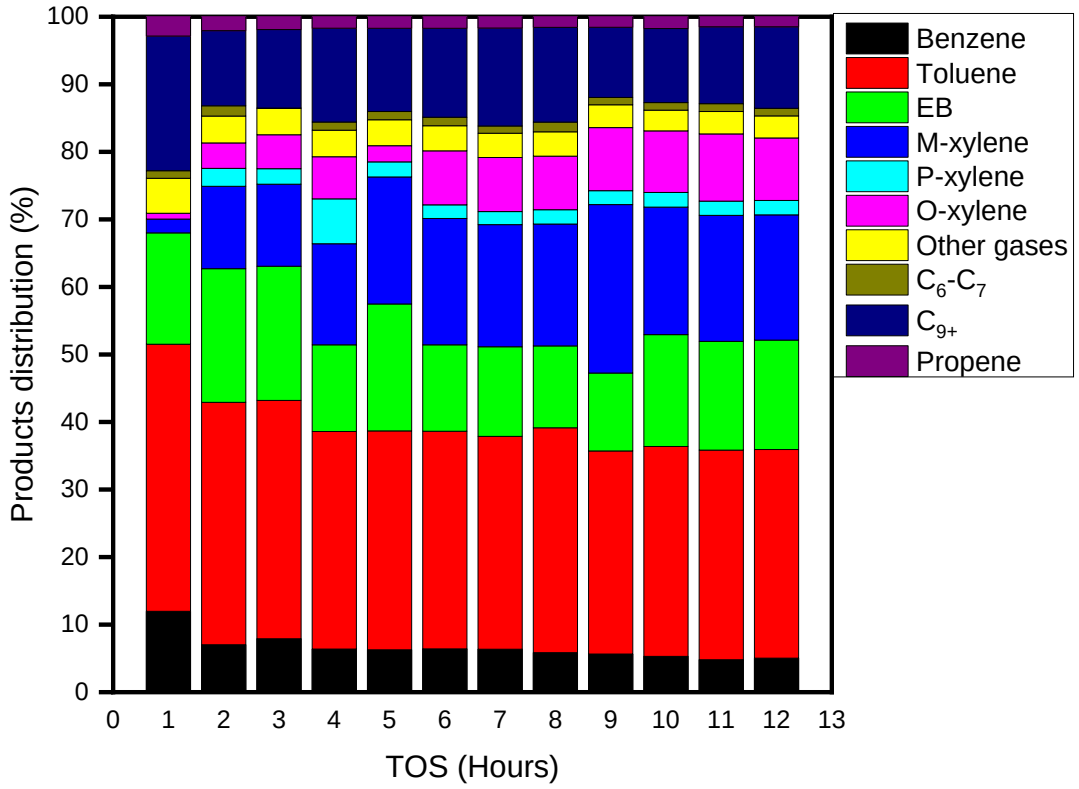


Figure 4.44: Products distribution of propane aromatization over Zn-3Ni/ZSM-5

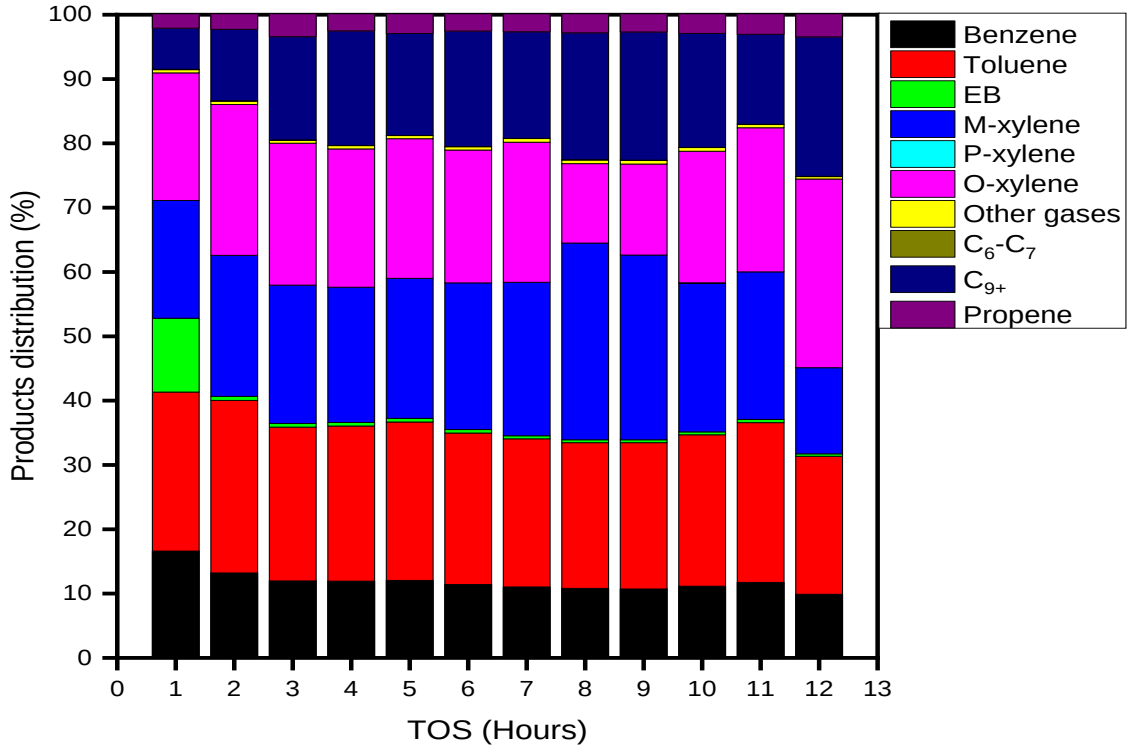


Figure 4.45: Products distribution of propane aromatization over Zn-3Cu/ZSM-5

General comparison was made based on undesired products to determine the best performing catalyst of different metal impregnation dosages. It was observed nickel followed by copper loaded with zinc on ZSM-5 had lower light gases showing that the possession of the same oxidation state and proximity to Zinc in the periodic table (close atomic size) played a very vital role in forming a bimetallic catalyst for enhanced dehydrogenation. Cobalt and iron Zn/ZSM-5 had higher light gases component because possession of +2 and +3 oxidation state. Equal Zn-Me composition on ZSM-5had little or no light gases as compared other bimetallic catalysts. It was also observed that Zn/ZSM-5 was losing activity with time on stream by the increase in the light gases formed. Zn-Ni/ZSM-5 also had the highest conversion and aromatic selectivity.

Table 4.5 shows the summary of catalyst performances and product selectivity.

Table 4.5: Catalyst aromatic favoured products

Catalyst	Aromatic products
HZSM-5	benzene
Zn/ZSM-5	m-xylene
Zn-1Fe/ZSM-5	toluene, ethylbenzene
Zn-2Fe/ZSM-5	m-xylene
Zn-3Fe/ZSM-5	m-xylene, benzene
Zn-1Co/ZSM-5	toluene, benzene
Zn-2Co/ZSM-5	toluene
Zn-3Co/ZSM-5	toluene
Zn-1Ni/ZSM-5	toluene, benzene
Zn-2Ni/ZSM-5	o-xylene
Zn-3Ni/ZSM-5	Ethylbenzene
Zn-1Cu/ZSM-5	m, o-xylene

Zn-2Cu/ZSM-5	m, o-xylene
Zn-3Cu/ZSM-5	m, o-xylene

4.4Effect ofChange in Process Conditions on Propane Conversion and Aromatic Selectivity over Zn-Ni/ZSM-5.

This section shows the effect of temperature and flowrate change on catalyst performance for propane aromatization.

4.4.1 Effect of temperature change on propane aromatization

Aromatization is an endothermic process; thus temperature has a key role effect on it. But higher temperature will lead to gas phase reaction leading to cracking of propane to lower alkanes. Figure 4.46 to Figure 4.48 show the effect of temperature on Zn-Ni/ZSM-5 of same weight percentage loading (2 wt. %) for propane aromatization. Increase in temperature as shown inFigure 4.46 increased propane conversion, aromatic yield and selectivity as aromatization is endothermic process which proceeds faster at higher temperature.

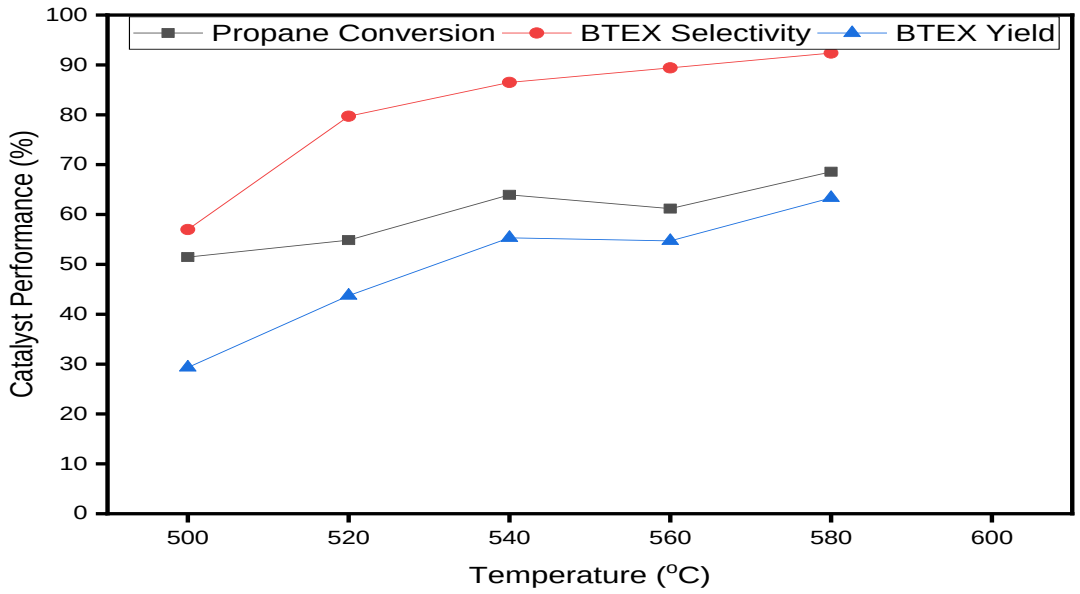


Figure 4.46:Effect of temperature on catalytic perfomance of propane aromatization over Zn-Ni/ZSM-5 catalyst

This further led to cracking of C_{9+}which are higher aromatic compounds to lower aromatic compounds which were clearly seen in increased toluene, benzene, o and m-xylene selectivity respectively. Increase in temperature favour dehydrogenation, oligomerization and cyclization as observed in products distribution in Figure 4.47. Lighter gases which are majorly propenewere utilized because of C_6-C_7 in the mixture were properly oligomerized, dehydrogenated, cyclized and dehydro-cyclized subsequently to formaromatic compound and as temperature increases. Compared to the previous reports, increase in temperature increased aromatic selectivity, propane conversion and stable products distribution (Al-Otaibi and Hutchings, 2010).

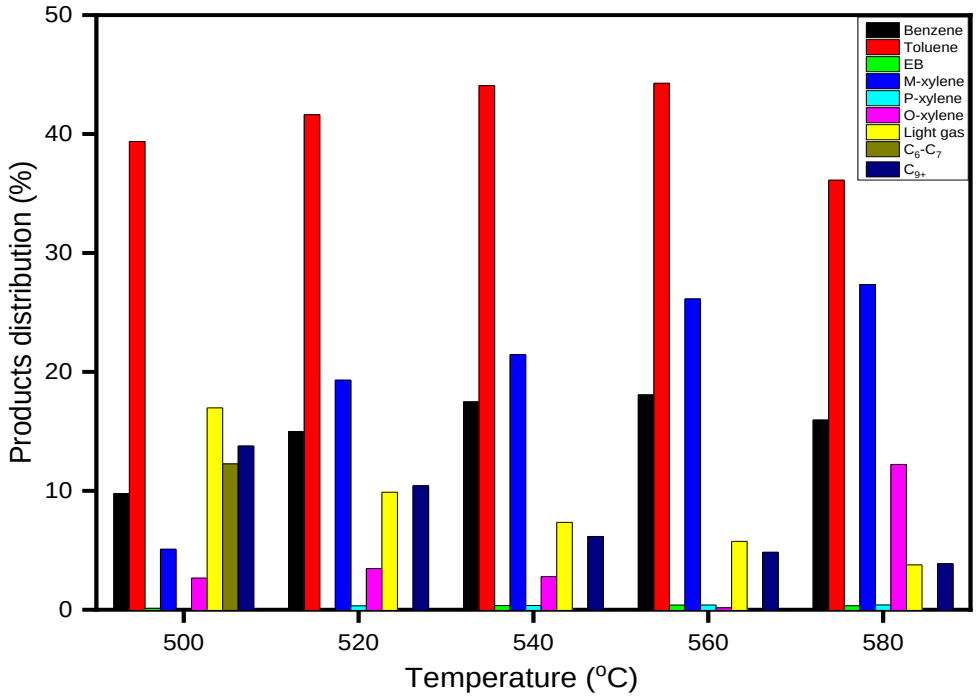


Figure 4.47: Effect of temperature on product distribution of propane aromatization over Zn-Ni/ZSM-5 catalyst

Figure 4.48 shows the lump of aromatic compounds and other products. It can be observed that the aromatic compounds increased with increase in temperature while the other products

reduced. This showed that temperature increased had favoured further conversion or utilization of product like propene and cyclo-hexanes in forming aromatic compounds alongside cracking of higher aromatic compounds to lower ones.

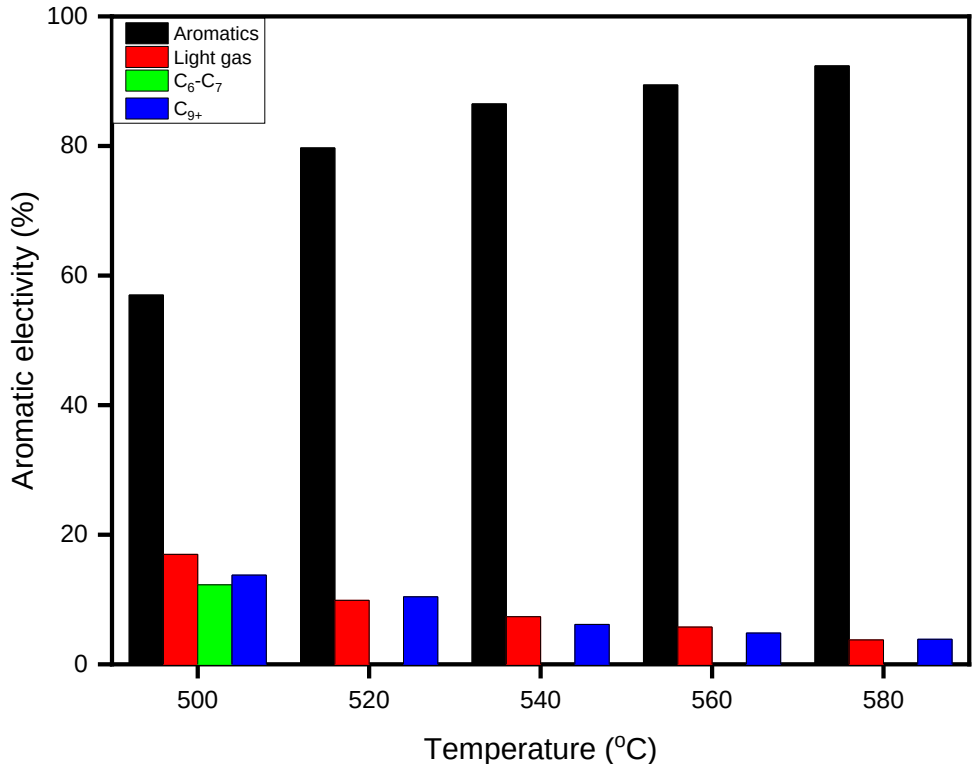


Figure 4.48: Effect of temperature on aromatic selectivity of propane aromatization over Zn-Ni/ZSM-5 catalyst.

4.4.2Effect of flow rate on propane aromatization

Increase in feed flow rate produced a major effect on both conversion and selectivity. This is presented in Figures 4.49 to Figure 4.51. Figure 4.49 showed conversion reduction as propane feed flow rate increased shorter residence time of propane with the catalyst surface at the reaction condition.Thus, increased aromatic selectivity because of shorter time of contact for cracking to take place and buildup of higher aromatics, C_{9+}.

Products distribution in Figure 4.50 shows reduction in light gases because the contact time was short to favour cracking or any form of secondary reactions but rapid oligomerization and isomerization. Shorter residence time also was responsible for declining $C_{9+}$with increase

propane flow rate. Thus, more toluene, benzene and m-xylene were formed. Increased light gases formed are as a result of unutilized propene.

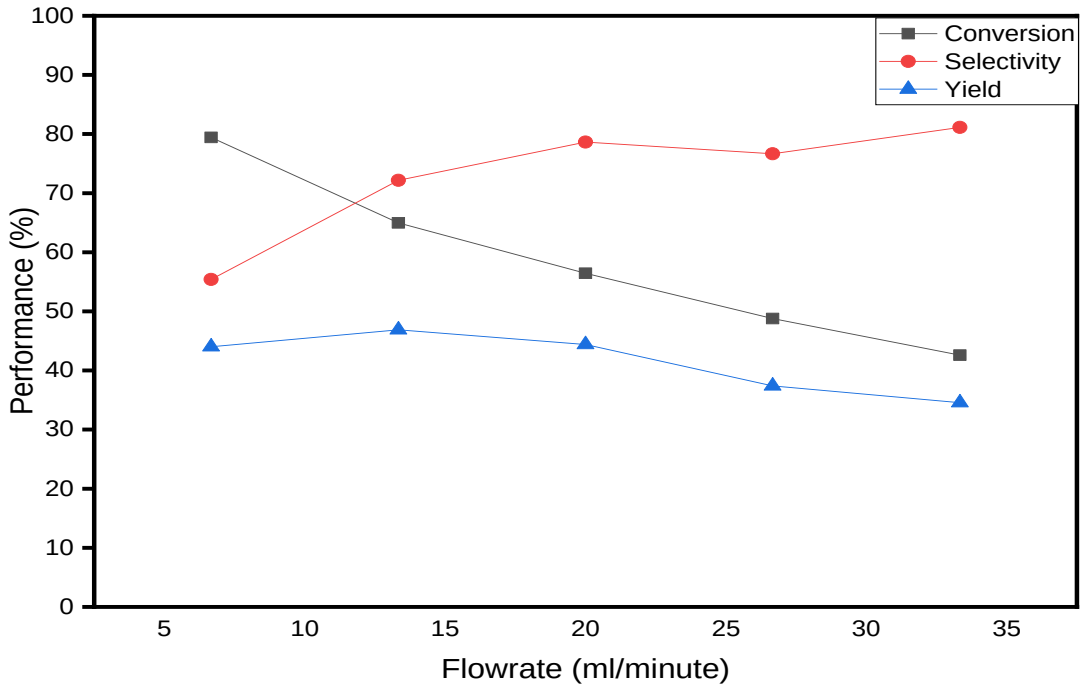


Figure 4.49: Effect of feed flowrate on catalytic performance of propane aromatization over Zn-Ni/ZSM-5 catalyst

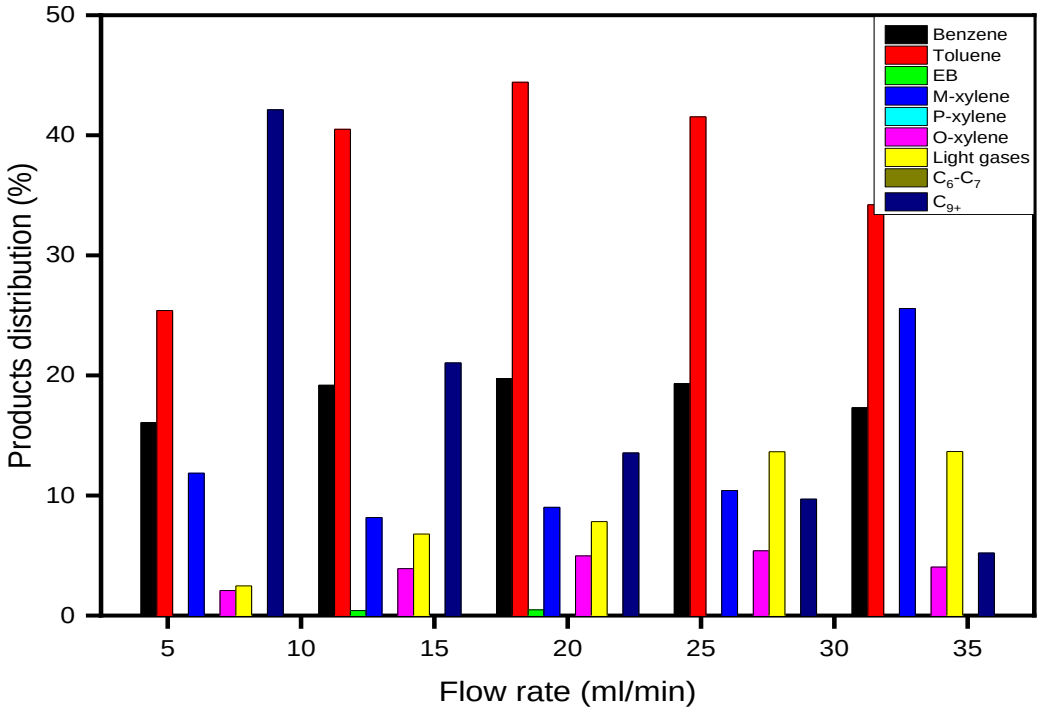


Figure 4.50: Effect of feed flow rate on product distribution of propane aromatization over Zn-Ni/ZSM-5 catalyst.

Figure 4.51 shows the lump of the aromatic compound in comparison with other products from the reactor. The increase in aromatic compound can be observed

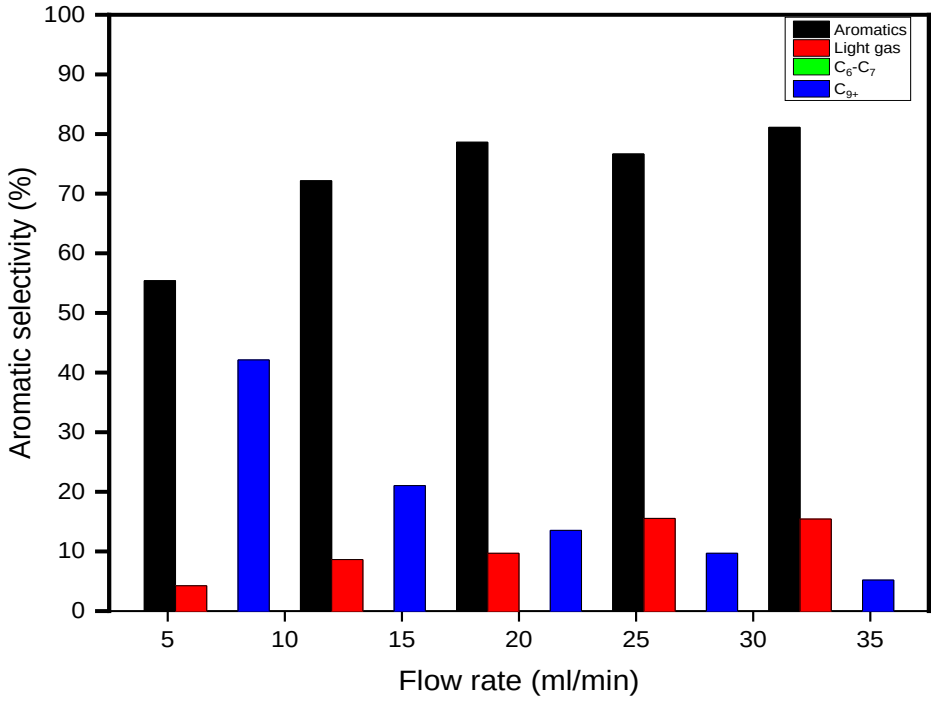


Figure 4.51: Effect of feed flow rate products distribution over Zn-Ni/ZSM-5 catalyst

CHAPTER FIVE

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

The following conclusions were deduced from this work:

i. Zinc-metal basedbimetallic catalysts comprising ofiron, cobalt, nickel and copper of loading range 1-3 wt. % as the second metal co-impregnated with 2 wt. % zinc on ZSM-5 were synthesized with physicochemical properties analysed using XRF, XRD, FTIR, Pyridine-FTIR, SEM, TEM, Nitrogen-adsorption, BET, Hydrogen-TPR and XPS.Analyses showed that synthesized catalysts had strong metal-metal interaction on ZSM-5, maintenance of ZSM-5 structure and are microporous as parent HZSM-5 (90 % microporosity) despite surface metal impregnation from the XRD, FTIR, H_2-TPR and XPS. The impregnated metal did not alter the structure of ZSM-5. Impregnated metals were properly dispersed with oxidation state of 2+ as shown by the XPS.

ii. Increase in metal loading from 1 and 3 wt. % with 2 wt. % Zn on ZSM-5 improved and sustained propane conversion and selectivity towards aromatics on twelve hours' time on stream (TOS). Aromatic yield on average increased for both Zn/ZSM-5 and all the bimetallic catalysts. Bimetallic catalysts of same 2 wt. % zinc showed sustained and improved selectivity on average of 85 % and yield 44-47 %as comparedto Zn/ZSM-5 with declining activity, aromatic selectivity and yield.

iii. Products analysis from the GC showedthe reaction path was not altered on account of metal impregnation when compared with parent HZSM-5. There is distinct,

progressive, sustained and improved selectivity of each aromatic compound as they were more favoured compared to light gases and hexanes (reduced undesired products) for all tested catalysts.

iv. Metal impregnated catalysts had selectivity for toluene but Zn-Co/ZSM-5 possessed improved selectivity for toluene (40-45%) of the total aromatic products.Zn-Cu/ZSM-5 is highly selective towards m and o-xylene. Zn-1Fe/ZSM-5, Zn-1Cu/ZSM-5 and Zn-3Ni/ZSM-5 is highly selective towards ethylbenzene (10-15 %). 2 and 3 wt. % loading of impregnated metals with zinc had good selectivity for benzene of about 10-15 % of the total aromatic products.

v. Zn-Ni/ZSM-5(2 wt. % each) gave the best performance of sustained conversion and selectivity of 55% and 85% respectively.Temperature increase from 500 to 580 ^{o}C was found to increase aromatic selectivity from 56 % to 92 % for Zn-Ni/ZSM-5 bimetallic catalyst. Increase in flow rate of propane reduces conversion and increases selectivity towards aromatics.Aromatic selectivity for the HZSM-5 catalyst to Zn and bimetallic catalysts generally follow this order based on the performance test:

Zn-Ni/ZSM-5 >Zn-Cu/ZSM-5>Zn-Co/ZSM-5 >Zn-Fe/ZSM-5 >Zn/ZSM-5 > HZSM-5

5.2 Recommendations

Here are the suggested recommendations to take this research study further:

i. Intra frame work impregnation ofzinc and promoting metals within zeolite walls should be investigated.

ii. Hierarchical form of bimetallic zinc based catalyst should be investigated for light alkane aromatization.

iii. Zinc based ZSM-5 bimetallic catalysts should be tested on other feedstocks in extension to study their application.

iv. Serial impregnation of metals should also be studied to investigate the effect on the mode of impregnation on catalyst performance.

v. The effect of equal weight percentage loading of metals impregnated on ZSM-5 should be investigated for light alkane aromatization.

vi. A pilot plant should be designed both for catalyst synthesis and fixed bed reactor for aromatics production.

vii. Nigerian government and appropriate scientific research bodies should invest in the further development findings of this research towards the commercialization of aromatization as an industrial process technology in the country.

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APPENDIX A

This section presents the carbon balance for the calculation of aromatic selectivity for catalyst used.

Table A1: HZSM-5

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.3884	0	0.000000	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	8.615382	16.043	0.537018	1	0.537018	11.3432
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	12.13033	42.081	0.288261	3	0.864784	18.26646
neo-pentane	1.36297	72.151	0.018891	5	0.094453	1.995081
n-pentane	1.297424	72.151	0.017982	5	0.08991	1.899137
Propane	27.09469	44.097	0.614434	6	3.686603	0
iso butane	3.55447	58.124	0.061153	6	0.366919	7.75028
n-Butane	1.24645	58.124	0.021445	7	0.150113	3.170764
i-Pentane	0.013597	72.151	0.000188	3	0.000565	0.011942
hexane	0.521155	86.178	0.006047	4	0.02419	0.510948
cyclohexane	0.073926	84.162	0.000878	4	0.003514	0.074215
n-heptane	28.54579	100.205	0.284874	5	1.42437	30.08634
Benzene	0.689072	78.114	0.008821	6	0.052928	1.11798
Toluene	10.60068	92.141	0.115048	7	0.805339	17.01083
EB	1.547251	106.168	0.014574	8	0.116589	2.462657
m-Xylene	1.381873	106.168	0.013016	8	0.104127	2.199435
P-xylene	0.372349	106.168	0.003507	8	0.028057	0.592642
O-Xylene	0.138181	106.168	0.001302	8	0.010412	0.219934
C9+	0.814416	120.19	0.006776	9	0.060985	1.288152
	100					
Total	100		2.014216		8.420876	
	Propane conversion		22.5			
	Aromatic sum		14.7294		1.117453	20.60347
	Total converted products		72.90531		4.734273	
	aromatics selectivity		20.20347			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.3884	0	0	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	12.61893	16.043	0.786569	1	0.786569	16.61436
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	3.617421	42.081	0.085963	3	0.25789	5.447295
neo-pentane	0.467859	72.151	0.006484	5	0.032422	0.684841
n-pentane	30.56583	72.151	0.423637	5	2.118185	44.7415
Propane	8.788156	44.097	0.199291	6	1.195749	0
iso butane	0.743572	58.124	0.012793	6	0.076757	1.621308
n-Butane	1.136297	58.124	0.01955	7	0.136847	2.890555
i-Pentane	0.20358	72.151	0.002822	3	0.008465	0.178797
hexane	16.89801	86.178	0.196083	4	0.78433	16.56707
cyclohexane	0.037846	84.162	0.00045	4	0.001799	0.037994
n-heptane	14.61395	100.205	0.14584	5	0.729202	15.40263
Benzene	2.709443	78.114	0.034686	6	0.208114	4.395912
Toluene	3.243297	92.141	0.035199	7	0.246395	5.204494
EB	1.005323	106.168	0.009469	8	0.075753	1.600106
m-Xylene	0.870693	106.168	0.008201	8	0.065609	1.385824
P-xylene	0.47318	106.168	0.004457	8	0.035655	0.75313
O-Xylene	0.056695	106.168	0.000534	8	0.004272	0.090238
C9+	2.159968	120.19	0.017971	9	0.161742	3.416396
	100					
Total	100		1.99		6.925755	
	Propane conversion		45.2			
	Aromatic sum		8.358631		0.635799	10.09595
	Total converted products		91.42189		5.730007	
	aromatics selectivity		9.142921			

input paramters		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.3884	0	0	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.789278	16.043	0.173863	1	0.173863	3.672425
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	4.711406	42.081	0.11196	3	0.335881	7.094674
neo-pentane	0.535021	72.151	0.007415	5	0.037076	0.78315
n-pentane	28.03349	72.151	0.388539	5	1.942696	41.03472
Propane	8.40949	44.097	0.190704	6	1.144226	0
iso butane	0.907017	58.124	0.015605	6	0.093629	1.977688
n-Butane	1.279489	58.124	0.022013	7	0.154092	3.254812
i-Pentane	0	72.151	0	3	0	0
hexane	17.50946	86.178	0.203178	4	0.812711	17.16655
cyclohexane	7.249721	84.162	0.08614	4	0.34456	7.277999
n-heptane	19.97323	100.205	0.199324	5	0.996618	21.05114
Benzene	3.456713	78.114	0.044252	6	0.265513	5.608315
Toluene	2.000976	92.141	0.021716	7	0.152015	3.210952
EB	0.909933	106.168	0.008571	8	0.068565	1.448279
m-Xylene	0.822459	106.168	0.007747	8	0.061974	1.309053
P-xylene	0.364533	106.168	0.003434	8	0.027468	0.580203
O-Xylene	0.065904	106.168	0.000621	8	0.004966	0.104895
C9+	4.613612	120.19	0.038386	9	0.345474	7.297296
	100.					
Total	100.		1.523468		6.961329	
	Propane conversion		54.7			
	Aromatic sum		7.620517		0.580502	9.979231
	Total converted products		95.22224		5.817103	
	aromatics selectivity		8.002876			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
1					

Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.3884	0	0	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	6.469782	42.081	0.153746	3	0.461238	9.742526
neo-pentane	0.455294	72.151	0.00631	5	0.031551	0.666447
n-pentane	25.33035	72.151	0.351074	5	1.755371	37.07793
Propane	8.493619	44.097	0.192612	6	1.155673	0
iso butane	0.84157	58.124	0.014479	6	0.086873	1.834985
n-Butane	1.16765	58.124	0.020089	7	0.140623	2.970312
i-Pentane	0	72.151	0	3	0	0
hexane	17.03311	86.178	0.19765	4	0.790602	16.69953
cyclohexane	7.12977	84.162	0.084715	4	0.338859	7.157579
n-heptane	18.88532	100.205	0.188467	5	0.942334	19.90452
Benzene	3.642574	78.114	0.046632	6	0.279789	5.909863
Toluene	2.198121	92.141	0.023856	7	0.166992	3.527309
EB	1.859292	106.168	0.017513	8	0.140102	2.959312
m-Xylene	1.663787	106.168	0.015671	8	0.12537	2.64814
P-xylene	0.784538	106.168	0.00739	8	0.059117	1.248697
O-Xylene	0.127169	106.168	0.001198	8	0.009582	0.202407
C9+	3.918044	120.19	0.032599	9	0.293389	6.197124
	100					
Total	100		1.354		6.777466	
	Propane conversion		48.9			
	Aromatic sum		10.27548		0.780953	13.89153
	Total converted products		91.50638		5.621793	
	aromatics selectivity		11.22925			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.3884	0	0	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.789278	16.043	0.173863	1	0.173863	3.672425
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	4.711406	42.081	0.11196	3	0.335881	7.094674
neo-pentane	0.535021	72.151	0.007415	5	0.037076	0.78315
n-pentane	28.03349	72.151	0.388539	5	1.942696	41.03472
Propane	8.40949	44.097	0.190704	6	1.144226	0
iso butane	0.907017	58.124	0.015605	6	0.093629	1.977688
n-Butane	1.279489	58.124	0.022013	7	0.154092	3.254812
i-Pentane	0	72.151	0	3	0	0
hexane	17.50946	86.178	0.203178	4	0.812711	17.16655
cyclohexane	7.249721	84.162	0.08614	4	0.34456	7.277999
n-heptane	19.97323	100.205	0.199324	5	0.996618	21.05114
Benzene	3.456713	78.114	0.044252	6	0.265513	5.608315
Toluene	2.000976	92.141	0.021716	7	0.152015	3.210952
EB	0.909933	106.168	0.008571	8	0.068565	1.448279
m-Xylene	0.822459	106.168	0.007747	8	0.061974	1.309053
P-xylene	0.364533	106.168	0.003434	8	0.027468	0.580203
O-Xylene	0.065904	106.168	0.000621	8	0.004966	0.104895
C9+	4.613612	120.19	0.038386	9	0.345474	7.297296
	103.6317					
Total	103.6317		1.523468		6.961329	
	Propane conversion		52.6			
	Aromatic sum		7.620517		0.580502	9.979231
	Total converted products		95.22224		5.817103	
	aromatics selectivity		8.002876			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.3884	0	0	

Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 6					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	6.782888	42.081	0.161186	3	0.483559	10.21402
neo-pentane	0.21504	72.151	0.00298	5	0.014902	0.31477
n-pentane	31.09137	72.151	0.430921	5	2.154605	45.51078
Propane	9.342177	44.097	0.211855	6	1.271131	0
iso butane	1.009868	58.124	0.017374	6	0.104246	2.201949
n-Butane	0.868315	58.124	0.014939	7	0.104573	2.208851
i-Pentane	0	72.151	0	3	0	0
hexane	15.85203	86.178	0.183945	4	0.735781	15.54158
cyclohexane	6.096071	84.162	0.072433	4	0.28973	6.119849
n-heptane	18.6865	100.205	0.186483	5	0.932414	19.69497
Benzene	4.334678	78.114	0.055492	6	0.33295	7.032761
Toluene	2.326899	92.141	0.025254	7	0.176776	3.733958
EB	0.99185	106.168	0.009342	8	0.074738	1.578662
m-Xylene	0.918472	106.168	0.008651	8	0.069209	1.461871
P-xylene	0.442757	106.168	0.00417	8	0.033363	0.704707
O-Xylene	0.075331	106.168	0.00071	8	0.005676	0.119899
C9+	0.965748	120.19	0.008035	9	0.072317	1.527512
	100					
Total	100		1.393771		6.85597	
	Propane conversion		53.02			
	Aromatic sum		9.089987		0.692712	12.40344
	Total converted products		90.65782		5.584839	
	aromatics selectivity		10.0267			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.3884	0	0	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	3.233065	30.07	0.107518	2	0.215036	4.542111
propene	3.831797	42.081	0.091058	3	0.273173	5.770114
neo-pentane	0.30773	72.151	0.004265	5	0.021325	0.450447
n-pentane	29.15823	72.151	0.404128	5	2.02064	42.6811
Propane	9.947773	44.097	0.225588	6	1.353531	0
iso butane	1.009174	58.124	0.017362	6	0.104175	2.200434
n-Butane	0.834479	58.124	0.014357	7	0.100498	2.122779
i-Pentane	0.30773	72.151	0.004265	3	0.012795	0.270268
hexane	16.63796	86.178	0.193065	4	0.77226	16.31212
cyclohexane	6.261587	84.162	0.074399	4	0.297597	6.28601
n-heptane	19.67591	100.205	0.196357	5	0.981783	20.73778
Benzene	3.968996	78.114	0.05081	6	0.304862	6.439464
Toluene	1.826161	92.141	0.019819	7	0.138734	2.930427
EB	0.907201	106.168	0.008545	8	0.06836	1.443931
m-Xylene	0.815248	106.168	0.007679	8	0.061431	1.297575
P-xylene	0.424088	106.168	0.003994	8	0.031956	0.674992
O-Xylene	0.067988	106.168	0.00064	8	0.005123	0.108212
C9+	0.784875	120.19	0.00653	9	0.058773	1.241427
	100					
Total	100		1.430381		6.822051	
	Propane conversion		48.00			
	Aromatic sum		8.009682		0.610466	11.16327
	Total converted products		90.05223		5.46852	
	aromatics selectivity		8.894485			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
1					
Propane	33.09	44.097	0.750391	3	2.251174

Nitrogen	66.91	28.014	2.3884	0	0	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	3.185141	30.07	0.105924	2	0.211848	4.474782
propene	4.2434	42.081	0.100839	3	0.302517	6.389926
neo-pentane	0.689457	72.151	0.009556	5	0.047779	1.009211
n-pentane	23.33266	72.151	0.323387	5	1.616933	34.15377
Propane	11.103	44.097	0.251786	6	1.510714	0
iso butane	1.008825	58.124	0.017356	6	0.104139	2.199675
n-Butane	0.091316	58.124	0.001571	7	0.010997	0.232293
i-Pentane	0.306929	72.151	0.004254	3	0.012762	0.269565
hexane	15.7723	86.178	0.18302	4	0.73208	15.46341
cyclohexane	9.739891	84.162	0.115728	4	0.462912	9.777881
n-heptane	22.3921	100.205	0.223463	5	1.117315	23.60055
Benzene	2.54977	78.114	0.032642	6	0.19585	4.136854
Toluene	2.324467	92.141	0.025227	7	0.176591	3.730056
EB	0.957222	106.168	0.009016	8	0.072129	1.523547
m-Xylene	0.865975	106.168	0.008157	8	0.065253	1.378315
P-xylene	0.463428	106.168	0.004365	8	0.03492	0.737607
O-Xylene	0.068099	106.168	0.000641	8	0.005131	0.108388
C9+	0.90602	120.19	0.007538	9	0.067844	1.433041
	100					
Total	100		1.42447		6.747714	
	Propane conversion		41.81			
	Aromatic sum		7.228962		0.549875	10.49981
	Total converted products		88.897		5.237	
	aromatics selectivity		8.13184			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.3884	0	0	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 10					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	3.483722	30.07	0.115854	2	0.231707	4.894256
propene	4.641184	42.081	0.110292	3	0.330875	6.98893
neo-pentane	0.754089	72.151	0.010452	5	0.052258	1.103816
n-pentane	21.61803	72.151	0.299622	5	1.49811	31.64393
Propane	12.14381	44.097	0.275389	6	1.652332	0
iso butane	1.103395	58.124	0.018983	6	0.113901	2.405876
n-Butane	0.537362	58.124	0.009245	7	0.064716	1.366961
i-Pentane	0.335601	72.151	0.004651	3	0.013954	0.294747
	15.7723	86.178	0.18302	4	0.73208	15.46341
	9.009891	84.162	0.107054	4	0.428217	9.045034
	22.3921	100.205	0.223463	5	1.117315	23.60055
Benzene	2.54977	78.114	0.032642	6	0.195850	4.136854
Toluene	2.324467	92.141	0.025227	7	0.176591	3.730056
EB	0.954222	106.168	0.008988	8	0.071903	1.518772
m-Xylene	0.705975	106.168	0.00665	8	0.053197	1.123654
P-xylene	0.463428	106.168	0.004365	8	0.034920	0.737607
O-Xylene	0.068099	106.168	0.000641	8	0.005131	0.108388
C9+	1.142581	120.19	0.009506	9	0.085558	1.807206
	100					
Total	100		1.446044		6.858614	
	Propane conversion		39.03			
	Aromatic sum		7.065962		0.537592	10.32584
	Total converted products		87.85621		5.206282	
	aromatics selectivity		8.042643			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				
Propane	33.09	44.097	0.750391	3	2.251174
Nitrogen	66.91	28.014	2.3884	0	0
Total	100		3.138791		2.251174

Output parameters	Catalyst Run 11					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	3.199601	30.07	0.106405	2	0.21281	4.495097
propene	4.262665	42.081	0.101297	3	0.30389	6.418936
neo-pentane	0.692588	72.151	0.009599	5	0.047996	1.013792
n-pentane	20.44715	72.151	0.283394	5	1.416969	29.93003
Propane	11.1534	44.097	0.252929	6	1.517573	0
iso butane	1.013405	58.124	0.017435	6	0.104611	2.209661
n-Butane	0.493536	58.124	0.008491	7	0.059438	1.255476
i-Pentane	0.308323	72.151	0.004273	3	0.01282	0.270789
Hexane	18.65564	86.178	0.216478	4	0.865912	18.29028
Cyclohexane	11.66693	84.162	0.138625	4	0.554499	11.71244
n-heptane	20.25295	100.205	0.202115	5	1.010576	21.34595
Benzene	2.509549	78.114	0.032127	6	0.19276	4.071596
Toluene	2.2878	92.141	0.024829	7	0.173805	3.671215
EB	0.942122	106.168	0.008874	8	0.070991	1.499513
m-Xylene	0.852315	106.168	0.008028	8	0.064224	1.356573
P-xylene	0.456117	106.168	0.004296	8	0.034369	0.725972
O-Xylene	0.067024	106.168	0.000631	8	0.00505	0.106678
C9+	1.08195	120.19	0.009002	9	0.081018	1.711307
	100					
Total	100		1.428828		6.729312	
	Propane conversion		49.28			
	Aromatic sum		7.114927		0.541201	10.38426
	Total converted products		89.18967		5.211739	
	aromatics selectivity		7.9773			

Table A2: Zn/ZSM-5

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	2.388400	0	0	
Total	100		3.138791		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.033888	42.081	0.048333	3	0.144998	1.999556
neo-pentane	0	72.151	0	5	0	0
n-pentane	0.017689	72.151	0.000245	5	0.001226	0.016905
Propane	4.275715	44.097	0.096962	6	0.581769	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.378943	58.124	0.00652	7	0.045637	0.629343
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.039786	100.205	0.000397	5	0.001985	0.027377
Benzene	14.67152	78.114	0.187822	6	1.126931	15.54063
Toluene	26.28286	92.141	0.285246	7	1.996722	27.53524
EB	0.667315	106.168	0.006285	8	0.050284	0.693424
m-Xylene	17.3954	106.168	0.163848	8	1.310783	18.07599
P-xylene	1.096912	106.168	0.010332	8	0.082655	1.139828
O-Xylene	18.52985	106.168	0.174533	8	1.396266	19.25482
C9+	14.61012	120.19	0.121559	9	1.094027	15.08688
	100					
Total	100		1.102081		7.833284	
	Propane conversion		27.00371			
	Aromatic sum		78.64385		5.963642	82.23994
	Total converted products		95.72429		7.251515	
	aromatics selectivity		82.15664			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	2				
Propane	33.09	44.097	0.750391	3	2.251174
Nitrogen	66.91	28.014	2.388400	0	0

Total	100		3.138791		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.821726	42.081	0.043290944	3	0.129873	1.792526
neo-pentane	0	72.151	0	5	0	0
n-pentane	0.355527	72.151	0.004927534	5	0.024638	0.340053
Propane	4.403616	44.097	0.099862032	6	0.599172	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.355527	58.124	0.00611669	7	0.042817	0.590965
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.018793	100.205	0.000187545	5	0.000938	0.012943
Benzene	16.21242	78.114	0.207548144	6	1.245289	17.18768
Toluene	29.14702	92.141	0.31633062	7	2.214314	30.56233
EB	0.719496	106.168	0.006776955	8	0.054216	0.748293
m-Xylene	16.43491	106.168	0.154801012	8	1.238408	17.09271
P-xylene	1.147363	106.168	0.010807052	8	0.086456	1.193286
O-Xylene	17.00293	106.168	0.16015114	8	1.281209	17.68346
C9+	12.38068	120.19	0.103009215	9	0.927083	12.79575
Total	100					
Total	100		1.113808882		7.844413	
	Propane conversion					
	Aromatic sum		80.66413428		6.119892	84.46776
	Total converted products		95.59638398		7.24524	
	aromatics selectivity		84.37990112			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	2					
Propane	33.09	44.097	0.750391183	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.13879100		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.821726	42.081	0.043290944	3	0.129873	1.792526
neo-pentane	0	72.151	0	5	0	0
n-pentane	0.355527	72.151	0.004927534	5	0.024638	0.340053
Propane	4.403616	44.097	0.099862032	6	0.599172	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.355527	58.124	0.00611669	7	0.042817	0.590965
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.018793	100.205	0.000187545	5	0.000938	0.012943
Benzene	16.21242	78.114	0.207548144	6	1.245289	17.18768
Toluene	29.14702	92.141	0.31633062	7	2.214314	30.56233
EB	0.719496	106.168	0.006776955	8	0.054216	0.748293
m-Xylene	16.43491	106.168	0.154801012	8	1.238408	17.09271
P-xylene	1.147363	106.168	0.010807052	8	0.086456	1.193286
O-Xylene	17.00293	106.168	0.16015114	8	1.281209	17.68346
C9+	12.38068	120.19	0.103009215	9	0.927083	12.79575
Total	100					
Total	100		1.113808882		7.844413	
	Propane conversion		24.412			
	Aromatic sum		80.66413428		6.119892	84.46776
	Total converted products		95.59638398		7.24524	
	aromatics selectivity		84.37990112			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	Run 3				
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0

Total	100			3.13879100		2.251174	
Output parameters	Catalyst Run 3						
Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane		0	16.043	0	1	0	0
ethylene		0	28.05	0	2	0	0
ethane		0	30.07	0	2	0	0
propene		1.856925	42.081	0.044127	3	0.132382	1.830596
neo-pentane		0	72.151	0	5	0	0
n-pentane		0	72.151	0	5	0	0
Propane		4.492012	44.097	0.101867	6	0.6112	0
iso butane		0	58.124	0	6	0	0
n-Butane		0.30252	58.124	0.005205	7	0.036433	0.503802
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane		0.00392	100.205	3.91E-05	5	0.000196	0.002705
Benzene		13.72845	78.114	0.175749	6	1.054494	14.58165
Toluene		25.96985	92.141	0.281849	7	1.972943	27.28207
EB		3.663998	106.168	0.034511	8	0.276091	3.81781
m-Xylene		16.69679	106.168	0.157268	8	1.258141	17.39771
P-xylene		1.07847	106.168	0.010158	8	0.081265	1.123744
O-Xylene		16.97348	106.168	0.159874	8	1.27899	17.68601
C9+		15.23358	120.19	0.126746	9	1.140713	15.7739
Total	100			1.097393		7.842847	
	Propane conversion			27.702			
	Aromatic sum			78.11104		5.921924	81.889
	Total converted products			95.50799		7.231647	
	aromatics selectivity			81.78482			

input paramters			Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	Run 4						
Propane	33.09		44.097	0.75039100	3	2.251174	
Nitrogen	66.91		28.014	2.38840000	0	0	
Total	100			3.13879100		2.251174	
Output parameters	Catalyst Run 4						
Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane		0	16.043	0	1	0	0
ethylene		0	28.05	0	2	0	0
ethane		0	30.07	0	2	0	0
propene		2.446434	42.081	0.058136	3	0.174409	2.443209
neo-pentane		0	72.151	0	5	0	0
n-pentane		0	72.151	0	5	0	0
Propane		5.616164	44.097	0.127359	6	0.764156	0
iso butane		0	58.124	0	6	0	0
n-Butane		0.36318	58.124	0.006248	7	0.043739	0.612712
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane		0	100.205	0	5	0	0
Benzene		11.41926	78.114	0.146187	6	0.877123	12.28718
Toluene		20.60502	92.141	0.223625	7	1.565374	21.92856
EB		0.547516	106.168	0.005157	8	0.041257	0.577944
m-Xylene		20.54652	106.168	0.193528	8	1.548227	21.68835
P-xylene		0.91306	106.168	0.0086	8	0.068801	0.963801
O-Xylene		17.68636	106.168	0.166588	8	1.332708	18.66925
C9+	19.85647		120.19	0.165209	9	1.486881	20.82899
Total	100						
Total	100			1.100639		7.902675	
	Propane conversion			32.78871			
	Aromatic sum			71.71775		5.43349	76.11509
	Total converted products			94.38384		7.138519	
	aromatics selectivity			75.9852			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	Run 5				
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0

Total	100			3.13879100		2.251174	
Output parameters	Catalyst Run 5						
Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane		0	16.043	0	1	0	0
ethylene		0	28.05	0	2	0	0
ethane		0	30.07	0	2	0	0
propene		3.091037	42.081	0.073454	3	0.220363	3.143702
neo-pentane		0	72.151	0	5	0	0
n-pentane		0	72.151	0	5	0	0
Propane		7.362002	44.097	0.16695	6	1.001701	0
iso butane		0	58.124	0	6	0	0
n-Butane		0.480484	58.124	0.008267	7	0.057866	0.825512
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane		0.003156	100.205	3.15E-05	5	0.000157	0.002246
Benzene		11.58749	78.114	0.148341	6	0.890045	12.69737
Toluene		22.06627	92.141	0.239484	7	1.676386	23.91531
EB		0.670048	106.168	0.006311	8	0.05049	0.720285
m-Xylene		20.08629	106.168	0.189193	8	1.513547	21.59226
P-xylene		0.857117	106.168	0.008073	8	0.064586	0.921379
O-Xylene		11.75539	106.168	0.110724	8	0.885795	12.63675
C9+		22.04072	120.19	0.183382	9	1.650441	23.54518
Total	100						
Total	100			1.134212		8.011377	
	Propane conversion			39.83343			
	Aromatic sum			67.0226		5.080849	72.48336
	Total converted products			92.638		7.009676	
	aromatics selectivity			72.34893			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	6				
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0
Total	100		3.13879100		2.251174

Output parameters	Catalyst Run 6						
Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane		0	16.043	0	1	0	0
ethylene		0	28.05	0	2	0	0
ethane		0	30.07	0	2	0	0
propene		3.139198	42.081	0.074599	3	0.223797	3.178929
neo-pentane		0	72.151	0	5	0	0
n-pentane		0	72.151	0	5	0	0
Propane		6.898996	44.097	0.15645	6	0.938703	0
iso butane		0	58.124	0	6	0	0
n-Butane		0.487588	58.124	0.008389	7	0.058721	0.834108
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane		0	100.205	0	5	0	0
Benzene		10.42938	78.114	0.133515	6	0.801089	11.37909
Toluene		20.02172	92.141	0.217294	7	1.521061	21.60595
EB		0.425947	106.168	0.004012	8	0.032096	0.45591
m-Xylene		19.6093	106.168	0.184701	8	1.477605	20.98869
P-xylene		0.68383	106.168	0.006441	8	0.051528	0.731933
O-Xylene		12.42056	106.168	0.11699	8	0.935918	13.29427
C9+		25.88349	120.19	0.215355	9	1.938193	27.53112
		0					
Total							
Total	100			1.117745		7.97871	
	Propane conversion			46.59771			
	Aromatic sum			63.59073		4.819296	68.45584
	Total converted products			93.101		7.040007	
	aromatics selectivity			68.30295			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	7				

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.13879100		2.251174	
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	3.126752	30.07	0.103982	2	0.207965	2.952656
propene	0	42.081	0	3	0	0
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	6.681167	44.097	0.151511	6	0.909064	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.5596	58.124	0.009628	7	0.067394	0.956848
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	10.04046	78.114	0.128536	6	0.771216	10.94961
Toluene	19.69574	92.141	0.213757	7	1.496296	21.24419
EB	0.69687	106.168	0.006564	8	0.052511	0.74554
m-Xylene	19.40907	106.168	0.182815	8	1.462517	20.76461
P-xylene	0.647333	106.168	0.006097	8	0.048778	0.692544
O-Xylene	11.80008	106.168	0.111145	8	0.889162	12.6242
C9+	27.34294	120.19	0.227498	9	2.047478	29.0698
Total						
Total	100		1.141532		7.952381	
	Propane conversion					
	Aromatic sum		62.28955		4.72048	67.0207
	Total converted products		93.31883		7.043317	
	aromatics selectivity		66.74917			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	8					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.13879100		2.251174	
Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	4.573155	42.081	0.108675	3	0.326025	4.675865
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	7.685981	44.097	0.174297	6	1.045783	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.510983	58.124	0.008791	7	0.061539	0.882592
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	9.398966	78.114	0.120324	6	0.721942	10.35412
Toluene	18.61213	92.141	0.201996	7	1.413974	20.27926
EB	0.659195	106.168	0.006209	8	0.049672	0.712396
m-Xylene	18.45944	106.168	0.17387	8	1.390961	19.94921
P-xylene	0.498115	106.168	0.004692	8	0.037534	0.538316
O-Xylene	11.48373	106.168	0.108166	8	0.865326	12.41053
C9+	28.1183	120.19	0.233949	9	2.105539	30.19771
Total						
Total	100		1.140969		8.018293	
	Propane conversion		44.35914			
	Aromatic sum		59.11158		4.479408	64.24383
	Total converted products		92.31402		6.97251	
	aromatics selectivity		64.03316			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	9					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.13879100		2.251174	

Output parameters	Catalyst Run 9					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	4.208679	42.081	0.100014	3	0.300041	4.292829
neo-pentane	0.079903	72.151	0.001107	5	0.005537	0.079224
n-pentane	0	72.151	0	5	0	0
Propane	7.546482	44.097	0.171134	6	1.026802	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.646642	58.124	0.011125	7	0.077876	1.114215
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	9.32982	78.114	0.119439	6	0.716631	10.25317
Toluene	18.38301	92.141	0.19951	7	1.396567	19.98133
EB	0.634554	106.168	0.005977	8	0.047815	0.684113
m-Xylene	18.74461	106.168	0.176556	8	1.412449	20.20856
P-xylene	0	106.168	0	8	0	0
O-Xylene	11.1792	106.168	0.105297	8	0.842378	12.05229
C9+	29.2471	120.19	0.243341	9	2.190065	31.33427
Total						
Total	100		1.133499		8.016162	
	Propane conversion		49.70114			
	Aromatic sum		58.27119		4.41584	63.17946
	Total converted products		92.45352		6.98936	
	aromatics selectivity		63.02756			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	10					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.13879100		2.251174	

Output parameters	Catalyst Run 10					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	4.684194	42.081	0.111314	3	0.333941	4.817927
neo-pentane	0.059493	72.151	0.000825	5	0.004123	0.059482
n-pentane	0	72.151	0	5	0	0
Propane	8.288563	44.097	0.187962	6	1.127772	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.649234	58.124	0.01117	7	0.078189	1.128065
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	9.059491	78.114	0.115978	6	0.695867	10.0396
Toluene	18.23724	92.141	0.197927	7	1.385492	19.98914
EB	0.500502	106.168	0.004714	8	0.037714	0.544117
m-Xylene	17.87073	106.168	0.168325	8	1.3466	19.42802
P-xylene	0.451995	106.168	0.004257	8	0.034059	0.491383
O-Xylene	10.85936	106.168	0.102285	8	0.818277	11.80567
C9+	29.33921	120.19	0.244107	9	2.196962	31.6966
Total						
Total	100		1.148864		8.058996	
	Propane conversion		46.58057			
	Aromatic sum		56.97931		4.318009	62.29793
	Total converted products		91.71144		6.931224	
	aromatics selectivity		62.1289			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	11				
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0

Total	100		3.13879100		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	5.587844	42.081	0.132788	3	0.398363	5.713462
neo-pentane	0.062285	72.151	0.000863	5	0.004316	0.061906
n-pentane	0	72.151	0	5	0	0
Propane	7.606087	44.097	0.172485	6	1.034912	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.533339	58.124	0.009176	7	0.064231	0.921224
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	7.686623	78.114	0.098403	6	0.590416	8.467941
Toluene	17.88751	92.141	0.194132	7	1.358923	19.49013
EB	0.750924	106.168	0.007073	8	0.056584	0.811544
m-Xylene	19.57806	106.168	0.184406	8	1.475251	21.15855
P-xylene	0.428886	106.168	0.00404	8	0.032318	0.463509
O-Xylene	12.33442	106.168	0.116178	8	0.929426	13.33015
C9+	27.54403	120.19	0.229171	9	2.062536	29.58159
Total						
Total	100		1.148715		8.007278	
	Propane conversion		36.13829			
	Aromatic sum		58.66642		4.442918	63.72182
	Total converted products		92.39391		6.972365	
	aromatics selectivity		63.49598			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	12					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.13879100		2.251174	
Output parameters	Catalyst Run 12					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	6.142231	42.081	0.145962	3	0.437886	6.80395
neo-pentane	0.087597	72.151	0.001214	5	0.00607	0.094323
n-pentane	0	72.151	0	5	0	0
Propane	14.58966	44.097	0.330854	6	1.985123	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.537723	58.124	0.009251	7	0.064759	1.006238
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	6.271706	78.114	0.080289	6	0.481735	7.485276
Toluene	13.33252	92.141	0.144697	7	1.012878	15.73827
EB	0.486391	106.168	0.004581	8	0.036651	0.569484
m-Xylene	13.35568	106.168	0.125798	8	1.006381	15.63731
P-xylene	0	106.168	0	8	0	0
O-Xylene	10.67529	106.168	0.100551	8	0.804407	12.49902
C9+	34.52121	120.19	0.287222	9	2.584998	40.16613
Total	100		1.230419		8.420888	
	Propane conversion					
	Aromatic sum		44.12158		3.342052	51.92936
	Total converted products		85.41034		6.435765	
	aromatics selectivity		51.65836			

Table A3: Zn-Fe/ZSM-5 (2-1 wt. %)

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				
Propane	33.09	44.097	0.75039100	3	2.251174

Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.13879100		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.407037	16.043	0.087704	1	0.087704	1.267036
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.389413	42.081	0.056781	3	0.170344	2.46091
neo-pentane	0.151883	72.151	0.002105	5	0.010525	0.152057
n-pentane	0.235065	72.151	0.003258	5	0.01629	0.235334
Propane	5.438699	44.097	0.123335	6	0.740009	0
iso butane	0.141263	58.124	0.00243	6	0.014582	0.210666
n-Butane	1.045706	58.124	0.017991	7	0.125937	1.819371
i-Pentane	0.010893	72.151	0.000151	3	0.000453	0.006543
hexane	0.032589	86.178	0.000378	4	0.001513	0.021853
cyclohexane	0	84.162	0	4	0	0
n-heptane	10.12037	100.205	0.100997	5	0.504983	7.295353
Benzene	7.524876	78.114	0.096332	6	0.577992	8.350086
Toluene	41.11989	92.141	0.446271	7	3.1239	45.1301
EB	1.892707	106.168	0.017827	8	0.14262	2.060388
m-Xylene	15.15145	106.168	0.142712	8	1.141696	16.49376
P-xylene	1.372384	106.168	0.012927	8	0.103412	1.493968
O-Xylene	8.541873	106.168	0.080456	8	0.64365	9.298624
C9+	3.423904	120.19	0.028487	9	0.256387	3.703949
	100					
Total	100		1.220143		7.661996	
	Propane conversion		53.94138			
	Aromatic sum		75.60318		5.733269	82.82693
	Total converted products		94.5613		6.921987	
	aromatics selectivity		79.9515			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.948745	16.043	0.12147	1	0.12147	1.754845
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.359178	42.081	0.056063	3	0.168188	2.42977
neo-pentane	0.184177	72.151	0.002553	5	0.012763	0.184387
n-pentane	0.270904	72.151	0.003755	5	0.018773	0.271214
Propane	5.329199	44.097	0.120852	6	0.72511	0
iso butane	0.159575	58.124	0.002745	6	0.016473	0.237974
n-Butane	1.173289	58.124	0.020186	7	0.141302	2.041346
i-Pentane	0.012797	72.151	0.000177	3	0.000532	0.007687
hexane	0.016325	86.178	0.000189	4	0.000758	0.010947
cyclohexane	0	84.162	0	4	0	0
n-heptane	10.01128	100.205	0.099908	5	0.49954	7.216713
Benzene	7.277983	78.114	0.093171	6	0.559028	8.076117
Toluene	31.8432	92.141	0.345592	7	2.419144	34.9487
EB	1.827377	106.168	0.017212	8	0.137697	1.98927
m-Xylene	14.88731	106.168	0.140224	8	1.121792	16.20622
P-xylene	2.509776	106.168	0.02364	8	0.189117	2.732125
O-Xylene	10.21049	106.168	0.096173	8	0.769383	11.11507
C9+	9.978409	120.19	0.083022	9	0.747198	10.79455
	100					
Total	100		1.226932		7.648269	
	Propane conversion		62.782			
	Aromatic sum		68.55612		5.196162	75.05479
	Total converted products		94.6708		6.923159	
	aromatics selectivity		72.41528			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
1					

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.581918	16.043	0.098605	1	0.098605	1.424517
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.775717	42.081	0.065961	3	0.197884	2.858773
neo-pentane	0.202978	72.151	0.002813	5	0.014066	0.20321
n-pentane	0.332865	72.151	0.004613	5	0.023067	0.333246
Propane	5.898185	44.097	0.133755	6	0.802529	0
iso butane	0.190901	58.124	0.003284	6	0.019706	0.284691
n-Butane	1.378501	58.124	0.023717	7	0.166016	2.398386
i-Pentane	0.014614	72.151	0.000203	3	0.000608	0.008778
hexane	0.025228	86.178	0.000293	4	0.001171	0.016917
cyclohexane	0.002656	84.162	3.16E-05	4	0.000126	0.001823
n-heptane	11.56635	100.205	0.115427	5	0.577135	8.337702
Benzene	8.154436	78.114	0.104391	6	0.626349	9.048686
Toluene	28.86481	92.141	0.313268	7	2.192875	31.67984
EB	1.658509	106.168	0.015622	8	0.124972	1.805442
m-Xylene	11.63815	106.168	0.10962	8	0.876961	12.66921
P-xylene	0.620901	106.168	0.005848	8	0.046786	0.675909
O-Xylene	10.51045	106.168	0.098998	8	0.791986	11.44161
C9+	14.58282	120.19	0.121331	9	1.091983	15.77557
	100					
Total	100		1.217781		7.652825	
	Propane conversion		65.56775			
	Aromatic sum		61.44726		4.65993	68.02523
	Total converted products		94.10181		6.850296	
	aromatics selectivity		65.2987			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.581918	16.043	0.098605	1	0.098605	1.424517
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.775717	42.081	0.065961	3	0.197884	2.858773
neo-pentane	0.202978	72.151	0.002813	5	0.014066	0.20321
n-pentane	0.332865	72.151	0.004613	5	0.023067	0.333246
Propane	5.898185	44.097	0.133755	6	0.802529	0
iso butane	0.190901	58.124	0.003284	6	0.019706	0.284691
n-Butane	1.378501	58.124	0.023717	7	0.166016	2.398386
i-Pentane	0.014614	72.151	0.000203	3	0.000608	0.008778
hexane	0.025228	86.178	0.000293	4	0.001171	0.016917
cyclohexane	0.002656	84.162	3.16E-05	4	0.000126	0.001823
n-heptane	11.56635	100.205	0.115427	5	0.577135	8.337702
Benzene	8.154436	78.114	0.104391	6	0.626349	9.048686
Toluene	28.86481	92.141	0.313268	7	2.192875	31.67984
EB	1.658509	106.168	0.015622	8	0.124972	1.805442
m-Xylene	11.63815	106.168	0.10962	8	0.876961	12.66921
P-xylene	0.620901	106.168	0.005848	8	0.046786	0.675909
O-Xylene	10.51045	106.168	0.098998	8	0.791986	11.44161
C9+	14.58282	120.19	0.121331	9	1.091983	15.77557
	100					
Total	100		1.217781		7.652825	
	Propane conversion		62.51413			
	Aromatic sum		61.44726		4.65993	68.02523
	Total converted products		94.10181		6.850296	
	aromatics selectivity		65.2987			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				
Propane	33.09	44.097	0.75039100	3	2.251174

Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.918561	16.043	0.119589	1	0.119589	1.727664
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.57461	42.081	0.061182	3	0.183547	2.651648
neo-pentane	0.211113	72.151	0.002926	5	0.01463	0.211354
n-pentane	0.305982	72.151	0.004241	5	0.021204	0.306332
Propane	5.54097	44.097	0.125654	6	0.753925	0
iso butane	0.1733	58.124	0.002982	6	0.017889	0.258442
n-Butane	1.382583	58.124	0.023787	7	0.166508	2.405487
i-Pentane	0.013453	72.151	0.000186	3	0.000559	0.008081
hexane	0.022328	86.178	0.000259	4	0.001036	0.014972
cyclohexane	0.002783	84.162	3.31E-05	4	0.000132	0.001911
n-heptane	13.02347	100.205	0.129968	5	0.649842	9.388079
Benzene	7.664212	78.114	0.098116	6	0.588694	8.504702
Toluene	28.2075	92.141	0.306134	7	2.142938	30.95843
EB	1.394741	106.168	0.013137	8	0.105097	1.518306
m-Xylene	11.32357	106.168	0.106657	8	0.853257	12.32676
P-xylene	0.355768	106.168	0.003351	8	0.026808	0.387287
O-Xylene	9.986646	106.168	0.094065	8	0.752516	10.87139
C9+	15.89841	120.19	0.132277	9	1.190496	17.19876
	100					
Total	100		1.224544		7.588667	
	Propane conversion		69.13575			
	Aromatic sum		58.93243		4.46931	65.39106
	Total converted products		94.45903		6.834742	
	aromatics selectivity		62.38941			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.661116	16.043	0.103541	1	0.103541	1.495835
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.68088	42.081	0.063708	3	0.191123	2.761098
neo-pentane	0.186445	72.151	0.002584	5	0.01292	0.186659
n-pentane	0.279313	72.151	0.003871	5	0.019356	0.279632
Propane	6.239628	44.097	0.141498	6	0.848987	0
iso butane	0.162992	58.124	0.002804	6	0.016825	0.243069
n-Butane	1.373086	58.124	0.023623	7	0.165364	2.388963
i-Pentane	0.046149	72.151	0.00064	3	0.001919	0.027721
hexane	0.03017	86.178	0.00035	4	0.0014	0.020231
cyclohexane	0	84.162	0	4	0	0
n-heptane	12.96924	100.205	0.129427	5	0.647136	9.348987
Benzene	7.340373	78.114	0.09397	6	0.56382	8.14535
Toluene	27.7567	92.141	0.301242	7	2.108691	30.46367
EB	1.688485	106.168	0.015904	8	0.127231	1.838073
m-Xylene	11.53443	106.168	0.108643	8	0.869145	12.5563
P-xylene	0.611236	106.168	0.005757	8	0.046058	0.665387
O-Xylene	9.779133	106.168	0.09211	8	0.73688	10.6455
C9+	16.63195	120.19	0.13838	9	1.245424	17.99229
	100.9713					
Total	100.9713		1.228053		7.705821	
	Propane conversion		67.07756			
	Aromatic sum		58.71036		4.451826	64.92538
	Total converted products		94.7317		6.856835	
	aromatics selectivity		61.97541			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	

Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.404671	16.043	0.087557	1	0.087557	1.264906
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.341558	42.081	0.055644	3	0.166932	2.411623
neo-pentane	0.201194	72.151	0.002789	5	0.013943	0.201424
n-pentane	0.234687	72.151	0.003253	5	0.016264	0.234956
Propane	4.971371	44.097	0.112737	6	0.676423	0
iso butane	0.124941	58.124	0.00215	6	0.012897	0.186324
n-Butane	1.188806	58.124	0.020453	7	0.143171	2.068345
i-Pentane	0.010304	72.151	0.000143	3	0.000428	0.00619
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	22.56962	100.205	0.225234	5	1.126172	16.2695
Benzene	9.670552	78.114	0.123801	6	0.742803	10.73107
Toluene	23.87878	92.141	0.259155	7	1.814083	26.20755
EB	1.368939	106.168	0.012894	8	0.103153	1.490217
m-Xylene	9.879926	106.168	0.093059	8	0.744475	10.75522
P-xylene	0.524594	106.168	0.004941	8	0.039529	0.571069
O-Xylene	8.248031	106.168	0.077688	8	0.621508	8.97875
C9+	13.38203	120.19	0.111341	9	1.002065	14.47656
	100					
Total	100		1.192838		7.311403	
	Propane conversion		67.97669			
	Aromatic sum		53.57082		4.065551	61.2745
	Total converted products		95.02863		6.63498	
	aromatics selectivity		56.37335			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.55154	16.043	0.096711	1	0.096711	1.397162
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.280449	42.081	0.054192	3	0.162576	2.348686
neo-pentane	0.181129	72.151	0.00251	5	0.012552	0.181336
n-pentane	0.257272	72.151	0.003566	5	0.017829	0.257567
Propane	5.581917	44.097	0.126583	6	0.759496	0
iso butane	0.13921	58.124	0.002395	6	0.01437	0.207604
n-Butane	1.178621	58.124	0.020278	7	0.141944	2.050625
i-Pentane	0.00941	72.151	0.00013	3	0.000391	0.005652
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	20.8817	100.205	0.20839	5	1.041949	15.05275
Benzene	9.658262	78.114	0.123643	6	0.741859	10.71743
Toluene	23.84749	92.141	0.258815	7	1.811706	26.17321
EB	1.349126	106.168	0.012707	8	0.10166	1.468649
m-Xylene	10.33163	106.168	0.097314	8	0.778512	11.24695
P-xylene	0.472047	106.168	0.004446	8	0.03557	0.513867
O-Xylene	8.363364	106.168	0.078775	8	0.630199	9.104301
C9+	13.91683	120.19	0.11579	9	1.042112	15.0551
	100					
Total	100		1.206246		7.389436	
	Propane conversion		64.038			
	Aromatic sum		54.02192		4.099505	61.83322
	Total converted products		94.41808		6.62994	
	aromatics selectivity		57.21565			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.681898	16.043	0.104837	1	0.104837	1.514549
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.744445	42.081	0.065218	3	0.195654	2.826565
neo-pentane	0.195802	72.151	0.002714	5	0.013569	0.196026
n-pentane	0.307021	72.151	0.004255	5	0.021276	0.307372
Propane	5.601657	44.097	0.12703	6	0.762182	0
iso butane	0.152891	58.124	0.00263	6	0.015783	0.228007
n-Butane	1.34229	58.124	0.023094	7	0.161655	2.335383
i-Pentane	0.013788	72.151	0.000191	3	0.000573	0.008282
hexane	0.017621	86.178	0.000204	4	0.000818	0.011816
cyclohexane	0	84.162	0	4	0	0
n-heptane	12.07098	100.205	0.120463	5	0.602314	8.701465
Benzene	7.574486	78.114	0.096967	6	0.581802	8.405137
Toluene	27.70379	92.141	0.300667	7	2.104672	30.4056
EB	1.603364	106.168	0.015102	8	0.120817	1.745411
m-Xylene	11.2539	106.168	0.106001	8	0.848007	12.25091
P-xylene	0.525667	106.168	0.004951	8	0.03961	0.572238
O-Xylene	9.641138	106.168	0.09081	8	0.726482	10.49528
C9+	17.56926	120.19	0.146179	9	1.315612	19.00627
	100					
Total	100		1.211315		7.615663	
	Propane conversion		70.59556			
	Aromatic sum		58.30234		4.42139	64.51305
	Total converted products		94.39834		6.853481	
	aromatics selectivity		61.76204			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.563476	16.043	0.097455	1	0.097455	1.40791
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.278964	42.081	0.054157	3	0.16247	2.347155
neo-pentane	0.193517	72.151	0.002682	5	0.013411	0.193738
n-pentane	0.271863	72.151	0.003768	5	0.01884	0.272174
Propane	5.210816	44.097	0.118167	6	0.709003	0
iso butane	0.121908	58.124	0.002097	6	0.012584	0.181802
n-Butane	1.204784	58.124	0.020728	7	0.145095	2.096143
i-Pentane	0.011487	72.151	0.000159	3	0.000478	0.0069
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	23.14097	100.205	0.230936	5	1.154681	16.68136
Benzene	9.682509	78.114	0.123954	6	0.743721	10.74433
Toluene	21.87243	92.141	0.23738	7	1.66166	24.00553
EB	1.284994	106.168	0.012103	8	0.096827	1.398836
m-Xylene	10.07744	106.168	0.09492	8	0.759358	10.97023
P-xylene	0.465493	106.168	0.004384	8	0.035076	0.506733
O-Xylene	8.058838	106.168	0.075906	8	0.607252	8.772796
C9+	14.56052	120.19	0.121146	9	1.090313	15.75144
	100					
Total	100		1.199943		7.308223	
	Propane conversion		67.90475			
	Aromatic sum		51.44170		3.903894	59.1569
	Total converted products		94.78918		6.59922	
	aromatics selectivity		54.26958			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.855802	16.043	0.115677	1	0.115677	1.67115
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.715505	42.081	0.06453	3	0.193591	2.796759
neo-pentane	0.225961	72.151	0.003132	5	0.015659	0.22622
n-pentane	0.322224	72.151	0.004466	5	0.02233	0.322593
Propane	5.64412	44.097	0.127993	6	0.76796	0
iso butane	0.14356	58.124	0.00247	6	0.014819	0.214091
n-Butane	1.434819	58.124	0.024685	7	0.172798	2.496369
i-Pentane	0.012875	72.151	0.000178	3	0.000535	0.007734
hexane	0.039524	86.178	0.000459	4	0.001835	0.026503
cyclohexane	0	84.162	0	4	0	0
n-heptane	13.20876	100.205	0.131817	5	0.659087	9.521644
Benzene	7.706012	78.114	0.098651	6	0.591905	8.551086
Toluene	26.15083	92.141	0.283813	7	1.986692	28.70119
EB	1.542917	106.168	0.014533	8	0.116262	1.679609
m-Xylene	12.03477	106.168	0.113356	8	0.906847	13.10097
P-xylene	0.509177	106.168	0.004796	8	0.038368	0.554287
O-Xylene	9.342962	106.168	0.088002	8	0.704013	10.17068
C9+	17.11018	120.19	0.142359	9	1.281235	18.50964
	100					
Total	100		1.220918		7.589614	
	Propane conversion		71.03925			
	Aromatic sum		57.28667		4.344088	63.68086
	Total converted products		94.35588		6.821654	
	aromatics selectivity		60.71341			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.325353	16.043	0.082613	1	0.082613	1.19348
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.424007	42.081	0.057603	3	0.17281	2.496538
neo-pentane	0.19801	72.151	0.002744	5	0.013722	0.198237
n-pentane	0.255024	72.151	0.003535	5	0.017673	0.255316
Propane	5.570733	44.097	0.126329	6	0.757974	0
iso butane	0.130115	58.124	0.002239	6	0.013431	0.194041
n-Butane	1.246878	58.124	0.021452	7	0.150164	2.16938
i-Pentane	0.01034	72.151	0.000143	3	0.00043	0.006211
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	23.43839	100.205	0.233904	5	1.169522	16.89575
Benzene	9.623148	78.114	0.123194	6	0.739162	10.67846
Toluene	21.68799	92.141	0.235378	7	1.647648	23.8031
EB	1.240582	106.168	0.011685	8	0.093481	1.350489
m-Xylene	10.01645	106.168	0.094345	8	0.754762	10.90384
P-xylene	0.415368	106.168	0.003912	8	0.031299	0.452166
O-Xylene	7.888534	106.168	0.074302	8	0.594419	8.587404
C9+	14.52908	120.19	0.120884	9	1.087959	15.71743
	100					
Total	100		1.194264		7.327068	
	Propane conversion		66.56506			
	Aromatic sum		50.87207		3.86077	58.77173
	Total converted products		94.42927		6.569094	
	aromatics selectivity		53.8732			

Table A4**:** Zn-Co/ZSM-5 (2-1 wt. %)

Run 1-12

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.552626	16.043	0.096779	1	0.096779	1.402699
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.476459	42.081	0.058850	3	0.176549	2.558877
neo-pentane	0.218899	72.151	0.003034	5	0.01517	0.219865
n-pentane	0.28455	72.151	0.003944	5	0.019719	0.285805
Propane	6.042712	44.097	0.137032	6	0.822194	0
iso butane	0.158985	58.124	0.002735	6	0.016412	0.237867
n-Butane	1.254439	58.124	0.021582	7	0.151075	2.189653
i-Pentane	0.01332	72.151	0.000185	3	0.000554	0.008027
hexane	0.033441	86.178	0.000388	4	0.001552	0.022497
cyclohexane	0	84.162	0	4	0	0
n-heptane	10.96286	100.205	0.109404	5	0.547021	7.928436
Benzene	8.753161	78.114	0.112056	6	0.672337	9.744746
Toluene	46.56797	92.141	0.505399	7	3.537793	51.27618
EB	1.693192	106.168	0.015948	8	0.127586	1.849208
m-Xylene	8.780737	106.168	0.082706	8	0.661648	9.589822
P-xylene	0	106.168	0	8	0	0
O-Xylene	3.509245	106.168	0.033054	8	0.26443	3.832598
C9+	8.157716	120.19	0.067873	9	0.610861	8.853724
	100					
Total	100		1.25097		7.72168	
	Propane conversion		55.82513			
	Aromatic sum		69.3043		5.263794	76.29255
	Total converted products		94.4176		6.899487	
	aromatics selectivity		73.40189			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.67716	16.043	0.104542	1	0.104542	1.515208
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.077357	42.081	0.049366	3	0.148097	2.146493
neo-pentane	0.194034	72.151	0.002689	5	0.013446	0.19489
n-pentane	0.320609	72.151	0.004444	5	0.022218	0.322023
Propane	5.280792	44.097	0.119754	6	0.718524	0
iso butane	0.172155	58.124	0.002962	6	0.017771	0.257572
n-Butane	1.233529	58.124	0.021222	7	0.148557	2.153154
i-Pentane	0.013519	72.151	0.000187	3	0.000562	0.008147
hexane	0.017773	86.178	0.000206	4	0.000825	0.011957
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.09178	100.205	0.090732	5	0.453659	6.575257
Benzene	6.715362	78.114	0.085969	6	0.515812	7.476098
Toluene	42.22914	92.141	0.45831	7	3.20817	46.49868
EB	1.420361	106.168	0.013378	8	0.107027	1.551238
m-Xylene	10.85715	106.168	0.102264	8	0.818111	11.85756
P-xylene	0.156385	106.168	0.001473	8	0.011784	0.170795
O-Xylene	8.139104	106.168	0.076662	8	0.6133	8.889066
C9+	10.40379	120.19	0.086561	9	0.779051	11.29143
	100					
Total	100		1.220721		7.681456	
	Propane conversion		63.20763			
	Aromatic sum		69.5175		5.274205	75.74689
	Total converted products		94.71921		6.962932	
	aromatics selectivity		73.39325			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.358234	16.043	0.084662	1	0.084662	1.227078
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.236161	42.081	0.053139	3	0.159418	2.310583
neo-pentane	0.224581	72.151	0.003113	5	0.015563	0.225572
n-pentane	0.310136	72.151	0.004298	5	0.021492	0.311503
Propane	5.311676	44.097	0.120454	6	0.722726	0
iso butane	0.155655	58.124	0.002678	6	0.016068	0.232886
n-Butane	1.241427	58.124	0.021358	7	0.149508	2.166939
i-Pentane	0.013723	72.151	0.00019	3	0.000571	0.00827
hexane	0.03294	86.178	0.000382	4	0.001529	0.02216
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.534441	100.205	0.095149	5	0.475747	6.895393
Benzene	6.887609	78.114	0.088174	6	0.529043	7.667858
Toluene	41.35047	92.141	0.448774	7	3.141417	45.53116
EB	1.34157	106.168	0.012636	8	0.10109	1.465187
m-Xylene	9.354195	106.168	0.088107	8	0.70486	10.21612
P-xylene	0.151293	106.168	0.001425	8	0.01140	0.165234
O-Xylene	8.025655	106.168	0.075594	8	0.604751	8.765164
C9+	12.47024	120.19	0.103754	9	0.933789	13.53418
	100					
Total	100		1.20389		7.673634	
	Propane conversion		63.54425			
	Aromatic sum		67.11079		5.092561	73.26469
	Total converted products		94.68832		6.950908	
	aromatics selectivity		70.87546			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.516961	16.043	0.094556	1	0.094556	1.370478
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.436085	42.081	0.05789	3	0.173671	2.51716
neo-pentane	0.244652	72.151	0.003391	5	0.016954	0.245731
n-pentane	0.331693	72.151	0.004597	5	0.022986	0.333155
Propane	5.51106	44.097	0.124976	6	0.749855	0
iso butane	0.163461	58.124	0.002812	6	0.016874	0.244564
n-Butane	1.337857	58.124	0.023017	7	0.161121	2.335261
i-Pentane	0.013856	72.151	0.000192	3	0.000576	0.00835
hexane	0.030725	86.178	0.000357	4	0.001426	0.02067
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.760762	100.205	0.097408	5	0.48704	7.059071
Benzene	5.753474	78.114	0.073655	6	0.441929	6.405245
Toluene	40.69922	92.141	0.441706	7	3.091941	44.81407
EB	1.388593	106.168	0.013079	8	0.104634	1.516542
m-Xylene	8.988113	106.168	0.084659	8	0.677275	9.816306
P-xylene	0.558559	106.168	0.005261	8	0.042089	0.610027
O-Xylene	8.073039	106.168	0.07604	8	0.608322	8.816915
C9+	13.19189	120.19	0.109759	9	0.987828	14.31741
	100					
Total	100		1.213356		7.679076	
	Propane conversion		64.55094			
	Aromatic sum		65.461		4.966189	71.67024
	Total converted products		94.48894		6.929221	
	aromatics selectivity		69.27901			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.408544	16.043	0.087798	1	0.087798	1.27253
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.389373	42.081	0.05678	3	0.170341	2.468893
neo-pentane	0.21946	72.151	0.003042	5	0.015208	0.220428
n-pentane	0.303394	72.151	0.004205	5	0.021025	0.304732
Propane	4.749983	44.097	0.107717	6	0.6463	0
iso butane	0.155703	58.124	0.002679	6	0.016073	0.232957
n-Butane	1.282106	58.124	0.022058	7	0.154407	2.237946
i-Pentane	0.012885	72.151	0.000179	3	0.000536	0.007765
hexane	0.028158	86.178	0.000327	4	0.001307	0.018943
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.837846	100.205	0.098177	5	0.490886	7.114819
Benzene	7.074483	78.114	0.090566	6	0.543397	7.875902
Toluene	40.43119	92.141	0.438797	7	3.071579	44.51895
EB	1.34589	106.168	0.012677	8	0.101416	1.469904
m-Xylene	8.92611	106.168	0.084075	8	0.672603	9.748589
P-xylene	0.587982	106.168	0.005538	8	0.044306	0.64216
O-Xylene	7.929241	106.168	0.074686	8	0.597486	8.659866
C9+	13.31765	120.19	0.110805	9	0.997245	14.4539
	100					
Total	100		1.200106		7.631912	
	Propane conversion		67.4665			
	Aromatic sum		66.2949		5.030786	72.0164
	Total converted products		95.25002		6.985612	
	aromatics selectivity		69.60093			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 6					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.418282	16.043	0.088405	1	0.088405	1.281328
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.728315	42.081	0.041071	3	0.123213	1.785835
neo-pentane	0.176244	72.151	0.002443	5	0.012214	0.177021
n-pentane	0.271751	72.151	0.003766	5	0.018832	0.272949
Propane	3.979349	44.097	0.090241	6	0.541445	0
iso butane	0.136611	58.124	0.00235	6	0.014102	0.204393
n-Butane	1.158556	58.124	0.019932	7	0.139527	2.022287
i-Pentane	0.010657	72.151	0.000148	3	0.000443	0.006422
hexane	0	86.178	0	4	0	0
cyclohexane	0.053392	84.162	0.000634	4	0.002538	0.036779
n-heptane	19.30068	100.205	0.192612	5	0.96306	13.95842
Benzene	8.453261	78.114	0.108217	6	0.649302	9.410872
Toluene	34.77541	92.141	0.377415	7	2.641906	38.29135
EB	1.135953	106.168	0.0107	8	0.085597	1.240623
m-Xylene	8.197911	106.168	0.077216	8	0.617731	8.953292
P-xylene	0.313584	106.168	0.002954	8	0.023629	0.342478
O-Xylene	7.000229	106.168	0.065935	8	0.527483	7.645252
C9+	11.88981	120.19	0.098925	9	0.890326	12.90424
	100					
Total	100		1.182965		7.339754	
	Propane conversion		70.09788			
	Aromatic sum		59.87635		4.545649	66.8644
	Total converted products		96.02065		6.798309	
	aromatics selectivity		62.35779			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.36839	16.043	0.085295	1	0.085295	1.236253
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.136689	42.081	0.050776	3	0.152327	2.2078
neo-pentane	0.228128	72.151	0.003162	5	0.015809	0.229134
n-pentane	0.309652	72.151	0.004292	5	0.021459	0.311017
Propane	4.747873	44.097	0.107669	6	0.646013	0
iso butane	0.167791	58.124	0.002887	6	0.017321	0.251043
n-Butane	1.329469	58.124	0.022873	7	0.160111	2.320619
i-Pentane	0.01306	72.151	0.000181	3	0.000543	0.00787
hexane	0.015271	86.178	0.000177	4	0.000709	0.010273
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.82222	100.205	0.098021	5	0.490106	7.103518
Benzene	6.552809	78.114	0.083888	6	0.503327	7.29513
Toluene	39.73562	92.141	0.431248	7	3.018736	43.75305
EB	1.45707	106.168	0.013724	8	0.109794	1.591329
m-Xylene	9.655349	106.168	0.090944	8	0.727553	10.54502
P-xylene	0.525682	106.168	0.004951	8	0.039611	0.57412
O-Xylene	8.141366	106.168	0.076684	8	0.61347	8.891537
C9+	13.79356	120.19	0.114765	9	1.032881	14.97041
	100					
Total	100		1.191536		7.635064	
	Propane conversion		64.20025			
	Aromatic sum		66.06790		5.012491	71.71919
	Total converted products		95.25213		6.989051	
	aromatics selectivity		69.36108			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.669577	16.043	0.104069	1	0.104069	1.508357
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.547792	42.081	0.060545	3	0.181635	2.632585
neo-pentane	0.237763	72.151	0.003295	5	0.016477	0.238812
n-pentane	0.3404	72.151	0.004718	5	0.023589	0.341901
Propane	6.141875	44.097	0.139281	6	0.835686	0
iso butane	0.168034	58.124	0.002891	6	0.017346	0.251407
n-Butane	1.453773	58.124	0.025012	7	0.175081	2.537596
i-Pentane	0.012706	72.151	0.000176	3	0.000528	0.007657
hexane	0.019883	86.178	0.000231	4	0.000923	0.013376
cyclohexane	0	84.162	0	4	0	0
n-heptane	11.24749	100.205	0.112245	5	0.561224	8.134289
Benzene	7.159395	78.114	0.091653	6	0.549919	7.970432
Toluene	39.89149	92.141	0.43294	7	3.030578	43.92468
EB	1.315967	106.168	0.012395	8	0.099161	1.437224
m-Xylene	9.596044	106.168	0.090385	8	0.723084	10.48025
P-xylene	0.147906	106.168	0.001393	8	0.011145	0.161535
O-Xylene	8.09084	106.168	0.076208	8	0.609663	8.836356
C9+	14.03247	120.19	0.116752	9	1.050772	15.22971
	104.0734					
Total	104.0734		1.274189		7.99088	
	Propane conversion		67.71412			
	Aromatic sum		66.20165		5.02355	70.20844
	Total converted products		97.93154		7.155193	
	aromatics selectivity		67.59992			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 9					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.706538	16.043	0.106373	1	0.106373	1.541749
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.035116	42.081	0.048362	3	0.145086	2.102847
neo-pentane	0.221816	72.151	0.003074	5	0.015372	0.222794
n-pentane	0.316929	72.151	0.004393	5	0.021963	0.318326
Propane	5.353908	44.097	0.121412	6	0.728472	0
iso butane	0.178659	58.124	0.003074	6	0.018443	0.267303
n-Butane	1.325423	58.124	0.022803	7	0.159624	2.313558
i-Pentane	0.011007	72.151	0.000153	3	0.000458	0.006633
hexane	0.019117	86.178	0.000222	4	0.000887	0.012861
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.564324	100.205	0.095448	5	0.477238	6.917005
Benzene	6.388709	78.114	0.081787	6	0.490722	7.112441
Toluene	38.25233	92.141	0.41515	7	2.906049	42.11979
EB	1.187988	106.168	0.01119	8	0.089518	1.297452
m-Xylene	10.20372	106.168	0.096109	8	0.768874	11.14392
P-xylene	0.292581	106.168	0.002756	8	0.022047	0.31954
O-Xylene	8.174547	106.168	0.076996	8	0.615971	8.927776
C9+	14.76729	120.19	0.122866	9	1.105796	16.02722
	100					
Total	100		1.212167		7.67289	
	Propane conversion		67.99712			
	Aromatic sum		64.49987		4.89318	70.46206
	Total converted products		94.64609		6.944418	
	aromatics selectivity		68.14848			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 10					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.634922	16.043	0.101909	1	0.101909	1.477048
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.210698	42.081	0.052534	3	0.157603	2.284272
neo-pentane	0.198153	72.151	0.002746	5	0.013732	0.199027
n-pentane	0.308646	72.151	0.004278	5	0.021389	0.310007
Propane	5.435438	44.097	0.123261	6	0.739566	0
iso butane	0.15324	58.124	0.002636	6	0.015819	0.229272
n-Butane	0.826049	58.124	0.014212	7	0.099483	1.441888
i-Pentane	0.01243	72.151	0.000172	3	0.000517	0.007491
hexane	0.027608	86.178	0.00032	4	0.001281	0.018573
cyclohexane	0	84.162	0	4	0	0
n-heptane	10.12555	100.205	0.101048	5	0.505242	7.322886
Benzene	6.10042	78.114	0.078096	6	0.468578	6.791494
Toluene	38.11338	92.141	0.413642	7	2.895493	41.96679
EB	1.419983	106.168	0.013375	8	0.106999	1.550824
m-Xylene	10.19994	106.168	0.096074	8	0.768589	11.1398
P-xylene	0.1614	106.168	0.00152	8	0.012162	0.176272
O-Xylene	8.140286	106.168	0.076674	8	0.613389	8.890357
C9+	14.93186	120.19	0.124235	9	1.118119	16.20583
	100					
Total	100		1.206733		7.639869	
	Propane conversion		67.37913			
	Aromatic sum		64.13541		4.86521	70.50719
	Total converted products		94.56456		6.900303	
	aromatics selectivity		67.82182			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 11					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.7206	16.043	0.107249	1	0.107249	1.554453
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.532916	42.081	0.060191	3	0.180574	2.617214
neo-pentane	0.216161	72.151	0.002996	5	0.01498	0.217114
n-pentane	0.319399	72.151	0.004427	5	0.022134	0.320807
Propane	5.412681	44.097	0.122745	6	0.736469	0
iso butane	0.152902	58.124	0.002631	6	0.015784	0.228766
n-Butane	0.886143	58.124	0.015246	7	0.10672	1.546784
i-Pentane	0.012527	72.151	0.000174	3	0.000521	0.00755
hexane	0.040335	86.178	0.000468	4	0.001872	0.027135
cyclohexane	0	84.162	0	4	0	0
n-heptane	12.36965	100.205	0.123443	5	0.617217	8.945841
Benzene	6.226105	78.114	0.079705	6	0.478232	6.931417
Toluene	36.71471	92.141	0.398462	7	2.789236	40.42671
EB	1.269082	106.168	0.011954	8	0.095628	1.386019
m-Xylene	9.685201	106.168	0.091225	8	0.729802	10.57763
P-xylene	0.153847	106.168	0.001449	8	0.011593	0.168023
O-Xylene	7.813541	106.168	0.073596	8	0.588768	8.533505
C9+	14.4742	120.19	0.120428	9	1.083849	15.70913
	100					
Total	100		1.216389		7.580629	
	Propane conversion		72.29788			
	Aromatic sum		61.86248		4.693259	68.5732
	Total converted products		94.58732		6.844159	
	aromatics selectivity		65.40251			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 12					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.553066	16.043	0.096806	1	0.096806	1.403097
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.109832	42.081	0.050137	3	0.150412	2.18005
neo-pentane	0.204985	72.151	0.002841	5	0.014205	0.205889
n-pentane	0.35765	72.151	0.004957	5	0.024785	0.359228
Propane	5.631579	44.097	0.127709	6	0.766253	0
iso butane	0.183233	58.124	0.003152	6	0.018915	0.274146
n-Butane	1.364503	58.124	0.023476	7	0.16433	2.381773
i-Pentane	0.01394	72.151	0.000193	3	0.00058	0.008401
hexane	0.031852	86.178	0.00037	4	0.001478	0.021428
cyclohexane	0	84.162	0	4	0	0
n-heptane	10.79032	100.205	0.107682	5	0.538412	7.803657
Benzene	6.191704	78.114	0.079265	6	0.47559	6.893119
Toluene	37.05541	92.141	0.40216	7	2.815119	40.80186
EB	1.391033	106.168	0.013102	8	0.104817	1.519207
m-Xylene	9.883515	106.168	0.093093	8	0.744745	10.79421
P-xylene	0.500578	106.168	0.004715	8	0.03772	0.546703
O-Xylene	8.123469	106.168	0.076515	8	0.612122	8.871991
C9+	14.61333	120.19	0.121585	9	1.094267	15.86013
	100					
Total	100		1.20776		7.660557	
	Propane conversion		69.01319			
	Aromatic sum		63.14571		4.790113	69.47928
	Total converted products		94.36842		6.894304	
	aromatics selectivity		66.91402			

Table A5: Zn-Ni/ZSM-5 (2-1 wt. %) Run 1-12

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.998354	16.043	0.124562	1	0.124562	1.795864
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.571335	42.081	0.061104	3	0.183313	2.642899
neo-pentane	0.155044	72.151	0.002149	5	0.010744	0.154907
n-pentane	0.263565	72.151	0.003653	5	0.018265	0.263331
Propane	5.374695	44.097	0.121883	6	0.731301	0
iso butane	0.108014	58.124	0.001858	6	0.01115	0.160754
n-Butane	0.959234	58.124	0.016503	7	0.115523	1.665535
i-Pentane	0.007555	72.151	0.000105	3	0.000314	0.004529
hexane	0.011586	86.178	0.000134	4	0.000538	0.007754
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.341461	100.205	0.093224	5	0.466118	6.720197
Benzene	8.799262	78.114	0.112646	6	0.675878	9.744403
Toluene	45.2227	92.141	0.490799	7	3.435592	49.53226
EB	1.376455	106.168	0.012965	8	0.103719	1.495357
m-Xylene	8.707806	106.168	0.082019	8	0.656153	9.460012
P-xylene	0	106.168	0	8	0	0
O-Xylene	6.945217	106.168	0.065417	8	0.523338	7.545166
C9+	8.157716	120.19	0.067873	9	0.610861	8.807027
	100					
Total	100		1.256896		7.66737	
	Propane conversion		57.58025			
	Aromatic sum		71.05144		5.39468	77.7772
	Total converted products		94.6253		6.936069	
	aromatics selectivity		75.08714			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.541228	16.043	0.096069	1	0.096069	1.385058
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.969083	42.081	0.046793	3	0.140378	2.023884
neo-pentane	0.160691	72.151	0.002227	5	0.011136	0.160548
n-pentane	0.294099	72.151	0.004076	5	0.020381	0.293838
Propane	3.890268	44.097	0.088221	6	0.529324	0
iso butane	0.10006	58.124	0.001721	6	0.010329	0.148916
n-Butane	0.932508	58.124	0.016043	7	0.112304	1.619129
i-Pentane	0.009664	72.151	0.000134	3	0.000402	0.005793
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	11.55829	100.205	0.115346	5	0.576732	8.314971
Benzene	8.637308	78.114	0.110573	6	0.663439	9.565052
Toluene	42.50453	92.141	0.461299	7	3.229091	46.55506
EB	1.046584	106.168	0.009858	8	0.078863	1.136991
m-Xylene	8.159204	106.168	0.076852	8	0.614815	8.864021
P-xylene	0.009783	106.168	9.21E-05	8	0.000737	0.010628
O-Xylene	6.989422	106.168	0.065834	8	0.526669	7.593189
C9+	12.19728	120.19	0.101483	9	0.91335	13.16812
	100					
Total	100		1.196621		7.524017	
	Propane conversion		67.84663			
	Aromatic sum		67.34683		5.113613	73.10704
	Total converted products		96.10973		6.994693	
	aromatics selectivity		70.07285			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	0	0	0	
Total	100		0.750391		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.696453	16.043	0.105744	1	0.105744	1.524554
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.196688	42.081	0.052201	3	0.156604	2.257825
neo-pentane	0.153507	72.151	0.002128	5	0.010638	0.153371
n-pentane	0.360521	72.151	0.004997	5	0.024984	0.360201
Propane	4.667826	44.097	0.105854	6	0.635122	0
iso butane	0.123757	58.124	0.002129	6	0.012775	0.184184
n-Butane	1.114301	58.124	0.019171	7	0.134198	1.93478
i-Pentane	0.010769	72.151	0.000149	3	0.000448	0.006455
hexane	0.02397	86.178	0.000278	4	0.001113	0.01604
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.060467	100.205	0.090419	5	0.452097	6.518051
Benzene	6.679133	78.114	0.085505	6	0.51303	7.396548
Toluene	39.79252	92.141	0.431866	7	3.023059	43.58461
EB	1.246021	106.168	0.011736	8	0.093891	1.353656
m-Xylene	10.19144	106.168	0.095994	8	0.767948	11.07181
P-xylene	0	106.168	0	8	0	0
O-Xylene	8.237182	106.168	0.077586	8	0.62069	8.948734
C9+	14.44544	120.19	0.120188	9	1.081695	15.59522
	100					
Total	100		1.205946		7.634034	
	Propane conversion		69.52175			
	Aromatic sum		66.1463		5.018618	71.70567
	Total converted products		95.33217		6.998913	
	aromatics selectivity		69.38508			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.583802	16.043	0.098722	1	0.098722	1.423318
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.932303	42.081	0.045919	3	0.137756	1.986081
neo-pentane	0.150347	72.151	0.002084	5	0.010419	0.150214
n-pentane	0.322758	72.151	0.004473	5	0.022367	0.322472
Propane	4.461732	44.097	0.10118	6	0.60708	0
iso butane	0.094925	58.124	0.001633	6	0.009799	0.141275
n-Butane	0.657154	58.124	0.011306	7	0.079143	1.141028
i-Pentane	0.010271	72.151	0.000142	3	0.000427	0.006157
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	13.29043	100.205	0.132632	5	0.663162	9.561061
Benzene	8.631175	78.114	0.110495	6	0.662968	9.558261
Toluene	39.90931	92.141	0.433133	7	3.031931	43.71253
EB	1.125728	106.168	0.010603	8	0.084826	1.222972
m-Xylene	7.548472	106.168	0.071099	8	0.568794	8.200531
P-xylene	0.091808	106.168	0.000865	8	0.006918	0.099739
O-Xylene	7.014752	106.168	0.066072	8	0.528578	7.620707
C9+	13.17503	120.19	0.109618	9	0.986566	14.2237
	100					
Total	100		1.199978		7.499455	
	Propane conversion		69.5565			
	Aromatic sum		64.32125		4.884015	70.86113
	Total converted products		95.53827		6.892375	
	aromatics selectivity		67.32511			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.200029	16.043	0.137133	1	0.137133	1.977104
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.473822	42.081	0.058787	3	0.176361	2.542672
neo-pentane	0.422066	72.151	0.00585	5	0.029249	0.421691
n-pentane	0.680042	72.151	0.009425	5	0.047126	0.679439
Propane	12.80105	44.097	0.290293	6	1.741758	0
iso butane	0.267419	58.124	0.004601	6	0.027605	0.397992
n-Butane	1.321463	58.124	0.022735	7	0.159147	2.294479
i-Pentane	0.023418	72.151	0.000325	3	0.000974	0.014039
hexane	0.012098	86.178	0.00014	4	0.000562	0.008096
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.030684	100.205	0.000306	5	0.001531	0.022074
Benzene	10.4188	78.114	0.133379	6	0.800277	11.5379
Toluene	37.23552	92.141	0.404115	7	2.828802	40.78394
EB	3.510609	106.168	0.033067	8	0.264532	3.813866
m-Xylene	6.417013	106.168	0.060442	8	0.483537	6.971333
P-xylene	0	106.168	0	8	0	0
O-Xylene	2.94495	106.168	0.027739	8	0.221909	3.199344
C9+	19.24101	120.19	0.160088	9	1.440795	20.77249
	100					
Total	100		1.348425		8.361297	
	Propane conversion		72.25413			
	Aromatic sum		60.5269		4.599057	69.47699
	Total converted products		87.19895		6.619539	
	aromatics selectivity		69.41242			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
1					
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0
Total	100		3.138791000		2.251174
Output parameters	Catalyst Run 6				
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.200029	16.043	0.137133	1	0.137133	1.977104
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.473822	42.081	0.058787	3	0.176361	2.542672
neo-pentane	0.422066	72.151	0.00585	5	0.029249	0.421691
n-pentane	0.680042	72.151	0.009425	5	0.047126	0.679439
Propane	12.80105	44.097	0.290293	6	1.741758	0
iso butane	0.267419	58.124	0.004601	6	0.027605	0.397992
n-Butane	1.321463	58.124	0.022735	7	0.159147	2.294479
i-Pentane	0.023418	72.151	0.000325	3	0.000974	0.014039
hexane	0.012098	86.178	0.00014	4	0.000562	0.008096
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.030684	100.205	0.000306	5	0.001531	0.022074
Benzene	10.4188	78.114	0.133379	6	0.800277	11.5379
Toluene	37.23552	92.141	0.404115	7	2.828802	40.78394
EB	3.510609	106.168	0.033067	8	0.264532	3.813866
m-Xylene	6.417013	106.168	0.060442	8	0.483537	6.971333
P-xylene	0	106.168	0	8	0	0
O-Xylene	2.94495	106.168	0.027739	8	0.221909	3.199344
C9+	19.24101	120.19	0.160088	9	1.440795	20.77249
	100					
Total	100		1.348425		8.361297	
	Propane conversion		72.981			
	Aromatic sum		60.5269		4.599057	69.47699
	Total converted products		87.19895		6.619539	
	aromatics selectivity		69.41242			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.834845	16.043	0.11437	1	0.11437	1.648923
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.520797	42.081	0.059903	3	0.17971	2.590954
neo-pentane	0.351197	72.151	0.004868	5	0.024338	0.350886
n-pentane	0.501669	72.151	0.006953	5	0.034765	0.501224
Propane	9.520113	44.097	0.21589	6	1.295342	0
iso butane	0.259087	58.124	0.004457	6	0.026745	0.385592
n-Butane	1.250037	58.124	0.021506	7	0.150545	2.170462
i-Pentane	0.019509	72.151	0.00027	3	0.000811	0.011695
hexane	0.012823	86.178	0.000149	4	0.000595	0.008581
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.036604	100.205	0.000365	5	0.001826	0.026333
Benzene	8.384412	78.114	0.107336	6	0.644014	9.284993
Toluene	29.61454	92.141	0.321405	7	2.249832	32.4367
EB	7.503613	106.168	0.070677	8	0.565414	8.151797
m-Xylene	8.696512	106.168	0.081913	8	0.655302	9.447742
P-xylene	0.161729	106.168	0.001523	8	0.012187	0.1757
O-Xylene	6.504419	106.168	0.061265	8	0.490123	7.06629
C9+	22.8281	120.19	0.189933	9	1.709401	24.64509
	100					
Total	100		1.262785		8.155319	
	Propane conversion		71.08638			
	Aromatic sum		60.86522		4.616871	67.30154
	Total converted products		90.47989		6.859978	
	aromatics selectivity		67.26934			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.404611	16.043	0.087553	1	0.087553	1.262284
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.114276	42.081	0.026479	3	0.079438	1.145288
neo-pentane	0.210797	72.151	0.002922	5	0.014608	0.21061
n-pentane	0.24918	72.151	0.003454	5	0.017268	0.248959
Propane	4.41514	44.097	0.100123	6	0.60074	0
iso butane	0.115342	58.124	0.001984	6	0.011906	0.171661
n-Butane	0.625056	58.124	0.010754	7	0.075277	1.085295
i-Pentane	0.008836	72.151	0.000122	3	0.000367	0.005297
hexane	0.013859	86.178	0.000161	4	0.000643	0.009274
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.034648	100.205	0.000346	5	0.001729	0.024926
Benzene	8.681545	78.114	0.111139	6	0.666837	9.614042
Toluene	33.22397	92.141	0.360578	7	2.524043	36.3901
EB	8.431062	106.168	0.079412	8	0.6353	9.159362
m-Xylene	6.919762	106.168	0.065177	8	0.52142	7.517511
P-xylene	4.076493	106.168	0.038397	8	0.307173	4.428632
O-Xylene	7.722259	106.168	0.072736	8	0.58189	8.389331
C9+	22.75399	120.19	0.189317	9	1.703851	24.56509
	100.0008					
Total	100.0008		1.150655		7.830042	
	Propane conversion		71.82762			
	Aromatic sum		69.05509		5.236661	72.43661
	Total converted products		95.58569		7.229302	
	aromatics selectivity		72.24418			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				
Propane	33.09	44.097	0.75039100	3	2.251174

Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 9					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.961466	16.043	0.122263	1	0.122263	1.762714
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.1743	42.081	0.051669	3	0.155008	2.234813
neo-pentane	0.29675	72.151	0.004113	5	0.020565	0.296486
n-pentane	0.428086	72.151	0.005933	5	0.029666	0.427706
Propane	6.463383	44.097	0.146572	6	0.879432	0
iso butane	0.218064	58.124	0.003752	6	0.02251	0.324538
n-Butane	1.084742	58.124	0.018663	7	0.130638	1.883456
i-Pentane	0.014516	72.151	0.000201	3	0.000604	0.008702
hexane	0.017853	86.178	0.000207	4	0.000829	0.011947
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.028473	100.205	0.000284	5	0.001421	0.020483
Benzene	7.418035	78.114	0.094964	6	0.569785	8.214816
Toluene	31.89725	92.141	0.346179	7	2.42325	34.93694
EB	7.483379	106.168	0.070486	8	0.56389	8.129816
m-Xylene	6.875131	106.168	0.064757	8	0.518057	7.469026
P-xylene	3.544471	106.168	0.033385	8	0.267084	3.850653
O-Xylene	7.231842	106.168	0.068117	8	0.544936	7.856549
C9+	22.86226	120.19	0.190218	9	1.711959	24.68198
	100					
Total	100		1.221764		7.961895	
	Propane conversion		77.20269			
	Aromatic sum		64.4501		4.887002	69.00144
	Total converted products		93.53662		7.082464	
	aromatics selectivity		68.90361			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 10					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.240929	16.043	0.139683	1	0.139683	2.01386
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.612783	42.081	0.062089	3	0.186268	2.6855
neo-pentane	0.345652	72.151	0.004791	5	0.023953	0.345345
n-pentane	0.472555	72.151	0.00655	5	0.032748	0.472135
Propane	8.10356	44.097	0.183767	6	1.1026	0
iso butane	0.250726	58.124	0.004314	6	0.025882	0.373149
n-Butane	1.299758	58.124	0.022362	7	0.156533	2.256792
i-Pentane	0.016704	72.151	0.000232	3	0.000695	0.010013
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.034438	100.205	0.000344	5	0.001718	0.024774
Benzene	8.017787	78.114	0.102642	6	0.615853	8.878989
Toluene	27.43244	92.141	0.297722	7	2.084057	30.04666
EB	8.136007	106.168	0.076633	8	0.613067	8.838819
m-Xylene	7.146237	106.168	0.067311	8	0.538485	7.76355
P-xylene	3.839906	106.168	0.036168	8	0.289346	4.171609
O-Xylene	7.351266	106.168	0.069242	8	0.553935	7.98629
C9+	22.69925	120.19	0.188861	9	1.699752	24.50599
	100					
Total	100		1.26271		8.064574	
	Propane conversion		77.84212			
	Aromatic sum		61.92365		4.694742	67.43407
	Total converted products		91.89644		6.961973	
	aromatics selectivity		67.38416			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	

Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 11					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.219729	16.043	0.138361	1	0.138361	1.994808
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.742092	42.081	0.065162	3	0.195487	2.818407
neo-pentane	0.312524	72.151	0.004332	5	0.021658	0.312247
n-pentane	0.432346	72.151	0.005992	5	0.029961	0.431962
Propane	9.618373	44.097	0.218119	6	1.308711	0
iso butane	0.195328	58.124	0.003361	6	0.020163	0.290701
n-Butane	1.21004	58.124	0.020818	7	0.145728	2.101014
i-Pentane	0.014965	72.151	0.000207	3	0.000622	0.008971
hexane	0.007689	86.178	8.92E-05	4	0.000357	0.005146
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.081565	100.205	0.000814	5	0.00407	0.058678
Benzene	7.956242	78.114	0.101854	6	0.611125	8.810833
Toluene	30.85213	92.141	0.334836	7	2.343852	33.79223
EB	7.69649	106.168	0.072493	8	0.579948	8.361335
m-Xylene	6.553939	106.168	0.061732	8	0.493854	7.120088
P-xylene	3.855686	106.168	0.036317	8	0.290535	4.188752
O-Xylene	6.545485	106.168	0.061652	8	0.493217	7.110903
C9+	19.70538	120.19	0.163952	9	1.475567	21.27382
	100					
Total	100		1.290092		8.153217	
	Propane conversion		82.468			
	Aromatic sum		63.45997		4.812532	70.31234
	Total converted products		90.38163		6.844506	
	aromatics selectivity		70.21335			

Table A6: Zn-Cu/ZSM-5 (2-1 wt. % each)

Run 1-12

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.677015	16.043	0.166865	1	0.166865	2.305058
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.946066	42.081	0.070009	3	0.210028	2.901312
neo-pentane	0.404927	72.151	0.005612	5	0.028061	0.387633
n-pentane	0.491985	72.151	0.006819	5	0.034094	0.470973
Propane	10.72708	44.097	0.243261	6	1.459566	0
iso butane	0.177722	58.124	0.003058	6	0.018346	0.253428
n-Butane	1.286184	58.124	0.022128	7	0.154898	2.139747
i-Pentane	0.020067	72.151	0.000278	3	0.000834	0.011526
hexane	0.010963	86.178	0.000127	4	0.000509	0.007029
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.010155	100.205	0.000101	5	0.000507	0.006999
Benzene	17.53785	78.114	0.224516	6	1.347097	18.60868
Toluene	30.1924	92.141	0.327676	7	2.293733	31.68543
EB	8.615111	106.168	0.081146	8	0.649168	8.967553
m-Xylene	8.023829	106.168	0.075577	8	0.604614	8.352082
P-xylene	0.196523	106.168	0.001851	8	0.014808	0.204562
O-Xylene	6.339623	106.168	0.059713	8	0.477705	6.598976
C9+	16.53028	120.19	0.137535	9	1.237811	17.09901
	100					
Total	100		1.426273		8.698644	
	Propane conversion		55.63133			
	Aromatic sum		70.90535		5.387125	74.41728
	Total converted products		95.4607		7.239078	
	aromatics selectivity		74.277			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.879912	16.043	0.11718	1	0.11718	1.618709
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.177717	42.081	0.051751	3	0.155252	2.144635
neo-pentane	0.361754	72.151	0.005014	5	0.025069	0.346304
n-pentane	0.503741	72.151	0.006982	5	0.034909	0.482227
Propane	7.994734	44.097	0.181299	6	1.087793	0
iso butane	0.181831	58.124	0.003128	6	0.01877	0.259287
n-Butane	1.228342	58.124	0.021133	7	0.147932	2.043518
i-Pentane	0.020766	72.151	0.000288	3	0.000863	0.011928
hexane	0.560015	86.178	0.006498	4	0.025993	0.35907
cyclohexane	0	84.162	0	4	0	0
n-heptane	9.55116	100.205	0.095316	5	0.476581	6.583449
Benzene	31.20401	78.114	0.399468	6	2.396805	33.10926
Toluene	8.095375	92.141	0.087859	7	0.61501	8.495693
EB	8.059138	106.168	0.075909	8	0.607274	8.388836
m-Xylene	0.16943	106.168	0.001596	8	0.012767	0.176362
P-xylene	6.579399	106.168	0.061972	8	0.495773	6.848561
O-Xylene	2.178848	106.168	0.020523	8	0.164181	2.267985
C9+	21.27703	120.19	0.177028	9	1.593254	22.00908
	100					
Total	100		1.312942		7.975407	
	Propane conversion		66.47442			
	Aromatic sum		56.2862		4.29181	62.31201
	Total converted products		94.02847		6.887614	
	aromatics selectivity		59.86081			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.035225	16.043	0.126861	1	0.126861	1.752441
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.603033	42.081	0.061858	3	0.185573	2.56349
neo-pentane	0.375004	72.151	0.005197	5	0.025987	0.358988
n-pentane	0.570204	72.151	0.007903	5	0.039515	0.545852
Propane	8.531239	44.097	0.193465	6	1.160792	0
iso butane	0.241621	58.124	0.004157	6	0.024942	0.344546
n-Butane	1.30897	58.124	0.02252	7	0.157642	2.177655
i-Pentane	0.022196	72.151	0.000308	3	0.000923	0.012749
hexane	0.035261	86.178	0.000409	4	0.001637	0.022609
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.090959	100.205	0.000908	5	0.004539	0.062696
Benzene	9.949742	78.114	0.127375	6	0.764248	10.55725
Toluene	28.57602	92.141	0.310134	7	2.170935	29.98911
EB	8.707391	106.168	0.082015	8	0.656122	9.063608
m-Xylene	8.210332	106.168	0.077333	8	0.618667	8.546215
P-xylene	0.166253	106.168	0.001566	8	0.012528	0.173054
O-Xylene	7.06028	106.168	0.066501	8	0.532008	7.349114
C9+	21.51627	120.19	0.179019	9	1.611169	22.25656
	100					
Total	100		1.267528		8.094086	
	Propane conversion		65.28008			
	Aromatic sum		62.67002		4.754507	68.57501
	Total converted products		91.46876		6.933295	
	aromatics selectivity		68.51521			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.316425	16.043	0.144389	1	0.144389	1.994571
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.371242	42.081	0.056349	3	0.169048	2.33522
neo-pentane	0.386526	72.151	0.005357	5	0.026786	0.370018
n-pentane	0.57144	72.151	0.00792	5	0.0396	0.547035
Propane	8.860604	44.097	0.200934	6	1.205606	0
iso butane	0.273784	58.124	0.00471	6	0.028262	0.39041
n-Butane	1.280628	58.124	0.022033	7	0.154229	2.130504
i-Pentane	0.019767	72.151	0.000274	3	0.000822	0.011353
hexane	0.025294	86.178	0.000294	4	0.001174	0.016218
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.088181	100.205	0.00088	5	0.0044	0.060782
Benzene	9.505996	78.114	0.121694	6	0.730163	10.08641
Toluene	27.40925	92.141	0.297471	7	2.082295	28.76464
EB	8.2137	106.168	0.077365	8	0.618921	8.549721
m-Xylene	9.105956	106.168	0.085769	8	0.686154	9.478479
P-xylene	0.156659	106.168	0.001476	8	0.011805	0.163068
O-Xylene	6.993492	106.168	0.065872	8	0.526976	7.279595
C9+	22.42106	120.19	0.186547	9	1.678921	23.19247
	100					
Total	100		1.279333		8.109551	
	Propane conversion		62.94383			
	Aromatic sum		61.38505		4.656314	67.44425
	Total converted products		91.1394		6.903945	
	aromatics selectivity		67.35293			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.021544	16.043	0.126008	1	0.126008	1.740661
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.351294	42.081	0.055875	3	0.167626	2.315575
neo-pentane	0.363828	72.151	0.005043	5	0.025213	0.348289
n-pentane	0.574696	72.151	0.007965	5	0.039826	0.550152
Propane	7.815317	44.097	0.17723	6	1.063381	0
iso butane	0.185893	58.124	0.003198	6	0.019189	0.26508
n-Butane	1.140632	58.124	0.019624	7	0.137369	1.8976
i-Pentane	0.026576	72.151	0.000368	3	0.001105	0.015264
hexane	0.069272	86.178	0.000804	4	0.003215	0.044416
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.04981	100.205	0.000497	5	0.002485	0.034333
Benzene	8.639931	78.114	0.110607	6	0.66364	9.167468
Toluene	27.28137	92.141	0.296083	7	2.07258	28.63044
EB	8.118794	106.168	0.076471	8	0.61177	8.450932
m-Xylene	9.673332	106.168	0.091113	8	0.728908	10.06907
P-xylene	0.161537	106.168	0.001522	8	0.012172	0.168146
O-Xylene	7.385072	106.168	0.06956	8	0.556482	7.687193
C9+	24.1411	120.19	0.200858	9	1.807721	24.9717
	100					
Total	100		1.242827		8.038689	
	Propane conversion		71.52358			
	Aromatic sum		61.26004		4.645551	66.59994
	Total converted products		92.18468		6.975309	
	aromatics selectivity		66.4536			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 6					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.760943	16.043	0.109764	1	0.109764	1.51627
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.352188	42.081	0.055897	3	0.16769	2.316455
neo-pentane	0.321781	72.151	0.00446	5	0.022299	0.308038
n-pentane	0.532407	72.151	0.007379	5	0.036895	0.509669
Propane	7.561379	44.097	0.171472	6	1.028829	0
iso butane	0.228371	58.124	0.003929	6	0.023574	0.325652
n-Butane	1.09395	58.124	0.018821	7	0.131747	1.819939
i-Pentane	0.02132	72.151	0.000295	3	0.000886	0.012245
hexane	0.019597	86.178	0.000227	4	0.00091	0.012565
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.013393	100.205	0.000134	5	0.000668	0.009231
Benzene	8.174353	78.114	0.104646	6	0.627879	8.673462
Toluene	31.22307	92.141	0.338862	7	2.372033	32.76705
EB	7.370326	106.168	0.069421	8	0.555371	7.671844
m-Xylene	8.894085	106.168	0.083774	8	0.67019	9.25794
P-xylene	0.249621	106.168	0.002351	8	0.018809	0.259833
O-Xylene	6.92238	106.168	0.065202	8	0.521617	7.205573
C9+	23.26084	120.19	0.193534	9	1.741805	24.06115
	100					
Total	100		1.230168		8.030966	
	Propane conversion		69.85333			
	Aromatic sum		62.83383		4.765898	68.06348
	Total converted products		92.43862		7.002137	
	aromatics selectivity		67.97357			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.859556	16.043	0.115911	1	0.115911	1.601181
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.278194	42.081	0.054138	3	0.162415	2.243585
neo-pentane	0.435188	72.151	0.006032	5	0.030158	0.416602
n-pentane	0.560245	72.151	0.007765	5	0.038824	0.536318
Propane	9.015356	44.097	0.204444	6	1.226662	0
iso butane	0.241606	58.124	0.004157	6	0.02494	0.344524
n-Butane	1.315792	58.124	0.022638	7	0.158464	2.189003
i-Pentane	0.022966	72.151	0.000318	3	0.000955	0.013191
hexane	0.030369	86.178	0.000352	4	0.00141	0.019472
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.043069	100.205	0.00043	5	0.002149	0.029687
Benzene	8.868064	78.114	0.113527	6	0.681163	9.40953
Toluene	27.83172	92.141	0.302056	7	2.11439	29.20801
EB	8.149762	106.168	0.076763	8	0.614103	8.483167
m-Xylene	9.985595	106.168	0.094055	8	0.752437	10.3941
P-xylene	0.256973	106.168	0.00242	8	0.019363	0.267486
O-Xylene	7.994514	106.168	0.075301	8	0.602405	8.321568
C9+	21.11103	120.19	0.175647	9	1.580824	21.83737
	100					
Total	100		1.255953		8.126575	
	Propane conversion		67.67958			
	Aromatic sum		63.08663		4.783862	69.33221
	Total converted products		90.98464		6.899912	
	aromatics selectivity		69.33766			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.38871	16.043	0.148894	1	0.148894	2.056812
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.25892	42.081	0.05368	3	0.161041	2.224605
neo-pentane	0.374726	72.151	0.005194	5	0.025968	0.358722
n-pentane	0.585598	72.151	0.008116	5	0.040581	0.560588
Propane	7.238166	44.097	0.164142	6	0.984852	0
iso butane	0.263367	58.124	0.004531	6	0.027187	0.375555
n-Butane	1.29616	58.124	0.0223	7	0.156099	2.156344
i-Pentane	0.023835	72.151	0.00033	3	0.000991	0.01369
hexane	0.026991	86.178	0.000313	4	0.001253	0.017306
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.029657	100.205	0.000296	5	0.00148	0.020442
Benzene	7.895496	78.114	0.101077	6	0.606459	8.377579
Toluene	25.94623	92.141	0.281593	7	1.971149	27.22928
EB	7.578456	106.168	0.071382	8	0.571054	7.888489
m-Xylene	9.724253	106.168	0.091593	8	0.732745	10.12207
P-xylene	0.262696	106.168	0.002474	8	0.019795	0.273443
O-Xylene	7.455957	106.168	0.070228	8	0.561823	7.760979
C9+	26.65078	120.19	0.221739	9	1.995649	27.56772
	100					
Total	100		1.247882		8.007019	
	Propane conversion		74.99717			
	Aromatic sum		58.86309		4.463025	63.55622
	Total converted products		92.76183		7.022168	
	aromatics selectivity		63.45615			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 9					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.937107	16.043	0.120745	1	0.120745	1.667957
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.414707	42.081	0.057382	3	0.172147	2.378025
neo-pentane	0.379316	72.151	0.005257	5	0.026286	0.363116
n-pentane	0.474803	72.151	0.006581	5	0.032903	0.454525
Propane	6.672533	44.097	0.151315	6	0.907889	0
iso butane	0.229863	58.124	0.003955	6	0.023728	0.327779
n-Butane	1.251065	58.124	0.021524	7	0.150668	2.081321
i-Pentane	0.019008	72.151	0.000263	3	0.00079	0.010918
hexane	0.023403	86.178	0.000272	4	0.001086	0.015006
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.024988	100.205	0.000249	5	0.001247	0.017223
Benzene	8.609973	78.114	0.110223	6	0.661339	9.135681
Toluene	28.29415	92.141	0.307075	7	2.149522	29.69331
EB	8.264244	106.168	0.077841	8	0.62273	8.602332
m-Xylene	10.60422	106.168	0.099881	8	0.799052	11.03803
P-xylene	0.286468	106.168	0.002698	8	0.021586	0.298188
O-Xylene	8.13066	106.168	0.076583	8	0.612664	8.463284
C9+	22.38349	120.19	0.186234	9	1.676108	23.15361
	100					
Total	100		1.228079		7.980491	
	Propane conversion		72.561			
	Aromatic sum		64.18972		4.866892	68.81332
	Total converted products		93.32747		7.072601	
	aromatics selectivity		68.77902			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 10					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.004085	16.043	0.12492	1	0.12492	1.725629
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.219568	42.081	0.052745	3	0.158235	2.18585
neo-pentane	0.378871	72.151	0.005251	5	0.026255	0.36269
n-pentane	0.494665	72.151	0.006856	5	0.03428	0.473539
Propane	8.863569	44.097	0.201002	6	1.20601	0
iso butane	0.21632	58.124	0.003722	6	0.02233	0.308467
n-Butane	1.213476	58.124	0.020877	7	0.146142	2.018788
i-Pentane	0.018277	72.151	0.000253	3	0.00076	0.010498
hexane	0.010558	86.178	0.000123	4	0.00049	0.00677
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.014515	100.205	0.000145	5	0.000724	0.010005
Benzene	7.828283	78.114	0.100216	6	0.601297	8.306262
Toluene	25.99147	92.141	0.282084	7	1.974585	27.27675
EB	7.5661	106.168	0.071265	8	0.570123	7.875628
m-Xylene	9.958184	106.168	0.093796	8	0.750372	10.36557
P-xylene	0.235021	106.168	0.002214	8	0.017709	0.244636
O-Xylene	7.86652	106.168	0.074095	8	0.59276	8.188337
C9+	25.12052	120.19	0.209007	9	1.881061	25.98481
	100					
Total	100		1.24857		8.108053	
	Propane conversion		67.34683			
	Aromatic sum		59.44558		4.506846	65.29728
	Total converted products		91.13643		6.902043	
	aromatics selectivity		65.22702			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 11					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.803957	16.043	0.112445	1	0.112445	1.553307
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.469189	42.081	0.058677	3	0.176031	2.431679
neo-pentane	0.294119	72.151	0.004076	5	0.020382	0.281558
n-pentane	0.528154	72.151	0.00732	5	0.036601	0.505598
Propane	7.608784	44.097	0.172547	6	1.035279	0
iso butane	0.244476	58.124	0.004206	6	0.025237	0.348617
n-Butane	1.282977	58.124	0.022073	7	0.154512	2.134412
i-Pentane	0.020455	72.151	0.000284	3	0.000851	0.011749
hexane	0.018747	86.178	0.000218	4	0.00087	0.01202
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.014738	100.205	0.000147	5	0.000735	0.010159
Benzene	8.619066	78.114	0.11034	6	0.662037	9.145329
Toluene	28.34204	92.141	0.307594	7	2.15316	29.74356
EB	7.87752	106.168	0.074199	8	0.593589	8.199788
m-Xylene	10.09404	106.168	0.095076	8	0.760609	10.50699
P-xylene	0.282924	106.168	0.002665	8	0.021319	0.294498
O-Xylene	7.669176	106.168	0.072236	8	0.57789	7.98292
C9+	22.8296	120.19	0.189946	9	1.709513	23.61507
	99.99999					
Total	99.99999		1.234048		8.04106	
	Propane conversion		70.30367			
	Aromatic sum		62.88477		4.768604	68.0667
	Total converted products		92.39118		7.005781	
	aromatics selectivity		68.06361			

		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
input paramters						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 12					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.803957	16.043	0.112445	1	0.112445	1.553307
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.469189	42.081	0.058677	3	0.176031	2.431679
neo-pentane	0.294119	72.151	0.004076	5	0.020382	0.281558
n-pentane	0.528154	72.151	0.00732	5	0.036601	0.505598
Propane	7.608784	44.097	0.172547	6	1.035279	0
iso butane	0.244476	58.124	0.004206	6	0.025237	0.348617
n-Butane	1.282977	58.124	0.022073	7	0.154512	2.134412
i-Pentane	0.020455	72.151	0.000284	3	0.000851	0.011749
hexane	0.018747	86.178	0.000218	4	0.00087	0.01202
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.014738	100.205	0.000147	5	0.000735	0.010159
Benzene	8.619066	78.114	0.11034	6	0.662037	9.145329
Toluene	28.34204	92.141	0.307594	7	2.15316	29.74356
EB	7.87752	106.168	0.074199	8	0.593589	8.199788
m-Xylene	10.09404	106.168	0.095076	8	0.760609	10.50699
P-xylene	0.282924	106.168	0.002665	8	0.021319	0.294498
O-Xylene	7.669176	106.168	0.072236	8	0.57789	7.98292
C9+	22.8296	120.19	0.189946	9	1.709513	23.61507
	99.99999					
Total	99.99999		1.234048		8.04106	
	Propane conversion		66.83			
	Aromatic sum		62.88477		4.768604	68.0667
	Total converted products		92.39118		7.005781	
	aromatics selectivity		68.06361			

Table A7: Zn-Fe/ZSM-5 (2 wt. % each)

Run 1-12

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.874548	42.081	0.044546	3	0.133639	1.880865
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	5.75182	44.097	0.130436	6	0.782614	0
iso butane	0.295195	58.124	0.005079	6	0.030472	0.428874
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.483669	100.205	0.014806	5	0.074032	1.041942
Benzene	15.24227	78.114	0.195129	6	1.170771	16.47776
Toluene	29.58056	92.141	0.321036	7	2.247251	31.62842
EB	0.451852	106.168	0.004256	8	0.034048	0.479202
m-Xylene	17.80072	106.168	0.167666	8	1.341324	18.87816
P-xylene	1.255758	106.168	0.011828	8	0.094624	1.331767
O-Xylene	26.21955	106.168	0.246963	8	1.975703	27.80658
C9+	0.044055	120.19	0.000367	9	0.003299	0.04643
Total	100					
Total	100		1.14211		7.887777	
	Propane conversion		43.55567			
	Aromatic sum		90.55071		6.863722	96.60189
	Total converted products		94.24818		7.105163	
	aromatics selectivity		96.07688			

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.817041	42.081	0.066943	3	0.20083	2.788952
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	5.089423	44.097	0.115414	6	0.692486	0
iso butane	0.171771	58.124	0.002955	6	0.017731	0.246239
n-Butane	0.443955	58.124	0.007638	7	0.053466	0.742496
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0.044746	84.162	0.000532	4	0.002127	0.029533
n-heptane	0.065143	100.205	0.00065	5	0.00325	0.04514
Benzene	14.39804	78.114	0.184321	6	1.105925	15.35813
Toluene	29.51781	92.141	0.320355	7	2.242484	31.14167
EB	2.865616	106.168	0.026991	8	0.215931	2.998659
m-Xylene	21.67033	106.168	0.204114	8	1.632909	22.67642
P-xylene	1.001888	106.168	0.009437	8	0.075495	1.048402
O-Xylene	20.78296	106.168	0.195755	8	1.566043	21.74785
C9+	1.131376	120.19	0.009413	9	0.084719	1.176505
	100.0001					
Total	100.0001		1.144519		7.893395	
	Propane conversion		55.02767			Selectivity
	Aromatic sum		90.23664		6.838786	94.97114
	Total converted products		94.91067		7.20091	
	aromatics selectivity		95.07534			

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	3.166958	16.043	0.197404	1	0.197404	2.841049
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	3.798057	42.081	0.090256	3	0.270768	3.896896
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	7.28886	44.097	0.165292	6	0.991749	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.816504	58.124	0.014048	7	0.098333	1.415216
i-Pentane	0	72.151	0	3	0	0
hexane	1.463068	86.178	0.016977	4	0.067909	0.97735
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.029204	100.205	0.000291	5	0.001457	0.020972
Benzene	12.07295	78.114	0.154556	6	0.927333	13.34621
Toluene	22.63639	92.141	0.245671	7	1.719699	24.74996
EB	1.952027	106.168	0.018386	8	0.14709	2.116919
m-Xylene	16.53772	106.168	0.155769	8	1.246155	17.9347
P-xylene	0.851943	106.168	0.008024	8	0.064196	0.923908
O-Xylene	15.83719	106.168	0.149171	8	1.193368	17.17499
C9+	13.54913	120.19	0.112731	9	1.014578	14.60184
	100					
Total	100		1.328577		7.940039	
	Propane conversion		52.40467			
	Aromatic sum		69.88822		5.29784	76.24667
	Total converted products		92.71114		6.94829	
	aromatics selectivity		75.38276			

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	1.72587	30.07	0.057395	2	0.11479	1.609497
propene	0	42.081	0	3	0	0
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	5.56435	44.097	0.126184	6	0.757106	0
iso butane	0.299732	58.124	0.005157	6	0.030941	0.433825
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.077606	100.205	0.000774	5	0.003872	0.054295
Benzene	9.232047	78.114	0.118187	6	0.709121	9.942733
Toluene	19.61896	92.141	0.212923	7	1.490462	20.89808
EB	0.419992	106.168	0.003956	8	0.031647	0.443734
m-Xylene	30.8897	106.168	0.290951	8	2.327609	32.63589
P-xylene	15.98194	106.168	0.150534	8	1.204276	16.8854
O-Xylene	14.90776	106.168	0.140417	8	1.123333	15.75049
C9+	1.282052	120.19	0.010667	9	0.096002	1.346063
	100					
Total	100		1.117146		7.889159	
	Propane conversion		55.27525			
	Aromatic sum		91.05039		6.886449	96.55632
	Total converted products		94.43565		7.132054	
	aromatics selectivity		96.41527			

Run 5

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.966082	42.081	0.070485	3	0.211455	3.033789
neo-pentane	0.054781	72.151	0.000759	5	0.003796	0.054466
n-pentane	0	72.151	0	5	0	0
Propane	7.724008	44.097	0.175159	6	1.050957	0
iso butane	0.324735	58.124	0.005587	6	0.033522	0.480942
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.110608	100.205	0.001104	5	0.005519	0.079184
Benzene	10.77491	78.114	0.137938	6	0.82763	11.87417
Toluene	23.51309	92.141	0.255186	7	1.786302	25.62842
EB	0.380838	106.168	0.003587	8	0.028697	0.411721
m-Xylene	21.39265	106.168	0.201498	8	1.611985	23.12747
P-xylene	0.639861	106.168	0.006027	8	0.048215	0.691749
O-Xylene	16.58184	106.168	0.156185	8	1.249479	17.92652
C9+	15.5366	120.19	0.129267	9	1.163403	16.69157
	100					
Total	100		1.142783		8.020959	
	Propane conversion		59.27517			
	Aromatic sum		73.28319		5.552307	79.66005
	Total converted products		92.27599		6.970002	
	aromatics selectivity		79.41739			

	Run 6					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 6					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	3.205545	42.081	0.076176	3	0.228527	3.296505
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	8.463691	44.097	0.191933	6	1.151601	0
iso butane	0.192274	58.124	0.003308	6	0.019848	0.286308
n-Butane	0.449044	58.124	0.007726	7	0.054079	0.780096
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.09668	100.205	0.000965	5	0.004824	0.069588
Benzene	10.79696	78.114	0.138221	6	0.829323	11.96301
Toluene	23.98766	92.141	0.260336	7	1.822355	26.28753
EB	0.396191	106.168	0.003732	8	0.029854	0.430643
m-Xylene	22.65294	106.168	0.213369	8	1.706951	24.62281
P-xylene	0.635084	106.168	0.005982	8	0.047855	0.690311
O-Xylene	16.85691	106.168	0.158776	8	1.270207	18.32277
C9+	12.26701	120.19	0.102063	9	0.918571	13.25042
	100					
Total	100		1.162586		8.083996	
	Propane conversion		56.89092			
	Aromatic sum		75.32576		5.706545	82.31708
	Total converted products		91.53631		6.932395	
	aromatics selectivity		82.29058			

	Run 7					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	3.330828	42.081	0.079153	3	0.237458	3.462068
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	9.346839	44.097	0.211961	6	1.271765	0
iso butane	0.403407	58.124	0.00694	6	0.041643	0.607138
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0.001703	86.178	1.98E-05	4	7.9E-05	0.001152
cyclohexane	0.139849	84.162	0.001662	4	0.006647	0.096906
n-heptane	0.03605	100.205	0.00036	5	0.001799	0.026226
Benzene	19.93254	78.114	0.255172	6	1.531035	22.32201
Toluene	21.72837	92.141	0.235816	7	1.650715	24.06691
EB	3.234895	106.168	0.03047	8	0.243757	3.553896
m-Xylene	16.21984	106.168	0.152775	8	1.222202	17.81932
P-xylene	0.650474	106.168	0.006127	8	0.049015	0.714619
O-Xylene	9.195315	106.168	0.086611	8	0.692888	10.10209
C9+	15.77989	120.19	0.131291	9	1.181621	17.22767
	100					
Total	100		1.198358		8.130623	
	Propane conversion		61.51117			
	Aromatic sum		70.96143		5.389611	78.57884
	Total converted products		90.65316		6.858858	
	aromatics selectivity		78.27794			

Run 8

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	

Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	4.046724	42.081	0.096165	3	0.288495	4.249239
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	10.41812	44.097	0.236255	6	1.417527	0
iso butane	0.246093	58.124	0.004234	6	0.025404	0.374168
n-Butane	0.438594	58.124	0.007546	7	0.052821	0.777996
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.347876	100.205	0.003472	5	0.017358	0.255669
Benzene	9.114926	78.114	0.116687	6	0.700125	10.31212
Toluene	20.41109	92.141	0.22152	7	1.550641	22.83934
EB	0.506397	106.168	0.00477	8	0.038158	0.562031
m-Xylene	19.07283	106.168	0.179648	8	1.437181	21.16819
P-xylene	2.038702	106.168	0.019203	8	0.153621	2.262677
O-Xylene	11.30647	106.168	0.106496	8	0.851968	12.54861
C9+	22.3496	120.19	0.185952	9	1.67357	24.64996
	100.2974					
Total	100.2974		1.181947		8.206869	
	Propane conversion		61.96283			
	Aromatic sum		62.45041		4.731694	69.69297
	Total converted products		89.87929		6.789342	
	aromatics selectivity		69.48253			

Run 9

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	

Output parameters	Catalyst Run 9					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	4.483002	42.081	0.106533	3	0.319598	4.729282
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	10.54359	44.097	0.2391	6	1.4346	0
iso butane	0.198167	58.124	0.003409	6	0.020456	0.302704
n-Butane	0.328341	58.124	0.005649	7	0.039543	0.585138
i-Pentane		72.151	0	3	0	0
hexane		86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.070445	100.205	0.000703	5	0.003515	0.052015
Benzene	9.270468	78.114	0.118679	6	0.712072	10.53695
Toluene	20.81686	92.141	0.225924	7	1.581468	23.40192
EB	0.329742	106.168	0.003106	8	0.024847	0.367672
m-Xylene	20.78525	106.168	0.195777	8	1.566216	23.17622
P-xylene	0.41827	106.168	0.00394	8	0.031518	0.466385
O-Xylene	12.35676	106.168	0.116389	8	0.93111	13.77819
C9+	20.3991	120.19	0.169724	9	1.527514	22.60352
	100					
Total	100		1.188932		8.192456	
	Propane conversion		62.357			
	Aromatic sum		63.97736		4.847231	71.72734
	Total converted products		89.45641		6.757857	
	aromatics selectivity		71.51791			

Run 10

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 10					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	7.36336	42.081	0.174981	3	0.524942	7.892201
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	11.68875	44.097	0.265069	6	1.590414	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.22665	58.124	0.003899	7	0.027296	0.410379
i-Pentane	0	72.151	0	3	0	0
hexane		86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.055215	100.205	0.000551	5	0.002755	0.041421
Benzene	9.109497	78.114	0.116618	6	0.699708	10.51971
Toluene	19.78362	92.141	0.21471	7	1.502972	22.59632
EB	0.264981	106.168	0.002496	8	0.019967	0.300192
m-Xylene	17.6392	106.168	0.166144	8	1.329154	19.98307
P-xylene	0.344254	106.168	0.003243	8	0.02594	0.389998
O-Xylene	17.6392	106.168	0.166144	8	1.329154	19.98307
C9+	15.88528	120.19	0.132168	9	1.189513	17.88364
	100					
Total	100		1.246023		8.241814	
	Propane conversion		64.59167			
	Aromatic sum		64.78075		4.906894	73.77236
	Total converted products		88.31125		6.6514	
	aromatics selectivity		73.35503			

Run 11

Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 11					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	5.390226	42.081	0.128092	3	0.384275	5.88773
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	13.39	44.097	0.303649	6	1.821892	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.220726	58.124	0.003797	7	0.026582	0.407288
i-Pentane	0	72.151	0	3	0	0
hexane		86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.081973	100.205	0.000818	5	0.00409	0.062669
Benzene	9.020012	78.114	0.115472	6	0.692834	10.61537
Toluene	19.73349	92.141	0.214166	7	1.499164	22.96967
EB	0.295091	106.168	0.002779	8	0.022236	0.340689
m-Xylene	18.14575	106.168	0.170915	8	1.367323	20.94966
P-xylene	0.335808	106.168	0.003163	8	0.025304	0.387697
O-Xylene	10.27698	106.168	0.096799	8	0.774394	11.865
C9+	23.10995	120.19	0.192278	9	1.730506	26.51422
	100					
Total	100		1.23193		8.348601	
	Propane conversion		62.5605			
	Aromatic sum		57.80713		4.381255	67.12809
	Total converted products		86.61		6.526709	
	aromatics selectivity		66.74417			

	Run 12					
Propane	33.09		44.097	0.75039100	3	2.251174
Nitrogen	66.91		28.014	2.38840000	0	0
Total	100			3.138791000		2.251174
Output parameters	Catalyst Run 12					
Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane		0	16.043	0	1	0	0
ethylene		0	28.05	0	2	0	0
ethane		0	30.07	0	2	0	0
propene		5.837994	42.081	0.138732	3	0.416197	6.364274
neo-pentane		0	72.151	0	5	0	0
n-pentane		0	72.151	0	5	0	0
Propane		13.37274	44.097	0.303257	6	1.819544	0
iso butane		0.18363	58.124	0.003159	6	0.018956	0.28986
n-Butane		0.32634	58.124	0.005615	7	0.039302	0.600985
i-Pentane		0	72.151	0	3	0	0
hexane			86.178	0	4	0	0
cyclohexane		0	84.162	0	4	0	0
n-heptane		0.099507	100.205	0.000993	5	0.004965	0.075925
Benzene		9.741844	78.114	0.124713	6	0.748279	11.44231
Toluene		21.23471	92.141	0.230459	7	1.613212	24.66843
EB		0.345041	106.168	0.00325	8	0.026	0.397573
m-Xylene		18.78531	106.168	0.17694	8	1.415516	21.64536
P-xylene		0.379896	106.168	0.003578	8	0.028626	0.437734
O-Xylene		10.78074	106.168	0.101544	8	0.812353	12.4221
C9+		18.91224	120.19	0.157353	9	1.416176	21.65545
	100					
Total	100			1.249593		8.359126	
	Propane conversion			66.93767			
	Aromatic sum			61.26755		4.643986	71.01351
	Total converted products			86.62726		6.539581	
	aromatics selectivity			70.72548			

Table A8: Zn-Co/ZSM-5 (2 wt. % each) Run 1

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.793631	42.081	0.04262329	3	0.12787	3.413934
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	50.43492	44.097	1.14372669	6	6.86236	
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	5.720333	78.114	0.07323057	6	0.439383	11.73088
Toluene	17.21335	92.141	0.18681529	7	1.307707	34.91382
EB	3.463869	106.168	0.0326263	8	0.26101	6.968588
m-Xylene	18.69669	106.168	0.17610477	8	1.408838	37.61387
P-xylene	0.148321	106.168	0.00139704	8	0.011176	0.298392
O-Xylene	0.373994	106.168	0.00352266	8	0.028181	0.752398
C9+	2.154898	120.19	0.0179291	9	0.161362	4.30812
	100					
Total	100		1.67797571		10.60789	
	Propane conversion		35.434330			
	Aromatic sum		45.6165554		3.456297	92.27795

Total converted products	49.5650844	3.745528	
aromatics selectivity	92.0336483		

Run 2

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 2						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	1.828588	28.05	0.06519	2	0.130381	3.222119
ethane	0	30.07	0	2	0	0
propene	0	42.081	0	3	0	0
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	46.46335	44.097	1.053662	6	6.321975	
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	6.32724	78.114	0.081	6	0.486	12.01061
Toluene	19.08632	92.141	0.207143	7	1.449998	35.83405
EB	0.638571	106.168	0.006015	8	0.048118	1.189143
m-Xylene	22.34657	106.168	0.210483	8	1.683865	41.61365
P-xylene	0.155943	106.168	0.001469	8	0.011751	0.290397
O-Xylene	0.383059	106.168	0.003608	8	0.028864	0.71333
C9+	2.770353	120.19	0.02305	9	0.207448	5.1267
Total	100					
Total	100		1.65162		10.3684	
	Propane conversion		35.36692			
	Aromatic sum		48.93771		3.708596	91.65118
	Total converted products		53.53665		4.046425	
	aromatics selectivity		91.40973			

Run 3

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 3						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	2.087179	28.05	0.074409	2	0.148818	4.196895
ethane	0	30.07	0	2	0	0
propene	0	42.081	0	3	0	0
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	53.12137	44.097	1.204648	6	7.227889	0
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	7.339952	78.114	0.093965	6	0.563788	15.89963
Toluene	21.02773	92.141	0.228213	7	1.597488	45.05146
EB	0.162231	106.168	0.001528	8	0.012224	0.344747
m-Xylene	11.1314	106.168	0.104847	8	0.838776	23.6547
P-xylene	0.168996	106.168	0.001592	8	0.012734	0.359123
O-Xylene	1.257591	106.168	0.011845	8	0.094762	2.672435
C9+	3.703546	120.19	0.030814	9	0.277327	7.821017
Total	100					
Total	100		1.751861		10.77381	
	Propane conversion		34.57325			
	Aromatic sum		41.0879		3.119773	87.98209

Total converted products		46.87863		3.545918
aromatics selectivity		87.64741		

Run 4

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 4						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	2.087179	28.05	0.074409	2	0.148818	4.196895
ethane	0	30.07	0	2	0	0
propene	0	42.081	0	3	0	0
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	53.12137	44.097	1.204648	6	7.227889	0
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	7.339952	78.114	0.093965	6	0.563788	15.89963
Toluene	21.02773	92.141	0.228213	7	1.597488	45.05146
EB	0.162231	106.168	0.001528	8	0.012224	0.344747
m-Xylene	11.1314	106.168	0.104847	8	0.838776	23.6547
P-xylene	0.168996	106.168	0.001592	8	0.012734	0.359123
O-Xylene	1.257591	106.168	0.011845	8	0.094762	2.672435
C9+	3.703546	120.19	0.030814	9	0.277327	7.821017
Total	100					
Total	100		1.751861		10.77381	
	Propane conversion		41.41117			
	Aromatic sum		41.0879		3.119773	87.98209
	Total converted products		46.87863		3.545918	
	aromatics selectivity		87.64741			

Run 5

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 5						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.911388	42.081	0.069185	3	0.207556	8.272806
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	66.69899	44.097	1.512552	6	9.07531	0
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	4.452863	78.114	0.057005	6	0.342028	13.63262
Toluene	11.01316	92.141	0.119525	7	0.836675	33.34837
EB	0	106.168	0	8	0	0
m-Xylene	8.1231	106.168	0.076512	8	0.612094	24.39696
P-xylene	0	106.168	0	8	0	0
O-Xylene	2.782332	106.168	0.026207	8	0.209655	8.356471
C9+	4.018167	120.19	0.033432	9	0.300886	11.99278
Total	100					
Total	100		1.894417		11.5842	
	Propane conversion		41.23817			
	Aromatic sum		26.37145		2.000453	79.73442

Total converted products		33.30101		2.508895	
aromatics selectivity		79.19116			

Run 6

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 6						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 6					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	3.035576	42.081	0.072136	3	0.216409	9.141336
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	68.56395	44.097	1.554844	6	9.329064	0
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	4.315139	78.114	0.055242	6	0.331449	14.00073
Toluene	10.34743	92.141	0.1123	7	0.786099	33.20556
EB	0	106.168	0	8	0	0
m-Xylene	7.440511	106.168	0.070082	8	0.560659	23.68277
P-xylene	0	106.168	0	8	0	0
O-Xylene	2.542236	106.168	0.023945	8	0.191563	8.091809
C9+	3.755158	120.19	0.031244	9	0.281192	11.87779
Total	100					
Total	100		1.919793		11.69644	
	Propane conversion		33.51367			
	Aromatic sum		24.64531		1.869771	78.98087
	Total converted products		31.43605		2.367373	
	aromatics selectivity		78.39826			

Run 7

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 7						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	2.466387	28.05	0.087928	2	0.175856	6.25541
ethane	0	30.07	0	2	0	0
propene	0	42.081	0	3	0	0
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	62.7727	44.097	1.423514	6	8.541085	0
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	5.535325	78.114	0.070862	6	0.425173	15.12387
Toluene	15.85778	92.141	0.172103	7	1.204724	42.85336
EB	0.122344	106.168	0.001152	8	0.009219	0.327926
m-Xylene	8.394592	106.168	0.079069	8	0.632552	22.50056
P-xylene	0.127446	106.168	0.0012	8	0.009603	0.341601
O-Xylene	0.948395	106.168	0.008933	8	0.071464	2.542045
C9+	3.77503	120.19	0.031409	9	0.28268	10.05523
Total	100					
Total	100		1.876171		11.35235	
	Propane conversion		36.83783			
	Aromatic sum		30.98588		2.352734	83.68936

	Total converted products	37.2273		2.81127	
	aromatics selectivity	83.2343			

Run 8

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 8						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0.885006	28.05	0.031551	2	0.063102	2.130957
ethane	0	30.07	0	2	0	0
propene	1.277408	42.081	0.030356	3	0.091068	3.075363
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	60.857	44.097	1.380071	6	8.280427	
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	6.814574	78.114	0.087239	6	0.523433	17.67635
Toluene	18.54791	92.141	0.201299	7	1.409094	47.58518
EB	0.158165	106.168	0.00149	8	0.011918	0.402476
m-Xylene	7.835148	106.168	0.0738	8	0.590396	19.9377
P-xylene	0.15438	106.168	0.001454	8	0.011633	0.392842
O-Xylene	1.466676	106.168	0.013815	8	0.110517	3.732176
C9+	2.003737	120.19	0.016671	9	0.150043	5.066948
Total	100					
Total	100		1.837746		11.24163	
	Propane conversion		34.14992			
	Aromatic sum		34.97685		2.656992	89.72673
	Total converted products		39.143		2.961204	
	aromatics selectivity		89.35659			

Run 9

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
Run 9						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 9					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.370269	42.081	0.056326	3	0.168979	5.765191
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	61.23044	44.097	1.38854	6	8.331239	0
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	6.695481	78.114	0.085714	6	0.514285	17.54628
Toluene	17.52796	92.141	0.19023	7	1.331608	45.43151
EB	0	106.168	0	8	0	0
m-Xylene	8.106512	106.168	0.076356	8	0.610844	20.84065
P-xylene	0	106.168	0	8	0	0
O-Xylene	1.248803	106.168	0.011763	8	0.0941	3.210489
C9+	2.82054	120.19	0.023467	9	0.211206	7.205884
Total	100					
Total	100		1.832395		11.26226	
	Propane conversion		34.81825			
	Aromatic sum		33.57875		2.550838	87.02892

	Total converted products			38.76956		2.931023
	aromatics selectivity			86.61112		

Run 10

input paramters			Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	Run 10						
Propane	33.09		44.097	0.75039100	3	2.251174	
Nitrogen	66.91		28.014	2.38840000	0	0	
Total	100			3.138791000		2.251174	
Output parameters	Catalyst Run 10						
Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0		16.043	0	1	0	0
ethylene	0		28.05	0	2	0	0
ethane	0		30.07	0	2	0	0
propene	2.424787		42.081	0.057622	3	0.172866	6.38886
neo-pentane	0		72.151	0	5	0	0
n-pentane	0		72.151	0	5	0	0
Propane	64.2128		44.097	1.456172	6	8.737029	0
iso butane	0		58.124	0	6	0	0
n-Butane	0		58.124	0	7	0	0
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane	0		100.205	0	5	0	0
Benzene		6.51052	78.114	0.083346	6	0.500078	18.48215
Toluene		18.15574	92.141	0.197043	7	1.379301	50.97691
EB		0.143949	106.168	0.001356	8	0.010847	0.400886
m-Xylene		3.383771	106.168	0.031872	8	0.254975	9.423492
P-xylene		0.143057	106.168	0.001347	8	0.01078	0.398402
O-Xylene		1.237224	106.168	0.011653	8	0.093228	3.445554
C9+		3.788156	120.19	0.031518	9	0.283663	10.48375
Total	100						
Total	100			1.87193		11.44277	
	Propane conversion			26.96633			
	Aromatic sum			29.57426		2.249208	83.12739
	Total converted products			35.7872		2.705737	
	aromatics selectivity			82.6392			

Run 11

input paramters			Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	Run 11						
Propane	33.09		44.097	0.75039100	3	2.251174	
Nitrogen	66.91		28.014	2.38840000	0	0	
Total	100			3.138791000		2.251174	
Output parameters	Catalyst Run 11						
Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0		16.043	0	1	0	0
ethylene	2.269858		28.05	0.080922	2	0.161844	5.626444
ethane	0		30.07	0	2	0	0
propene	0		42.081	0	3	0	0
neo-pentane	0		72.151	0	5	0	0
n-pentane	0		72.151	0	5	0	0
Propane	61.93447		44.097	1.404505	6	8.427032	0
iso butane	0		58.124	0	6	0	0
n-Butane	0		58.124	0	7	0	0
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane	0		100.205	0	5	0	0
Benzene		6.308661	78.114	0.080762	6	0.484573	16.84603
Toluene		16.76318	92.141	0.18193	7	1.273507	44.27306
EB		0	106.168	0	8	0	0
m-Xylene		3.858412	106.168	0.036343	8	0.29074	10.10748
P-xylene		0	106.168	0	8	0	0
O-Xylene		4.170117	106.168	0.039278	8	0.314228	10.92402
C9+		4.695307	120.19	0.039066	9	0.351591	12.22296
Total	100						
Total	100			1.862806		11.30352	

	Propane conversion		29.00100			
	Aromatic sum		31.10037		2.363049	82.1506
	Total converted products		38.06553		2.876484	
	aromatics selectivity		81.70217			

Run 12

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	Run 12					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 12					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	1.247795	28.05	0.044485	2	0.088969	3.537228
ethane	0	30.07	0	2	0	0
propene	0	42.081	0	3	0	0
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	66.82271	44.097	1.515357	6	9.092144	
iso butane	0	58.124	0	6	0	0
n-Butane	0	58.124	0	7	0	0
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0	100.205	0	5	0	0
Benzene	7.293104	78.114	0.093365	6	0.560189	22.27191
Toluene	18.31539	92.141	0.198776	7	1.391429	55.32023
EB	0	106.168	0	8	0	0
m-Xylene	1.792613	106.168	0.016885	8	0.135077	5.370389
P-xylene	0	106.168	0	8	0	0
O-Xylene	0.99727	106.168	0.009393	8	0.075147	2.987666
C9+	3.531117	120.19	0.029379	9	0.264415	10.51257
Total	100					
Total	100		1.90764		11.60737	
	Propane conversion		35.15667			
	Aromatic sum		28.39837		2.161843	85.9502
	Total converted products		33.17729		2.515227	
	aromatics selectivity		85.59583			

Table A9: Zn-Ni (2 wt. % each)

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst A run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.964788	42.081	0.070454	3	0.211363	2.945985
neo-pentane	0	72.151	0	5	0	0
n-pentane	0.048661	72.151	0.000674	5	0.003372	0.047001
Propane	5.45402	44.097	0.123682	6	0.742094	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.545687	58.124	0.009388	7	0.065718	0.915984
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.047436	100.205	0.000473	5	0.002367	0.032991
Benzene	15.77166	78.114	0.201906	6	1.211434	16.88502
Toluene	31.8424	92.141	0.345583	7	2.419084	33.71729
EB	0.493713	106.168	0.00465	8	0.037202	0.518528
m-Xylene	18.92519	106.168	0.178257	8	1.426056	19.87642
P-xylene	0.964706	106.168	0.009087	8	0.072693	1.013195
O-Xylene	15.73789	106.168	0.148236	8	1.185886	16.52892
C9+	7.203849	120.19	0.059937	9	0.539435	7.51866
Total	100					
Total	100		1.152329		7.916704	
	Propane conversion		55.6715			
	Aromatic sum		83.73556		6.352355	88.53938

	Total converted products		94.54598		7.17461	
	aromatics selectivity		88.56596			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
			2			
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.737265	42.081	0.065048	3	0.195143	2.735347
neo-pentane	0	72.151	0	5	0	0
n-pentane	0.039533	72.151	0.000548	5	0.00274	0.038401
Propane	5.927245	44.097	0.134414	6	0.806483	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.588755	58.124	0.010129	7	0.070905	0.993888
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.049812	100.205	0.000497	5	0.002486	0.03484
Benzene	13.21606	78.114	0.169189	6	1.015137	14.22934
Toluene	28.04574	92.141	0.304378	7	2.130649	29.86567
EB	0.507786	106.168	0.004783	8	0.038263	0.536337
m-Xylene	18.73473	106.168	0.176463	8	1.411704	19.7881
P-xylene	0.801225	106.168	0.007547	8	0.060374	0.846274
O-Xylene	18.68778	106.168	0.176021	8	1.408167	19.73851
C9+	10.66407	120.19	0.088727	9	0.798541	11.19329
Total	100					
Total	100		1.137744		7.94059	
	Propane conversion		52.42133			
	Aromatic sum		79.99332		6.064294	85.00424
	Total converted products		94.07275		7.134108	
	aromatics selectivity		85.03346			

input paramters			3 Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1						
Propane	33.09		44.097	0.75039100	3	2.251174	
Nitrogen	66.91		28.014	2.38840000	0	0	
Total	100			3.138791000		2.251174	
Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0		16.043	0	1	0	0
ethylene	0		28.05	0	2	0	0
ethane	0		30.07	0	2	0	0
propene	3.185934		42.081	0.07571	3	0.227129	3.204387
neo-pentane	0		72.151	0	5	0	0
n-pentane	0.029186		72.151	0.000405	5	0.002023	0.028535
Propane		6.406628	44.097	0.145285	6	0.871709	0
iso butane	0		58.124	0	6	0	0
n-Butane		0.467557	58.124	0.008044	7	0.056309	0.794421
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane	0.026639		100.205	0.000266	5	0.001329	0.018753
Benzene	12.12998		78.114	0.155286	6	0.931714	13.14484
Toluene	25.55258		92.141	0.27732	7	1.941243	27.38752
EB	0.465525		106.168	0.004385	8	0.035078	0.494894
m-Xylene	20.35913		106.168	0.191763	8	1.534107	21.64355
P-xylene	0.88785		106.168	0.008363	8	0.066902	0.943863
O-Xylene	19.20126		106.168	0.180857	8	1.446858	20.41263
C9+	11.28937		120.19	0.093929	9	0.845364	11.9266
Total	100.0016						
Total	100.0016			1.141612		7.959764	
	Propane conversion			52.97017			
	Aromatic sum			78.59632		5.955901	84.0273
	Total converted products			93.59501		7.088055	
	aromatics selectivity			83.97491			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0
Total	100		3.138791000		2.251174

			4			
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.437929	42.081	0.057934	3	0.173803	2.437771
neo-pentane	0.063084	72.151	0.000874	5	0.004372	0.061317
n-pentane	0.037353	72.151	0.000518	5	0.002589	0.036307
Propane	5.758762	44.097	0.130593	6	0.783558	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.382197	58.124	0.006576	7	0.046029	0.645604
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.28624	100.205	0.002857	5	0.014283	0.200331
Benzene	12.37689	78.114	0.158446	6	0.950679	13.3343
Toluene	26.09829	92.141	0.283243	7	1.982701	27.80954
EB	0.459731	106.168	0.00433	8	0.034642	0.485889
m-Xylene	20.46044	106.168	0.192718	8	1.541741	21.62459
P-xylene	0.805103	106.168	0.007583	8	0.060666	0.850912
O-Xylene	19.48923	106.168	0.18357	8	1.468558	20.59812
C9+	11.34476	120.19	0.09439	9	0.849512	11.91532
Total	100					
Total	100		1.123632		7.91313	
	Propane conversion		59.45325			
	Aromatic sum		79.68968		6.038986	84.70335
	Total converted products		94.24124		7.129572	
	aromatics selectivity		84.55925			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0
Total	100		3.138791000		2.251174

			5			
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	3.087119	42.081	0.073361	3	0.220084	3.115541
neo-pentane	0.072451	72.151	0.001004	5	0.005021	0.071075
n-pentane	0.03574	72.151	0.000495	5	0.002477	0.035062
Propane	6.655374	44.097	0.150926	6	0.905555	
iso butane	0	58.124	0	6	0	0
n-Butane	0.426788	58.124	0.007343	7	0.051399	0.727612
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.035465	100.205	0.000354	5	0.00177	0.025051
Benzene	11.39215	78.114	0.14584	6	0.87504	12.38719
Toluene	23.57608	92.141	0.25587	7	1.791087	25.35489
EB	0.415101	106.168	0.00391	8	0.031279	0.442787
m-Xylene	21.03838	106.168	0.198161	8	1.58529	22.44159
P-xylene	0.78364	106.168	0.007381	8	0.059049	0.835907
O-Xylene	19.74992	106.168	0.186025	8	1.488201	21.06719
C9+	12.7318	120.19	0.105931	9	0.953375	13.49611
Total	100					
Total	100		1.136601		7.969626	
	Propane conversion		57.13967			
	Aromatic sum		76.95527		5.829946	82.52954
	Total converted products		93.34463		7.064071	
	aromatics selectivity		82.4421			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	

6

Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane		0	16.043	0	1	0	0
ethylene		0	28.05	0	2	0	0
ethane		0	30.07	0	2	0	0
propene		3.466141	42.081	0.082368	3	0.247105	3.492596
neo-pentane		0	72.151	0	5	0	0
n-pentane		0.02895	72.151	0.000401	5	0.002006	0.028356
Propane		6.510407	44.097	0.147638	6	0.88583	
iso butane		0	58.124	0	6	0	0
n-Butane		0.471773	58.124	0.008117	7	0.056817	0.80305
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane		0.033005	100.205	0.000329	5	0.001647	0.023277
Benzene		10.94057	78.114	0.140059	6	0.840354	11.87762
Toluene		23.05057	92.141	0.250166	7	1.751164	24.75105
EB		0.423763	106.168	0.003991	8	0.031932	0.451322
m-Xylene		21.72138	106.168	0.204594	8	1.636756	23.134
P-xylene		0.730528	106.168	0.006881	8	0.055047	0.778036
O-Xylene		19.57643	106.168	0.184391	8	1.475128	20.84955
C9+		13.04935	120.19	0.108573	9	0.977154	13.81115
Total	100.0029						
Total	100.0029			1.13751		7.960939	
	Propane conversion			57.8345			
	Aromatic sum			76.44324		5.790381	81.84157
	Total converted products			93.49247		7.07511	
	aromatics selectivity			81.76407			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	

7

Component	Wt%		Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane		0	16.043	0	1	0	0
ethylene		0	28.05	0	2	0	0
ethane		0	30.07	0	2	0	0
propene		2.414239	42.081	0.057371	3	0.172114	2.43828
neo-pentane		0.031399	72.151	0.000435	5	0.002176	0.030825
n-pentane		0.033044	72.151	0.000458	5	0.00229	0.03244
Propane		6.782985	44.097	0.15382	6	0.922918	
iso butane		0	58.124	0	6	0	0
n-Butane		0.292752	58.124	0.005037	7	0.035257	0.499471
i-Pentane	0		72.151	0	3	0	0
hexane	0		86.178	0	4	0	0
cyclohexane	0		84.162	0	4	0	0
n-heptane		0.059326	100.205	0.000592	5	0.00296	0.041937
Benzene		13.39443	78.114	0.171473	6	1.028837	14.57521
Toluene		27.71195	92.141	0.300756	7	2.105291	29.82498
EB		0.503148	106.168	0.004739	8	0.037913	0.537106
m-Xylene		20.8452	106.168	0.196342	8	1.570733	22.25207
P-xylene		0.874186	106.168	0.008234	8	0.065872	0.933186
O-Xylene		19.71441	106.168	0.185691	8	1.485526	21.04496
C9+		7.342931	120.19	0.061094	9	0.549849	7.789537
Total	100						
Total	100			1.146041		7.981736	
	Propane conversion			59.503			
	Aromatic sum			83.04332		6.294172	89.16751
	Total converted products			93.21701		7.058818	
	aromatics selectivity			89.08602			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0
Total	100		3.138791000		2.251174

		8				
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.201356	42.081	0.052312	3	0.156937	2.249695
neo-pentane	0.057339	72.151	0.000795	5	0.003974	0.056961
n-pentane	0.021705	72.151	0.000301	5	0.001504	0.021562
Propane	5.784838	44.097	0.131184	6	0.787106	
iso butane	0	58.124	0	6	0	0
n-Butane	0.329506	58.124	0.005669	7	0.039683	0.568858
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.083885	100.205	0.000837	5	0.004186	0.060002
Benzene	10.75851	78.114	0.137728	6	0.82637	11.84602
Toluene	22.5062	92.141	0.244258	7	1.709808	24.51012
EB	0.383469	106.168	0.003612	8	0.028895	0.414214
m-Xylene	18.93798	106.168	0.178377	8	1.42702	20.45635
P-xylene	8.265753	106.168	0.077855	8	0.622843	8.928466
O-Xylene	17.13838	106.168	0.161427	8	1.291416	18.51246
C9+	11.52878	120.19	0.095921	9	0.863292	12.3753
Total	97.9977					
Total	97.9977		1.090278		7.763033	
	Propane conversion		58.606			
	Aromatic sum		77.99029		5.906351	84.66762
	Total converted products		92.21286		6.975927	
	aromatics selectivity		84.57637			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole
	1				
Propane	33.09	44.097	0.75039100	3	2.251174
Nitrogen	66.91	28.014	2.38840000	0	0
Total	100		3.138791000		2.251174

		9				
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.566749	42.081	0.060995	3	0.182986	2.587142
neo-pentane	0	72.151	0	5	0	0
n-pentane	0.027382	72.151	0.00038	5	0.001898	0.026829
Propane	6.755287	44.097	0.153192	6	0.919149	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.686565	58.124	0.011812	7	0.082685	1.169031
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.02906	100.205	0.00029	5	0.00145	0.020501
Benzene	11.88148	78.114	0.152104	6	0.912626	12.90312
Toluene	24.36821	92.141	0.264467	7	1.851266	26.17402
EB	0.524984	106.168	0.004945	8	0.039559	0.559299
m-Xylene	21.74006	106.168	0.20477	8	1.638163	23.16107
P-xylene	0.861258	106.168	0.008112	8	0.064898	0.917553
O-Xylene	19.29357	106.168	0.181727	8	1.453815	20.55468
C9+	11.26539	120.19	0.09373	9	0.843569	11.92675
Total	100					
Total	100		1.136524		7.992062	
	Propane conversion		56.868			
	Aromatic sum		78.66956		5.960326	84.26975
	Total converted products		93.24471		7.072913	
	aromatics selectivity		84.36893			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	

		10				
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.647346	42.081	0.062911	3	0.188732	2.668379
neo-pentane	0	72.151	0	5	0	0
n-pentane	0.027842	72.151	0.000386	5	0.001929	0.027279
Propane	7.210721	44.097	0.16352	6	0.981117	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.697031	58.124	0.011992	7	0.083945	1.186851
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.306549	100.205	0.003059	5	0.015296	0.216263
Benzene	11.46758	78.114	0.146806	6	0.880834	12.45363
Toluene	23.4965	92.141	0.255006	7	1.785041	25.23771
EB	0.402248	106.168	0.003789	8	0.03031	0.42854
m-Xylene	22.28305	106.168	0.209885	8	1.679079	23.73956
P-xylene	0.731818	106.168	0.006893	8	0.055144	0.779652
O-Xylene	19.35304	106.168	0.182287	8	1.458296	20.61803
C9+	11.37627	120.19	0.094652	9	0.851872	12.04414
Total	100					
Total	100		1.141185		8.011596	
	Propane conversion		56.36			
	Aromatic sum		77.73424		5.888704	83.75965
	Total converted products		92.78928		7.030479	
	aromatics selectivity		83.77502			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	

		11				
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	3.107257	42.081	0.07384	3	0.22152	2.911017
neo-pentane	0	72.151	0	5	0	0
n-pentane	0.032678	72.151	0.000453	5	0.002265	0.029759
Propane	8.463406	44.097	0.191927	6	1.151562	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.818123	58.124	0.014075	7	0.098528	1.294772
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.035786	100.205	0.000357	5	0.001786	0.023465
Benzene	12.35292	78.114	0.15814	6	0.948838	12.46879
Toluene	25.3105	92.141	0.274693	7	1.922852	25.26843
EB	0.433302	106.168	0.004081	8	0.03265	0.429062
m-Xylene	24.00337	106.168	0.226089	8	1.808708	23.76846
P-xylene	0.788316	106.168	0.007425	8	0.059401	0.780601
O-Xylene	20.84715	106.168	0.19636	8	1.57088	20.64313
C9+	12.58353	120.19	0.104697	9	0.942273	12.38252
Total	108.7763					
Total	108.7763		1.252137		8.761263	
	Propane conversion		58.9615			
	Aromatic sum		83.73556		6.34333	83.35846
	Total converted products		100.3129		7.609701	
	aromatics selectivity		83.47434			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
			12			
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0.860699	28.05	0.030684	2	0.061369	0.877254
ethane	0	30.07	0	2	0	0
propene	2.187848	42.081	0.051991	3	0.155974	2.22961
neo-pentane	0	72.151	0	5	0	0
n-pentane	0	72.151	0	5	0	0
Propane	7.627462	44.097	0.17297	6	1.037821	0
iso butane	0	58.124	0	6	0	0
n-Butane	0.721015	58.124	0.012405	7	0.086833	1.241262
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.239646	100.205	0.002392	5	0.011958	0.170934
Benzene	10.34884	78.114	0.132484	6	0.794903	11.36294
Toluene	21.32023	92.141	0.231387	7	1.619709	23.15335
EB	0.373717	106.168	0.00352	8	0.02816	0.402546
m-Xylene	24.7299	106.168	0.232932	8	1.863454	26.63762
P-xylene	0.61067	106.168	0.005752	8	0.046015	0.657778
O-Xylene	15.65776	106.168	0.147481	8	1.179848	16.86564
C9+	15.32221	120.19	0.127483	9	1.147349	16.40108
Total	100					
Total	100		1.151481		8.033394	
	Propane conversion		59.433			
	Aromatic sum		73.04112		5.53209	79.07986
	Total converted products		92.37254		6.995573	
	aromatics selectivity		79.07233			

Table A10: Zn-Cu (2 wt. % each)

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.313374	42.081	0.054974	3	0.164923	2.337775
neo-pentane	0.089292	72.151	0.001238	5	0.006188	0.087712
n-pentane	0.050823	72.151	0.000704	5	0.003522	0.049924
Propane	6.64451	44.097	0.150679	6	0.904076	
iso butane	0	58.124	0	6	0	0
n-Butane	0.241794	58.124	0.00416	7	0.02912	0.412771
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.018793	100.205	0.000188	5	0.000938	0.013292
Benzene	10.36891	78.114	0.132741	6	0.796445	11.28956
Toluene	21.57403	92.141	0.234141	7	1.63899	23.23261
EB	0.480914	106.168	0.00453	8	0.036238	0.513672
m-Xylene	26.86864	106.168	0.253077	8	2.024613	28.69879
P-xylene	0.855857	106.168	0.008061	8	0.064491	0.914154
O-Xylene	17.99998	106.168	0.169542	8	1.356339	19.22604
C9+	12.45825	120.19	0.103655	9	0.932892	13.22369
Total	100					
Total	100		1.11769		7.958775	

	Propane conversion		32.23422			
	Aromatic sum		78.14834		5.917117	83.87483
	Total converted products		93.32067		7.054699	
	aromatics selectivity		83.74173			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	2					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.224762	42.081	0.052869	3	0.158606	2.208738
neo-pentane	0.226651	72.151	0.003141	5	0.015707	0.218731
n-pentane	0.048677	72.151	0.000675	5	0.003373	0.046976
Propane	4.869061	44.097	0.110417	6	0.662502	
iso butane	0	58.124	0	6	0	0
n-Butane	0.028312	58.124	0.000487	7	0.00341	0.047483
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.053447	100.205	0.000533	5	0.002667	0.037139
Benzene	11.42664	78.114	0.146282	6	0.87769	12.22268
Toluene	22.61369	92.141	0.245425	7	1.717974	23.92445
EB	0.547539	106.168	0.005157	8	0.041258	0.574562
m-Xylene	28.99385	106.168	0.273094	8	2.184752	30.42479
P-xylene	1.020821	106.168	0.009615	8	0.076921	1.071202
O-Xylene	13.30063	106.168	0.125279	8	1.002233	13.95707
C9+	14.63965	120.19	0.121804	9	1.096238	15.26618
Total	99.99373					
Total	99.99373		1.094778		7.84333	
	Propane conversion		40.57189			
	Aromatic sum		77.90317		5.900828	82.17476
	Total converted products		95.12467		7.180828	
	aromatics selectivity		81.89587			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	3					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.895811	42.081	0.045051	3	0.135154	1.872197
neo-pentane	0.23999	72.151	0.003326	5	0.016631	0.230379
n-pentane	0.03611	72.151	0.0005	5	0.002502	0.034664
Propane	4.441686	44.097	0.100725	6	0.604352	
iso butane	0	58.124	0	6	0	0
n-Butane	0.024509	58.124	0.000422	7	0.002952	0.040888
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.062113	100.205	0.00062	5	0.003099	0.042932
Benzene	12.82834	78.114	0.164226	6	0.985355	13.64942
Toluene	25.77044	92.141	0.279685	7	1.957794	27.11992
EB	0.575442	106.168	0.00542	8	0.043361	0.600647
m-Xylene	27.15544	106.168	0.255778	8	2.046224	28.34488
P-xylene	1.055962	106.168	0.009946	8	0.079569	1.102215
O-Xylene	12.51691	106.168	0.117897	8	0.943177	13.06516
C9+	13.39725	120.19	0.111467	9	1.003205	13.89669
Total	100					
Total	100		1.095064		7.823377	
	Propane conversion		45.63233			
	Aromatic sum		79.90253		6.055481	83.88225

	Total converted products		95.55831		7.219025	
	aromatics selectivity		83.61651			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	4					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.56122	42.081	0.060864	3	0.182592	2.539358
neo-pentane	0.28845	72.151	0.003998	5	0.019989	0.277997
n-pentane	0.047935	72.151	0.000664	5	0.003322	0.046198
Propane	4.76482	44.097	0.108053	6	0.648319	
iso butane	0	58.124	0	6	0	0
n-Butane	0.022016	58.124	0.000379	7	0.002651	0.036874
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.067853	100.205	0.000677	5	0.003386	0.047086
Benzene	12.69535	78.114	0.162523	6	0.97514	13.56153
Toluene	24.98783	92.141	0.271191	7	1.898338	26.4007
EB	0.526928	106.168	0.004963	8	0.039705	0.552191
m-Xylene	27.52838	106.168	0.259291	8	2.074326	28.84821
P-xylene	1.015788	106.168	0.009568	8	0.076542	1.064489
O-Xylene	11.70084	106.168	0.110211	8	0.881685	12.26183
C9+	13.79259	120.19	0.114757	9	1.032809	14.36355
Total	100					
Total	100		1.107139		7.838805	
	Propane conversion		44.40178			
	Aromatic sum		78.45512		5.945737	82.68894
	Total converted products		95.23518		7.190486	
	aromatics selectivity		82.3804			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	5					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.966712	42.081	0.046736	3	0.140209	1.946708
neo-pentane	0.286866	72.151	0.003976	5	0.01988	0.276014
n-pentane	0.054097	72.151	0.00075	5	0.003749	0.05205
Propane	4.676123	44.097	0.106042	6	0.636251	
iso butane	0	58.124	0	6	0	0
n-Butane	0.0335	58.124	0.000576	7	0.004034	0.056016
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.055996	100.205	0.000559	5	0.002794	0.038794
Benzene	13.10834	78.114	0.16781	6	1.006862	13.97961
Toluene	25.8007	92.141	0.280013	7	1.960093	27.21458
EB	0.54407	106.168	0.005125	8	0.040997	0.569214
m-Xylene	28.4239	106.168	0.267726	8	2.141805	29.73754
P-xylene	1.048832	106.168	0.009879	8	0.079032	1.097305
O-Xylene	12.08148	106.168	0.113796	8	0.910367	12.63983
C9+	11.91939	120.19	0.099171	9	0.892541	12.39234
Total	100					
Total	100		1.102159		7.838613	
	Propane conversion		46.24378			
	Aromatic sum		81.00731		6.139155	85.23808
	Total converted products		95.32388		7.202363	
	aromatics selectivity		84.98114			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	6					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 6					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.376139	42.081	0.056466	3	0.169398	2.299748
neo-pentane	0.287943	72.151	0.003991	5	0.019954	0.270899
n-pentane	0.083756	72.151	0.001161	5	0.005804	0.078799
Propane	4.975728	44.097	0.112836	6	0.677016	
iso butane	0	58.124	0	6	0	0
n-Butane	0.03062	58.124	0.000527	7	0.003688	0.050064
i-Pentane	0.003099	72.151	4.3E-05	3	0.000129	0.001749
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.054356	100.205	0.000542	5	0.002712	0.036822
Benzene	11.79314	78.114	0.150973	6	0.905841	12.29773
Toluene	22.51185	92.141	0.24432	7	1.710237	23.21825
EB	0.567209	106.168	0.005343	8	0.04274	0.580246
m-Xylene	29.9538	106.168	0.282136	8	2.257087	30.6423
P-xylene	1.096909	106.168	0.010332	8	0.082655	1.122122
O-Xylene	13.77829	106.168	0.129778	8	1.038225	14.09499
C9+	15.05645	120.19	0.125272	9	1.127449	15.30629
Total	102.5693					
Total	102.5693		1.123719		8.042934	
	Propane conversion		38.81056			
	Aromatic sum		79.7012		6.036785	81.95563
	Total converted products		97.59356		7.365918	
	aromatics selectivity		81.66645			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	7					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
			3.138791000			
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.452041	42.081	0.05827	3	0.174809	2.575215
neo-pentane	0.320876	72.151	0.004447	5	0.022236	0.327579
n-pentane	0.103472	72.151	0.001434	5	0.007171	0.105634
Propane	5.388393	44.097	0.122194	6	0.733165	
iso butane	0	58.124	0	6	0	0
n-Butane	0.037828	58.124	0.000651	7	0.004556	0.067113
i-Pentane	0.005815	72.151	8.06E-05	3	0.000242	0.003562
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.066904	100.205	0.000668	5	0.003338	0.049179
Benzene	12.5116	78.114	0.160171	6	0.961027	14.15748
Toluene	24.94285	92.141	0.270703	7	1.894922	27.91527
EB	0.593246	106.168	0.005588	8	0.044702	0.658539
m-Xylene	27.0407	106.168	0.254697	8	2.037578	30.01683
P-xylene	1.048822	106.168	0.009879	8	0.079031	1.164257
O-Xylene	10.98981	106.168	0.103513	8	0.828107	12.19936
C9+	9.754086	120.19	0.081156	9	0.7304	10.75998
Total						
Total	95.25645		1.073451		7.521283	
	Propane conversion		46.36211			
	Aromatic sum		77.12703		5.845367	86.11174
	Total converted products		89.86805		6.788118	
	aromatics selectivity		85.82252			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	8					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.218589	42.081	0.052722	3	0.158166	2.147263
neo-pentane	0.27834	72.151	0.003858	5	0.019289	0.261865
n-pentane	0.062738	72.151	0.00087	5	0.004348	0.059024
Propane	4.731408	44.097	0.107295	6	0.643773	
iso butane	0	58.124	0	6	0	0
n-Butane	0.040135	58.124	0.000691	7	0.004834	0.065621
i-Pentane	0.003681	72.151	5.1E-05	3	0.000153	0.002078
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.063919	100.205	0.000638	5	0.003189	0.043299
Benzene	12.84769	78.114	0.164474	6	0.986842	13.3974
Toluene	25.20892	92.141	0.273591	7	1.915135	25.99995
EB	0.648082	106.168	0.006104	8	0.048834	0.662979
m-Xylene	30.81638	106.168	0.290261	8	2.322084	31.52471
P-xylene	1.188798	106.168	0.011197	8	0.089579	1.216123
O-Xylene	11.8969	106.168	0.112057	8	0.896459	12.17036
C9+	12.84798	120.19	0.106897	9	0.962075	13.06117
Total	100					
Total	100		1.130705		8.054758	
	Propane conversion		48.156			
	Aromatic sum		82.60677		6.258932	84.45479
	Total converted products		98.12216		7.410986	
	aromatics selectivity		84.18769			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	9					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 9					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.969686	42.081	0.046807	3	0.140421	1.962616
neo-pentane	0.312167	72.151	0.004327	5	0.021633	0.302356
n-pentane	0.063206	72.151	0.000876	5	0.00438	0.061219
Propane	5.216175	44.097	0.118289	6	0.709732	
iso butane	0	58.124	0	6	0	0
n-Butane	0.037349	58.124	0.000643	7	0.004498	0.062868
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.068793	100.205	0.000687	5	0.003433	0.047976
Benzene	11.32677	78.114	0.145003	6	0.870018	12.15994
Toluene	21.99897	92.141	0.238753	7	1.671273	23.3588
EB	0.513624	106.168	0.004838	8	0.038703	0.540935
m-Xylene	30.49596	106.168	0.287243	8	2.29794	32.1175
P-xylene	1.08783	106.168	0.010246	8	0.08197	1.145672
O-Xylene	11.68464	106.168	0.110058	8	0.880464	12.30594
C9+	15.22483	120.19	0.126673	9	1.140057	15.93418
Total	100					
Total	100		1.094441		7.864523	
	Propane conversion		43.26733			
	Aromatic sum		77.10779		5.840369	81.62879
	Total converted products		94.78382		7.154791	
	aromatics selectivity		81.35121			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	10					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 10					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.218589	42.081	0.052722	3	0.158166	2.147263
neo-pentane	0.27834	72.151	0.003858	5	0.019289	0.261865
n-pentane	0.062738	72.151	0.00087	5	0.004348	0.059024
Propane	4.731408	44.097	0.107295	6	0.643773	
iso butane	0	58.124	0	6	0	0
n-Butane	0.040135	58.124	0.000691	7	0.004834	0.065621
i-Pentane	0.003681	72.151	5.1E-05	3	0.000153	0.002078
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.063919	100.205	0.000638	5	0.003189	0.043299
Benzene	12.84769	78.114	0.164474	6	0.986842	13.3974
Toluene	25.20892	92.141	0.273591	7	1.915135	25.99995
EB	0.648082	106.168	0.006104	8	0.048834	0.662979
m-Xylene	30.81638	106.168	0.290261	8	2.322084	31.52471
P-xylene	1.188798	106.168	0.011197	8	0.089579	1.216123
O-Xylene	11.8969	106.168	0.112057	8	0.896459	12.17036
C9+	12.84798	120.19	0.106897	9	0.962075	13.06117
Total	100					
Total	100		1.130705		8.054758	
	Propane conversion		45.32222			
	Aromatic sum		82.60677		6.258932	84.45479
	Total converted products		98.12216		7.410986	
	aromatics selectivity		84.18769			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	11					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 11					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.969686	42.081	0.046807	3	0.140421	1.962616
neo-pentane	0.312167	72.151	0.004327	5	0.021633	0.302356
n-pentane	0.063206	72.151	0.000876	5	0.00438	0.061219
Propane	5.216175	44.097	0.118289	6	0.709732	
iso butane	0	58.124	0	6	0	0
n-Butane	0.037349	58.124	0.000643	7	0.004498	0.062868
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.068793	100.205	0.000687	5	0.003433	0.047976
Benzene	11.32677	78.114	0.145003	6	0.870018	12.15994
Toluene	21.99897	92.141	0.238753	7	1.671273	23.3588
EB	0.513624	106.168	0.004838	8	0.038703	0.540935
m-Xylene	30.49596	106.168	0.287243	8	2.29794	32.1175
P-xylene	1.08783	106.168	0.010246	8	0.08197	1.145672
O-Xylene	11.68464	106.168	0.110058	8	0.880464	12.30594
C9+	15.22483	120.19	0.126673	9	1.140057	15.93418
Total	100					
Total	100		1.094441		7.864523	
	Propane conversion		47.30311			
	Aromatic sum		77.10779		5.840369	81.62879
	Total converted products		94.78382		7.154791	
	aromatics selectivity		81.35121			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	12					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 12					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	0	16.043	0	1	0	0
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.969686	42.081	0.046807	3	0.140421	1.962616
neo-pentane	0.312167	72.151	0.004327	5	0.021633	0.302356
n-pentane	0.063206	72.151	0.000876	5	0.00438	0.061219
Propane	5.216175	44.097	0.118289	6	0.709732	
iso butane	0	58.124	0	6	0	0
n-Butane	0.037349	58.124	0.000643	7	0.004498	0.062868
i-Pentane	0	72.151	0	3	0	0
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.068793	100.205	0.000687	5	0.003433	0.047976
Benzene	11.32677	78.114	0.145003	6	0.870018	12.15994
Toluene	21.99897	92.141	0.238753	7	1.671273	23.3588
EB	0.513624	106.168	0.004838	8	0.038703	0.540935
m-Xylene	30.49596	106.168	0.287243	8	2.29794	32.1175
P-xylene	1.08783	106.168	0.010246	8	0.08197	1.145672
O-Xylene	11.68464	106.168	0.110058	8	0.880464	12.30594
C9+	15.22483	120.19	0.126673	9	1.140057	15.93418
Total	100					
Total	100		1.094441		7.864523	
	Propane conversion		51.56389			
	Aromatic sum		77.10779		5.840369	81.52871
	Total converted products		94.78382		7.154791	
	aromatics selectivity		81.45122			

Table A11: Zn-Ni/ZSM-5 (2-3 wt. %) Run 1-12

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 1					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	4.048565	16.043	0.252357	1	0.252357	3.534459
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.721219	42.081	0.064666	3	0.193999	2.717103
neo-pentane	0.055365	72.151	0.000767	5	0.003837	0.053737
n-pentane	0.032869	72.151	0.000456	5	0.002278	0.031902
Propane	4.884624	44.097	0.11077	6	0.66462	0
iso butane	0.111456	58.124	0.001918	6	0.011505	0.161141
n-Butane	0.671272	58.124	0.011549	7	0.080843	1.132266
i-Pentane	0.006558	72.151	9.09E-05	3	0.000273	0.003819
hexane	0	86.178	0	4	0	0
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.062028	100.205	0.010599	5	0.052993	0.742205
Benzene	11.38304	78.114	0.145723	6	0.874341	12.24583
Toluene	37.6181	92.141	0.408267	7	2.857867	40.02666
EB	15.68096	106.168	0.147699	8	1.181596	16.54918
m-Xylene	1.939146	106.168	0.018265	8	0.146119	2.046512
P-xylene	0	106.168	0	8	0	0
O-Xylene	0.821554	106.168	0.007738	8	0.061906	0.867042
C9+	18.96325	120.19	0.157777	9	1.419995	19.88815
	100					
Total	100		1.338642		7.804527	
	Propane conversion		74.17933			
	Aromatic sum		67.4428		5.121828	71.73522
	Total converted products		95.11538		7.139907	
	aromatics selectivity		70.9063			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 2					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.82661	16.043	0.113857	1	0.113857	1.594658
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.988967	42.081	0.047265	3	0.141796	1.985959
neo-pentane	0.20971	72.151	0.002907	5	0.014533	0.203542
n-pentane	0.279827	72.151	0.003878	5	0.019392	0.271597
Propane	3.181199	44.097	0.072141	6	0.432846	0
iso butane	0.236367	58.124	0.004067	6	0.0244	0.341736
n-Butane	1.272376	58.124	0.021891	7	0.153235	2.146177
i-Pentane	0.025943	72.151	0.00036	3	0.001079	0.015108
hexane	0.020277	86.178	0.000235	4	0.000941	0.013182
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.451834	100.205	0.014489	5	0.072443	1.014624
Benzene	6.798095	78.114	0.087028	6	0.522167	7.313362
Toluene	34.74967	92.141	0.377136	7	2.639951	36.97458
EB	19.16345	106.168	0.180501	8	1.444009	20.22449
m-Xylene	11.8057	106.168	0.111198	8	0.889586	12.45935
P-xylene	2.56939	106.168	0.024201	8	0.193609	2.711651
O-Xylene	3.648117	106.168	0.034362	8	0.274894	3.850105
C9+	10.77247	120.19	0.089629	9	0.806658	11.29787
	100					
Total	100		1.185144		7.745395	
	Propane conversion		78.4795			
	Aromatic sum		78.73442		5.964217	81.56139
	Total converted products		96.8188		7.31255	
	aromatics selectivity		81.32142			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 3					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.718995	16.043	0.107149	1	0.107149	1.500709
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.870237	42.081	0.044444	3	0.133331	1.867409
neo-pentane	0.2073	72.151	0.002873	5	0.014366	0.201203
n-pentane	0.2879	72.151	0.00399	5	0.019951	0.279432
Propane	3.411253	44.097	0.077358	6	0.464148	0
iso butane	0.246452	58.124	0.00424	6	0.025441	0.356316
n-Butane	1.276467	58.124	0.021961	7	0.153728	2.153077
i-Pentane	0.024981	72.151	0.000346	3	0.001039	0.014548
hexane	0.014899	86.178	0.000173	4	0.000692	0.009686
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.006772	100.205	6.76E-05	5	0.000338	0.004733
Benzene	7.637227	78.114	0.09777	6	0.586622	8.216096
Toluene	34.0915	92.141	0.369993	7	2.589949	36.27427
EB	19.18859	106.168	0.180738	8	1.445904	20.25102
m-Xylene	11.72929	106.168	0.110479	8	0.883829	12.37871
P-xylene	2.21201	106.168	0.020835	8	0.16668	2.334484
O-Xylene	4.849496	106.168	0.045678	8	0.365421	5.118001
C9+	11.22663	120.19	0.093407	9	0.840666	11.77419
	100					
Total	100		1.181502		7.799251	
	Propane conversion		77.33233			
	Aromatic sum		79.70811		6.038404	82.32199
	Total converted products		96.58875		7.335104	
	aromatics selectivity		82.52319			

input paramters	Mol.wt (g/mol)	mole	No of carbon	Carbon mole

	1					
Propane	33.09	44.097	0.75039100	3	2.251173549	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251173549	
Output parameters	Catalyst Run 4					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.96097	16.043	0.122232	1	0.122232118	1.711957
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.624423	42.081	0.038602	3	0.115806857	1.621966
neo-pentane	0.206005	72.151	0.002855	5	0.014275934	0.199946
n-pentane	0.287187	72.151	0.00398	5	0.019901792	0.27874
Propane	3.020371	44.097	0.068494	6	0.410962814	0
iso butane	0.207126	58.124	0.003564	6	0.021381158	0.29946
n-Butane	1.179692	58.124	0.020296	7	0.14207287	1.989842
i-Pentane	0.023692	72.151	0.000328	3	0.000985083	0.013797
hexane	0.019782	86.178	0.00023	4	0.000918174	0.01286
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.162599	100.205	0.011602	5	0.058011031	0.81249
Benzene	6.186348	78.114	0.079196	6	0.475178401	6.655246
Toluene	31.21478	92.141	0.338772	7	2.371402979	33.21336
EB	12.4377	106.168	0.117151	8	0.937209103	13.12635
m-Xylene	14.51378	106.168	0.136706	8	1.093646248	15.31737
P-xylene	6.442455	106.168	0.060682	8	0.48545362	6.799159
O-Xylene	6.041305	106.168	0.056903	8	0.455226019	6.375798
C9+	13.47179	120.19	0.112087	9	1.008786875	14.12885
	100					
Total	100		1.173681		7.733451075	
	Propane conversion		77.33917			
	Aromatic sum		76.83637		5.81811637	79.45546
	Total converted products		96.97963		7.322488261	
	aromatics selectivity		79.22939			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.750391	3	2.251174	
Nitrogen	66.91	28.014	0	0	0	
Total	100		0.750391		2.251174	
Output parameters	Catalyst Run 5					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.819101	16.043	0.113389	1	0.113389	1.588103
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.654339	42.081	0.039313	3	0.11794	1.651837
neo-pentane	0.198405	72.151	0.00275	5	0.013749	0.192569
n-pentane	0.277265	72.151	0.003843	5	0.019214	0.26911
Propane	3.064389	44.097	0.069492	6	0.416952	0
iso butane	0.21778	58.124	0.003747	6	0.022481	0.314863
n-Butane	1.178612	58.124	0.020278	7	0.141943	1.988021
i-Pentane	0.024116	72.151	0.000334	3	0.001003	0.014044
hexane	0.014701	86.178	0.000171	4	0.000682	0.009557
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.166373	100.205	0.01164	5	0.058199	0.815127
Benzene	6.075444	78.114	0.077777	6	0.46666	6.535936
Toluene	31.42222	92.141	0.341023	7	2.387163	33.43409
EB	18.21922	106.168	0.171607	8	1.37286	19.22798
m-Xylene	18.23762	106.168	0.171781	8	1.374246	19.24739
P-xylene	2.166459	106.168	0.020406	8	0.163248	2.286411
O-Xylene	2.321249	106.168	0.021864	8	0.174911	2.449771
C9+	11.94271	120.19	0.099365	9	0.894287	12.52519
	100					
Total	100		1.168779		7.738926	
	Propane conversion		77.80533			
	Aromatic sum		78.44221		5.939087	81.11319
	Total converted products		96.93561		7.321974	
	aromatics selectivity		80.92198			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 6					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.774904	16.043	0.110634	1	0.110634	1.549519
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.64807	42.081	0.039164	3	0.117493	1.645578
neo-pentane	0.150081	72.151	0.00208	5	0.0104	0.145667
n-pentane	0.265292	72.151	0.003677	5	0.018384	0.257489
Propane	3.280249	44.097	0.074387	6	0.446323	0
iso butane	0.222358	58.124	0.003826	6	0.022953	0.321481
n-Butane	1.156948	58.124	0.019905	7	0.139334	1.951479
i-Pentane	0.02573	72.151	0.000357	3	0.00107	0.014984
hexane	0.021261	86.178	0.000247	4	0.000987	0.013821
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.190529	100.205	0.011881	5	0.059405	0.832009
Benzene	6.19932	78.114	0.079362	6	0.476175	6.669202
Toluene	31.17088	92.141	0.338295	7	2.368068	33.16665
EB	12.37275	106.168	0.116539	8	0.932315	13.0578
m-Xylene	18.0894	106.168	0.170385	8	1.363077	19.09097
P-xylene	1.959891	106.168	0.01846	8	0.147682	2.068406
O-Xylene	7.73016	106.168	0.072811	8	0.582485	8.158161
C9+	12.74218	120.19	0.106017	9	0.954153	13.36366
	100					
Total	100		1.168027		7.750938	
	Propane conversion		74.57717			
	Aromatic sum		77.52240		5.869802	80.35744
	Total converted products		96.71975		7.304615	
	aromatics selectivity		80.15157			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 7					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.486136	16.043	0.092635	1	0.092635	1.297419
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.615004	42.081	0.038378	3	0.115135	1.612561
neo-pentane	0.218851	72.151	0.003033	5	0.015166	0.212414
n-pentane	0.285715	72.151	0.00396	5	0.0198	0.277311
Propane	2.700107	44.097	0.061231	6	0.367387	0
iso butane	0.229479	58.124	0.003948	6	0.023689	0.331777
n-Butane	1.22429	58.124	0.021063	7	0.147444	2.065067
i-Pentane	0.025388	72.151	0.000352	3	0.001056	0.014785
hexane	0.014493	86.178	0.000168	4	0.000673	0.009422
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.032822	100.205	0.010307	5	0.051535	0.721795
Benzene	6.194652	78.114	0.079303	6	0.475816	6.664181
Toluene	30.67957	92.141	0.332963	7	2.330743	32.64388
EB	12.9103	106.168	0.121603	8	0.97282	13.62511
m-Xylene	17.60224	106.168	0.165796	8	1.326369	18.57684
P-xylene	1.891782	106.168	0.017819	8	0.14255	1.996525
O-Xylene	7.784673	106.168	0.073324	8	0.586593	8.215692
C9+	14.1045	120.19	0.117352	9	1.056165	14.79242
	100					
Total	100		1.143235		7.725575	
	Propane conversion		74.97767			
	Aromatic sum		77.06322		5.834891	79.29793
	Total converted products		97.29989		7.358189	
	aromatics selectivity		79.20175			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 8					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	2.725402	16.043	0.169881	1	0.169881	2.379317
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	2.464335	42.081	0.058562	3	0.175685	2.460608
neo-pentane	0.269456	72.151	0.003735	5	0.018673	0.26153
n-pentane	0.437739	72.151	0.006067	5	0.030335	0.424864
Propane	4.989807	44.097	0.113155	6	0.678932	0
iso butane	0.350374	58.124	0.006028	6	0.036168	0.506565
n-Butane	1.81113	58.124	0.03116	7	0.218118	3.054918
i-Pentane	0.040916	72.151	0.000567	3	0.001701	0.023828
hexane	0.008462	86.178	9.82E-05	4	0.000393	0.005501
cyclohexane	0	84.162	0	4	0	0
n-heptane	0.592476	100.205	0.005913	5	0.029563	0.414056
Benzene	5.381838	78.114	0.068897	6	0.413383	5.789758
Toluene	30.60322	92.141	0.332135	7	2.324943	32.56265
EB	11.15007	106.168	0.105023	8	0.840183	11.76742
m-Xylene	16.58777	106.168	0.156241	8	1.249926	17.50619
P-xylene	1.945198	106.168	0.018322	8	0.146575	2.052899
O-Xylene	7.29378	106.168	0.0687	8	0.549603	7.69762
C9+	13.34803	120.19	0.111058	9	0.99952	13.99906
	100					
Total	100		1.255541		7.883582	
	Propane conversion		74.52217			
	Aromatic sum		72.96187		5.524613	76.68121
	Total converted products		95.01019		7.204651	
	aromatics selectivity		76.79373			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
1						
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 9					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.721243	16.043	0.107289	1	0.107289	1.502672
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.521921	42.081	0.036166	3	0.108499	1.519619
neo-pentane	0.153533	72.151	0.002128	5	0.01064	0.149018
n-pentane	0.209017	72.151	0.002897	5	0.014485	0.202869
Propane	2.733951	44.097	0.061999	6	0.371991	0
iso butane	0.184801	58.124	0.003179	6	0.019077	0.267183
n-Butane	0.998724	58.124	0.017183	7	0.120279	1.684596
i-Pentane	0.016028	72.151	0.000222	3	0.000666	0.009334
hexane	0.018531	86.178	0.000215	4	0.00086	0.012047
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.044609	100.205	0.010425	5	0.052124	0.730032
Benzene	5.498349	78.114	0.070389	6	0.422333	5.9151
Toluene	29.24338	92.141	0.317376	7	2.221635	31.11574
EB	11.21857	106.168	0.105668	8	0.845345	11.83972
m-Xylene	24.25445	106.168	0.228453	8	1.827628	25.59736
P-xylene	1.999431	106.168	0.018833	8	0.150662	2.110135
O-Xylene	9.090109	106.168	0.08562	8	0.68496	9.593408
C9+	10.09335	120.19	0.083978	9	0.755804	10.58563
	100					
Total	100		1.152021		7.714277	
	Propane conversion		73.70367			
	Aromatic sum		81.30429		6.152562	83.79629
	Total converted products		97.26605		7.342285	
	aromatics selectivity		83.58959			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 10					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.405614	16.043	0.087615	1	0.087615	1.227122
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.695582	42.081	0.040293	3	0.12088	1.693017
neo-pentane	0.163982	72.151	0.002273	5	0.011364	0.159159
n-pentane	0.195762	72.151	0.002713	5	0.013566	0.190005
Propane	2.634458	44.097	0.059742	6	0.358454	0
iso butane	0.184655	58.124	0.003177	6	0.019062	0.266971
n-Butane	1.022305	58.124	0.017588	7	0.123118	1.724369
i-Pentane	0.015254	72.151	0.000211	3	0.000634	0.008883
hexane	0.024715	86.178	0.000287	4	0.001147	0.016067
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.702895	100.205	0.016994	5	0.084971	1.190079
Benzene	5.11623	78.114	0.065497	6	0.392982	5.504019
Toluene	30.03161	92.141	0.325931	7	2.281517	31.95443
EB	16.00143	106.168	0.150718	8	1.205744	16.8874
m-Xylene	18.24412	106.168	0.171842	8	1.374736	19.25426
P-xylene	2.100047	106.168	0.01978	8	0.158243	2.216322
O-Xylene	8.801823	106.168	0.082905	8	0.663237	9.28916
C9+	10.65951	120.19	0.088689	9	0.7982	11.17941
	100					
Total	100		1.136257		7.695471	
	Propane conversion		74.64058			
	Aromatic sum		80.29527		6.07646	82.81922
	Total converted products		97.36554		7.337017	
	aromatics selectivity		82.46785			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 11					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.565974	16.043	0.097611	1	0.097611	1.36712
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.440454	42.081	0.034231	3	0.102692	1.438275
neo-pentane	0.173852	72.151	0.00241	5	0.012048	0.168739
n-pentane	0.207545	72.151	0.002877	5	0.014383	0.201441
Propane	2.692132	44.097	0.06105	6	0.366301	0
iso butane	0.196063	58.124	0.003373	6	0.020239	0.283465
n-Butane	1.060488	58.124	0.018245	7	0.127717	1.788776
i-Pentane	0.016172	72.151	0.000224	3	0.000672	0.009418
hexane	0.016815	86.178	0.000195	4	0.00078	0.010931
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.117993	100.205	0.011157	5	0.055785	0.781317
Benzene	4.670401	78.114	0.05979	6	0.358737	5.024398
Toluene	30.20066	92.141	0.327766	7	2.29436	32.13431
EB	15.67419	106.168	0.147636	8	1.181085	16.54203
m-Xylene	18.1481	106.168	0.170938	8	1.367501	19.15292
P-xylene	2.052941	106.168	0.019337	8	0.154694	2.166607
O-Xylene	9.687494	106.168	0.091247	8	0.729975	10.22387
C9+	11.07872	120.19	0.092177	9	0.829591	11.61907
	100					
Total	100		1.140262		7.714172	
	Propane conversion		75.55667			
	Aromatic sum		80.43379		6.086352	82.83151
	Total converted products		97.30787		7.34787	
	aromatics selectivity		82.65908			

input paramters		Mol.wt (g/mol)	mole	No of carbon	Carbon mole	
	1					
Propane	33.09	44.097	0.75039100	3	2.251174	
Nitrogen	66.91	28.014	2.38840000	0	0	
Total	100		3.138791000		2.251174	
Output parameters	Catalyst Run 12					
Component	Wt%	Mol.wt (g/mol)	Mole	No of carbon	Carbon mole	Selectivity
methane	1.671901	16.043	0.104214	1	0.104214	1.459595
ethylene	0	28.05	0	2	0	0
ethane	0	30.07	0	2	0	0
propene	1.450456	42.081	0.034468	3	0.103405	1.448263
neo-pentane	0.158723	72.151	0.0022	5	0.010999	0.154055
n-pentane	0.200401	72.151	0.002778	5	0.013888	0.194507
Propane	2.586339	44.097	0.058651	6	0.351907	0
iso butane	0.162918	58.124	0.002803	6	0.016818	0.235544
n-Butane	0.998568	58.124	0.01718	7	0.12026	1.684332
i-Pentane	0.015039	72.151	0.000208	3	0.000625	0.008758
hexane	0.016596	86.178	0.000193	4	0.00077	0.010789
cyclohexane	0	84.162	0	4	0	0
n-heptane	1.079294	100.205	0.010771	5	0.053854	0.754272
Benzene	4.904274	78.114	0.062784	6	0.376701	5.275997
Toluene	30.07921	92.141	0.326448	7	2.285134	32.00509
EB	15.77959	106.168	0.148628	8	1.189028	16.65327
m-Xylene	18.05993	106.168	0.170107	8	1.360857	19.05987
P-xylene	2.080227	106.168	0.019594	8	0.15675	2.195405
O-Xylene	9.007563	106.168	0.084843	8	0.67874	9.506291
C9+	11.74896	120.19	0.097753	9	0.879779	12.322
	100					
Total	100		1.143622		7.703729	
	Propane conversion		75.23483			
	Aromatic sum		79.9108		6.04721	82.25458
	Total converted products		97.41366		7.351822	
	aromatics selectivity		82.03244			

APPENDIXB

These BET equations were used to to determine the monolayer absorbed gas volume.

$$\frac{1}{v[\left(\frac{po}{p}\right)-1]} = \frac{c-1}{v_m c}\left(\frac{p}{p_o}\right) + \frac{1}{v_m c} \text{b.1}$$

v = adsorbed gas quantity

po = saturation pressure of adsorbate

p = equilibrium pressure of adsorbate

c = BET constant = exp ($\frac{E_1 - E_L}{RT}$)b.2

E_1 = heat of adsorption for the first layer

E_L = heat of vaporization

Plotting $\frac{1}{v[\left(\frac{po}{p}\right)-1]}$ against $\left(\frac{p}{p_o}\right)$ leaves $\frac{1}{v_m c}$ as intercept and $\frac{c-1}{v_m c}$ as slope.

Total surface area S_t is calculated by:

$$S_t = \frac{v_m N s}{V} \text{b.3}$$

St = total surface area of sample material

vm= monolayer absorbed gas volume

N = Avogadro's number = 6.02 x 10^{23} molecules/mol.

s = cross-sectional area of adsorbed gas molecule

V = molar volume of adsorbed gas

$S_{BET} = \frac{S_t}{a}$(m^2/g)b.4

S_{BET} = specific surface area

a = mass of sample

APPENDIX C

C.1 Conferences and Paper Publications

This sections presents the lists of conferences as at completion of this research.

- ✓ *Effect of Iron Metal Addition on Aromatization of Propane over Zn-Fe/ZSM-5 Catalyst*: International Conference and Materials Congress, (NIMACON 2018) Materials Science and Technology Society of Nigeria (MSN). Abuja, 2018.
- ✓ *Propane Aromatization Over Zinc-cobalt Bimetallic/Zsm-5 Catalyst*: National Engineering Conference, Faculty of Engineering ABU, Zaria 2019.
- ✓ *Improved Selectivity Effect of Cobalt and Nickel Second Metal Co-impregnation with Zinc on ZSM-5 for Aromatization of Propane*. 49th Annual Conference of Nigerian Society of Chemical Engineers, Kaduna, 2019.

- ✓ *Light Alkane Aromatization over Zn-Co/ZSM-5 Catalyst: Effect of Temperature and Flowrate*. Material Science and Technology Society of Nigeria Kaduna (MSN), November, 2019.

Publications

This sections presents the lists of paper publications as at completion of this research.

- ✓ *Increasing the catalytic stability by optimizing the formation of Zinc/ZSM-5 with Copper for propane aromatization* (Published: Journal of King-Saud University-Engineering Science. Elsevier, 2020, https://doi.org/10.1007/s13203-020-00245-9.).
- ✓ *Highly Selective and Stable Zn-Fe/ZSM-5 Catalyst for Aromatization of Propane* (Published: Applied Petrochemical Research Journal Springer, 10(2), 55-65, 2020).
- ✓ *Improved Selectivity Effect of Cobalt and Nickel Second Metal Co-impregnation with Zinc on ZSM-5 for Aromatization of Propane*. (Published: Nigeria Society of Chemical Engineers, NSChE Journal, 35(1), 17-17, 2020).
- ✓ *Synergistic Effect of Zn with Ni On ZSM-5 as Propane Aromatization.*(JFUE-D-21-01071).