A PROJECT REPORT

ON

“STUDY ON ESTERIFICATION OF ETHYLENE GLYCOL WITH ACETIC ACID IN THE PRESENCE OF SERALITE SRC-120 AND MOLECULAR SIEVE 13X CATALYST”

A Thesis Submitted in Partial Fulfillment of the Requirements for the Degree of

Master of Technology

In

Chemical Engineering

Submitted By

VISHNU PRASAD YADAW

(208CH-101)

DEPARTMENT OF CHEMICAL ENGINEERING

NATIONAL INSTITUTE OF TECHNOLOGY

ROURKELA-769008

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Under the guidance of

PROF. (Dr.) R. K. SINGH

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CERTIFICATE

This is to certify that the thesis of the project entitled, "***STUDY ON ESTERIFICATION OF ETHYLENE GLYCOL WITH ACETIC ACID IN THE PRESENCE OF SERALITE SRC-120 AND MOLECULAR SIEVE 13X CATALYST***" submitted by Vishnu Prasad Yadaw (208CH-101) in partial fulfillment of the requirements for the award of Master of Technology Degree in Chemical Engineering at the National Institute of Technology, Rourkela is an authentic work carried out by him under my supervision and guidance

To the best of my knowledge, the matter embodied in the thesis has not been submitted to any other University/Institute for the award of any Degree.

Place: Rourkela

Date:

PROF. (Dr.) R. K SINGH
(Department of Chemical Engineering)
National institute of technology
Rourkela-769008

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ABSTRACT

There is an increasing the trend of chemical industries toward new processes that should meets more requirement such as generation of nearly zero waste chemicals, less energy, and sufficient uses of product chemicals in various application. Esterification is the general name for a chemical reaction in which two reactants ethylene glycol and acetic acid form an ester as a product. Since the reaction was occurred in equilibrium and reversible manner, the reaction was become slowly without catalyst.

The reaction was carried out in the presence of Seralite SRC-120 and Molecular Sieve 13x as acid catalyst with investigated temperature range from 333 to 363 K and varying amount of 0.5wt% to 2.0wt% catalyst load. It was found that as increase reaction time as increase mole fraction of product, conversion of reactant and selectivity of ethylene glycol di-acetate (EGDA) but decrease the selectivity of ethylene glycol mono-acetate (EGMA). The maximum conversion of acetic acid and ethylene glycol were obtained 46.12% and 100% during 10 hour reaction time with 1.5wt% amount of catalyst loading respectively. But Molecular sieve 13x has been given only 78% conversion of ethylene glycol with 4.0 wt% catalyst loading The selectivity of ethylene glycol di-acetate has been observed 66 percentages with amount of 0.5wt% Seralite SRC-120 as a catalyst. However the product selectivity with Molecular Sieve 13X was found to be very less. In the present work, parameter estimation has been done by using non-linear least square method with the help of Matlab modeling software. Best fit equilibrium constant and activation energy was found for reaction system.

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NOMENCLATURE :

K_1	Forward reaction equilibrium rate constant, lit/mol min
K_{-1}	Reverse reaction equilibrium rate constant, lit/mol min
K_2	Forward reaction equilibrium rate constant, lit/mol min
K_{-2}	Reverse reaction equilibrium rate constant, lit/mol min
C_{EG}	Concentration of ethylene glycol mol/lit
C_{HAC}	Concentration of ethylene glycol mol/lit
C_{EGMA}	Concentration of ethylene glycol mol/lit
C_{EGDA}	Concentration of ethylene glycol mol/lit
K_0	Pre-exponatial factor
E	Activation energy, KJ/mol
R	Real gas constant
T	Reaction temperature, K

ABBREVIATIONS :

EG	Ethylene glycol
AA	Acetic acid
EGMA	Ethylene glycol mono-acetate
EGDA	Ethylene glycol di-acetate

CHAPTER 1

INTRODUCTION

INTRODUCTION

1.1 Introduction

There is an increasing the inclination of chemical industries toward new processes that should meets requirement such as generation of nearly zero waste chemicals, less energy, and sufficient uses of product chemicals in various application. Hence the esterification is widely employed reaction in the organic process industry. The reaction is carried out between carboxylic acid and alcohol at with or without present of different acid catalyst under such specific condition. Ethylene glycol was first prepared in 1859 by the French chemist Charles Wurtz. It was produced on a small scale during World War I as a coolant and as an ingredient in explosives. Widespread industrial production began in 1937, when its precursor ethylene oxide became cheaply available. When first introduced it created a minor revolution in aircraft design because when used in place of water as a radiator coolant, its higher boiling point allowed for smaller radiators operating at higher temperatures. Ethylene glycol is produced from ethylene, via the intermediate ethylene oxide [1]. Major derevatives of ethylene glycol by various reaction processes are ethylene glycol, mono ethylene glycol, diethylene glycol, triethylene glycol, and tetraethylene glycol.

1.2 Available industrial chemical process

There are different chemical reaction processes are available:

Isomerization

In chemistry isomerisation is the process by which one molecule is transformed into another molecule which has exactly the same atoms, but the atoms are rearranged. In some molecules and under some conditions, isomerisation occurs spontaneously. Many isomers are equal or roughly equal in bond energy, and so exist in roughly equal amounts, provided that they can interconvert relatively freely, that is the energy barrier between the two isomers is not too high. When the isomerisation occurs intramolecularly it is considered a rearrangement reaction an intramolecular isomerization that involves the breaking or making of bonds is a special case of a molecular rearrangement [2].

Dehydration

Dehydration is defined as an excessive loss of body fluid. It is literally the removal of water from reaction system which forms during reaction process. In the case of ethylene glycol and acetic acid reaction system the dehydration play vital role because during reaction excess water has been losses [3].

Etherification

Etherification of glycol is defined acid catalyzed reaction with formation of mono-, di- and tri-alkyl glycol ethers. Since etherification reactions are carried out in the liquid phase, reaction becomes slightly slow without catalyst. Hence the etherification of ethylene and propylene glycols with isobutylene was carried out in the presence of cation exchange resin catalysts. In the case of ethylene glycol, the mixture of mono- and di-ethers of corresponding glycol is obtained. The mono-ether of ethylene glycol has good miscibility with water and is used for coating solvents and as a solvent for paints [4].

Acetylation

Acetylation also called ethanoylation is described as a reaction that introduces an acetyl functional group into a chemical compound. A reaction involving the replacement of the hydrogen atom of a hydroxyl group with an acetyl group (CH_3 CO) yields a specific ester, the acetate. Acetic anhydride is commonly used as an acetylating agent reacting with free hydroxyl groups [5].

Esterification

Esterification is the chemical process for making esters, which are compounds of the chemical structure R-COOR', where R and R' are either alkyl or aryl groups. The most common method for preparing esters is to heat a carboxylic acid with an alcohol while removing the water that is formed. A mineral acid catalyst is usually needed to make the reaction occur at a useful rate. Esters can also be formed by various other reactions. These include the reaction of an alcohol with an acid chloride or an anhydride. The chemical structure of the alcohol, the acid, and the acid catalyst used in the esterification reaction all effect its rate. Simple alcohols such as methanol and ethanol react very fast because they are relatively small and contain no carbon atom side chains that would hinder their reaction. These differing rates of reaction were first reported by Nikolay Menschutkin in 1879-83. German chemists, during World War II, developed solid acid catalysts or ion exchange resins for use in the manufacture of esters. These solid catalysts work well with acid sensitive esters because they can be separated from the product by filtration and therefore, the catalyst does not spend very much time in contact with the acid unstable product. The esterification process has a broad spectrum of uses from the preparation of highly specialized esters in the chemical laboratory to the production of millions of tons of commercial ester products. These commercial compounds are manufactured by either a batch or a continuous synthetic process. The continuous process for making esters was first patented in 1921 and has been used extensively in the manufacture of large quantities of esters.

[6].

1.3 Industrial application

In present markets point of view organic esters are valuable intermediates in several branch of chemical industry. It has been wide applications in plasticizers, solvents, perfumery also used as flavoring agents and preservative in the food industry chemicals and as precursors to a gamut of pharmaceuticals, agrochemicals, and other fine chemicals. Ethylene glycol mono and di-acetate are major product of esterification of ethylene glycol with acetic acid and they have widely used as an engine coolant and antifreeze. Due to its low freezing point, it has also been used as a deicing fluid for windshields and jet engines. The antifreeze capabilities of ethylene glycol derivatives have made it’s an important component of vitrification mixtures for low-temperature preservation of biological tissues and organs. Minor uses of ethylene glycol include the manufacture of capacitors and as a chemical intermediate in the manufacture of 1, 4-dioxane.

1.4 Purpose of project work

Esterification of carboxlic acids with alcohols in the presence of acid catalysts has been done by many researchers, but the ethylene glycol and acetic acid reaction system has not been studied more. Therefore present work is considered as esterification reaction between ethylene glycol with acetic acid at presence of different catalysts. Hence the main objective of this work is to find out the effects of various parameters such as temperature, catalyst type, catalyst loading, reaction time and variable molar ratio of reactant on the five component reaction system. Also have studied on percentage conversion for ethylene glycol and acetic acid, and have to find out the selectivity of ethylene glycol mono acetate and di-acetate.

1.5 Organization of thesis

Chapter 1: This section is divided in several parts introduction, industrial process available, industrial application of product, physical property of reactant, product and catalyst and finally purpose of project work.

Chapter 2: This section is literature review section in which has explained previous work done with different alcohol and also with ethylene glycol in presence of different catalysts.

Chapter 3: This section shows the present work esterification mechanism and chemistry.

Chapter 4: This section shows experimental setup.

Chapter 5: In this section result has been shown which include effect of reaction time, temperature, catalyst loading, molar ratio of reactant and type of catalyst.

Chapter 6: Discussion of result has been done in this section.

Chapter 7: Conclusion has been explained in this section.

CHAPTER 2

LITERATURE REVIEW

This Literature review represents the esterification of acetic acid with various alcohols in the presence of several acid and ion- exchange catalyst.

2.1 Esterification of acetic acid with butanol

Esterification of acetic acid is well established chemical process, through which methyl, ethyl, butyl and ethylene glycol acetate are formed. Several catalysts are used to synthesis acetate in this process. Mesoporous Al-MCM-41 molecular sieves in the Si/Al ratios 33, 52, 72 and 114 (Rabindran et al. 2005) and 25, 50, 75 and 100 were synthesized under hydrothermal condition. The acidity and surface area of catalyst were measured with the help FTIR using pyridine as the diagnostic base and BET showed surface areas between 900 and $1000m^2/g$ and pore diameter around 26 °A units. Rabindran et al. (2005) was studied the effect of reaction temperature, mole ratio of the reactant, time and catalyst loading on *n*-butanol conversion and selectivity of *n*-butyl acetate was studied. Al-MCM-41 (33 and 25) was found to be more active than the other catalysts owing to its high density of Bronsted acid sites. The reaction was also studied over H-Mordenite, H-beta, H-ZSM-5 and HY zeolites, and the results are compared. *n*-Butyl acetate was the major product obtained which is facilitated by weak and moderate Bronsted acid sites. The low reaction period and low amount of catalyst were required for converting a major amount of the reactants to product with high selectivity. The reaction over as-prepared catalyst showed conversion 68% less than that of calcined sample. Hence the reaction is proposed to occur mainly within the pores of the catalyst. The catalytic activity of the materials was tested for the vapour phase esterification of acetic acidwith n-butyl alcohol (NBA), isobutyl alcohol (IBA) and tertiary butyl alcohol (TBA) under autogeneous condition at 100, 150, 175 and 200 ^{0}C.NBAconversion was found to be higher than IBA and TBA. The hydrophobic properties of catalyst, alcohols and the stearic properties of alcohols were suggested to play important roles in the esterification. Another esterification reaction were carried out between the propionic acid with *n*-butanol over Amberlyst 15, Amberlyst 35, Amberlyst 39, and HZSM-5 catalysts at the temperatures range from 353 to 383 K in a stirred batch reactor (Liu et al., 2001). The literature elaborated experimental results that indicated the Amberlyst resins such as Amberlysts 15wet, 35wet, and 39wet are effective catalysts than HZSM-5 for this reaction. The activation energy of the forward reaction was found to be 14.1 kcal/mol. A propionic acid molecule is adsorbed on the acid site of the resin and protonated first and then reacted with an *n*-butanol molecule in the bulk liquid to form *n*-butyl propionate and water. The heat of reaction determined from the experimental data is quite small, indicating that this reaction is essentially isothermal. However, the reversible esterification of acetic acid with 1-butanol under the temperature range of 353.15 K to 393.15 K (Grob and Hasse, 2005) was investigated. Based on the final product as 1-butyl acetate and water result different modeling approaches *G*E models NRTL, UNIQUAC, PC-SAFT as well as COSMO-RS are compared.

Heteropolyacids supported on activated carbon have been shown to be efficient solid catalysts for the esterification of acrylic acid by butanol in liquid phase (DuPont et al., 1995). The reaction was carried out under batch and flow conditions. The authors have explained the supported heteropolyacids shown better activity per proton than do conventional catalysts such as sulfuric acid or resins. It was also proved that under flow conditions deactivation of the catalyst was low from 43 to 32% conversion. The formation of *n*-butyl acetate in the presence of heterogeneous catalysts was also esterified *n*-butanol with acetic acid (Blagova et al., 1995) at temperature varying between 100 and 120^{0}C. Three ion-exchange resin catalysts CT-269 mono-sulfonated, Amberlyst-46 surface-sulfonated and Amberlyst-48 bi-sulfonated are similar matrix but different sulfonation. It is concluded that the esterification occurs mainly on or near the external surface of catalysts particles whereas side reactions occur mainly in the pores. In this study shows that the ion-exchange capacity of A-46 is nearly five times lower than that of CT-269. A detailed study of the esterification of propanoic acid by butanol or 2-ethylhexanol over hetero- polyacids catalyst (DuPont and Lefebvre, 1996) has been carried out under homogeneous reaction phase. It was also showing that the reaction rate is proportional to the concentration of protons, and the activity loss increases with the surface area of the carbon support. Two heteropolyacids such as 12-tungstophosphoric and 12-tungstosilicic acids were chosen for the esterification reaction which is totally selective for the formation of the ester and water and can be performed until a conversion of 100% is reached by elimination of water by azeotropic distillation.

Esterification of acrylic acid with 1-butanol has been studied (Chen et al., 1999) in a heterogeneous solid liquid reaction system using a variety of solid acids. Cs2.5H0.5PW12O40 exhibited the highest catalytic activity in the unit of catalyst weight among the solid oxide catalysts, while the activity of Cs2.5H0.5PW12O40 was less than those of organic resins such as Nafion and Amberlyst 15.

2.2 Esterification of acetic acid with methanol

To investigate the similarities and differences between heterogeneous and homogeneous catalyzed esterification, the kinetics of acetic acid esterification with methanol (Liu et al., 2006) were investigated using a commercial Nafion/silica nanocomposite catalyst (SAC-13) and H_2SO4, respectively. Reactions were carried out in an isothermal well-mixed batch reactor at 60^0C. It was found that the resin/silica composite is strongly acidic, with highly accessible sites and sufficient robustness to withstand reasonably high temperatures upto 200^0C and attrition stress. Reaction on SAC-13 appears to involve single-site catalysis with a probable rate-controlling Eley-Rideal surface reaction, which reaction mechanism involving a nucleophilic attack between adsorbed carboxylic acid and un-adsorbed alcohol as the rate limiting step.

The adsorption equilibrium constants, dispersion coefficients and kinetic parameters were obtained as most three different useful applications of the reversible reaction (Yu et al. (2004)) of acetic acid and methanol catalyzed by Amberlyst-15 ion exchange resins. Experiments were conducted in a packed bed reactor in the temperature range 313–323K using a rectangular pulse input. The synthesis of methyl acetate, it has found that idea of recovery of dilute acetic acid from wastewater, and the hydrolysis of methyl acetate. The quasi-homogeneous kinetic model and linear adsorption isotherm are much applicable because of the solvent, methanol or water is present at a large excess concentration. It was also found that, with the increase of temperature, adsorption constants decrease, both the forward and backward reaction rate constants increase, and the reaction equilibrium constants for the forward reaction decrease while that for the backward reactions increase. Another esterification isothermal batch experiments carried out between acetic acid with methanol in the presence of hydrogen iodide (Ronnback et al., 1997) at temperature of 30-60^0C. The catalyst concentration was varied between 0.05 and 10.0 wt%. It was explained that the protolysis equilibria of the acids and the influence of the activity coefficients on the equilibria. Another paper has reported the impact of carboxylic acid chain length on the kinetics of liquid-phase acid-catalyzed esterification over sulfuric acid and a commercial Nafion/silica composite solid acid catalystSAC-13(Liu et al., 2006). Initial kinetics was measured for the reactions of a series of linear chain carboxylic acids such as acetic, propionic, butyric, hexanoic, and caprylic acid with methanol at 60^0C. It was shown that reaction rate decreased as the number of carbons in the linear alkyl chain increased for both H_2SO4 and SAC-13. It has done work on a set of linear-chain carboxylic acids (acetic acid [HAc], propionic acid [HPr], butyric acid [HBu], hexanoic acid [HHx], caprylic acid [HCp]).The same author (Liu et al., 2006) report the impact of water on liquid-phase sulfuric acid catalyzed esterification of acetic acid with methanol at 60^0C. In order to diminish the effect of water on the catalysis initial reaction kinetics were measured using a low concentration of sulfuric acid and different initial water concentrations. The decrease in initial reaction kinetics with increasing concentration of water indicated that catalysis is impaired as esterification proceeds and water is continuously produced from the condensation of carboxylic acids and alcohols. The negative impact of water on catalysis was found to be essentially independent of temperature or molar ratio of methanol-to-acetic acid under the experimental conditions used. The simultaneous water removal during reaction should not only inhibit the reverse hydrolysis reaction, but also preserve high activity of the catalytic protons throughout reaction. Esterification kinetics of propanoic acid with methanol in the presence of a fibrous polymer-supported sulphonic acid catalyst as well as a conventional resin catalyst (Lilja et al., 2002) was reported. Kinetic experiments were carried out in a batch reactor isothermally at 55, 60 and 63^0C and with different initial molar ratios of propanoic acid and methanol to 1:1, 2:3 and 3:2 with the conventional catalyst, Amberlyst 15. It was found that the reaction rate was higher with the fibre catalyst than with the Amberlyst 15 and achieved apparent second-order rate constant equal to $1.82 \times 10{-}3$ $dm^3/(mol^2$ g min) at 60^0C with the initial molar ratio 1:1 and $7.03 \times 10{-}4$ $dm^3/(mol^2$ g min) for the conventional catalyst under comparable conditions. The author and their co-workers were demonstrated the ability of the fibrous polymer-supported sulphonic acid catalyst in the esterification of propanoic acid with methanol and to develop an advanced kinetic model for the esterification. The reaction rate was higher over the fibre catalyst as Smopex-101than over a conventional resin catalyst asAmberlyst-15. It has reported that the increase of the temperature as well as the initial molar ratio of propanoic acid and methanol increased the esterification rate. The degree of cross-linking of the fibre catalyst and different fibre dimensions did not affect the reaction rate.

2.3 Esterification of acetic acid with ethanol

Most of the commercial processes for ethyl acetate production are via liquid-phase esterification (Wu et al., 2004). The reactions were conducted at temperature range of 363 to 400 K, with molar ratio of ethanol to acetic acid 1.5. Author has reported that the temperature is critical parameters in this novel EAc synthesis process and the one-pass ethanol conversion was successfully improved from 67 to 85 mol%. It has found maximum yield for ethyl acetate to not more than 67%. The equilibrium constant is almost constant and is independent of the reaction temperature while the ethanol concentration in the products flow decreased from 14 to 6.5 wt%. The reduction of ethanol concentration is advantageous for further purification processes.

Ethanol is converted into ethyl acetate with high selectivity over Cu-ZnO-ZrO_2-Al_2O_3 catalyst, together with low selectivity to methyl ethyl ketone. The ethyl acetate production ability of catalyst is roughly proportional to the Cu surface area of the Cu-ZnO-ZrO_2-Al_2O_3 catalyst. The highest ethanol conversion, the highest ethyl acetate selectivity, and the highest space-time yield of ethyl acetate were achieved at Cu content of 70 mol%. The additive oxides as ZnO, ZrO_2, and Al_2O_3 (Inui et al., 2002) are necessary for the selective ethyl acetate formation.

The kinetics of esterification of maleic acid with ethanol over cheap and easily available catalysts, ion-exchange resins and clay supported heteropoly acids (Yadav and Thathagar, 2002) over detail study has been done by authors and achieved the order of catalytic activity as

Amberlyst-36, Amberlyst-15, Indion-170, Amberlyst-18, Amberlite IRA SL 400, Filtrol-24.20% and DTP/K-10. A pseudo-homogeneous kinetic model was developed and the activation energy was found to be 14.2 kcal.

The esterification of acetic acid with ethanol, catalyzed both homogeneously by the acetic acid, and heterogeneously by Amberlyst 15, has been carried out at (Calvar et al., 2007) several temperatures between 303.15 and 353.15K and at various starting reactant compositions. The influence of feed composition and reflux ratio has been analyzed in packed column which is filled by Amberlyst 15. The best results have been obtained using the ASOG method to calculate the activity coefficients.

Another esterification process was reported by Yang et al. (2004) which occurred between the lactic acid and ethanol over five different cation-exchange resins. The effect of catalyst type, catalyst loading, and temperature on reaction kinetics was evaluated. In order to study in this paper the authors has analysed that which components is the strongest adsorption strength on the resin surface. It also has studied to simplified two mechanisms based on Lanwt%uir– Hinselwood model. The thermal stability and mechanical strength of the resin catalysts were tested by SEM. The order of catalytic activity was found to be: D002<D001<Amberlyst-15< NKC<002. Activation energies were found to be 51.58 KJ/mol and 52.26 KJ/mol, which suggested that this reaction was kinetically controlled. Pervaporation-aided esterification of acetic acid with ethanol was reported by some authors (Tanaka et al., 2001) at 343K over zeolite T membranes. Almost complete conversion was reached within 8 h when initial molar ratios of alcohol to acetic acid were 1.5 and 2.

2.4 Esterification of acetic acid with other alcohol

The kinetic behavior of the heterogeneous esterification of acetic acid with amyl alcohol over an acidic cation-exchange resin and Dowex 50Wx8-100 was (Wu and Lin, 2000) reported. The experiments were conducted in a fixed-bed reactor at temperatures from 323 to 393 K and at molar ratios of feed (amyl alcohol to acetic acid) vary from 1 to 10. Report has shown equilibrium conversion of acetic acid increase with increasing reaction temperature. The kinetic data were correlated with the quasi-homogeneous, Langmuir-Hinshelwood, Eley-Rideal, and modified Langmuir-Hinshelwood models. The modified Langmuir-Hinshelwood model yielded the best representation for the kinetic behavior of the reaction over wide ranges of temperature and feed composition. The formation of a gaseous phase, when the reactor operated at 393 K, is also of great advantage for the forward reaction esterification.

The esterification rate constant of the most active modification of the new catalyst was obtained at 55^{0}C, which clearly exceeds the corresponding value obtained with a traditional polyvinylbenzene supported catalyst. The esterification of acetic acid with methanol (Arvela et al., 1999) was selected to the model system. They have been determined the kinetic parameters both by using the activity coeficients and without the activity coeficients.. The apparent activation energies are for Amberlyst 15 was found 106 kJ/mol, for Smopex 101 133 kJ/mol, and for PE-UHS 86kJ/mol. The value of the equilibrium constant was estimated to be 4.0 to 5.0 at the reference temperature 55^{0}C. The values of the kinetic parameters also confirm that Smopex 101 is an efficient esterification catalyst.

However, Kinetics of heterogeneous catalysed esterification of acetic acid with isoamyl alcohol was studied over cation-exchange resin catalyst, Purolite CT-175, in a stirred batch reactor to produced isoamyl acetate (Teo and Saha, 2004). The equilibrium conversion of acetic acid was found to increase slightly with an increase in temperature from 333 to 363 K and also it increased appreciably with an excess of isoamyl alcohol in the reacting system. In their report it has explained towards understanding the chemistry of the reaction and obtaining a suitable rate expression and checking its validity under different experimental conditions as molar feed ratios (of isoamyl alcohol to acetic acid) of 1:1 to 10:1. LHHW model gave a better representation of the kinetic behaviour for all practical purposes on the reaction kinetics studied under the given conditions. According to the LHHW mechanism, acetic acid adsorbed on one catalytic centre reacts with isoamyl alcohol adsorbed on another catalytic centre to give isoamyl acetate and water each adsorbed on one centre.

Isopropyl lactate is a very important pharmaceutical intermediate. The current paper deals with the application of heterogeneous catalysts Indion-130, Ambelyst-36, Amberlyst-15, Amberlite-120, Dowex 50W, Filtrol-44, 20% DTPA/K-10 Amongst these Amberlyst-36, Amberlyst-15 and Indion-130 were observed to be most effective. The emphasis of the work by Yadav and Kulkarni (2000) were well study in detail the kinetics of esterification of lactic acid with isopropanol over cheap and easily available catalysts, ion-exchange resins and clays and clay supported heteropoly acids. The Amberlyst-36 was found to be the best catalyst. Aim of this literature (Corma et al., 1989) is to establish the relationship between the characteristics of HY zeolite and its catalytic activity in the esterification of carboxylic esters. A more precise understanding of the factors governing the catalytic properties of these inorganic materials has been obtained, and some progress has been made in the design of more adequate zeolites for general organic syntheses.The best materials are, therefore, obtained by dealuminating the zeolite to a framework Si/Al ratio of at least 15. These dealuminated materials have an average activity per acid site very similar to that found for sulfuric acid. Additionally these heterogeneous catalysts can overcome equilibrium limitations due to the hydrophobicity of their surfaces, where the concentration of water must be quite small. zeolite catalysts have been found to be especially valuable for the direct esterification of phenols. Yeramian et al. (1968) proposed the vapor-phase reactions catalyzed by ion exchange resins with isopropyl alcohol with acetic acid. The esterification reactions have been done at three different temperatures 110^0, 116^0 and 120°C. In this case it was found that the experimental data are explained fairly well by a Hinshelwood-Langmuir model. He has found that the influence of both reactants much important and no general order of reaction with respect to them can be deduced, he has been also found that both esterification and dehydration reactions proceed through the same rate mechanism. Chakrabarti and Sharma (1991) have studied on esterification of acetic acid with styrene in the presence of cation exchange resins as catalysts in the temperature range 20-60°C. The reaction was accompanied by dimerization of styrene. The selectivity with respect to the ester was greatly influenced by the catalyst, solvent and operating conditions. Monodisperse K2661 was found to be the best catalyst amongst those studied.

Dynamics of a chromatographic reactor and develope a kinetic model for the esterification of acetic acid with methanol in presence of homogeneous acid catalyst (Mazzotti et al. and Ronnback et al., (1997)) was studied. The synthesis of ethyl acetate and water from ethanol and acetic acid on a commercial polystyrene-divinylbenzene acidic resin is considered. The chromatographic reactor exhibits a rather rich dynamical behavior, which is a consequence of the dual role, as a catalyst and as a selective sorbent, played by the resin. The esterification kinetics was studied with isothermal batch an experiment at 30^0-60^0C and catalyst concentration was varied between 0.05 and 10.0 wt%. The experiments revealed that besides the main reaction, the esterification of acetic acid, a side reaction appeared. Tzong Liu et al. (2001) was determined the kinetic data on the esterification of propionic acid with *n*-butanol catalyzed by Amberlyst 15, Amberlyst 35, Amberlyst 39, and HZSM-5 pellets and at the temperatures from 353 to 383 K in a stirred batch reactor. The data indicated that the Amberlyst series resins were all effective to carry out this esterification. The activation energy of the forward reaction was found to be 14.1 kcal/mol and, kinetic model devlopedaccording Rideal-Eley theory. Also he has found that activity-based equilibrium constant increase slightly with an increase in temperature.

the esterification of acetic acid with isobutanol under uncatalyzed and heterogeneously catalyzed reactions condition using a stirred batch reactor in dioxane has been addressed. The equilibrium constant, which is independent of temperature ranging from 318 to 368 K, was found to be 4. It was also studied as excess of glycol diacetate (Shlechter et al. and Ince, 2002) equivalent to the amount which would be present in an extract layer from a liquid extractton column, using butylene glycol diacetate as a solvent for the recovery of glycol. (Gangadwala et al., Gelosa et al. and Altokka et al. (2003)) were reported esterification of acetic acid with butanol and glycerol with acetic acid and acetic acid with isobutanol in the presence of amberlyst catalyst respectively. Pseudohomogeneous, Eley-Rideal, Langmuir-Hinshelwood-Hougen-Watson (LHHW), and modified LHHW models were developed. The kinetics for the side-reaction etherification was also investigated. The equilibrium constant, which is independent of temperature ranging from 318 to 368 K, was found to be 4. Reactive chromatography is an attractive method for chemical synthesis because chemical reactions and product separation occur simultaneously in the same unit. In this work, the synthesis of triacetine, starting from glycerol and acetic acid, using reactive chromatography on acidic polymeric resins is investigated. The obtained data was compared with the predictions of a mathematical model, which kinetic and equilibrium parameters were estimated from the batch experiments mentioned above. Teo et al. and Kirumakki et al. (2004) have studied on esterification of acetic acid with isoamyl alcohol and benzyl alcohol over heterogeneous catalysed as zeolites H, HY and HZSM5 were studied in this report. The equilibrium conversion of acetic acid was found to increase slightly with an increase in temperature from 333 to 363 K and also it increased appreciably with an excess of isoamyl alcohol in the reacting system. The pore architecture seems to influence the product selectivity.

The reaction kinetics of the reversible liquid-phase esterification of acetic acid with 1-butanol was investigated at temperatures between 353.15 and 393.15 K using sulfuric acid as catalyst. Different thermodynamic models are compared: NRTL, UNIQUAC, and PC-SAFT. The weight-based activity of the heterogeneous catalysts decreases in the following order: Smopex-101 > Amberlyst 15 > sulphated ZrO2 > H-USY-20 > H-BETA-12.5 > H-MOR-45 > Nb2O5 > H-ZSM-5-12.5. The low activity of ZSM-5 is a result the influence of the Si/Al ratio Grob et al. and Peters et al. (2006). Liquid-phase esterification of acetic acid with isobutanol catalyzed by ion-exchange resins and manganese nodule leached residue was explained (Izci et al. Das et al. and parida (2007)). As a result, it was found that the weight-based activity of the heterogeneous catalysts increases in the following order: Dowex 50 Wx_2 > Amberlite IR- 120 and these catalysts were effectively for the synthesis of isobutyl acetate under these experimental conditions (Izci et al. Das et al. and parida (2007)). Water-washed manganese nodule leached residue (WMNLR) calcined at 400 ◦C shows highest catalytic activity with 76.6% conversion having 100% selectivity towards *n*-butyl acetate.

Schmid et al. (2008) was studied on esterification of ethylene glycol with acetic acid catalyzed by amberlyst 36 and has found the reaction kinetics and the chemical equilibrium at various temperatures, range from 333.15 to 363.15 K and starting compositions. Liao et al. (2009) was presented review on triacetylglycerol with glycerol by two steps such as esterification and acetylation. A two-step method is proposed to obtain high selectivity and high conversion rate for producing additive triacetylglycerol of biofuel from its byproduct glycerol. Amberlyst-35 was found to be an excellent catalyst. The optimal conditions are temperature of 105 °C and an acetic acid to glycerol molar ratio of 9:1 with 0.5 g catalyst. After the 4 hour reaction of the optimal condition, the selectivity of triacetylglycerol reaches almost 100% in 15 min by adding thereto acid anhydride.

CHAPTER 3

THE PRESENT WORKS AND APPLIED REACTION MECHANISM

THE PRESENT WORKS AND APPLIED REACTION MECHANISM

3.1 Present works

The esterification reaction is widely used in the chemical reaction process to form ester. Esterification reaction is generally carried out between alcohol and carboxylic acid with or without presence of acid catalyst. There are many work has been done previous with different alcohol and acetic acid reaction system to form value added products, but ethylene glycol and acetic acid reaction system has been found limited work in few literature . However the valuable products as ethylene glycol mono and di-acetate obtained from ethylene glycol and acetic acid reaction system, which is used as different application in many chemical and other industries.

Present work is an esterification of ethylene glycol with acetic acid in the presence of SERALITE SRC-120 and molecular sieve 13X as catalysts. The aim of present work to analyzes the effect of amount of catalyst loading, reactant molar ratio and reaction temperature on the product selectivity and reactant conversion. However some simulation work also has been done to obtain the value of chemical equilibrium constant, activation energy and rate of reaction. The equilibrium constant K1, K-1, K2 and K-2 has been calculated based on mole fraction and also determined the percentage selectivity and conversion of product and reactant respectively.

3.2 Reaction Mechanism

Acetic acid reacts with ethylene glycol in the presence of ion-exchange resin as a catalyst to produce the ester as ethylene glycol mono and di-acetate. Esterification reaction is very slow at without catalyst and it is also a type of reversible reaction. Due to reverse reaction it produce excess amount of water during reaction and the water reduces formation of ester as a products. This reverse reaction is following as hydrolysis reaction.

The experimental reaction was carried out in generally following two steps, first the reaction between ethylene glycol and acetic acid over acid catalyst and formation of ethylene glycol mono-acetate, second following consecutive step is ethylene glycol mono-acetate to ethylene glycol di-acetate. This reaction mechanism can be understood with help scheme 1. The equilibrium constant K1, K-1, K2 and K-2 has been calculated in mole fraction basis and also determined the percentage selectivity and conversion of product and reactant respectively.

$$\mathbf{C_2H_6O_2 + C_2H_4O_2 \xrightleftharpoons[K_{-1}]{K_1} C_4H_8O_3 + H_2O \ldots\ldots\ldots\ldots I}$$

$$\mathbf{C_4H_8O_3 + C_2H_4O_2 \xrightleftharpoons[K_{-2}]{K_2} C_6H_{10}O_4 + H_2O \ldots\ldots\ldots\ldots II}$$

Scheme 1

$$\boldsymbol{\frac{dC_{EG}}{dt} = -K_1 C_{EG} C_{AA} + K_{-1} C_{EGMA} C_{H_2O} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \mathbf{III}}$$

$$\boldsymbol{\frac{dC_{EGDA}}{dt} = K_2 C_{EGMA} C_{AA} - K_{-2} C_{EGDA} C_{H_2O} \ldots\ldots\ldots\ldots\ldots\ldots\ldots. \ldots. \mathbf{IV}}$$

Arrhenius equation:

$$\mathbf{K = K_0 e^{-\frac{E}{RT}}}$$

For equation III:

Rate of forward reaction = K_1 [C_{EG}] [C_{HAC}]

Rate of reverse reaction = K_{-1} [C_{EGMA}] [C_{H_2O}]

For equation IV:

Rate of forward reaction = K_2 [C_{EGMA}] [C_{HAC}]

Rate of reverse reaction = K_{-2} [C_{EGDA}] [C_{H_2O}]

CHAPTER 4

EXPERIMENTAL SETUP

4.1 Experimental Apparatus and gas-liquid chromatograph

Figure. 4.1. Experimental setup, gas-liquid chromatography and chemicals

4.2 Chemicals and catalyst material

Ethylene glycol and acetic acid (aldehyde free) were purchased from Merck Specialisties Pvt. ltd. Mumbai (India). The conversion of ethylene glycol with acetic acid was catalysed in the presence ion-exchange resin SERALITE SRC-120 and Molecular Sieve 13x purified from Sisco Research Laboratories Pvt Ltd Mumbai (India). The final product ethylene glycol mono acetate and di-acetate has been analyzed by liquid-gas chromatograph. The average pore diameter of Molecular sieve 13x with 10 A^0 and SERALITE SRC-120 with 8% crosslinking have been used in experiment.

4.3 Physical and chemical properties[6]

Component / Property	Ethylene glycol	Acetic acid	Ethylene glycol mono-acetate	Ethylene glycol di-acetate
Formula	$C_2H_6O_2$	$C_2H_4O_2$	$CH_3COOCH_2CH_2OH$	$CH_3COOCH_2CH_2OOCCH_3$
Physical state	Clear liquid	Clear liquid	Clear liquid	Clear liquid
Molecular weight	62.07	60.05	104.11	146.14
Boiling point (^0C)	195	118	186 - 189	186 - 191
Specific gravity	1.115	1.049	1.15	1.20
Flash point (^0C)	111	39	102	82
Stability	Stable under ordinary conditions	Stable under ordinary conditions	Stable under ordinary condition	Stable under ordinary conditions

4.4 Catalyst property[7]

<table>
<tr><td>Name of catalyst</td><td>Physically</td><td>Loss on drying</td><td>Ionic form</td><td>pH range</td><td>Particle size</td><td>Cross linking</td></tr>
<tr><td>SERALITE SRC-120 Standard grade</td><td>Yellow-brown resinous beads</td><td>Max 45-50%</td><td>H^+</td><td>0-14</td><td>20-50mesh</td><td>8%</td></tr>
<tr><td colspan="7">Molecular Sieve 13X[8]</td></tr>
<tr><td colspan="4">Physically</td><td colspan="3">Pale brown granules or pellets,</td></tr>
<tr><td colspan="4">Normal pore diameter</td><td colspan="3">9 A^0 (0.9 micron)</td></tr>
<tr><td colspan="4">Type of crystal structure</td><td colspan="3">Hexagonal</td></tr>
<tr><td colspan="4">Bulk density</td><td colspan="3">680 g/l</td></tr>
<tr><td colspan="4">Equilibrium water capacity at 20 C./55 % R.H.</td><td colspan="3">25 % wt.</td></tr>
<tr><td colspan="4">Water content</td><td colspan="3">1.5% wt. (max.)</td></tr>
<tr><td colspan="4">Heat of adsorption</td><td colspan="3">4200 KJ/Kg water (max.)</td></tr>
<tr><td colspan="4">Specific heat (approx.)</td><td colspan="3">1.07 KJ/Kg ^{0}C</td></tr>
<tr><td colspan="4">Pellets Size Normal</td><td colspan="3">1.5mm 3mm</td></tr>
<tr><td colspan="4">Beads sizes normal</td><td colspan="3">1.5 mm 3 mm</td></tr>
</table>

4.5 Procedure

All kinetic experiments have been carried out in a three necked glass reactor with a volume of 250 cm^3. Experimental setup has consists of magnetic stirrer, condenser, temperature sensor and thermometer. To maintain the preselected constant temperature within ±0.2 K the reactor is equipped with temperature controller with sensor. Magnetic stirrer and temperature controller are equipped together. However magnetic stirrer has used to well mix-up the reactant mixture during reaction process and temperature controller has to maintain the temperature at constant. Temperature sensor is applied for set the temperature with help of thermometer, which is deep inside in the reaction mixture. The temperature can be measured with ± 0.02 K in the investigated temperature range. For all experiment ethylene glycol and acetic acid should be consists with certain molar ratio, also catalyst should be certain amount. For that purpose have been used pipette, measuring cylinder and weighing machine. To start the experiment first of all certain amount of ethylene glycol and catalyst were placed in the reactor and wait until the desired temperature reached. When desired temperature reached it should be kept constant, after that second reactant acetic acid was place in reactor with the help of funnel, and then stirrer was start immediately. After temperature constancy was reached, the reactants were mixed and time measurement was started. To achieve the chemical equilibrium, the experiment was carried out about 10 to 12 hour, during reaction period of time 10 to 12 samples were taken and kept inside sample bottle. The samples were analyzed by liquid-gas chromatography with oven temperature programmed as start from 60^0C with increasing 15^0C per minute up to 200^0C. Sample has injected in chromatograph with amount of 2µl. To obtained proper correct results, each sample was analyzed three times and average value was taken for further calculation. The experiment has been carried out at 333, 343, 353 and 363K reaction temperature and 0.5, 1.0, 1.5 and 2.0gm of catalyst with different molar ratio 0.66, 1.5 and 3.0 of reactant.

CHAPTER 5

RESULTS

5.1 Observation table on different catalyst loading, reaction temperature and molar ratio with reaction time:

Table 5.1 Variation of different parameter at 0.5wt% catalyst loading, 333K reaction temperature and 3.0 molar ratio of AA to EG

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	74.5000	0.2500	0.8571	24.1829	0.2100
15.0000	73.5000	0.7600	1.8639	23.3661	0.5100
30.0000	71.7800	2.1600	2.8507	22.1833	1.0260
60.0000	67.9000	5.6000	4.6752	19.6348	2.1900
120.0000	64.4000	8.1600	7.0948	17.1052	3.2400
240.0000	61.8700	10.9700	7.4768	15.6842	3.9990
360.0000	58.7600	12.7300	10.3601	13.2179	4.9320
480.0000	57.8000	13.8500	10.4285	12.7015	5.2200
600.0000	57.0500	14.6800	10.5460	12.2790	5.4450

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.00	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.00	0.7510	0.0010	0.0050	0.0071	0.2359	0.9308	2.4885	70.6450	29.3550
15.00	0.7409	0.0031	0.0108	0.0171	0.2279	2.2606	5.7819	63.2550	36.7450
30.00	0.7236	0.0089	0.0166	0.0345	0.2164	4.5478	10.5513	48.0891	51.9109
60.00	0.6845	0.0232	0.0272	0.0736	0.1915	9.7074	20.8275	36.9486	63.0514
120.00	0.6492	0.0338	0.0413	0.1089	0.1669	14.3617	31.0273	37.8994	62.1006
240.00	0.6237	0.0454	0.0435	0.1344	0.1530	17.7260	36.7573	32.3597	67.6403
360.00	0.5923	0.0527	0.0603	0.1657	0.1289	21.8617	46.7020	36.3563	63.6437
480.00	0.5827	0.0574	0.0606	0.1754	0.1239	23.1383	48.7842	34.5772	65.4228
600.00	0.5751	0.0608	0.0613	0.1830	0.1198	24.1356	50.4879	33.5219	66.4781

Table 5.2 Variation of different parameter at 0.5wt% catalyst loading, 343K reaction temperature and 3.0 molar ratio of AA to EG

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.00	75.20	0.00	0.00	24.80	0.00
5.00	73.75	0.65	1.59	23.58	0.44
15.00	72.65	1.36	2.48	22.74	0.77
30.00	70.90	3.03	3.14	21.64	1.29
60.00	65.07	7.50	6.87	17.52	3.04
120.00	62.40	9.77	8.27	15.72	3.84
240.00	58.90	12.76	10.07	13.38	4.89
360.00	56.57	13.98	12.38	11.49	5.59
480.00	54.87	15.49	13.17	10.37	6.10
600.00	54.20	16.52	12.86	10.12	6.30

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	**EGDA**	**EGMA**	**Water**	**EG**	**AA**	**EG**	**EGMA**	**EGDA**
0.00	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.00	0.7434	0.0027	0.0092	0.0146	0.2300	1.9282	4.9286	63.1549	36.8451
15.00	0.7324	0.0056	0.0144	0.0257	0.2219	3.3909	8.2961	56.1640	43.8360
30.00	0.7147	0.0126	0.0182	0.0433	0.2111	5.7181	12.7282	42.0832	57.9168
60.00	0.6559	0.0311	0.0400	0.1021	0.1709	13.4707	29.3658	39.1471	60.8529
120.00	0.6290	0.0405	0.0481	0.1290	0.1534	17.0213	36.6038	37.2645	62.7355
240.00	0.5938	0.0529	0.0586	0.1643	0.1305	21.6755	46.0673	35.6584	64.3416
360.00	0.5703	0.0579	0.0720	0.1878	0.1120	24.7739	53.6866	38.3230	61.6770
480.00	0.5531	0.0642	0.0766	0.2049	0.1012	27.0346	58.1843	37.3757	62.6243
600.00	0.5464	0.0684	0.0748	0.2117	0.0987	27.9255	59.2122	35.3424	64.6576

Table 5.3. Variation of different parameter at 0.5wt% catalyst loading and 353K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	72.7500	1.2000	2.5370	22.7779	0.7350
15.0000	71.3400	2.2000	3.5564	21.7456	1.1580
30.0000	67.5500	5.4000	5.5668	19.1882	2.2950
60.0000	63.6300	8.8900	7.3894	16.6196	3.4710
120.0000	61.1200	10.9200	8.8480	14.8879	4.2240
240.0000	57.9600	13.8000	10.2224	12.8456	5.1720
360.0000	55.3400	15.1500	12.8404	10.7116	5.9580
480.0000	53.7000	16.7500	13.4036	9.6964	6.4500
600.0000	52.3100	17.5000	14.7445	8.5785	6.8670

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.0000	0.7334	0.0050	0.0148	0.0247	0.2222	3.2580	8.1535	59.7425	40.2575
15.0000	0.7192	0.0091	0.0207	0.0389	0.2121	5.1330	12.3161	53.1547	46.8453
30.0000	0.6809	0.0224	0.0324	0.0771	0.1872	10.1728	22.6283	41.9821	58.0179
60.0000	0.6414	0.0368	0.0430	0.1166	0.1621	15.3856	32.9856	36.8465	63.1535
120.0000	0.6161	0.0452	0.0515	0.1419	0.1452	18.7234	39.9680	36.2546	63.7454
240.0000	0.5843	0.0572	0.0595	0.1738	0.1253	22.9255	48.2031	34.2084	65.7916
360.0000	0.5579	0.0628	0.0747	0.2002	0.1045	26.4096	56.8081	37.3008	62.6992
480.0000	0.5413	0.0694	0.0780	0.2167	0.0946	28.5904	60.9017	35.9668	64.0332
600.0000	0.5273	0.0725	0.0858	0.2307	0.0837	30.4388	65.4092	37.1622	62.8378

Table 5.4. Variation of different parameter at 0.5wt% catalyst loading and 363K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% of Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	71.5800	2.4000	2.8555	22.0785	1.0860
15.0000	69.0400	4.5000	4.2663	20.3456	1.8480
30.0000	65.2500	7.3500	6.7754	17.6396	2.9850
60.0000	60.7500	10.9800	9.4039	14.5311	4.3350
120.0000	58.0000	13.2800	10.8938	12.6661	5.1600
240.0000	56.5800	14.5900	11.4889	11.7551	5.5860
360.0000	53.8100	16.3600	13.7686	9.6444	6.4170
480.0000	52.7000	17.5200	14.0400	8.9900	6.7500
600.0000	50.6900	18.5000	16.1278	7.3292	7.3530

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.0000	0.7216	0.0099	0.0166	0.0365	0.2154	4.8138	10.9737	45.5079	54.4921
15.0000	0.6960	0.0186	0.0248	0.0621	0.1985	8.1915	17.9611	39.9571	60.0429
30.0000	0.6578	0.0304	0.0394	0.1003	0.1721	13.2314	28.8726	39.2853	60.7147
60.0000	0.6124	0.0455	0.0547	0.1457	0.1418	19.2154	41.4069	37.5455	62.4545
120.0000	0.5847	0.0550	0.0634	0.1734	0.1236	22.8723	48.9269	36.5402	63.4598
240.0000	0.5704	0.0604	0.0668	0.1877	0.1147	24.7606	52.6004	35.5972	64.4028
360.0000	0.5424	0.0678	0.0801	0.2156	0.0941	28.4441	61.1112	37.1361	62.8639
480.0000	0.5313	0.0726	0.0817	0.2268	0.0877	29.9202	63.7499	35.9999	64.0001
600.0000	0.5110	0.0766	0.0938	0.2471	0.0715	32.5931	70.4468	37.9621	62.0379

Table 5.5. Variation of different parameter at 1.0wt% catalyst loading and 333K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	73.5800	0.7000	1.8107	23.4233	0.4860
15.0000	72.0800	1.7000	2.9860	22.2979	0.9360
30.0000	70.0000	3.5000	4.0270	20.9130	1.5600
60.0000	63.6500	8.8000	7.4830	16.6020	3.4650
120.0000	59.2700	12.2000	10.2311	13.5198	4.7790
240.0000	55.6000	15.0300	12.5607	10.9293	5.8800
360.0000	51.5400	17.3000	16.3641	7.6979	7.0980
480.0000	50.2000	18.3400	17.2051	6.7549	7.5000
600.0000	49.3600	18.9700	17.7635	6.1544	7.7520

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000		
5.0000	0.7417	0.0029	0.0105	0.0163	0.2285	2.1542	5.5513	64.4846	35.5154
15.0000	0.7266	0.0070	0.0174	0.0315	0.2175	4.1489	10.0890	55.2157	44.7843
30.0000	0.7056	0.0145	0.0234	0.0524	0.2040	6.9149	15.6734	44.6784	55.3216
60.0000	0.6416	0.0365	0.0435	0.1164	0.1620	15.3590	33.0564	37.3776	62.6224
120.0000	0.5975	0.0505	0.0595	0.1606	0.1319	21.1835	45.4845	37.0533	62.9467
240.0000	0.5605	0.0623	0.0730	0.1976	0.1066	26.0638	55.9303	36.9723	63.0277
360.0000	0.5196	0.0717	0.0952	0.2385	0.0751	31.4627	68.9600	39.9020	60.0980
480.0000	0.5060	0.0760	0.1001	0.2520	0.0659	33.2447	72.7625	39.7041	60.2959
600.0000	0.4976	0.0786	0.1033	0.2605	0.0600	34.3617	75.1837	39.6602	60.3398

Table 5.6. Variation of different parameter at 1.0wt% catalyst loading and 343K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	72.5100	1.7000	2.2407	22.7423	0.8070
15.0000	70.2500	3.2000	4.0211	21.0439	1.4850
30.0000	65.5000	7.3000	6.4133	17.8767	2.9100
60.0000	59.9200	12.1000	9.2469	14.1490	4.5840
120.0000	53.9000	14.5000	16.2624	8.9476	6.3900
240.0000	50.8000	16.9300	18.1738	6.7761	7.3200
360.0000	48.1200	19.7800	18.7589	5.2171	8.1240
480.0000	47.6000	20.1000	19.2043	4.8156	8.2800
600.0000	46.8000	21.1000	19.1664	4.4136	8.5200

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.0000	0.7309	0.0070	0.0130	0.0271	0.2219	3.5771	8.2973	48.0569	51.9431
15.0000	0.7082	0.0133	0.0234	0.0499	0.2053	6.5824	15.1455	46.8657	53.1343
30.0000	0.6603	0.0302	0.0373	0.0978	0.1744	12.8989	27.9166	38.1442	61.8558
60.0000	0.6040	0.0501	0.0538	0.1540	0.1380	20.3191	42.9474	34.9135	65.0865
120.0000	0.5433	0.0601	0.0946	0.2147	0.0873	28.3244	63.9211	44.0478	55.9522
240.0000	0.5121	0.0701	0.1057	0.2460	0.0661	32.4468	72.6769	42.9710	57.0290
360.0000	0.4851	0.0819	0.1091	0.2730	0.0509	36.0106	78.9634	39.9647	60.0353
480.0000	0.4798	0.0833	0.1117	0.2782	0.0470	36.7021	80.5821	40.1429	59.8571
600.0000	0.4718	0.0874	0.1115	0.2863	0.0431	37.7659	82.2031	38.9349	61.0651

Table 5.7. Variation of different parameter at 1.0wt% catalyst loading and 353K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	71.5000	2.2000	3.2791	21.9109	1.1100
15.0000	70.0000	3.7000	3.7421	20.9979	1.5600
30.0000	63.2000	8.7000	8.4054	16.0945	3.6000
60.0000	59.2000	11.8000	10.9223	13.2776	4.8000
120.0000	52.8000	16.3000	15.6047	8.5753	6.7200
240.0000	49.9000	17.8000	18.4944	6.2156	7.5900
360.0000	47.4000	18.7000	21.5455	4.0144	8.3400
480.0000	46.6000	21.5000	18.9432	4.3768	8.5800
600.0000	46.1000	21.8000	19.3824	3.9876	8.7300

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.0000	0.7208	0.0091	0.0191	0.0373	0.2138	4.9202	11.6495	51.1289	48.8711
15.0000	0.7056	0.0153	0.0218	0.0524	0.2048	6.9149	15.3310	41.5172	58.4828
30.0000	0.6371	0.0360	0.0489	0.1210	0.1570	15.9574	35.1027	40.4109	59.5891
60.0000	0.5968	0.0489	0.0635	0.1613	0.1295	21.2766	46.4611	39.3835	60.6165
120.0000	0.5323	0.0675	0.0908	0.2258	0.0837	29.7872	65.4223	40.1907	59.8093
240.0000	0.5030	0.0737	0.1076	0.2550	0.0606	33.6436	74.9371	42.1733	57.8267
360.0000	0.4778	0.0775	0.1253	0.2802	0.0392	36.9681	83.8127	44.7127	55.2873
480.0000	0.4698	0.0891	0.1102	0.2883	0.0427	38.0319	82.3515	38.2124	61.7876
600.0000	0.4647	0.0903	0.1127	0.2933	0.0389	38.6968	83.9211	38.4267	61.5733

Table 5.8. Variation of different parameter at 1.0wt% catalyst loading and 363K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	70.5000	3.0000	3.8727	21.2173	1.4100
15.0000	68.5000	4.5000	5.2023	19.7876	2.0100
30.0000	61.7000	10.8000	8.0137	15.4363	4.0500
60.0000	53.2200	15.7800	15.6175	8.7884	6.5940
120.0000	47.6000	18.8000	21.0564	4.2636	8.2800
240.0000	45.3500	20.9000	21.9646	2.8304	8.9550
360.0000	44.0000	21.9300	22.8372	1.8728	9.3600
480.0000	43.7000	22.9000	21.9753	1.9747	9.4500
600.0000	42.9000	23.6000	22.3647	1.4453	9.6900

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000		
5.0000	0.7107	0.0124	0.0225	0.0474	0.2070	6.2500	14.4463	47.5369	52.4631
15.0000	0.6905	0.0186	0.0303	0.0675	0.1930	8.9096	20.2111	44.7964	55.2036
30.0000	0.6220	0.0447	0.0466	0.1361	0.1506	17.9521	37.7568	34.2465	65.7535
60.0000	0.5365	0.0654	0.0908	0.2216	0.0857	29.2287	64.5627	40.9924	59.0076
120.0000	0.4798	0.0779	0.1225	0.2782	0.0416	36.7021	82.8081	44.0143	55.9857
240.0000	0.4572	0.0866	0.1277	0.3009	0.0276	39.6941	88.5872	42.4519	57.5481
360.0000	0.4435	0.0909	0.1328	0.3145	0.0183	41.4893	92.4485	42.2286	57.7714
480.0000	0.4405	0.0949	0.1278	0.3175	0.0193	41.8883	92.0376	40.2478	59.7522
600.0000	0.4325	0.0978	0.1301	0.3256	0.0141	42.9521	94.1723	39.9465	60.0535

Table 5.9. Variation of different parameter at 1.5wt% catalyst loading and 333K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.00	75.20	0.00	0.00	24.80	0
5.00	72.01	1.20	3.82	22.01	0.957014
15.00	67.50	4.00	7.65	18.54	2.310014
30.00	65.00	5.30	10.13	16.51	3.060014
60.00	57.40	10.57	15.79	10.90	5.340014
120.00	53.60	14.76	16.41	8.75	6.480014
240.00	51.60	17.30	16.26	7.76	7.080014
360.00	49.50	18.55	18.12	6.12	7.710014
480.00	48.89	19.90	17.25	6.06	7.893014
600.00	47.78	20.60	18.18	5.21	8.226014

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.0000	0.7259	0.0050	0.0222	0.0322	0.2148	4.2420	11.2368	69.0813	30.9187
15.0000	0.6804	0.0166	0.0445	0.0776	0.1809	10.2393	25.2339	57.3029	42.6971
30.0000	0.6552	0.0220	0.0589	0.1028	0.1611	13.5638	33.4246	57.2924	42.7076
60.0000	0.5786	0.0438	0.0919	0.1794	0.1063	23.6702	56.0673	51.1928	48.8072
120.0000	0.5403	0.0611	0.0954	0.2177	0.0853	28.7234	64.7259	43.8356	56.1644
240.0000	0.5202	0.0717	0.0946	0.2379	0.0757	31.3830	68.7100	39.7492	60.2508
360.0000	0.4990	0.0768	0.1054	0.2591	0.0597	34.1755	75.3196	40.6748	59.3252
480.0000	0.4928	0.0824	0.1003	0.2652	0.0592	34.9867	75.5496	37.8329	62.1672
600.0000	0.4817	0.0853	0.1057	0.2764	0.0509	36.4627	78.9759	38.2512	61.7488

Table 5.10. Variation of different parameter at 1.5wt% catalyst loading and 343K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% of Water
0.00	75.20	0.00	0.00	24.80	0.00
5.00	71.50	2.03	3.52	21.84	1.110014
15.00	65.40	6.30	8.01	17.35	2.940014
30.00	63.30	8.38	8.69	16.06	3.570014
60.00	55.30	14.30	14.12	10.31	5.970014
120.00	51.32	17.00	17.17	7.34	7.164014
240.00	48.23	19.47	19.01	5.20	8.091014
360.00	47.02	20.78	19.24	4.51	8.454014
480.00	46.02	21.28	20.26	3.68	8.754014
600.00	45.49	22.10	20.01	3.48	8.913014

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.0000	0.7208	0.0084	0.0205	0.0373	0.2130	4.9202	11.9406	54.9054	45.0947
15.0000	0.6593	0.0261	0.0466	0.0988	0.1692	13.0319	30.0456	47.1623	52.8377
30.0000	0.6381	0.0347	0.0505	0.1200	0.1567	15.8244	35.2339	42.1203	57.8797
60.0000	0.5575	0.0592	0.0821	0.2006	0.1006	26.4627	58.4303	40.9375	59.0625
120.0000	0.5173	0.0704	0.0999	0.2407	0.0716	31.7553	70.3903	41.4882	58.5118
240.0000	0.4862	0.0807	0.1106	0.2719	0.0507	35.8643	79.0359	40.6646	59.3354
360.0000	0.4740	0.0861	0.1119	0.2841	0.0439	37.4734	81.8344	39.3915	60.6085
480.0000	0.4639	0.0882	0.1178	0.2942	0.0359	38.8032	85.1449	40.0602	59.9398
600.0000	0.4586	0.0916	0.1164	0.2995	0.0340	39.5080	85.9491	38.8610	61.1390

Table 5.11. Variation of different parameter at 1.5wt% catalyst loading and 353K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.00	75.82	0.00	0.00	24.18	0.00
5.00	69.90	3.20	4.63	20.68	1.590014
15.00	64.00	7.20	9.16	16.28	3.360014
30.00	61.90	9.21	9.93	14.97	3.990014
60.00	53.97	15.48	14.74	9.44	6.369014
120.00	50.07	18.00	17.91	6.48	7.539014
240.00	46.40	20.30	21.00	3.66	8.640014
360.00	45.60	21.40	20.82	3.30	8.880014
480.00	44.70	22.90	20.24	3.01	9.150014
600.00	43.80	23.50	20.95	2.33	9.420014

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7520	0.0000	0.0060	0.0060	0.2359	0.0000	0.0000	0.0000	0.0000
5.0000	0.7046	0.0133	0.0269	0.0534	0.2018	7.0478	16.6038	50.3746	49.6254
15.0000	0.6452	0.0298	0.0532	0.1129	0.1589	14.8936	34.3378	47.1623	52.8377
30.0000	0.6240	0.0382	0.0578	0.1341	0.1460	17.6861	39.6460	43.0837	56.9164
60.0000	0.5441	0.0641	0.0858	0.2140	0.0921	28.2314	61.9514	40.0692	59.9308
120.0000	0.5047	0.0746	0.1042	0.2533	0.0632	33.4175	73.8863	41.1280	58.8720
240.0000	0.4677	0.0841	0.1221	0.2903	0.0357	38.2979	85.2396	42.0662	57.9338
360.0000	0.4597	0.0887	0.1211	0.2984	0.0322	39.3617	86.6894	40.5775	59.4225
480.0000	0.4506	0.0949	0.1177	0.3075	0.0293	40.5585	87.8709	38.2888	61.7113
600.0000	0.4415	0.0974	0.1218	0.3165	0.0228	41.7553	90.5935	38.4870	61.5130

Table 5.12. Variation of different parameter at 1.5wt% catalyst loading and 363K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.00	75.82	0.00	0.00	24.18	0
5.00	68.20	4.50	5.72	19.48	2.100014
15.00	63.03	8.08	9.58	15.66	3.651014
30.00	56.90	11.43	15.44	10.74	5.490014
60.00	49.62	17.00	20.12	5.59	7.674014
120.00	46.00	19.46	22.89	2.89	8.760014
240.00	43.93	20.47	25.04	1.18	9.381014
360.00	43.40	21.73	24.16	1.17	9.540014
480.00	43.00	23.60	22.19	1.55	9.660014
600.00	42.10	24.10	23.04	0.83	9.930014

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7520	0.0000	0.0060	0.0060	0.2359	0.0000	0.0000	0.0000	0.0000
5.0000	0.6875	0.0186	0.0333	0.0706	0.1900	9.3085	21.4611	47.1623	52.8377
15.0000	0.6354	0.0335	0.0557	0.1227	0.1527	16.1835	36.8726	45.4305	54.5695
30.0000	0.5736	0.0474	0.0898	0.1845	0.1048	24.3351	56.6780	48.6638	51.3362
60.0000	0.5002	0.0704	0.1170	0.2579	0.0545	34.0159	77.4737	45.3768	54.6232
120.0000	0.4637	0.0806	0.1331	0.2944	0.0282	38.8298	88.3447	45.2242	54.7758
240.0000	0.4428	0.0848	0.1456	0.3152	0.0115	41.5824	95.2402	46.1955	53.8045
360.0000	0.4375	0.0900	0.1405	0.3206	0.0114	42.2872	95.2910	43.8356	56.1644
480.0000	0.4335	0.0978	0.1291	0.3246	0.0151	42.8191	93.7556	39.7600	60.2400
600.0000	0.4244	0.0998	0.1340	0.3337	0.0081	44.0159	96.6495	40.1564	59.8436

Table 5.13. Variation of different parameter at 2.0wt% catalyst loading and 333K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% of Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	69.5200	3.2100	5.2721	20.2938	1.7040
15.0000	65.5000	5.0400	9.6330	16.9170	2.9100
30.0000	62.3000	7.1600	12.1594	14.5106	3.8700
60.0000	56.1000	11.3700	16.9083	9.8917	5.7300
120.0000	52.9700	14.9300	17.2618	8.1692	6.6690
240.0000	49.5800	19.8600	16.1143	6.7597	7.6860
360.0000	47.3600	20.5500	18.9793	4.7587	8.3520
480.0000	46.2000	20.9000	20.4913	3.7087	8.7000
600.0000	45.3700	21.6300	20.8900	3.1610	8.9490

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000	0.0000	0.0000
5.0000	0.7008	0.0133	0.0307	0.0573	0.1980	7.5532	18.1700	53.5499	46.4501
15.0000	0.6603	0.0209	0.0560	0.0978	0.1650	12.8989	31.7864	57.2941	42.7059
30.0000	0.6280	0.0297	0.0707	0.1300	0.1416	17.1542	41.4896	54.3803	45.6197
60.0000	0.5655	0.0471	0.0983	0.1925	0.0965	25.3989	60.1141	51.0722	48.9278
120.0000	0.5340	0.0619	0.1004	0.2241	0.0797	29.5612	67.0598	44.7987	55.2013
240.0000	0.4998	0.0823	0.0937	0.2583	0.0659	34.0691	72.7431	36.2869	63.7131
360.0000	0.4774	0.0851	0.1104	0.2806	0.0464	37.0213	80.8116	39.3304	60.6696
480.0000	0.4657	0.0866	0.1192	0.2923	0.0362	38.5638	85.0456	40.7652	59.2348
600.0000	0.4574	0.0896	0.1215	0.3007	0.0308	39.6675	87.2539	40.4020	59.5980

Table 5.14. Variation of different parameter at 2.0wt% catalyst loading and 343K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% of Water
0.0000	75.2000	0.0000	0.0000	24.8000	0.0000
5.0000	67.8500	4.3500	6.5427	19.0523	2.2050
15.0000	64.0800	6.8100	9.5727	16.2013	3.3360
30.0000	60.6400	9.6700	11.4609	13.8611	4.3680
60.0000	53.8700	15.6600	14.6618	9.4092	6.3990
120.0000	50.8900	17.6400	17.0063	7.1706	7.2930
240.0000	47.8300	20.9900	17.5377	5.4312	8.2110
360.0000	45.6600	21.5700	20.4728	3.4352	8.8620
480.0000	44.1900	22.3800	21.8668	2.2602	9.3030
600.0000	43.1200	23.0500	22.7669	1.4390	9.6240

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7581	0.0000	0.0000	0.0000	0.2419	0.0000	0.0000		
5.0000	0.6840	0.0180	0.0381	0.0741	0.1859	9.7739	23.1763	51.3558	48.6442
15.0000	0.6460	0.0282	0.0557	0.1121	0.1581	14.7872	34.6723	49.6648	50.3352
30.0000	0.6113	0.0401	0.0667	0.1468	0.1352	19.3617	44.1084	45.4124	54.5876
60.0000	0.5430	0.0649	0.0853	0.2150	0.0918	28.3643	62.0598	39.6566	60.3434
120.0000	0.5130	0.0731	0.0989	0.2451	0.0700	32.3271	71.0861	40.3593	59.6407
240.0000	0.4822	0.0870	0.1020	0.2759	0.0530	36.3963	78.0998	36.9672	63.0328
360.0000	0.4603	0.0894	0.1191	0.2978	0.0335	39.2819	86.1483	39.9838	60.0162
480.0000	0.4455	0.0927	0.1272	0.3126	0.0220	41.2367	90.8863	40.6819	59.3181
600.0000	0.4347	0.0955	0.1324	0.3234	0.0140	42.6596	94.1974	40.9438	59.0562

Table 5.15. Variation of different parameter at 2.0wt% catalyst loading and 353K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% of Water
0.0000	75.8200	0.0000	0.0000	24.1800	0.0000
5.0000	67.3500	4.8300	6.7255	18.7394	2.3550
15.0000	63.0800	7.6600	10.0951	15.5289	3.6360
30.0000	59.4800	11.2100	11.2776	13.3164	4.7160
60.0000	52.6700	16.7100	15.2459	8.6150	6.7590
120.0000	48.9500	19.2300	18.1038	5.8412	7.8750
240.0000	46.8300	21.2500	18.9007	4.5083	8.5110
360.0000	43.6600	23.3400	21.4178	2.1202	9.4620
480.0000	42.0900	24.9000	21.9167	1.1603	9.9330
600.0000	41.0000	25.0800	23.5496	0.1104	10.2600

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7520	0.0000	0.0060	0.0060	0.2359	0.0000	0.0000	0.0000	0.0000
5.0000	0.6789	0.0200	0.0391	0.0791	0.1828	10.4388	24.4377	49.4284	50.5716
15.0000	0.6359	0.0317	0.0587	0.1222	0.1515	16.1170	37.3835	48.0536	51.9464
30.0000	0.5996	0.0464	0.0656	0.1585	0.1299	20.9042	46.3047	41.3886	58.6114
60.0000	0.5309	0.0692	0.0887	0.2271	0.0840	29.9601	65.2619	39.0401	60.9599
120.0000	0.4934	0.0797	0.1053	0.2646	0.0570	34.9069	76.4468	39.7886	60.2114
240.0000	0.4721	0.0880	0.1099	0.2860	0.0440	37.7260	81.8213	38.4358	61.5642
360.0000	0.4401	0.0967	0.1246	0.3179	0.0207	41.9415	91.4508	39.1770	60.8230
480.0000	0.4243	0.1032	0.1275	0.3338	0.0113	44.0292	95.3213	38.1886	61.8114
600.0000	0.4133	0.1039	0.1370	0.3448	0.0011	45.4787	99.5547	39.7260	60.2740

Table 5.16. Variation of different parameter at 2.0wt% catalyst loading and 363K reaction temperature

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.0000	75.7200	0.0000	0.0000	24.2834	0.0000
5.0000	66.5200	5.0800	7.8080	17.9879	2.6040
15.0000	61.6800	7.9300	12.1371	14.1969	4.0560
30.0000	57.8500	10.2600	15.4563	11.2287	5.2050
60.0000	49.5300	15.8200	21.9565	4.9924	7.7010
120.0000	46.0900	18.4500	24.1724	2.5546	8.7330
240.0000	44.1100	19.8600	25.5956	1.1074	9.3270
360.0000	42.9000	21.1000	25.9264	0.3836	9.6900
480.0000	41.1100	25.4100	22.8888	0.3642	10.2270
600.0000	39.8800	27.7500	21.6871	0.0869	10.5960

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.7530	0.0000	0.0050	0.0050	0.2369	0.0000	0.0000	0.0000	0.0000
5.0000	0.6706	0.0210	0.0454	0.0875	0.1755	11.5425	27.4680	51.8969	48.1031
15.0000	0.6218	0.0329	0.0706	0.1363	0.1385	17.9787	42.7545	51.7913	48.2087
30.0000	0.5832	0.0425	0.0899	0.1749	0.1095	23.0718	54.7231	51.3955	48.6045
60.0000	0.4993	0.0655	0.1277	0.2588	0.0487	34.1356	79.8692	49.3465	50.6535
120.0000	0.4646	0.0764	0.1406	0.2934	0.0249	38.7101	89.6991	47.9066	52.0934
240.0000	0.4447	0.0823	0.1489	0.3134	0.0108	41.3431	95.5347	47.4966	52.5034
360.0000	0.4325	0.0874	0.1508	0.3256	0.0037	42.9521	98.4531	46.3081	53.6919
480.0000	0.4144	0.1053	0.1331	0.3436	0.0036	45.3324	98.5313	38.7359	61.2641
600.0000	0.4020	0.1150	0.1261	0.3560	0.0008	46.9681	99.6495	35.4240	64.5760

Table 5.17. Variation of different parameter at 2.0wt% catalyst loading, 333K reaction temperature and 1.5 molar ratio of AA to EG

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% Water
0.0000	58.8785	0.0000	0.0000	41.1215	0.0000
5.0000	55.8100	0.2000	5.0338	38.0357	0.9206
15.0000	51.9000	2.5000	8.5344	34.9720	2.0936
30.0000	47.6000	7.6000	8.7220	32.6945	3.3836
60.0000	43.4300	8.6000	14.5253	28.8101	4.6346
120.0000	38.4300	9.6000	21.7673	24.0681	6.1346
240.0000	36.6000	10.7000	23.3722	22.6442	6.6836
360.0000	35.7000	11.3000	24.0774	21.9690	6.9536
480.0000	34.0690	12.0000	25.9072	20.5809	7.4429
600.0000	33.1800	12.6000	26.5933	19.9171	7.7096

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.5967	0.0000	0.0000	0.0000	0.4033	0.0000	0.0000	0.0000	0.0000
5.0000	0.5656	0.0008	0.0294	0.0311	0.3730	5.2115	7.5042	94.6428	5.3572
15.0000	0.5260	0.0104	0.0499	0.0707	0.3430	11.8523	14.9543	70.5553	8.8189
30.0000	0.4824	0.0317	0.0510	0.1143	0.3207	19.1555	20.4930	44.6151	22.6325
60.0000	0.4401	0.0358	0.0849	0.1566	0.2826	26.2379	29.9390	54.2447	22.2490
120.0000	0.3895	0.0400	0.1273	0.2072	0.2360	34.7300	41.4707	61.4132	21.4588
240.0000	0.3709	0.0446	0.1367	0.2258	0.2221	37.8381	44.9333	60.5246	22.7837
360.0000	0.3618	0.0471	0.1408	0.2349	0.2155	39.3666	46.5753	59.9298	23.5131
480.0000	0.3453	0.0500	0.1515	0.2514	0.2018	42.1368	49.9509	60.2450	23.9795
600.0000	0.3363	0.0525	0.1555	0.2604	0.1953	43.6466	51.5653	59.7013	24.6458

Table 5.18. Variation of different parameter at 2.0wt% catalyst loading, 333K reaction temperature and 0.66 molar ratio of AA to EG

Reaction time	Wt% of AA	Wt% of EGDA	Wt% of EGMA	Wt% of EG	Wt% of Water
0.00	38.89	0.00	0.00	61.11	0
5.00	36.50	0.72	3.11	58.95	0.71672
15.00	35.24	1.36	4.39	57.92	1.09472
30.00	33.50	3.41	4.48	56.99	1.61672
60.00	28.40	6.20	9.35	52.91	3.14672
120.00	22.30	11.00	13.08	48.64	4.97672
240.00	21.00	13.23	12.16	48.24	5.36672
360.00	19.60	16.00	10.64	47.97	5.78672
480.00	17.20	18.30	11.52	46.47	6.50672
600.00	16.40	19.70	10.91	46.24	6.74672

Reaction time	Mol Fraction					Conversion%		Selectivity%	
	AA	EGDA	EGMA	Water	EG	AA	EG	EGMA	EGDA
0.0000	0.3967	0.0000	0.0000	0.0000	0.6033	0.0000	0.0000	0.0000	0.0000
5.0000	0.3723	0.0030	0.0183	0.0244	0.5819	6.1427	3.5390	8.0302	2.6444
15.0000	0.3595	0.0057	0.0258	0.0372	0.5718	9.3827	5.2248	10.7072	2.7973
30.0000	0.3417	0.0143	0.0264	0.0550	0.5626	13.8570	6.7424	10.1901	6.7212
60.0000	0.2897	0.0260	0.0550	0.1070	0.5223	26.9713	13.4273	17.6942	10.8887
120.0000	0.2275	0.0461	0.0770	0.1692	0.4802	42.6570	20.4064	20.6343	17.0909
240.0000	0.2142	0.0555	0.0716	0.1825	0.4763	45.9999	21.0549	18.5193	20.0627
360.0000	0.1999	0.0671	0.0626	0.1968	0.4736	49.5999	21.4973	15.6272	23.6523
480.0000	0.1755	0.0767	0.0678	0.2212	0.4588	55.7714	23.9573	15.9500	25.9329
600.0000	0.1673	0.0826	0.0642	0.2294	0.4565	57.8285	24.3371	14.8241	27.5371

Table 5.19. Comparison of experimental data with simulated data at 0.5wt% catalyst loading and temperature at 333K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	AA	EGMA	EGDA	Water	EG	AA	EGMA	EGDA	Water
0	4	12.5333	0	0	0	4	12.533	0	0	0
5	3.9005	12.4167	0.0824	0.0171	0.1167	3.955	12.486	0.043	0.002	0.047
10	3.8346	12.3333	0.1308	0.0346	0.2	3.911	12.435	0.081	0.008	0.098
15	3.7687	12.25	0.1792	0.0521	0.2833	3.867	12.382	0.115	0.018	0.151
20	3.7051	12.1544	0.2109	0.084	0.3789	3.824	12.327	0.146	0.03	0.206
25	3.6415	12.0589	0.2425	0.116	0.4744	3.782	12.269	0.173	0.045	0.264
30	3.5779	11.9633	0.2741	0.148	0.57	3.74	12.211	0.197	0.063	0.322
35	3.5094	11.8556	0.3033	0.1872	0.6778	3.699	12.151	0.219	0.082	0.382
40	3.4409	11.7478	0.3326	0.2265	0.7856	3.659	12.09	0.238	0.103	0.443
45	3.3724	11.64	0.3618	0.2658	0.8933	3.62	12.028	0.255	0.125	0.505
50	3.3039	11.5322	0.3911	0.305	1.0011	3.581	11.966	0.271	0.148	0.567
55	3.2354	11.4244	0.4203	0.3443	1.1089	3.543	11.904	0.285	0.172	0.629
60	3.1669	11.3167	0.4495	0.3836	1.2167	3.506	11.842	0.298	0.196	0.691
65	3.1329	11.2681	0.4689	0.3982	1.2653	3.469	11.781	0.31	0.221	0.752
70	3.0989	11.2194	0.4883	0.4128	1.3139	3.433	11.72	0.321	0.246	0.813
75	3.0649	11.1708	0.5077	0.4274	1.3625	3.398	11.659	0.331	0.272	0.874
80	3.0309	11.1222	0.5271	0.442	1.4111	3.363	11.599	0.34	0.297	0.934
85	2.9969	11.0736	0.5465	0.4566	1.4597	3.329	11.54	0.349	0.322	0.993
90	2.9629	11.025	0.5659	0.4712	1.5083	3.295	11.482	0.358	0.347	1.051
95	2.9289	10.9764	0.5853	0.4858	1.5569	3.262	11.424	0.367	0.371	1.109
100	2.8949	10.9278	0.6046	0.5005	1.6056	3.23	11.368	0.375	0.395	1.165
150	2.7016	10.6279	0.6914	0.607	1.9054	2.936	10.863	0.458	0.606	1.67
200	2.6061	10.4522	0.7067	0.6872	2.0811	2.691	10.464	0.55	0.759	2.069
250	2.4966	10.2685	0.742	0.7614	2.2649	2.485	10.151	0.647	0.868	2.382
300	2.3308	10.0525	0.8575	0.8116	2.4808	2.315	9.903	0.741	0.945	2.63
350	2.1651	9.8365	0.9731	0.8619	2.6968	2.173	9.706	0.826	1.001	2.827
400	2.1042	9.74	0.9984	0.8975	2.7933	2.057	9.548	0.901	1.042	2.985
450	2.0695	9.6733	1.0011	0.9295	2.86	1.961	9.421	0.965	1.074	3.112
500	2.0373	9.6125	1.0046	0.9581	2.9208	1.883	9.318	1.02	1.098	3.215
550	2.0089	9.5604	1.0093	0.9818	2.9729	1.819	9.236	1.065	1.116	3.297
600	1.9805	9.5083	1.014	1.0055	3.025	1.767	9.169	1.103	1.131	3.364

Table 5.20. Comparison of experimental data with simulated data at 0.5wt% catalyst loading and temperature at 343K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	**AA**	**EGMA**	**EGDA**	**Water**	**EG**	**AA**	**EGMA**	**EGDA**	**Water**
0	4	12.53333	0	0	0	4	12.533	0	0	0
5	3.83428	12.32692	0.12443	0.04129	0.20758	3.907	12.436	0.09	0.003	0.097
10	3.73925	12.20419	0.19174	0.069	0.33032	3.817	12.337	0.171	0.013	0.196
15	3.67195	12.1052	0.23133	0.10068	0.4293	3.729	12.235	0.243	0.028	0.298
20	3.6086	12.01018	0.25905	0.13235	0.52432	3.645	12.131	0.307	0.047	0.402
25	3.53733	11.89932	0.28676	0.17195	0.63518	3.564	12.026	0.365	0.071	0.507
30	3.45814	11.77262	0.33032	0.2155	0.76188	3.486	11.922	0.416	0.098	0.611
35	3.36312	11.63405	0.37387	0.26301	0.90045	3.411	11.817	0.462	0.127	0.716
40	3.26414	11.48756	0.42534	0.31052	1.04695	3.339	11.714	0.503	0.158	0.819
45	3.17308	11.35294	0.47285	0.35407	1.18156	3.27	11.612	0.539	0.191	0.921
50	3.08993	11.2302	0.5164	0.38971	1.3043	3.204	11.511	0.571	0.225	1.022
55	3.01075	11.11538	0.55995	0.42534	1.41912	3.14	11.413	0.6	0.26	1.12
60	2.9474	11.02036	0.59559	0.46097	1.51414	3.079	11.317	0.627	0.295	1.216
65	2.88801	10.93326	0.6233	0.48869	1.60124	3.02	11.224	0.65	0.329	1.309
70	2.8405	10.86199	0.64706	0.51244	1.67251	2.964	11.133	0.672	0.364	1.4
75	2.79695	10.79864	0.67081	0.53224	1.7319	2.911	11.046	0.691	0.398	1.487
80	2.75735	10.73925	0.69061	0.55204	1.79129	2.859	10.961	0.71	0.431	1.572
85	2.72964	10.6957	0.70249	0.56787	1.8388	2.81	10.88	0.726	0.463	1.653
90	2.69796	10.64819	0.71833	0.58371	1.88631	2.763	10.801	0.742	0.495	1.732
95	2.67025	10.6086	0.7302	0.59559	1.9259	2.718	10.726	0.757	0.525	1.807
100	2.64649	10.569	0.74208	0.60747	1.96154	2.675	10.654	0.771	0.554	1.879
150	2.45249	10.2681	0.83314	0.71437	2.2664	2.334	10.091	0.89	0.776	2.442
200	2.29016	10.02262	0.90837	0.79751	2.50792	2.117	9.753	0.986	0.897	2.78
250	2.13971	9.80882	0.99152	0.86086	2.72568	1.982	9.555	1.058	0.96	2.978
300	2.00905	9.63066	1.07466	0.91233	2.90385	1.899	9.439	1.107	0.993	3.094
350	1.89423	9.47624	1.14989	0.95192	3.05826	1.849	9.371	1.139	1.011	3.162
400	1.79921	9.34163	1.20532	0.99152	3.19287	1.82	9.331	1.159	1.021	3.202
450	1.72794	9.23077	1.23699	1.03111	3.29977	1.802	9.308	1.171	1.027	3.225
500	1.68043	9.14367	1.24887	1.0707	3.39084	1.791	9.294	1.178	1.03	3.239
550	1.65271	9.08428	1.24887	1.09842	3.45023	1.785	9.286	1.183	1.032	3.247
600	1.64084	9.0526	1.24095	1.11821	3.4819	1.781	9.281	1.185	1.033	3.252

Table 5.21. Comparison of experimental data with simulated data at 0.5wt% catalyst loading and temperature at 353K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	**AA**	**EGMA**	**EGDA**	**Water**	**EG**	**AA**	**EGMA**	**EGDA**	**Water**
0	4.0000	12.5330	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5	3.7274	12.1923	0.1997	0.0690	0.3422	3.8720	12.3990	0.1230	0.0060	0.1340
10	3.5928	12.0102	0.2868	0.1165	0.5243	3.7490	12.2610	0.2300	0.0210	0.2720
15	3.4819	11.8518	0.3501	0.1680	0.6827	3.6330	12.1210	0.3220	0.0450	0.4120
20	3.3631	11.6736	0.4055	0.2274	0.8609	3.5220	11.9800	0.4030	0.0750	0.5530
25	3.2483	11.4955	0.4610	0.2868	1.0390	3.4170	11.8390	0.4720	0.1110	0.6940
30	3.1414	11.3292	0.5085	0.3462	1.2053	3.3170	11.6990	0.5330	0.1510	0.8340
35	3.0543	11.1867	0.5520	0.3976	1.3479	3.2220	11.5620	0.5850	0.1930	0.9710
40	2.9712	11.0600	0.5877	0.4412	1.4746	3.1330	11.4290	0.6300	0.2370	1.1040
45	2.9039	10.9570	0.6154	0.4808	1.5775	3.0490	11.2990	0.6690	0.2820	1.2340
50	2.8484	10.8660	0.6391	0.5124	1.6686	2.9690	11.1740	0.7030	0.3280	1.3590
55	2.7930	10.7789	0.6629	0.5402	1.7557	2.8940	11.0540	0.7340	0.3730	1.4790
60	2.7455	10.7076	0.6867	0.5679	1.8230	2.8230	10.9390	0.7610	0.4160	1.5940
65	2.7019	10.6442	0.7065	0.5916	1.8903	2.7560	10.8300	0.7850	0.4590	1.7030
70	2.6703	10.5888	0.7183	0.6075	1.9457	2.6930	10.7260	0.8080	0.5000	1.8070
75	2.6386	10.5413	0.7342	0.6273	1.9932	2.6330	10.6280	0.8280	0.5390	1.9050
80	2.6069	10.4898	0.7500	0.6431	2.0407	2.5770	10.5350	0.8470	0.5760	1.9980
85	2.5792	10.4502	0.7619	0.6550	2.0803	2.5240	10.4470	0.8660	0.6100	2.0860
90	2.5515	10.4146	0.7738	0.6708	2.1199	2.4740	10.3640	0.8830	0.6430	2.1690
95	2.5317	10.3790	0.7817	0.6827	2.1555	2.4270	10.2870	0.8990	0.6730	2.2460
100	2.5079	10.3433	0.7936	0.6946	2.1872	2.3830	10.2140	0.9150	0.7020	2.3190
150	2.3298	10.0662	0.8767	0.7896	2.4644	2.0600	9.7030	1.0500	0.8900	2.8300
200	2.1833	9.8405	0.9401	0.8688	2.6901	1.8860	9.4490	1.1440	0.9700	3.0840
250	2.0447	9.6346	1.0192	0.9361	2.8959	1.7950	9.3240	1.2000	1.0040	3.2090
300	1.9022	9.4446	1.1063	0.9915	3.0860	1.7490	9.2620	1.2320	1.0200	3.2710
350	1.7834	9.2822	1.1855	1.0311	3.2523	1.7250	9.2310	1.2480	1.0270	3.3020
400	1.6844	9.1397	1.2410	1.0747	3.3948	1.7130	9.2150	1.2560	1.0310	3.3180
450	1.6092	9.0249	1.2766	1.1143	3.5096	1.7070	9.2070	1.2610	1.0320	3.3260
500	1.5339	8.9140	1.3162	1.1499	3.6205	1.7040	9.2030	1.2630	1.0330	3.3300
550	1.4627	8.8190	1.3637	1.1736	3.7155	1.7020	9.2010	1.2640	1.0340	3.3320
600	1.4152	8.7240	1.4350	1.1895	3.8105	1.7010	9.2000	1.2650	1.0340	3.3330

Table 5.22. Comparison of experimental data with simulated data at 0.5wt% catalyst loading and temperature at 363K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	**AA**	**EGMA**	**EGDA**	**Water**	**EG**	**AA**	**EGMA**	**EGDA**	**Water**
0	4	12.53333	0	0	0	4	12.533	0	0	0
5	3.63235	12.02206	0.22738	0.14027	0.51244	3.805	12.325	0.181	0.014	0.208
10	3.42647	11.72511	0.33824	0.23133	0.80939	3.624	12.107	0.326	0.05	0.426
15	3.27602	11.50735	0.41346	0.3026	1.02715	3.456	11.887	0.442	0.102	0.646
20	3.13744	11.30147	0.48869	0.36991	1.23303	3.3	11.668	0.534	0.166	0.865
25	3.00283	11.10747	0.55995	0.4293	1.42308	3.157	11.454	0.607	0.236	1.079
30	2.88801	10.93326	0.6233	0.48869	1.59729	3.025	11.249	0.666	0.309	1.284
35	2.78507	10.78281	0.67873	0.5362	1.7517	2.903	11.054	0.715	0.382	1.479
40	2.694	10.64423	0.72624	0.58371	1.88631	2.791	10.872	0.756	0.453	1.661
45	2.61482	10.52545	0.76584	0.61934	2.00509	2.688	10.701	0.791	0.52	1.832
50	2.54355	10.42251	0.80147	0.65498	2.10803	2.594	10.544	0.823	0.583	1.989
55	2.4802	10.32749	0.83314	0.68665	2.20701	2.507	10.399	0.852	0.641	2.134
60	2.42873	10.2483	0.86086	0.71437	2.2862	2.426	10.266	0.88	0.694	2.267
65	2.37726	10.17308	0.88462	0.73812	2.36143	2.353	10.145	0.906	0.741	2.388
70	2.33767	10.10973	0.90441	0.75792	2.42081	2.285	10.034	0.931	0.784	2.499
75	2.30204	10.05826	0.92421	0.77771	2.47624	2.223	9.934	0.956	0.822	2.599
80	2.2664	10.00679	0.94005	0.79355	2.52771	2.165	9.843	0.979	0.855	2.69
85	2.24265	9.96324	0.95192	0.80939	2.57127	2.113	9.76	1.002	0.885	2.773
90	2.21097	9.92364	0.96776	0.82127	2.61086	2.064	9.686	1.024	0.912	2.847
95	2.19118	9.88801	0.97568	0.83314	2.64649	2.02	9.618	1.046	0.935	2.915
100	2.16742	9.85633	0.98756	0.84502	2.67817	1.979	9.557	1.066	0.955	2.976
150	2.02885	9.63857	1.0509	0.92025	2.89593	1.719	9.188	1.217	1.064	3.345
200	1.94174	9.50396	1.0905	0.96776	3.03054	1.614	9.049	1.289	1.098	3.484
250	1.84276	9.36538	1.14197	1.01131	3.16912	1.572	8.995	1.319	1.11	3.538
300	1.72398	9.1991	1.21324	1.05882	3.33145	1.555	8.975	1.331	1.114	3.558
350	1.61708	9.04468	1.28054	1.10633	3.48982	1.549	8.966	1.335	1.116	3.567
400	1.52998	8.92195	1.3241	1.14593	3.61256	1.547	8.963	1.337	1.116	3.57
450	1.46663	8.82296	1.35577	1.1776	3.71154	1.546	8.962	1.338	1.117	3.571
500	1.3914	8.7121	1.39932	1.21324	3.8224	1.545	8.962	1.338	1.117	3.571
550	1.29242	8.58541	1.46663	1.24095	3.94514	1.545	8.961	1.338	1.117	3.572
600	1.14989	8.42704	1.55373	1.25679	4.06391	1.545	8.961	1.338	1.117	3.572

Table 5.23. Comparison of experimental data with simulated data at 1.0wt% catalyst loading and temperature at 333K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	AA	EGMA	EGDA	Water	EG	AA	EGMA	EGDA	Water
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.7780	12.2633	0.1741	0.0480	0.2700	3.8980	12.4250	0.0960	0.0060	0.1080
10.0000	3.6872	12.1383	0.2306	0.0822	0.3950	3.7990	12.3090	0.1780	0.0230	0.2240
15.0000	3.5964	12.0133	0.2871	0.1164	0.5200	3.7040	12.1880	0.2470	0.0490	0.3450
20.0000	3.5220	11.8978	0.3205	0.1575	0.6356	3.6120	12.0640	0.3060	0.0810	0.4690
25.0000	3.4475	11.7822	0.3539	0.1986	0.7511	3.5240	11.9370	0.3560	0.1200	0.5960
30.0000	3.3731	11.6667	0.3872	0.2397	0.8667	3.4390	11.8100	0.3990	0.1620	0.7230
35.0000	3.2572	11.4903	0.4426	0.3002	1.0431	3.3570	11.6830	0.4360	0.2070	0.8500
40.0000	3.1413	11.3139	0.4980	0.3607	1.2194	3.2780	11.5570	0.4670	0.2550	0.9760
45.0000	3.0254	11.1375	0.5534	0.4212	1.3958	3.2020	11.4320	0.4950	0.3030	1.1010
50.0000	2.9095	10.9611	0.6088	0.4817	1.5722	3.1290	11.3110	0.5190	0.3520	1.2220
55.0000	2.7936	10.7847	0.6641	0.5422	1.7486	3.0590	11.1920	0.5410	0.4000	1.3410
60.0000	2.6777	10.6083	0.7195	0.6027	1.9250	2.9920	11.0770	0.5610	0.4480	1.4560
65.0000	2.6363	10.5475	0.7415	0.6222	1.9858	2.9260	10.9650	0.5790	0.4940	1.5680
70.0000	2.5949	10.4867	0.7636	0.6416	2.0467	2.8640	10.8580	0.5970	0.5390	1.6750
75.0000	2.5535	10.4258	0.7856	0.6610	2.1075	2.8030	10.7540	0.6140	0.5830	1.7790
80.0000	2.5120	10.3650	0.8076	0.6804	2.1683	2.7450	10.6540	0.6310	0.6240	1.8790
85.0000	2.4706	10.3042	0.8296	0.6998	2.2292	2.6890	10.5580	0.6470	0.6640	1.9750
90.0000	2.4292	10.2433	0.8516	0.7192	2.2900	2.6350	10.4660	0.6640	0.7010	2.0670
95.0000	2.3878	10.1825	0.8737	0.7386	2.3508	2.5820	10.3780	0.6800	0.7370	2.1550
100.0000	2.3463	10.1217	0.8957	0.7580	2.4117	2.5320	10.2940	0.6970	0.7710	2.2390
150.0000	2.0762	9.7254	1.0398	0.8841	2.8079	2.1150	9.6310	0.8680	1.0170	2.9020
200.0000	1.9021	9.4706	1.1331	0.9648	3.0628	1.8200	9.2050	1.0320	1.1480	3.3280
250.0000	1.7194	9.2103	1.2382	1.0424	3.3231	1.6120	8.9230	1.1670	1.2220	3.6100
300.0000	1.5022	8.9283	1.3906	1.1072	3.6050	1.4640	8.7310	1.2700	1.2660	3.8020
350.0000	1.2850	8.6464	1.5430	1.1720	3.8869	1.3600	8.6000	1.3470	1.2930	3.9330
400.0000	1.1909	8.5156	1.6004	1.2087	4.0178	1.2870	8.5080	1.4020	1.3110	4.0250
450.0000	1.1275	8.4225	1.6341	1.2384	4.1108	1.2350	8.4450	1.4420	1.3230	4.0880
500.0000	1.0734	8.3433	1.6633	1.2634	4.1900	1.1990	8.4000	1.4700	1.3310	4.1330
550.0000	1.0330	8.2850	1.6857	1.2813	4.2483	1.1730	8.3690	1.4900	1.3370	4.1640
600.0000	0.9927	8.2267	1.7080	1.2993	4.3067	1.1550	8.3480	1.5040	1.3410	4.1850

Table 5.24. Comparison of experimental data with simulated data at 1.0wt% catalyst loading and temperature at 343K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	AA	EGMA	EGDA	Water	EG	AA	EGMA	EGDA	Water
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.6681	12.0850	0.2155	0.1164	0.4483	3.7990	12.3180	0.1870	0.0140	0.2150
10.0000	3.5311	11.8967	0.3011	0.1678	0.6367	3.6110	12.0930	0.3380	0.0510	0.4400
15.0000	3.3942	11.7083	0.3866	0.2192	0.8250	3.4360	11.8640	0.4590	0.1050	0.6690
20.0000	3.2239	11.4444	0.4633	0.3128	1.0889	3.2740	11.6360	0.5550	0.1710	0.8970
25.0000	3.0536	11.1806	0.5400	0.4064	1.3528	3.1230	11.4120	0.6340	0.2440	1.1210
30.0000	2.8833	10.9167	0.6167	0.5000	1.6167	2.9820	11.1940	0.6980	0.3200	1.3390
35.0000	2.7831	10.7617	0.6621	0.5548	1.7717	2.8500	10.9860	0.7520	0.3980	1.5470
40.0000	2.6829	10.6067	0.7075	0.6096	1.9267	2.7280	10.7870	0.7980	0.4740	1.7460
45.0000	2.5827	10.4517	0.7529	0.6644	2.0817	2.6140	10.6000	0.8390	0.5470	1.9330
50.0000	2.4825	10.2967	0.7983	0.7192	2.2367	2.5070	10.4250	0.8770	0.6160	2.1080
55.0000	2.3823	10.1417	0.8437	0.7740	2.3917	2.4080	10.2600	0.9120	0.6800	2.2730
60.0000	2.2821	9.9867	0.8891	0.8288	2.5467	2.3140	10.1080	0.9460	0.7400	2.4250
65.0000	2.2122	9.9031	0.9453	0.8425	2.6303	2.2270	9.9660	0.9790	0.7940	2.5670
70.0000	2.1423	9.8194	1.0016	0.8562	2.7139	2.1450	9.8340	1.0120	0.8430	2.6990
75.0000	2.0724	9.7358	1.0578	0.8699	2.7975	2.0680	9.7130	1.0450	0.8880	2.8200
80.0000	2.0025	9.6522	1.1140	0.8836	2.8811	1.9950	9.6000	1.0770	0.9280	2.9330
85.0000	1.9325	9.5686	1.1702	0.8973	2.9647	1.9270	9.4960	1.1090	0.9640	3.0370
90.0000	1.8626	9.4850	1.2264	0.9110	3.0483	1.8630	9.4000	1.1410	0.9960	3.1330
95.0000	1.7927	9.4014	1.2826	0.9247	3.1319	1.8030	9.3100	1.1720	1.0250	3.2230
100.0000	1.7228	9.3178	1.3388	0.9384	3.2156	1.7460	9.2280	1.2030	1.0510	3.3050
150.0000	1.3556	8.8542	1.6096	1.0348	3.6792	1.3280	8.6620	1.4720	1.1990	3.8710
200.0000	1.2097	8.6389	1.6862	1.1041	3.8944	1.0920	8.3700	1.6520	1.2550	4.1630
250.0000	1.0720	8.4294	1.7522	1.1759	4.1039	0.9580	8.2110	1.7620	1.2800	4.3220
300.0000	0.9672	8.2433	1.7756	1.2572	4.2900	0.8810	8.1210	1.8270	1.2920	4.4120
350.0000	0.8624	8.0572	1.7991	1.3385	4.4761	0.8360	8.0700	1.8650	1.2990	4.4630
400.0000	0.8199	7.9911	1.8180	1.3621	4.5422	0.8110	8.0410	1.8870	1.3030	4.4920
450.0000	0.7929	7.9550	1.8359	1.3712	4.5783	0.7960	8.0240	1.8990	1.3050	4.5090
500.0000	0.7659	7.9111	1.8460	1.3881	4.6222	0.7870	8.0150	1.9070	1.3060	4.5180
550.0000	0.7389	7.8556	1.8444	1.4167	4.6778	0.7830	8.0090	1.9110	1.3060	4.5240
600.0000	0.7119	7.8000	1.8429	1.4452	4.7333	0.7800	8.0060	1.9130	1.3070	4.5270

Table 5.25. Comparison of experimental data with simulated data at 1.0wt% catalyst loading and temperature at 353K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	**AA**	**EGMA**	**EGDA**	**Water**	**EG**	**AA**	**EGMA**	**EGDA**	**Water**
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.5340	11.9167	0.3153	0.1507	0.6167	3.7850	12.3030	0.1990	0.0160	0.2300
10.0000	3.4604	11.7917	0.3376	0.2021	0.7417	3.5860	12.0620	0.3570	0.0570	0.4710
15.0000	3.3868	11.6667	0.3598	0.2534	0.8667	3.4010	11.8180	0.4830	0.1160	0.7150
20.0000	3.1231	11.2889	0.5093	0.3676	1.2444	3.2300	11.5760	0.5830	0.1870	0.9570
25.0000	2.8595	10.9111	0.6588	0.4817	1.6222	3.0710	11.3400	0.6650	0.2640	1.1930
30.0000	2.5959	10.5333	0.8082	0.5959	2.0000	2.9240	11.1140	0.7330	0.3430	1.4190
35.0000	2.5202	10.4222	0.8486	0.6313	2.1111	2.7870	10.8990	0.7920	0.4210	1.6340
40.0000	2.4445	10.3111	0.8889	0.6667	2.2222	2.6600	10.6970	0.8440	0.4960	1.8360
45.0000	2.3687	10.2000	0.9292	0.7021	2.3333	2.5410	10.5090	0.8930	0.5660	2.0240
50.0000	2.2930	10.0889	0.9696	0.7374	2.4444	2.4310	10.3340	0.9390	0.6300	2.1990
55.0000	2.2173	9.9778	1.0099	0.7728	2.5556	2.3280	10.1730	0.9840	0.6880	2.3600
60.0000	2.1416	9.8667	1.0502	0.8082	2.6667	2.2320	10.0240	1.0280	0.7400	2.5090
65.0000	2.0784	9.7778	1.0877	0.8339	2.7556	2.1420	9.8880	1.0720	0.7870	2.6450
70.0000	2.0152	9.6889	1.1253	0.8596	2.8444	2.0570	9.7620	1.1150	0.8280	2.7710
75.0000	1.9519	9.6000	1.1628	0.8853	2.9333	1.9780	9.6470	1.1580	0.8640	2.8860
80.0000	1.8887	9.5111	1.2003	0.9110	3.0222	1.9040	9.5410	1.2010	0.8960	2.9920
85.0000	1.8255	9.4222	1.2378	0.9366	3.1111	1.8340	9.4440	1.2430	0.9230	3.0890
90.0000	1.7623	9.3333	1.2753	0.9623	3.2000	1.7680	9.3540	1.2840	0.9480	3.1790
95.0000	1.6991	9.2444	1.3129	0.9880	3.2889	1.7070	9.2710	1.3240	0.9690	3.2620
100.0000	1.6359	9.1556	1.3504	1.0137	3.3778	1.6490	9.1940	1.3640	0.9880	3.3390
150.0000	1.2880	8.6792	1.5699	1.1421	3.8542	1.2240	8.6690	1.6870	1.0890	3.8640
200.0000	1.1294	8.4778	1.6857	1.1849	4.0556	0.9860	8.3950	1.8890	1.1250	4.1380
250.0000	0.9729	8.2819	1.8028	1.2243	4.2514	0.8510	8.2430	2.0090	1.1410	4.2900
300.0000	0.8250	8.1083	1.9250	1.2500	4.4250	0.7730	8.1580	2.0780	1.1480	4.3750
350.0000	0.6771	7.9347	2.0472	1.2757	4.5986	0.7290	8.1090	2.1190	1.1520	4.4240
400.0000	0.6670	7.8556	1.9883	1.3448	4.6778	0.7030	8.0810	2.1430	1.1550	4.4520
450.0000	0.6913	7.8000	1.8840	1.4247	4.7333	0.6880	8.0650	2.1560	1.1560	4.4680
500.0000	0.6955	7.7528	1.8285	1.4760	4.7806	0.6790	8.0560	2.1640	1.1560	4.4770
550.0000	0.6693	7.7181	1.8461	1.4846	4.8153	0.6750	8.0510	2.1690	1.1570	4.4820
600.0000	0.6432	7.6833	1.8637	1.4932	4.8500	0.6720	8.0480	2.1710	1.1570	4.4850

Table 5.26. Comparison of experimental data with simulated data at 1.0wt% catalyst loading and temperature at 363K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	**AA**	**EGMA**	**EGDA**	**Water**	**EG**	**AA**	**EGMA**	**EGDA**	**Water**
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.4222	11.7500	0.3724	0.2055	0.7833	3.6510	12.1290	0.2940	0.0550	0.4040
10.0000	3.3069	11.5833	0.4363	0.2569	0.9500	3.3430	11.6950	0.4750	0.1810	0.8380
15.0000	3.1916	11.4167	0.5002	0.3082	1.1167	3.0720	11.2680	0.5920	0.3370	1.2650
20.0000	2.9576	11.0389	0.5903	0.4521	1.4944	2.8310	10.8710	0.6750	0.4940	1.6620
25.0000	2.7237	10.6611	0.6804	0.5959	1.8722	2.6180	10.5130	0.7450	0.6370	2.0200
30.0000	2.4897	10.2833	0.7705	0.7397	2.2500	2.4270	10.1980	0.8120	0.7620	2.3350
35.0000	2.3110	10.0478	0.8924	0.7966	2.4856	2.2550	9.9230	0.8800	0.8650	2.6100
40.0000	2.1323	9.8122	1.0143	0.8534	2.7211	2.1000	9.6830	0.9490	0.9510	2.8500
45.0000	1.9536	9.5767	1.1361	0.9103	2.9567	1.9600	9.4730	1.0200	1.0200	3.0600
50.0000	1.7749	9.3411	1.2580	0.9671	3.1922	1.8330	9.2900	1.0910	1.0760	3.2430
55.0000	1.5962	9.1056	1.3798	1.0240	3.4278	1.7170	9.1270	1.1610	1.1220	3.4060
60.0000	1.4175	8.8700	1.5017	1.0808	3.6633	1.6100	8.9830	1.2300	1.1600	3.5500
65.0000	1.3567	8.7919	1.5453	1.0981	3.7414	1.5130	8.8550	1.2960	1.1910	3.6780
70.0000	1.2959	8.7139	1.5889	1.1153	3.8194	1.4240	8.7390	1.3590	1.2170	3.7940
75.0000	1.2350	8.6358	1.6324	1.1325	3.8975	1.3410	8.6350	1.4190	1.2390	3.8980
80.0000	1.1742	8.5578	1.6760	1.1498	3.9756	1.2660	8.5410	1.4760	1.2580	3.9920
85.0000	1.1134	8.4797	1.7196	1.1670	4.0536	1.1960	8.4550	1.5300	1.2740	4.0780
90.0000	1.0526	8.4017	1.7632	1.1843	4.1317	1.1310	8.3770	1.5810	1.2880	4.1560
95.0000	0.9918	8.3236	1.8068	1.2015	4.2097	1.0720	8.3050	1.6280	1.3000	4.2280
100.0000	0.9310	8.2456	1.8503	1.2187	4.2878	1.0170	8.2400	1.6730	1.3100	4.2930
150.0000	0.6299	7.8396	2.0465	1.3236	4.6938	0.6430	7.8090	1.9900	1.3670	4.7240
200.0000	0.5336	7.6833	2.0829	1.3836	4.8500	0.4600	7.6060	2.1530	1.3870	4.9270
250.0000	0.4436	7.5396	2.1190	1.4374	4.9938	0.3680	7.5050	2.2360	1.3960	5.0280
300.0000	0.3793	7.4458	2.1539	1.4668	5.0875	0.3210	7.4550	2.2790	1.4000	5.0780
350.0000	0.3149	7.3521	2.1889	1.4962	5.1813	0.2970	7.4290	2.3020	1.4010	5.1040
400.0000	0.3075	7.3167	2.1683	1.5242	5.2167	0.2850	7.4150	2.3130	1.4020	5.1180
450.0000	0.3144	7.2958	2.1337	1.5519	5.2375	0.2780	7.4080	2.3190	1.4030	5.1250
500.0000	0.3043	7.2611	2.1193	1.5765	5.2722	0.2750	7.4050	2.3220	1.4030	5.1280
550.0000	0.2687	7.2056	2.1349	1.5965	5.3278	0.2730	7.4030	2.3240	1.4030	5.1300
600.0000	0.2331	7.1500	2.1505	1.6164	5.3833	0.2720	7.4020	2.3240	1.4030	5.1310

Table 5.27. Comparison of experimental data with simulated data at 1.5wt% catalyst loading and temperature at 333K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	**AA**	**EGMA**	**EGDA**	**Water**	**EG**	**AA**	**EGMA**	**EGDA**	**Water**
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.5505	12.0017	0.3673	0.0822	0.5317	3.7090	12.2300	0.2790	0.0120	0.3030
10.0000	3.2706	11.6258	0.5513	0.1781	0.9075	3.4470	11.9360	0.5090	0.0440	0.5970
15.0000	2.9906	11.2500	0.7354	0.2740	1.2833	3.2110	11.6530	0.6980	0.0910	0.8800
20.0000	2.8814	11.1111	0.8149	0.3037	1.4222	2.9980	11.3830	0.8530	0.1490	1.1500
25.0000	2.7722	10.9722	0.8944	0.3333	1.5611	2.8070	11.1270	0.9790	0.2140	1.4060
30.0000	2.6630	10.8333	0.9740	0.3630	1.7000	2.6360	10.8860	1.0810	0.2830	1.6470
35.0000	2.5121	10.6222	1.0648	0.4232	1.9111	2.4820	10.6610	1.1650	0.3540	1.8720
40.0000	2.3611	10.4111	1.1556	0.4833	2.1222	2.3430	10.4510	1.2330	0.4250	2.0820
45.0000	2.2102	10.2000	1.2463	0.5435	2.3333	2.2180	10.2580	1.2880	0.4940	2.2750
50.0000	2.0592	9.9889	1.3371	0.6037	2.5444	2.1060	10.0790	1.3340	0.5600	2.4540
55.0000	1.9083	9.7778	1.4279	0.6638	2.7556	2.0050	9.9140	1.3720	0.6240	2.6190
60.0000	1.7573	9.5667	1.5187	0.7240	2.9667	1.9130	9.7630	1.4040	0.6830	2.7700
65.0000	1.7285	9.5139	1.5237	0.7479	3.0194	1.8310	9.6260	1.4310	0.7380	2.9070
70.0000	1.6996	9.4611	1.5286	0.7718	3.0722	1.7560	9.5000	1.4540	0.7890	3.0330
75.0000	1.6707	9.4083	1.5336	0.7957	3.1250	1.6890	9.3860	1.4750	0.8360	3.1470
80.0000	1.6419	9.3556	1.5385	0.8196	3.1778	1.6280	9.2820	1.4930	0.8790	3.2510
85.0000	1.6130	9.3028	1.5435	0.8436	3.2306	1.5720	9.1870	1.5100	0.9180	3.3460
90.0000	1.5841	9.2500	1.5484	0.8675	3.2833	1.5220	9.1020	1.5250	0.9530	3.4310
95.0000	1.5553	9.1972	1.5534	0.8914	3.3361	1.4760	9.0240	1.5390	0.9850	3.5090
100.0000	1.5264	9.1444	1.5583	0.9153	3.3889	1.4350	8.9540	1.5510	1.0140	3.5790
150.0000	1.3711	8.8500	1.5744	1.0545	3.6833	1.1790	8.5370	1.6450	1.1760	3.9960
200.0000	1.3047	8.7111	1.5683	1.1269	3.8222	1.0790	8.3860	1.6940	1.2260	4.1470
250.0000	1.2296	8.5708	1.5784	1.1921	3.9625	1.0400	8.3310	1.7180	1.2420	4.2020
300.0000	1.1194	8.4250	1.6529	1.2277	4.1083	1.0250	8.3110	1.7270	1.2480	4.2220
350.0000	1.0093	8.2792	1.7273	1.2634	4.2542	1.0190	8.3030	1.7310	1.2490	4.2300
400.0000	0.9842	8.2161	1.7145	1.3014	4.3172	1.0170	8.3000	1.7330	1.2500	4.2330
450.0000	0.9803	8.1738	1.6798	1.3399	4.3596	1.0160	8.2990	1.7330	1.2500	4.2340
500.0000	0.9552	8.1175	1.6738	1.3710	4.4158	1.0160	8.2980	1.7340	1.2510	4.2350
550.0000	0.8981	8.0404	1.7110	1.3910	4.4929	1.0160	8.2980	1.7340	1.2510	4.2350
600.0000	0.8410	7.9633	1.7481	1.4110	4.5700	1.0160	8.2980	1.7340	1.2510	4.2350

Table 5.28. Comparison of experimental data with simulated data at 1.5wt% catalyst loading and temperature at 343K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	**AA**	**EGMA**	**EGDA**	**Water**	**EG**	**AA**	**EGMA**	**EGDA**	**Water**
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.5224	11.9167	0.3386	0.1390	0.6167	3.6670	12.1740	0.3080	0.0250	0.3590
10.0000	3.1603	11.4083	0.5545	0.2853	1.1250	3.3700	11.8140	0.5400	0.0900	0.7190
15.0000	2.7982	10.9000	0.7703	0.4315	1.6333	3.1070	11.4610	0.7140	0.1790	1.0720
20.0000	2.7290	10.7833	0.7920	0.4790	1.7500	2.8730	11.1240	0.8450	0.2820	1.4090
25.0000	2.6598	10.6667	0.8137	0.5265	1.8667	2.6650	10.8080	0.9450	0.3900	1.7250
30.0000	2.5906	10.5500	0.8354	0.5740	1.9833	2.4800	10.5150	1.0230	0.4980	2.0180
35.0000	2.4360	10.3278	0.9225	0.6416	2.2056	2.3140	10.2470	1.0870	0.6000	2.2860
40.0000	2.2814	10.1056	1.0095	0.7091	2.4278	2.1650	10.0040	1.1410	0.6940	2.5290
45.0000	2.1267	9.8833	1.0966	0.7767	2.6500	2.0320	9.7850	1.1890	0.7790	2.7480
50.0000	1.9721	9.6611	1.1836	0.8443	2.8722	1.9110	9.5890	1.2330	0.8550	2.9440
55.0000	1.8174	9.4389	1.2707	0.9119	3.0944	1.8030	9.4140	1.2750	0.9220	3.1190
60.0000	1.6628	9.2167	1.3578	0.9795	3.3167	1.7050	9.2570	1.3150	0.9800	3.2760
65.0000	1.6229	9.1614	1.3822	0.9949	3.3719	1.6160	9.1180	1.3540	1.0310	3.4150
70.0000	1.5831	9.1061	1.4067	1.0103	3.4272	1.5350	8.9940	1.3910	1.0740	3.5390
75.0000	1.5432	9.0508	1.4311	1.0257	3.4825	1.4620	8.8840	1.4280	1.1110	3.6490
80.0000	1.5033	8.9956	1.4556	1.0411	3.5378	1.3950	8.7850	1.4630	1.1420	3.7480
85.0000	1.4635	8.9403	1.4800	1.0565	3.5931	1.3340	8.6980	1.4970	1.1690	3.8350
90.0000	1.4236	8.8850	1.5045	1.0719	3.6483	1.2790	8.6190	1.5290	1.1930	3.9140
95.0000	1.3837	8.8297	1.5290	1.0873	3.7036	1.2280	8.5490	1.5600	1.2120	3.9840
100.0000	1.3439	8.7744	1.5534	1.1027	3.7589	1.1820	8.4860	1.5890	1.2290	4.0470
150.0000	1.0979	8.4246	1.6954	1.2067	4.1088	0.8910	8.1130	1.7980	1.3110	4.4200
200.0000	0.9538	8.2100	1.7690	1.2772	4.3233	0.7710	7.9700	1.8950	1.3340	4.5630
250.0000	0.8292	8.0215	1.8297	1.3410	4.5118	0.7210	7.9120	1.9370	1.3420	4.6210
300.0000	0.7826	7.9375	1.8390	1.3784	4.5958	0.7000	7.8880	1.9540	1.3450	4.6450
350.0000	0.7360	7.8535	1.8482	1.4158	4.6799	0.6920	7.8780	1.9620	1.3470	4.6550
400.0000	0.6825	7.7811	1.8828	1.4347	4.7522	0.6880	7.8740	1.9650	1.3470	4.6590
450.0000	0.6273	7.7117	1.9237	1.4490	4.8217	0.6860	7.8720	1.9660	1.3470	4.6610
500.0000	0.5888	7.6553	1.9443	1.4669	4.8781	0.6860	7.8710	1.9670	1.3470	4.6620
550.0000	0.5754	7.6185	1.9343	1.4903	4.9149	0.6850	7.8710	1.9670	1.3470	4.6620
600.0000	0.5620	7.5817	1.9243	1.5137	4.9517	0.6850	7.8710	1.9670	1.3480	4.6620

Table 5.29. Comparison of experimental data with simulated data at 1.5wt% catalyst loading and temperature at 353K

Reaction time	**Experimental Concentration, kmol/m^3**					**Simulation Concentration, kmol/m^3**				
	EG	**AA**	**EGMA**	**EGDA**	**Water**	**EG**	**AA**	**EGMA**	**EGDA**	**Water**
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.3359	11.6500	0.4450	0.2192	0.8833	3.6380	12.1160	0.3080	0.0540	0.4170
10.0000	2.9812	11.1583	0.6627	0.3562	1.3750	3.3200	11.6720	0.4990	0.1810	0.8610
15.0000	2.6265	10.6667	0.8804	0.4932	1.8667	3.0420	11.2380	0.6220	0.3370	1.2950
20.0000	2.5557	10.5500	0.9053	0.5390	1.9833	2.7970	10.8350	0.7080	0.4950	1.6980
25.0000	2.4849	10.4333	0.9301	0.5849	2.1000	2.5810	10.4740	0.7790	0.6400	2.0590
30.0000	2.4142	10.3167	0.9550	0.6308	2.2167	2.3890	10.1560	0.8440	0.7660	2.3770
35.0000	2.2655	10.0964	1.0322	0.7024	2.4369	2.2180	9.8790	0.9100	0.8720	2.6540
40.0000	2.1168	9.8761	1.1093	0.7740	2.6572	2.0650	9.6390	0.9760	0.9590	2.8940
45.0000	1.9681	9.6558	1.1864	0.8456	2.8775	1.9280	9.4320	1.0420	1.0290	3.1010
50.0000	1.8194	9.4356	1.2635	0.9171	3.0978	1.8040	9.2510	1.1090	1.0870	3.2820
55.0000	1.6707	9.2153	1.3407	0.9887	3.3181	1.6930	9.0930	1.1750	1.1330	3.4400
60.0000	1.5219	8.9950	1.4178	1.0603	3.5383	1.5910	8.9540	1.2380	1.1710	3.5790
65.0000	1.4822	8.9408	1.4432	1.0747	3.5925	1.5000	8.8310	1.2990	1.2020	3.7020
70.0000	1.4424	8.8867	1.4686	1.0890	3.6467	1.4160	8.7220	1.3560	1.2280	3.8110
75.0000	1.4026	8.8325	1.4940	1.1034	3.7008	1.3400	8.6240	1.4110	1.2490	3.9090
80.0000	1.3628	8.7783	1.5194	1.1178	3.7550	1.2710	8.5370	1.4610	1.2670	3.9960
85.0000	1.3230	8.7242	1.5448	1.1322	3.8092	1.2080	8.4590	1.5090	1.2830	4.0740
90.0000	1.2833	8.6700	1.5702	1.1466	3.8633	1.1510	8.3880	1.5530	1.2960	4.1450
95.0000	1.2435	8.6158	1.5956	1.1610	3.9175	1.0990	8.3250	1.5940	1.3070	4.2080
100.0000	1.2037	8.5617	1.6210	1.1753	3.9717	1.0510	8.2670	1.6320	1.3170	4.2660
150.0000	0.9310	8.1921	1.7967	1.2723	4.3413	0.7470	7.9110	1.8850	1.3680	4.6220
200.0000	0.7418	7.9372	1.9203	1.3379	4.5961	0.6180	7.7660	1.9960	1.3850	4.7670
250.0000	0.5856	7.7222	2.0177	1.3967	4.8111	0.5630	7.7050	2.0450	1.3920	4.8290
300.0000	0.5614	7.6667	2.0105	1.4281	4.8667	0.5400	7.6780	2.0660	1.3950	4.8550
350.0000	0.5373	7.6111	2.0033	1.4595	4.9222	0.5290	7.6670	2.0750	1.3960	4.8660
400.0000	0.5167	7.5500	1.9833	1.5000	4.9833	0.5250	7.6620	2.0790	1.3960	4.8710
450.0000	0.4970	7.4875	1.9602	1.5428	5.0458	0.5230	7.6600	2.0810	1.3960	4.8730
500.0000	0.4670	7.4250	1.9577	1.5753	5.1083	0.5220	7.6590	2.0810	1.3960	4.8740
550.0000	0.4216	7.3625	1.9859	1.5925	5.1708	0.5220	7.6580	2.0820	1.3960	4.8750
600.0000	0.3763	7.3000	2.0142	1.6096	5.2333	0.5220	7.6580	2.0820	1.3960	4.8750

Table 5.30. Comparison of experimental data with simulated data at 1.5wt% catalyst loading and temperature at 363K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	AA	EGMA	EGDA	Water	EG	AA	EGMA	EGDA	Water
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.1416	11.3667	0.5502	0.3082	1.1667	3.4220	11.8820	0.5060	0.0720	0.6510
10.0000	2.8333	10.9358	0.7359	0.4308	1.5975	2.9520	11.2510	0.8130	0.2340	1.2820
15.0000	2.5251	10.5050	0.9215	0.5534	2.0283	2.5690	10.6760	1.0050	0.4260	1.8570
20.0000	2.2610	10.1644	1.1091	0.6299	2.3689	2.2540	10.1750	1.1350	0.6110	2.3580
25.0000	1.9970	9.8239	1.2967	0.7064	2.7094	1.9910	9.7500	1.2350	0.7740	2.7830
30.0000	1.7329	9.4833	1.4842	0.7829	3.0500	1.7700	9.3960	1.3220	0.9070	3.1370
35.0000	1.5942	9.2811	1.5593	0.8465	3.2522	1.5830	9.1030	1.4040	1.0130	3.4300
40.0000	1.4556	9.0789	1.6344	0.9101	3.4544	1.4230	8.8620	1.4820	1.0950	3.6710
45.0000	1.3170	8.8767	1.7094	0.9736	3.6567	1.2860	8.6620	1.5570	1.1570	3.8710
50.0000	1.1783	8.6744	1.7845	1.0372	3.8589	1.1670	8.4950	1.6290	1.2040	4.0380
55.0000	1.0397	8.4722	1.8595	1.1008	4.0611	1.0630	8.3560	1.6960	1.2400	4.1770
60.0000	0.9011	8.2700	1.9346	1.1644	4.2633	0.9730	8.2380	1.7590	1.2680	4.2950
65.0000	0.8648	8.2197	1.9568	1.1784	4.3136	0.8940	8.1380	1.8160	1.2890	4.3950
70.0000	0.8286	8.1694	1.9790	1.1925	4.3639	0.8250	8.0530	1.8690	1.3060	4.4800
75.0000	0.7923	8.1192	2.0012	1.2065	4.4142	0.7650	7.9790	1.9170	1.3180	4.5540
80.0000	0.7561	8.0689	2.0234	1.2206	4.4644	0.7120	7.9160	1.9600	1.3290	4.6170
85.0000	0.7199	8.0186	2.0455	1.2346	4.5147	0.6650	7.8610	1.9980	1.3370	4.6720
90.0000	0.6836	7.9683	2.0677	1.2486	4.5650	0.6230	7.8130	2.0330	1.3440	4.7200
95.0000	0.6474	7.9181	2.0899	1.2627	4.6153	0.5870	7.7710	2.0640	1.3490	4.7620
100.0000	0.6112	7.8678	2.1121	1.2767	4.6656	0.5550	7.7340	2.0920	1.3540	4.7990
150.0000	0.3973	7.5804	2.2526	1.3502	4.9529	0.3790	7.5380	2.2460	1.3740	4.9950
200.0000	0.2823	7.4367	2.3387	1.3790	5.0967	0.3260	7.4790	2.2950	1.3800	5.0540
250.0000	0.1902	7.3143	2.4005	1.4093	5.2190	0.3090	7.4620	2.3100	1.3810	5.0710
300.0000	0.1894	7.2775	2.3654	1.4452	5.2558	0.3040	7.4560	2.3140	1.3810	5.0770
350.0000	0.1885	7.2407	2.3303	1.4812	5.2926	0.3030	7.4540	2.3160	1.3820	5.0790
400.0000	0.2088	7.2111	2.2601	1.5311	5.3222	0.3020	7.4540	2.3160	1.3820	5.0790
450.0000	0.2344	7.1833	2.1812	1.5844	5.3500	0.3020	7.4540	2.3160	1.3820	5.0790
500.0000	0.2305	7.1417	2.1474	1.6222	5.3917	0.3020	7.4540	2.3160	1.3820	5.0790
550.0000	0.1823	7.0792	2.1813	1.6364	5.4542	0.3020	7.4540	2.3160	1.3820	5.0790
600.0000	0.1340	7.0167	2.2153	1.6507	5.5167	0.3020	7.4540	2.3160	1.3820	5.0790

Table 5.31. Comparison of experimental data with simulated data at 2.0wt% catalyst loading and temperature at 333K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	AA	EGMA	EGDA	Water	EG	AA	EGMA	EGDA	Water
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.2732	11.5867	0.5069	0.2199	0.9467	3.6240	12.1430	0.3610	0.0140	0.3900
10.0000	3.0009	11.2517	0.7166	0.2825	1.2817	3.2960	11.7770	0.6520	0.0520	0.7560
15.0000	2.7285	10.9167	0.9263	0.3452	1.6167	3.0080	11.4350	0.8850	0.1060	1.0980
20.0000	2.5992	10.7389	1.0072	0.3936	1.7944	2.7570	11.1170	1.0710	0.1720	1.4160
25.0000	2.4698	10.5611	1.0882	0.4420	1.9722	2.5370	10.8240	1.2180	0.2460	1.7090
30.0000	2.3404	10.3833	1.1692	0.4904	2.1500	2.3440	10.5540	1.3330	0.3230	1.9790
35.0000	2.2163	10.2111	1.2453	0.5385	2.3222	2.1750	10.3070	1.4240	0.4010	2.2260
40.0000	2.0921	10.0389	1.3214	0.5865	2.4944	2.0270	10.0810	1.4950	0.4780	2.4520
45.0000	1.9679	9.8667	1.3975	0.6346	2.6667	1.8960	9.8760	1.5500	0.5540	2.6570
50.0000	1.8438	9.6944	1.4736	0.6827	2.8389	1.7820	9.6890	1.5930	0.6250	2.8440
55.0000	1.7196	9.5222	1.5497	0.7307	3.0111	1.6800	9.5200	1.6260	0.6930	3.0130
60.0000	1.5954	9.3500	1.6258	0.7788	3.1833	1.5910	9.3670	1.6520	0.7570	3.1660
65.0000	1.5723	9.3065	1.6286	0.7991	3.2268	1.5120	9.2290	1.6730	0.8160	3.3040
70.0000	1.5491	9.2631	1.6315	0.8194	3.2703	1.4410	9.1040	1.6880	0.8700	3.4290
75.0000	1.5260	9.2196	1.6343	0.8397	3.3138	1.3790	8.9920	1.7010	0.9200	3.5410
80.0000	1.5028	9.1761	1.6371	0.8601	3.3572	1.3230	8.8900	1.7110	0.9660	3.6430
85.0000	1.4797	9.1326	1.6400	0.8804	3.4007	1.2740	8.8000	1.7190	1.0070	3.7330
90.0000	1.4565	9.0892	1.6428	0.9007	3.4442	1.2300	8.7180	1.7250	1.0450	3.8150
95.0000	1.4334	9.0457	1.6456	0.9210	3.4876	1.1900	8.6450	1.7310	1.0790	3.8880
100.0000	1.4102	9.0022	1.6485	0.9413	3.5311	1.1550	8.5790	1.7360	1.1090	3.9540
150.0000	1.2608	8.6871	1.6322	1.1070	3.8463	0.9520	8.2010	1.7640	1.2840	4.3320
200.0000	1.1661	8.4517	1.5862	1.2477	4.0817	0.8830	8.0770	1.7790	1.3390	4.4560
250.0000	1.0634	8.2325	1.5724	1.3642	4.3008	0.8580	8.0360	1.7860	1.3560	4.4970
300.0000	0.9289	8.0783	1.6872	1.3839	4.4550	0.8500	8.0220	1.7890	1.3610	4.5110
350.0000	0.7944	7.9242	1.8020	1.4036	4.6092	0.8470	8.0170	1.7900	1.3630	4.5160
400.0000	0.7111	7.8289	1.8734	1.4155	4.7044	0.8460	8.0160	1.7910	1.3630	4.5170
450.0000	0.6405	7.7483	1.9340	1.4255	4.7850	0.8460	8.0150	1.7910	1.3630	4.5180
500.0000	0.5835	7.6769	1.9767	1.4398	4.8564	0.8460	8.0150	1.7910	1.3630	4.5180
550.0000	0.5467	7.6193	1.9927	1.4607	4.9140	0.8460	8.0150	1.7910	1.3630	4.5180
600.0000	0.5098	7.5617	2.0087	1.4815	4.9717	0.8460	8.0150	1.7910	1.3630	4.5180

Table 5.32. Comparison of experimental data with simulated data at 2.0wt% catalyst loading and temperature at 343K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	AA	EGMA	EGDA	Water	EG	AA	EGMA	EGDA	Water
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.0730	11.3083	0.6291	0.2980	1.2250	3.5760	12.0860	0.4000	0.0240	0.4470
10.0000	2.8430	10.9942	0.7748	0.3822	1.5392	3.2120	11.6600	0.7030	0.0850	0.8730
15.0000	2.6131	10.6800	0.9205	0.4664	1.8533	2.8980	11.2610	0.9320	0.1700	1.2720
20.0000	2.4873	10.4889	0.9810	0.5317	2.0444	2.6280	10.8910	1.1030	0.2690	1.6420
25.0000	2.3615	10.2978	1.0415	0.5970	2.2356	2.3940	10.5520	1.2320	0.3740	1.9810
30.0000	2.2357	10.1067	1.1020	0.6623	2.4267	2.1910	10.2440	1.3300	0.4800	2.2890
35.0000	2.1160	9.9186	1.1533	0.7307	2.6147	2.0140	9.9650	1.4040	0.5820	2.5680
40.0000	1.9963	9.7306	1.2046	0.7991	2.8028	1.8600	9.7150	1.4610	0.6780	2.8180
45.0000	1.8766	9.5425	1.2559	0.8675	2.9908	1.7250	9.4910	1.5070	0.7670	3.0420
50.0000	1.7570	9.3544	1.3072	0.9358	3.1789	1.6070	9.2920	1.5440	0.8480	3.2410
55.0000	1.6373	9.1664	1.3585	1.0042	3.3669	1.5030	9.1150	1.5760	0.9210	3.4180
60.0000	1.5176	8.9783	1.4098	1.0726	3.5550	1.4110	8.9580	1.6030	0.9860	3.5750
65.0000	1.4875	8.9369	1.4286	1.0839	3.5964	1.3300	8.8200	1.6270	1.0430	3.7130
70.0000	1.4574	8.8956	1.4474	1.0952	3.6378	1.2580	8.6980	1.6490	1.0930	3.8350
75.0000	1.4273	8.8542	1.4662	1.1065	3.6792	1.1940	8.5900	1.6700	1.1370	3.9430
80.0000	1.3973	8.8128	1.4849	1.1178	3.7206	1.1370	8.4950	1.6890	1.1750	4.0380
85.0000	1.3672	8.7714	1.5037	1.1291	3.7619	1.0860	8.4110	1.7070	1.2070	4.1220
90.0000	1.3371	8.7300	1.5225	1.1404	3.8033	1.0400	8.3380	1.7240	1.2360	4.1950
95.0000	1.3070	8.6886	1.5413	1.1517	3.8447	1.0000	8.2730	1.7400	1.2600	4.2600
100.0000	1.2769	8.6472	1.5601	1.1630	3.8861	0.9640	8.2160	1.7550	1.2810	4.3170
150.0000	1.0864	8.3542	1.6480	1.2656	4.1792	0.7570	7.9080	1.8610	1.3820	4.6250
200.0000	0.9695	8.1417	1.6693	1.3612	4.3917	0.6870	7.8150	1.9070	1.4050	4.7180
250.0000	0.8492	7.9415	1.7098	1.4410	4.5918	0.6640	7.7850	1.9250	1.4120	4.7480
300.0000	0.7150	7.7908	1.8274	1.4575	4.7425	0.6560	7.7750	1.9310	1.4140	4.7580
350.0000	0.5809	7.6401	1.9450	1.4741	4.8932	0.6530	7.7710	1.9330	1.4140	4.7620
400.0000	0.4909	7.5283	2.0132	1.4959	5.0050	0.6520	7.7700	1.9340	1.4150	4.7630
450.0000	0.4119	7.4263	2.0691	1.5190	5.1071	0.6520	7.7700	1.9340	1.4150	4.7630
500.0000	0.3425	7.3353	2.1170	1.5405	5.1981	0.6510	7.7700	1.9340	1.4150	4.7630
550.0000	0.2873	7.2610	2.1531	1.5597	5.2724	0.6510	7.7700	1.9340	1.4150	4.7630
600.0000	0.2321	7.1867	2.1891	1.5788	5.3467	0.6510	7.7700	1.9340	1.4150	4.7630

Table 5.33. Comparison of experimental data with simulated data at 2.0wt% catalyst loading and temperature at 353K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	AA	EGMA	EGDA	Water	EG	AA	EGMA	EGDA	Water
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	3.0225	11.2250	0.6467	0.3308	1.3083	3.5290	12.0270	0.4350	0.0360	0.5060
10.0000	2.7636	10.8692	0.8087	0.4277	1.6642	3.1310	11.5400	0.7450	0.1240	0.9930
15.0000	2.5047	10.5133	0.9707	0.5247	2.0200	2.7930	11.0830	0.9640	0.2430	1.4500
20.0000	2.3857	10.3133	1.0086	0.6057	2.2200	2.5050	10.6630	1.1200	0.3750	1.8700
25.0000	2.2668	10.1133	1.0465	0.6868	2.4200	2.2590	10.2830	1.2320	0.5090	2.2500
30.0000	2.1478	9.9133	1.0844	0.7678	2.6200	2.0470	9.9420	1.3150	0.6380	2.5910
35.0000	2.0214	9.7242	1.1480	0.8306	2.8092	1.8640	9.6390	1.3790	0.7570	2.8940
40.0000	1.8951	9.5350	1.2116	0.8934	2.9983	1.7050	9.3730	1.4300	0.8650	3.1600
45.0000	1.7687	9.3458	1.2752	0.9562	3.1875	1.5660	9.1390	1.4750	0.9600	3.3940
50.0000	1.6423	9.1567	1.3388	1.0190	3.3767	1.4440	8.9350	1.5140	1.0420	3.5980
55.0000	1.5159	8.9675	1.4024	1.0817	3.5658	1.3370	8.7570	1.5510	1.1130	3.7760
60.0000	1.3895	8.7783	1.4660	1.1445	3.7550	1.2420	8.6020	1.5850	1.1730	3.9310
65.0000	1.3522	8.7267	1.4889	1.1589	3.8067	1.1580	8.4670	1.6180	1.2240	4.0660
70.0000	1.3150	8.6750	1.5118	1.1733	3.8583	1.0830	8.3490	1.6490	1.2670	4.1840
75.0000	1.2777	8.6233	1.5347	1.1877	3.9100	1.0170	8.2470	1.6790	1.3040	4.2860
80.0000	1.2404	8.5717	1.5576	1.2021	3.9617	0.9580	8.1570	1.7080	1.3340	4.3760
85.0000	1.2031	8.5200	1.5805	1.2164	4.0133	0.9050	8.0790	1.7350	1.3590	4.4540
90.0000	1.1658	8.4683	1.6034	1.2308	4.0650	0.8580	8.0100	1.7610	1.3810	4.5230
95.0000	1.1285	8.4167	1.6263	1.2452	4.1167	0.8160	7.9500	1.7860	1.3990	4.5830
100.0000	1.0913	8.3650	1.6492	1.2596	4.1683	0.7780	7.8970	1.8090	1.4140	4.6360
150.0000	0.8884	8.0700	1.7599	1.3517	4.4633	0.5580	7.6090	1.9610	1.4810	4.9240
200.0000	0.7988	7.9228	1.7918	1.4094	4.6106	0.4800	7.5160	2.0230	1.4970	5.0170
250.0000	0.6951	7.7610	1.8375	1.4674	4.7724	0.4530	7.4840	2.0450	1.5020	5.0490
300.0000	0.5346	7.5408	1.9384	1.5271	4.9925	0.4430	7.4720	2.0530	1.5040	5.0610
350.0000	0.3741	7.3207	2.0392	1.5867	5.2126	0.4390	7.4680	2.0560	1.5040	5.0650
400.0000	0.2904	7.1894	2.0754	1.6343	5.3439	0.4380	7.4670	2.0570	1.5040	5.0660
450.0000	0.2259	7.0804	2.0954	1.6788	5.4529	0.4380	7.4660	2.0580	1.5040	5.0670
500.0000	0.1589	6.9847	2.1335	1.7075	5.5486	0.4380	7.4660	2.0580	1.5040	5.0670
550.0000	0.0884	6.9090	2.1990	1.7127	5.6243	0.4380	7.4660	2.0580	1.5040	5.0670
600.0000	0.0178	6.8333	2.2644	1.7178	5.7000	0.4380	7.4660	2.0580	1.5040	5.0670

Table 5.34. Comparison of experimental data with simulated data at 2.0wt% catalyst loading and temperature at 363K

Reaction time	Experimental Concentration, kmol/m^3					Simulation Concentration, kmol/m^3				
	EG	AA	EGMA	EGDA	Water	EG	AA	EGMA	EGDA	Water
0.0000	4.0000	12.5333	0.0000	0.0000	0.0000	4.0000	12.5330	0.0000	0.0000	0.0000
5.0000	2.9013	11.0867	0.7508	0.3480	1.4467	3.3870	11.8380	0.5310	0.0820	0.6950
10.0000	2.5956	10.6833	0.9589	0.4456	1.8500	2.8960	11.1660	0.8410	0.2630	1.3670
15.0000	2.2898	10.2800	1.1670	0.5432	2.2533	2.4990	10.5600	1.0300	0.4720	1.9730
20.0000	2.1302	10.0672	1.2734	0.5964	2.4661	2.1740	10.0380	1.1580	0.6690	2.4950
25.0000	1.9707	9.8544	1.3798	0.6495	2.6789	1.9050	9.6010	1.2590	0.8370	2.9320
30.0000	1.8111	9.6417	1.4862	0.7027	2.8917	1.6790	9.2400	1.3490	0.9720	3.2930
35.0000	1.6434	9.4106	1.5904	0.7662	3.1228	1.4880	8.9450	1.4360	1.0760	3.5880
40.0000	1.4758	9.1794	1.6945	0.8297	3.3539	1.3250	8.7020	1.5190	1.1560	3.8310
45.0000	1.3082	8.9483	1.7987	0.8932	3.5850	1.1840	8.5020	1.6000	1.2160	4.0310
50.0000	1.1405	8.7172	1.9029	0.9566	3.8161	1.0630	8.3350	1.6770	1.2610	4.1980
55.0000	0.9729	8.4861	2.0070	1.0201	4.0472	0.9570	8.1950	1.7490	1.2950	4.3380
60.0000	0.8052	8.2550	2.1112	1.0836	4.2783	0.8640	8.0770	1.8150	1.3200	4.4560
65.0000	0.7725	8.2072	2.1290	1.0986	4.3261	0.7830	7.9760	1.8770	1.3400	4.5570
70.0000	0.7397	8.1594	2.1467	1.1136	4.3739	0.7120	7.8890	1.9330	1.3550	4.6440
75.0000	0.7069	8.1117	2.1645	1.1286	4.4217	0.6490	7.8140	1.9840	1.3680	4.7190
80.0000	0.6742	8.0639	2.1822	1.1436	4.4694	0.5930	7.7490	2.0300	1.3770	4.7840
85.0000	0.6414	8.0161	2.2000	1.1586	4.5172	0.5440	7.6920	2.0710	1.3850	4.8410
90.0000	0.6086	7.9683	2.2177	1.1736	4.5650	0.5000	7.6420	2.1080	1.3910	4.8910
95.0000	0.5759	7.9206	2.2355	1.1886	4.6128	0.4620	7.5980	2.1420	1.3970	4.9350
100.0000	0.5431	7.8728	2.2533	1.2037	4.6606	0.4270	7.5590	2.1720	1.4010	4.9740
150.0000	0.3537	7.5992	2.3585	1.2878	4.9342	0.2350	7.3470	2.3440	1.4210	5.1860
200.0000	0.2564	7.4617	2.4155	1.3281	5.0717	0.1720	7.2790	2.4020	1.4260	5.2540
250.0000	0.1689	7.3349	2.4638	1.3674	5.1985	0.1510	7.2560	2.4210	1.4280	5.2770
300.0000	0.1202	7.2508	2.4770	1.4027	5.2825	0.1440	7.2490	2.4280	1.4280	5.2840
350.0000	0.0716	7.1668	2.4903	1.4381	5.3665	0.1420	7.2460	2.4300	1.4280	5.2870
400.0000	0.0608	7.0506	2.3956	1.5436	5.4828	0.1410	7.2450	2.4310	1.4280	5.2880
450.0000	0.0595	6.9263	2.2739	1.6666	5.6071	0.1410	7.2450	2.4310	1.4280	5.2880
500.0000	0.0513	6.8175	2.1816	1.7671	5.7158	0.1400	7.2450	2.4310	1.4280	5.2880
550.0000	0.0327	6.7321	2.1334	1.8339	5.8013	0.1400	7.2450	2.4310	1.4280	5.2880
600.0000	0.0140	6.6467	2.0853	1.9007	5.8867	0.1400	7.2450	2.4310	1.4280	5.2880

Table 5.35. Estimated parameters at 0.5 wt% catalyst loading

T K	K1 Lit/Mol Min	K-1 Lit/Mol Min	K2 Lit/Mol Min	K-2 Lit/Mol Min
333	1.81E-04	5.37E-04	1.06E-03	3.73E-03
343	3.79E-04	1.61E-03	1.18E-03	3.86E-03
353	5.23E-04	1.94E-03	1.42E-03	4.80E-03
363	8.06E-04	2.33E-03	2.34E-03	7.01E-03

Table 5.36. Estimated parameters at 1.0wt% catalyst loading

T, K	K1 Lit/Mol Min	K-1 Lit/Mol Min	K2 Lit/Mol Min	K-2 Lit/Mol Min
333	4.15E-04	5.88E-04	1.98E-03	4.42E-03
343	8.31E-04	5.94E-04	2.31E-03	5.98E-03
353	8.89E-04	4.89E-04	2.43E-03	8.18E-03
363	1.48E-03	2.49E-04	5.65E-03	1.35E-02

Catalyst Wt%	E KJ/mol	K_0
0.5	47.32176	5357.593
	25.27386	8.989795
1.0	38.04532	429.8043
	31.32745	144.321

Table 5.37. Estimated parameters at 1.5 wt% catalyst loading

T, K	K1 Lit/Mol Min	K-1 Lit/Mol Min	K2 Lit/Mol Min	K-2 Lit/Mol Min
333	1.22E-03	1.40E-03	1.34E-03	3.64E-03
343	1.41E-03	8.29E-04	2.54E-03	6.26E-03
353	1.54E-03	6.06E-04	5.38E-03	1.26E-02
363	2.51E-03	3.58E-04	6.59E-03	1.70E-02

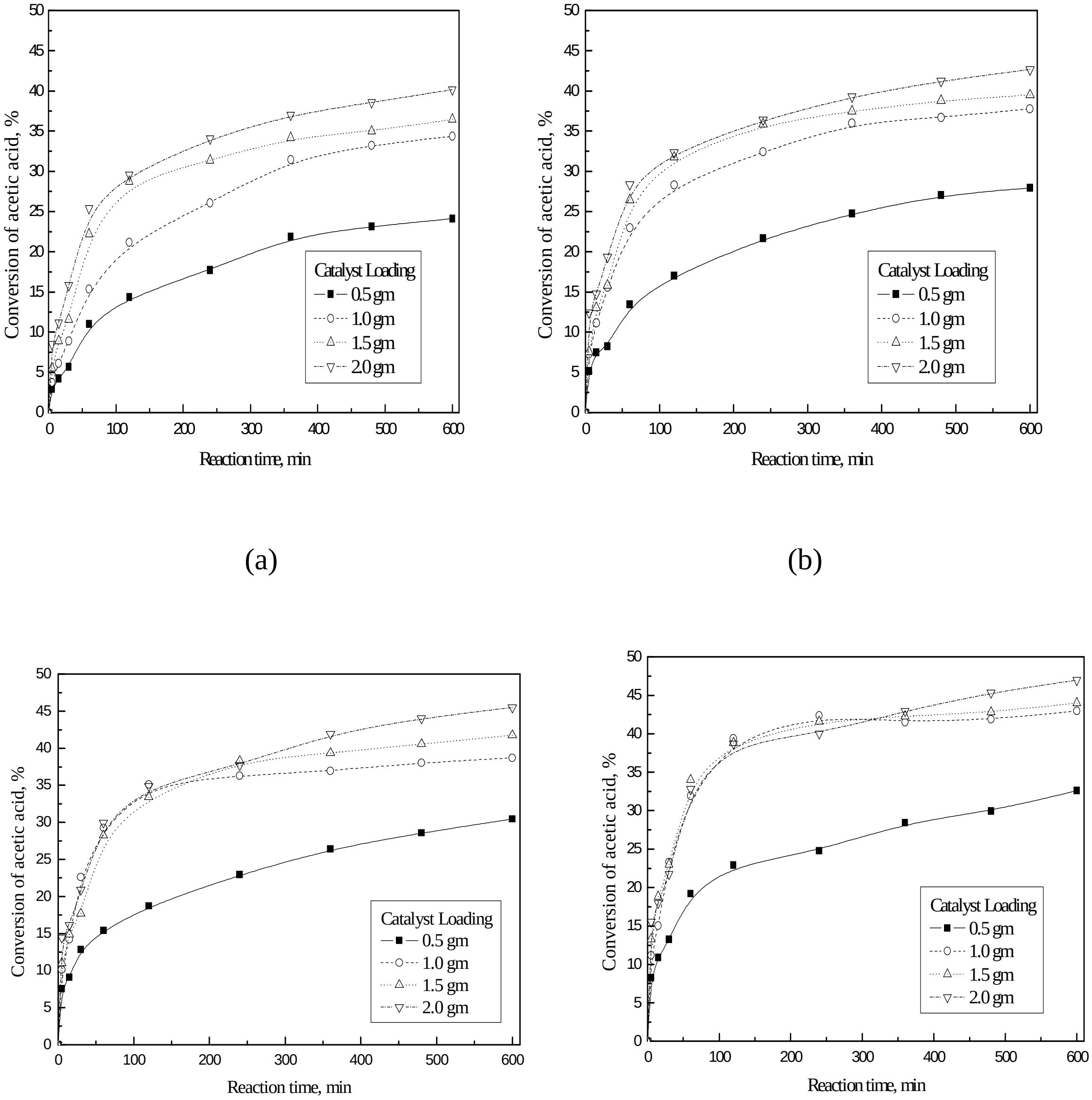
Table 5.38. Estimated parameters at 2.0wt% catalyst loading

T, K	K1 Lit/Mol Min	K-1 Lit/Mol Min	K2 Lit/Mol Min	K-2 Lit/Mol Min
333	1.60E-03	1.34E-03	1.24E-03	2.89E-03
343	1.82E-03	1.00E-03	1.87E-03	4.17E-03
353	2.04E-03	6.39E-04	2.56E-03	5.16E-03
363	2.73E-03	2.16E-04	4.76E-03	1.11E-02

Catalyst Wt%	E KJ/mol	K_0
1.5	22.15049	3.430274
	54.80678	574939.4
2.0	16.92696	0.70335
	42.86498	6407.92

5.2 Effect of catalyst loading on different parameters

5.2.1 Effect on conversion of acetic acid

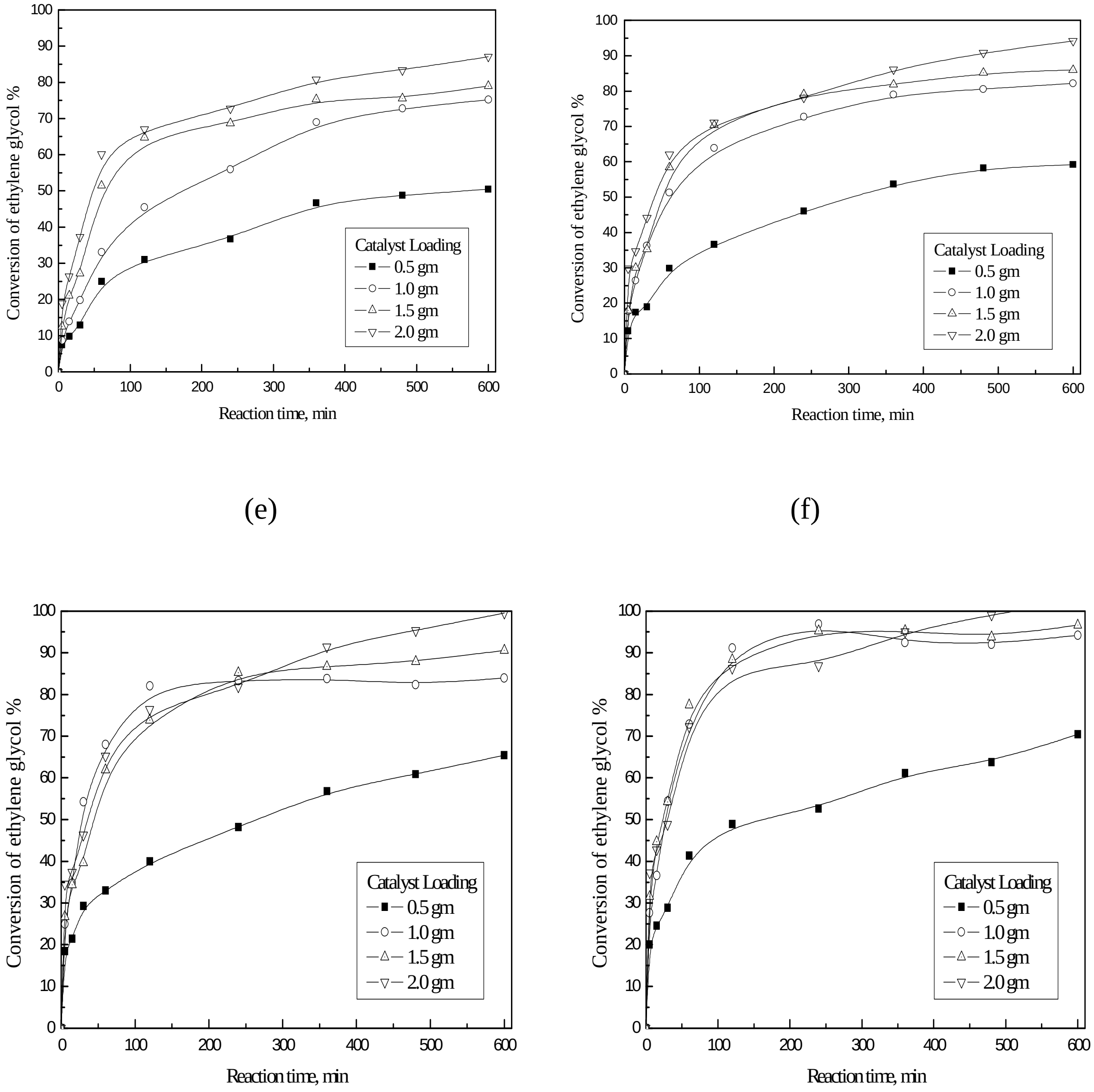


(a) (b)

(c) (d)

Fig.5.2.1. Plots (a), (b), (c) and (d) show the effect of catalyst loading on conversion of acetic acid at varying reaction time and temperature at 333, 343, 353 and 363 K

5.2.2 Effect on conversion of ethylene glycol



(e)

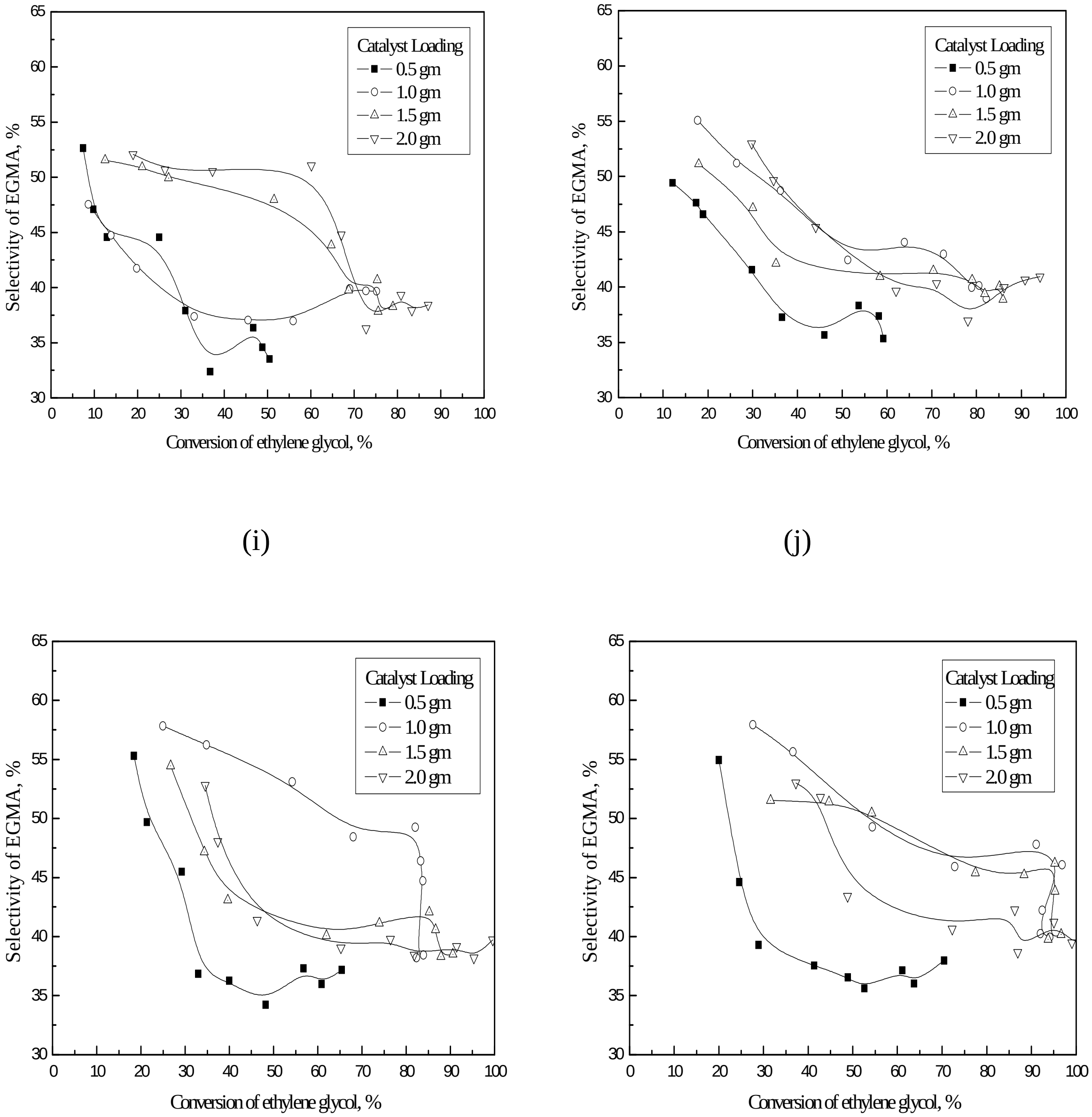
(f)

(g)

(h)

Fig.5.2.2. Plots (a), (b), (c) and (d) show the effect of catalyst loading on conversion of ethylene glycol at varying reaction time and temperature at 333, 343, 353 and 363 K

5.2.3 Effect on selectivity of ethylene glycol mono-acetate

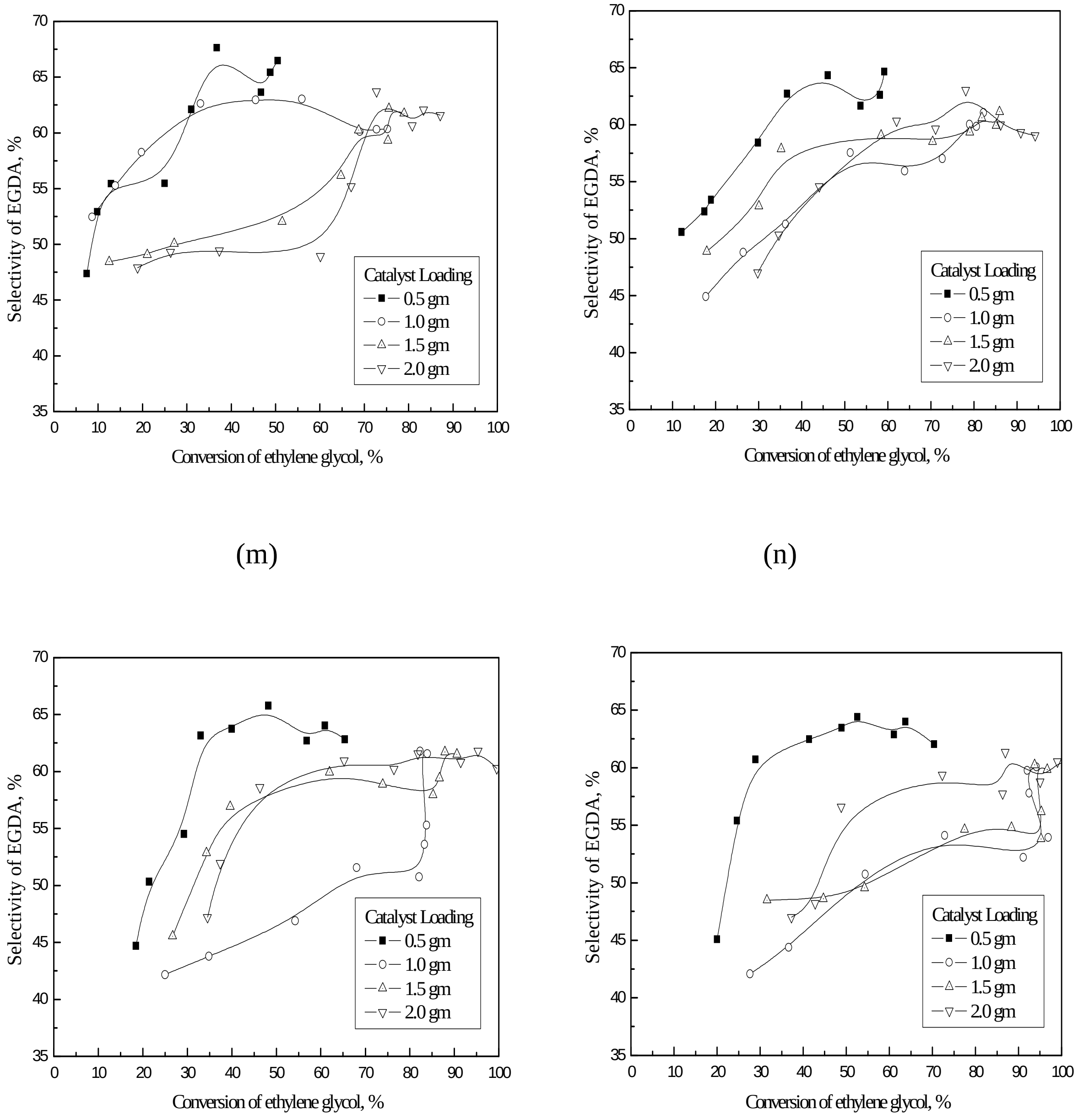


(i) (j)

(k) (l)

Fig.5.2.3. Plots (i), (j), (k) and (l) show the effect of catalyst loading on selectivity of ethylene glycol mono-acetate at varying ethylene glycol conversion and temperature at 333, 343, 353 and 363 K

5.2.4 Effect on selectivity of ethylene glycol di-acetate



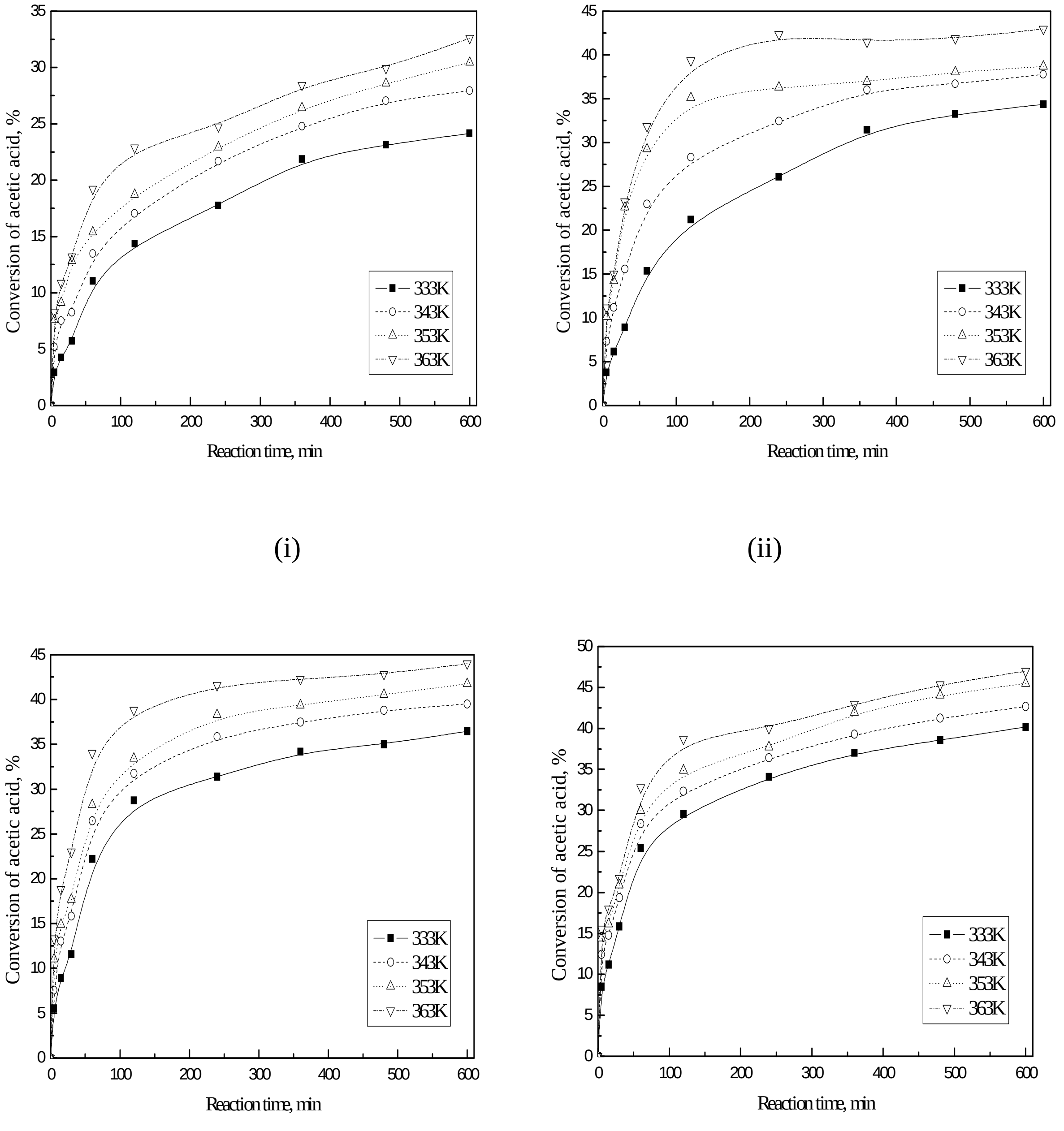
(m) (n)

(o) (p)

Fig.5.2.4. Plots (m), (n), (o) and (p) show the effect of catalyst loading on selectivity of ethylene glycol di-acetate at varying ethylene glycol conversion and temperature at 333, 343, 353 and 363 K

5.3 Effect of reaction temperature on various parameters

5.3.1 Effect on conversion of acetic acid

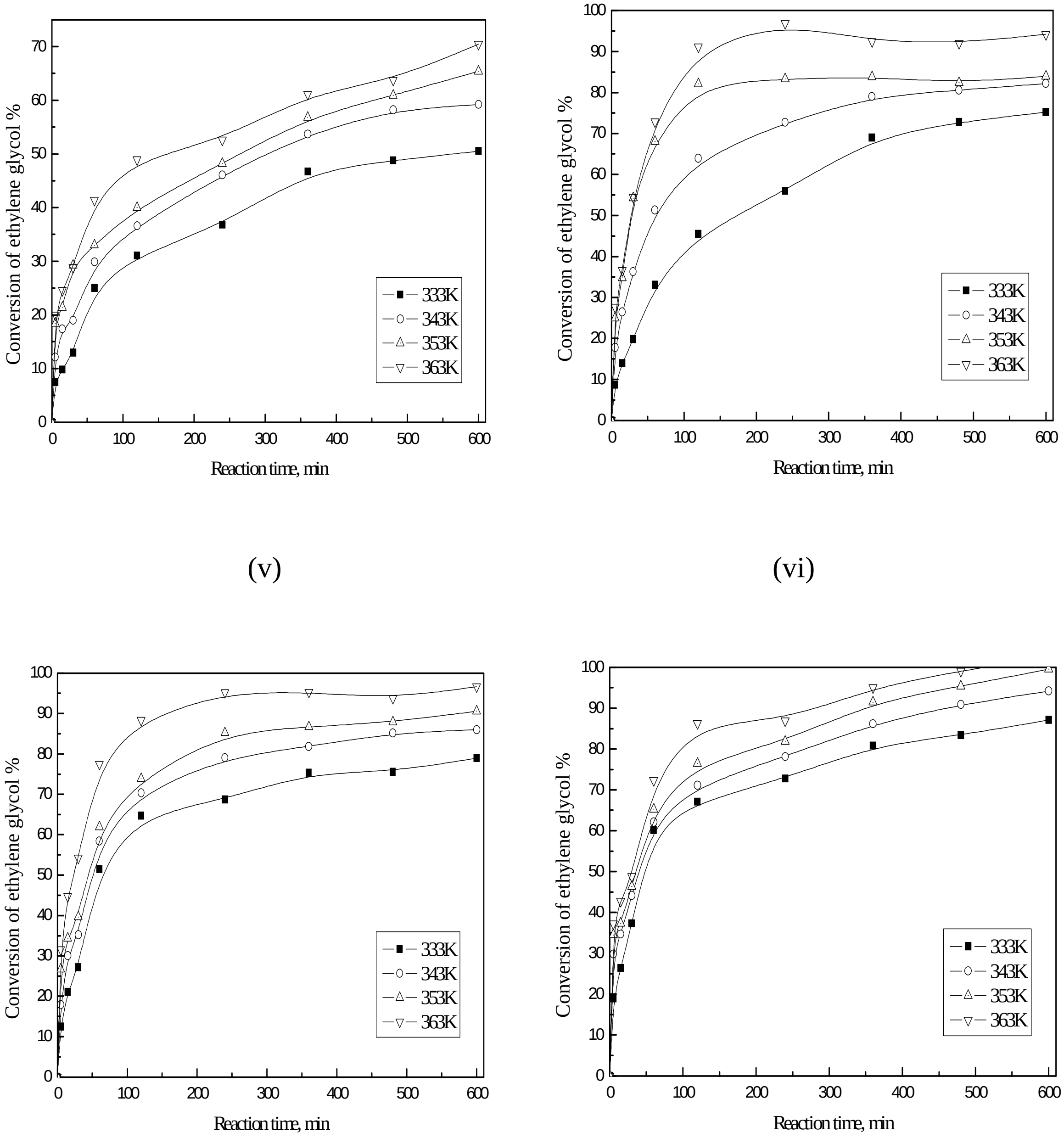


(i) (ii)

(iii) (iv)

Fig.5.3.1. Plots (i), (ii), (iii) and (iv) show the effect of reaction temperature on conversion of acetic acid with varying reaction time and catalyst loading of 0.5, 1.0, 1.5 and 2.0wt%

5.3.2 Effect on conversion of ethylene glycol



(v)

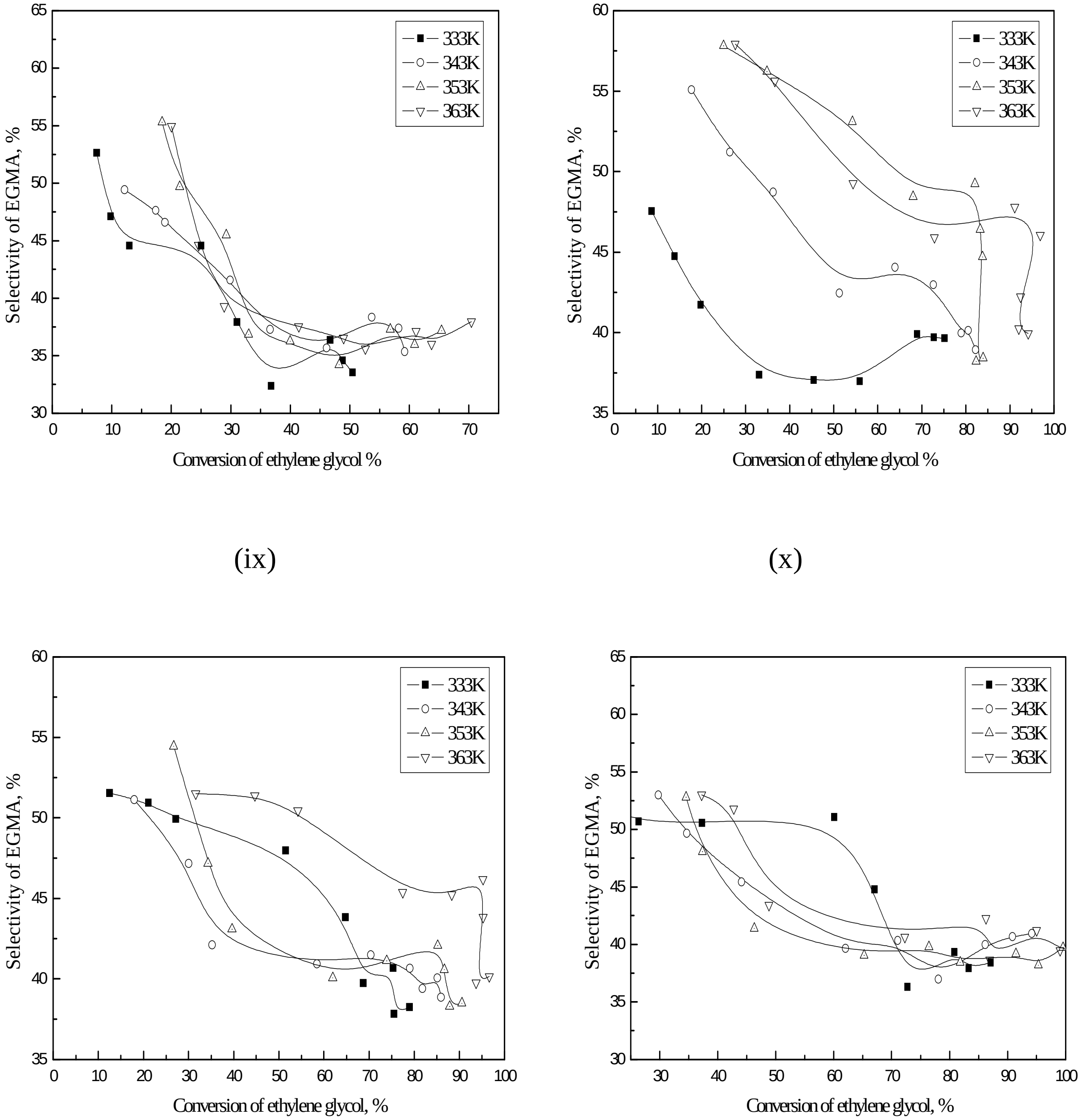
(vi)

(vii)

(viii)

Fig.5.3.2. Plots (v), (vi), (vii) and (viii) show the effect of reaction temperature on conversion of ethylene glycol with varying reaction time and catalyst loading of 0.5, 1.0, 1.5 and 2.0wt%

5.3.3 Effect on selectivity of ethylene glycol mono-acetate



(ix)

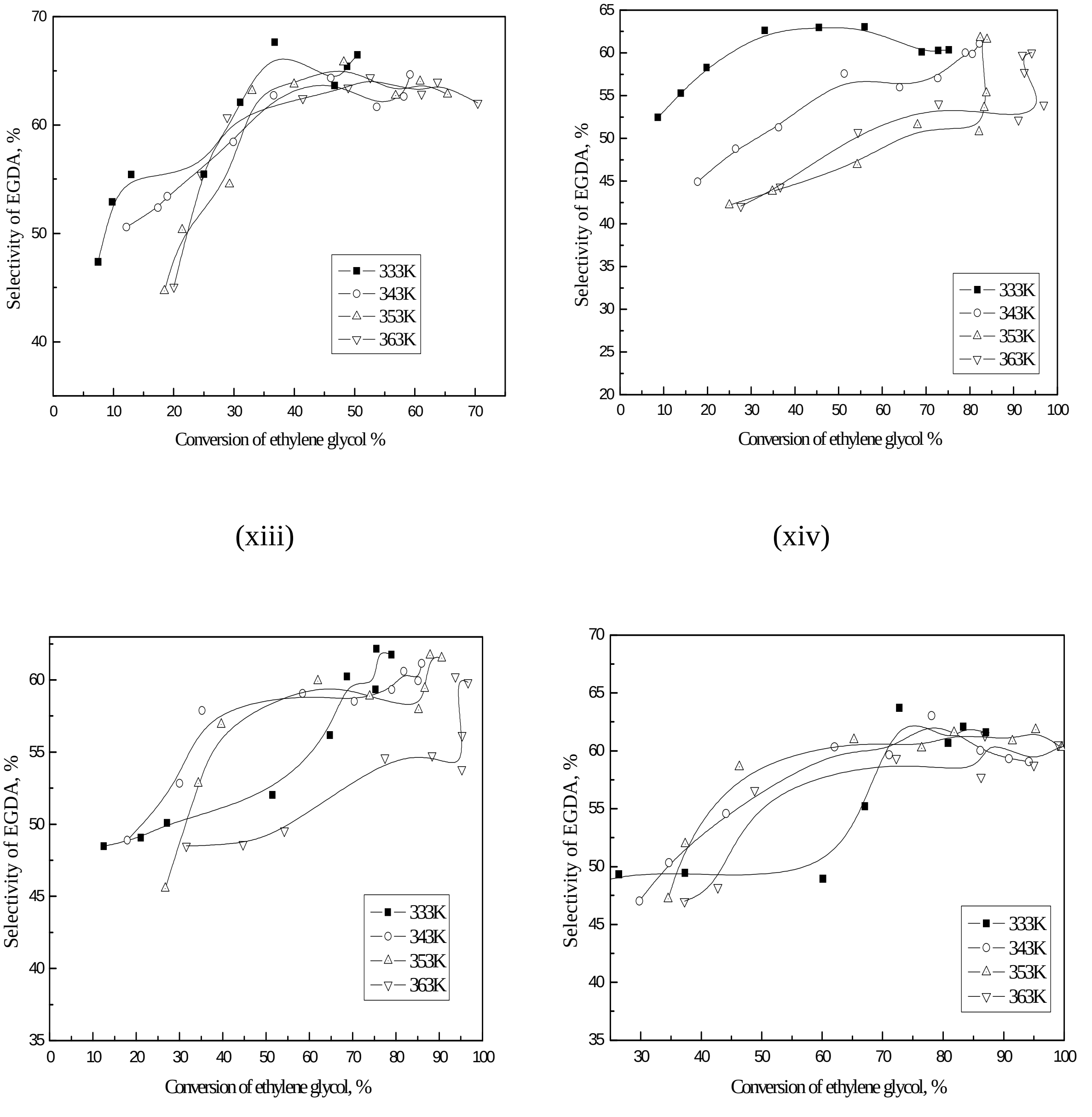
(x)

(xi)

(xii)

Fig.5.3.3. Plots (ix), (x), (xi) and (xii) show the effect of reaction temperature on selectivity of ethylene glycol mono-acetate with varying ethylene glycol conversion and catalyst loading of 0.5, 1.0, 1.5 and 2.0wt%

5.3.4 Effect on selectivity of ethylene glycol di-acetate

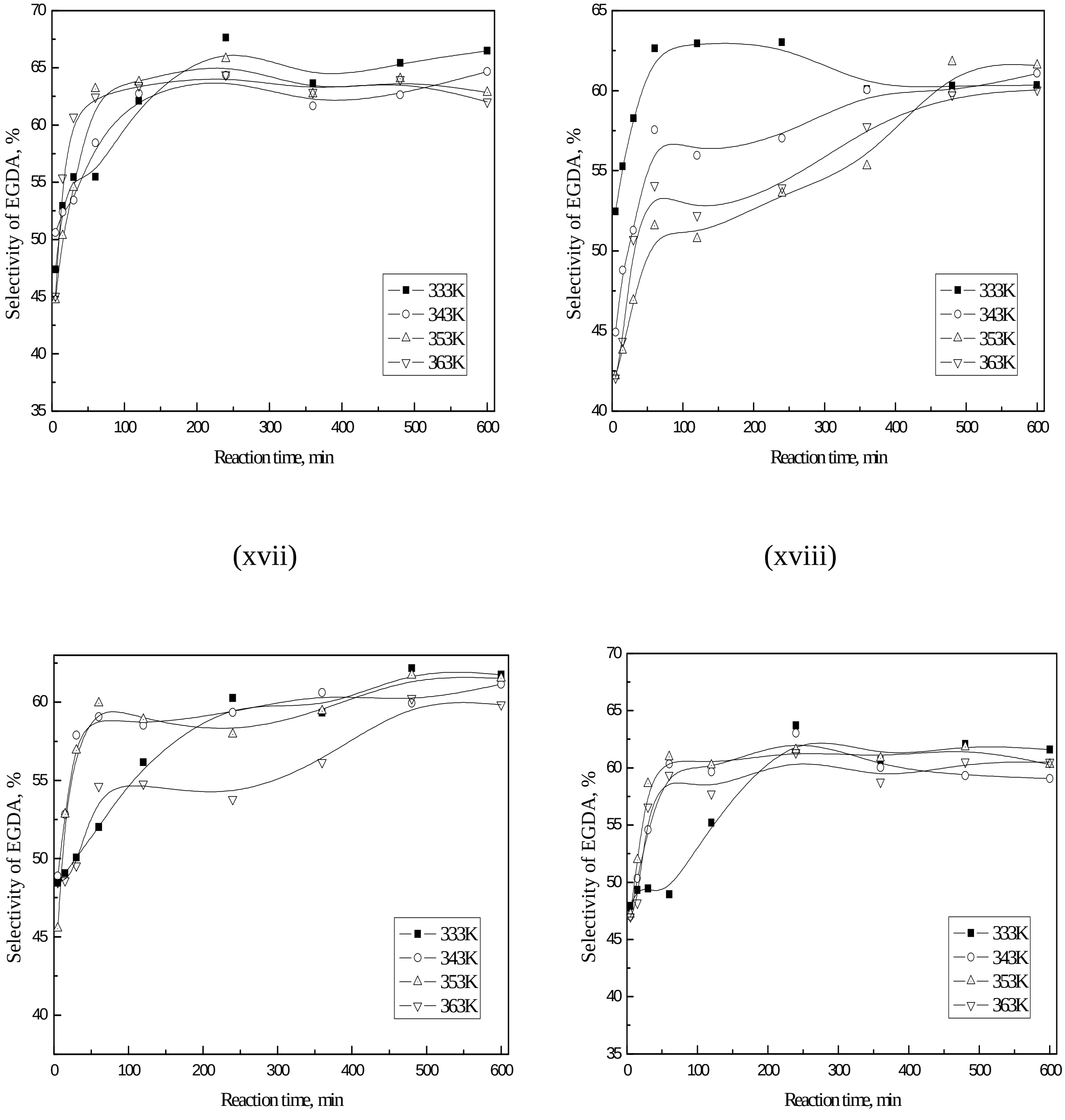


(xiii) (xiv)

(xv) (xvi)

Fig.5.3.4. Plots (xiii), (xiv), (xv) and (xvi) show the effect of reaction temperature on selectivity of ethylene glycol di-acetate with varying ethylene glycol conversion and catalyst loading of 0.5, 1.0, 1.5 and 2.0wt%

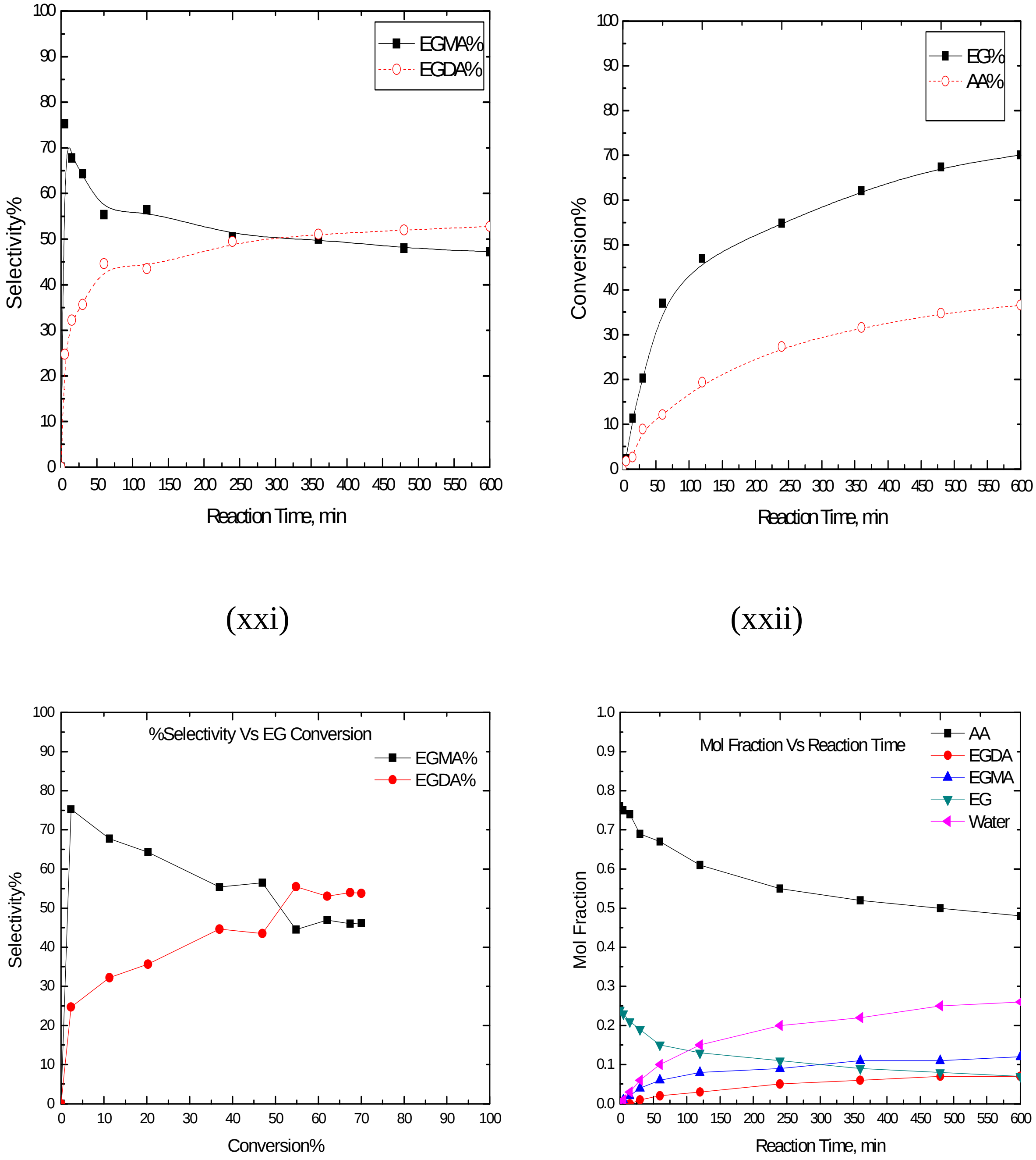
5.3.5 Effect on selectivity of ethylene glycol di-acetate with reaction time



(xvii) (xviii)

(xix) (xx)

Fig.5.3.5. Plots (xvii), (xviii), (xix) and (xx) show the effect of reaction temperature on selectivity of ethylene glycol di-acetate with varying reaction time and catalyst loading of 0.5, 1.0, 1.5 and 2.0wt%



(xxi) (xxii)

(xxiii) (xxiv)

Fig.5.3.6. Plots (xxi), (xxii), (xxiii) and (xxiv) show the effect of reaction time on selectivity of EGDA and mol fraction of used reaction system, also effect of EG conversion on selectivity of EGDA at molecular sieve 13X catalyst loading of, 4.0wt%

5.4 Parameter estimation

Rate equation based on the individual component of the five component reaction system, included ethylene glycol, acetic acid as reactant and ethylene glycol mono-acetate, ethylene glycol di-acetate and water as product has been written in following manner:

$$EG + AA \underset{K_{-1}}{\overset{K_1}{\rightleftharpoons}} EGMA + H_2O \ldots.\ldots\ldots\ldots\ldots\ldots\ldots...i$$

$$EGMA + AA \underset{K_{-2}}{\overset{K_2}{\rightleftharpoons}} EGDA + H_2O \ldots\ldots\ldots\ldots\ldots\ldots\ldots ii$$

$$\frac{dC_{EG}}{dt} = -K_1C_{EG}C_{AA} + K_{-1}C_{EGMA}C_{H_2O} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..1$$

$$\frac{dC_{AA}}{dt} = -K_1C_{EG}C_{AA} + K_{-1}C_{EGMA}C_{H_2O} - K_2C_{EGMA}C_{AA} + K_{-2}C_{EGDA}C_{H_2O} \ldots..2$$

$$\frac{dC_{EGMA}}{dt} = K_1C_{EG}C_{AA} - K_{-1}C_{EGMA}C_{H_2O} - K_2C_{EGMA}C_{AA} + K_{-2}C_{EGDA}C_{H_2O} \ldots.3$$

$$\frac{dC_{EGDA}}{dt} = K_2C_{EGMA}C_{AA} - K_{-2}C_{EGDA}C_{H_2O} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 4$$

$$\frac{dC_{H_2O}}{dt} = K_1C_{EG}C_{AA} - K_{-1}C_{EGMA}C_{H_2O} + K_2C_{EGMA}C_{AA} - K_{-2}C_{EGDA}C_{H_2O} \ldots\ldots 5$$

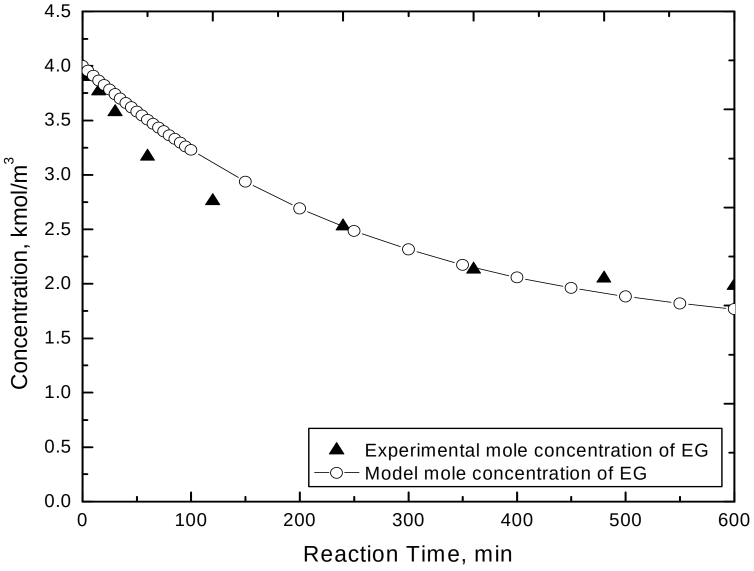


Fig.5.4.1. Plot shows the comparison between experimental and model EG concentration data with reaction time

From slope of concentration profile has been determined the rate of reaction at each point. All Parameter was estimated by non-linear least square method. The following function was optimized or minimized during parameter estimation

$$Erorr = \sum_{i=1}^{N} \frac{(C^{EG}_{expt.i} - C^{EG}_{model\,i})^2}{C^{EG}_{expt.i}} + \sum_{i=1}^{N} \frac{(C^{AA}_{expt.i} - C^{AA}_{model\,i})^2}{C^{AA}_{expt.i}} + \sum_{i=1}^{N} \frac{(C^{EGMA}_{expt.i} - C^{EGMA}_{model\,i})^2}{C^{EGMA}_{expt.i}} + \sum_{i=1}^{N} \frac{(C^{EGDA}_{expt.i} - C^{EGDA}_{model\,i})^2}{C^{EGDA}_{expt.i}} + \sum_{i=1}^{N} \frac{(C^{H_2O}_{expt.i} - C^{H_2O}_{model\,i})^2}{C^{H_2O}_{expt.i}}$$

Where,

N= Number of experimental data.

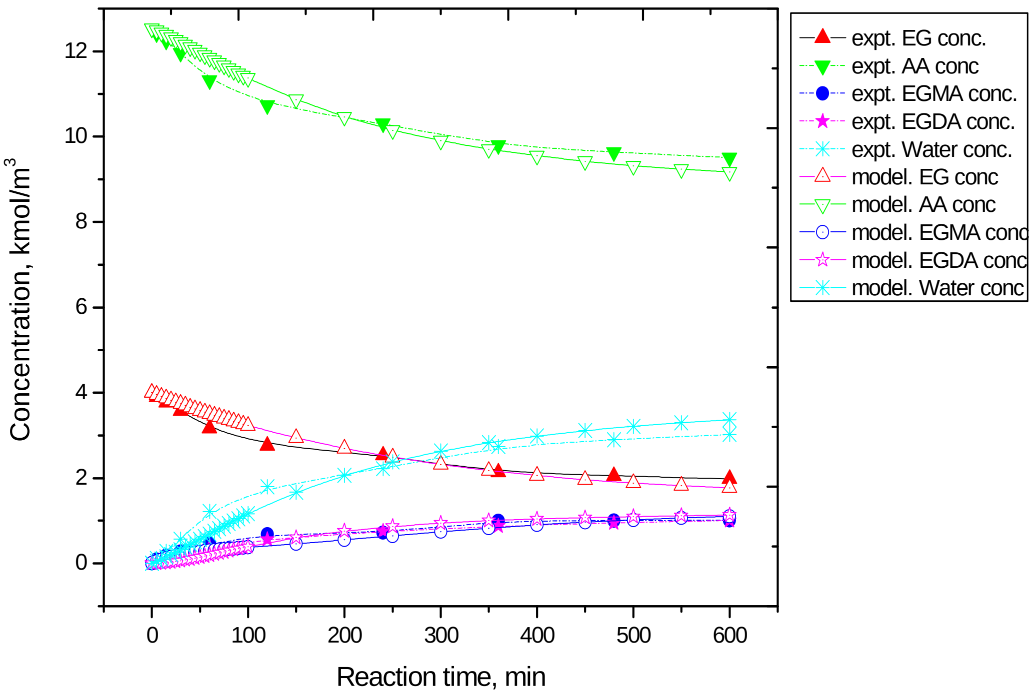
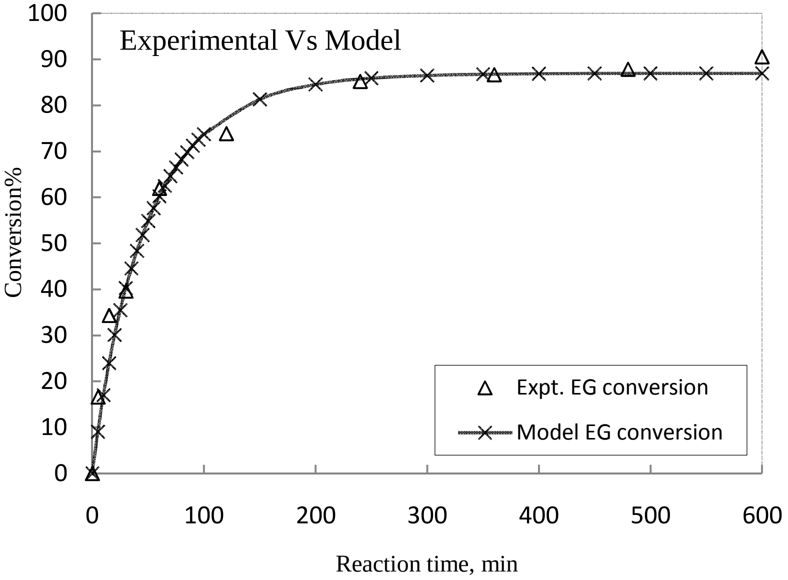


Fig.5.4.2. Plot shows the comparison between experimental and model of five component reaction system concentration data with reaction time



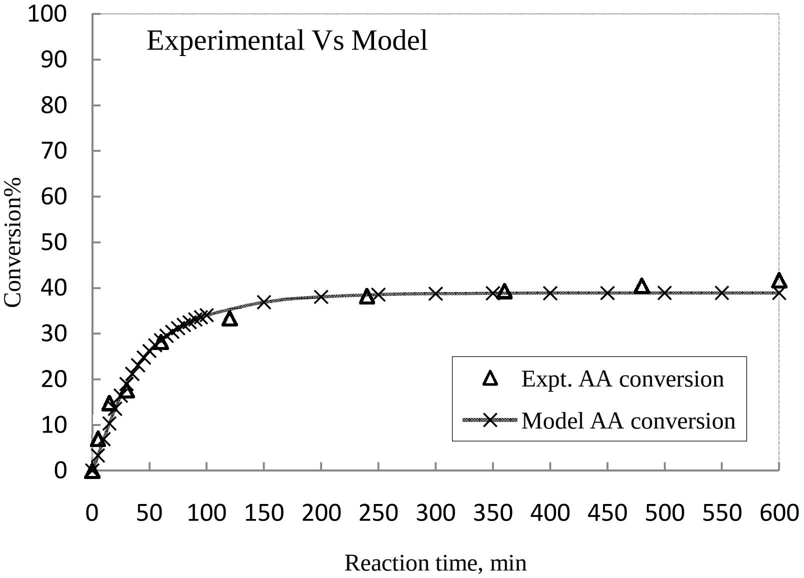


Fig.5.4.3. Comparison of experimental and model data for conversion of EG and AA with varying reaction time and catalyst loading of 1.5wt%

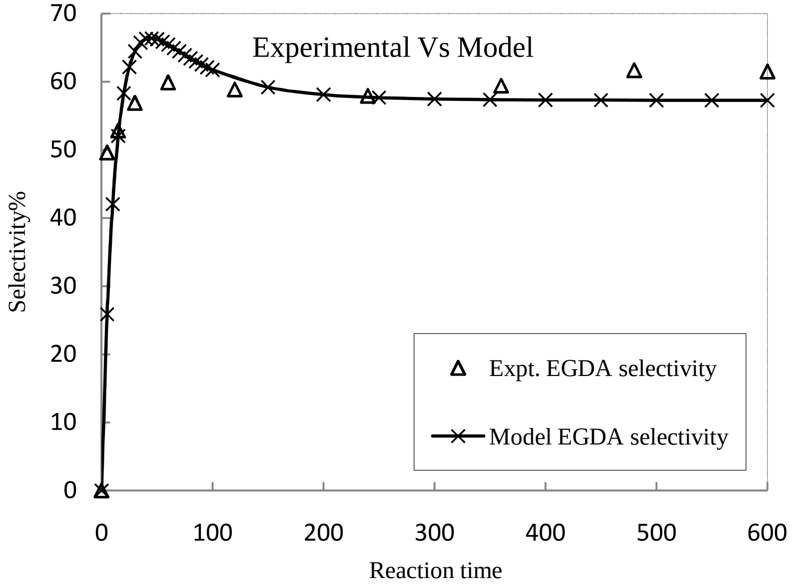


Fig.5.4.4. Comparison of experimental and model data for selectivity of EGDA with varying reaction time and catalyst loading of 1.5

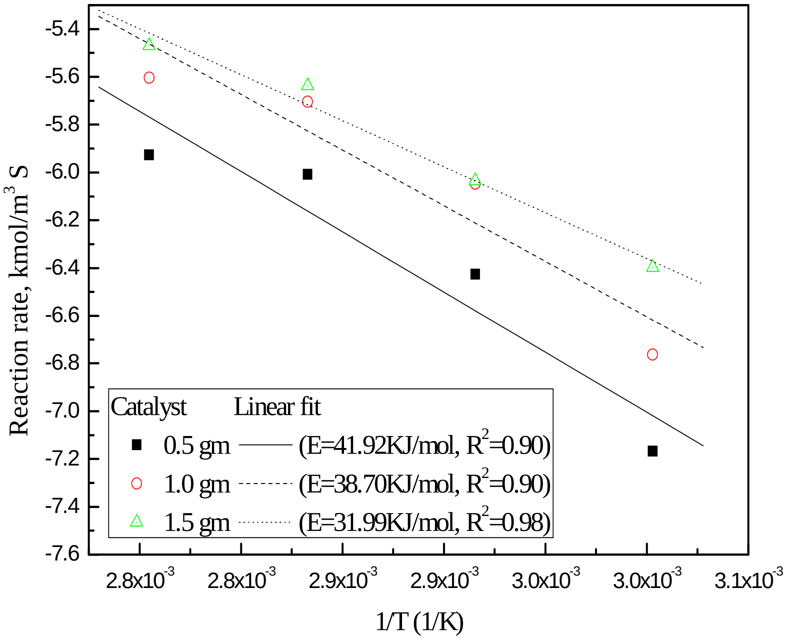


Fig.5.4.5. Plot shows the activation energy at 0.5, 1.0 and 1.5wt% catalyst loading

CHAPTER 6

DISCUSSION

Esterification of ethylene glycol with acetic acid has been carried out in the presence of Seralite SRC-120 (as type of Amberlite-120 ion exchange resin) and Molecular Sieve 13x(as Zeolite). The effect of various parameters has been found for five component reaction system and Therefore results were divided into several section due to purpose of easily understand. It was obtained that form reaction time curve profile that as increase reaction time as increase mole fraction of product, conversion of reactant and selectivity of ethylene glycol di-acetate (EGDA) but decrease in selectivity of ethylene glycol mono-acetate (EGMA) after 60 min . Observation table on different catalyst loading, reaction temperature, molar ratio and varying reaction time were shown in table from 5.1 to 5.18 and table 5.19 to 5.34 were represents the experimental and simulated data based on concentration of five component reactant and products system. Similarly the parameters have been estimated with different catalyst loading reported in table 5.35 to 5.38. Parameters as the rate of reaction, activation energy; pre-exponential factor and equilibrium rate constant were analyzed for best fit in five component reaction systems. In section 5.2 to 5.4 experimental and estimated data was graphically represented the effect of reaction time on conversion and selectivity of reactant and product respectively. Here it was found that as initially as from 60 to 120 min) increase the reaction time, suddenly increased the conversion of acetic acid (AA) and ethylene glycol (EG) because of the molecule of both reactant collide rapidly in presence of ion exchange acid catalyst. Maximum conversion of acetic acid was found to be 46.12 to 47 percentages at 353 to 363 K with 1.5 wt% and 2.0 wt% catalysts respectively. It was found that no much greater effect on reactant conversion either increases temperature or catalyst loading after 2 hour of the reaction time. Similarly the conversion of ethylene glycol was investigated and obtained 100 percentage conversions at 353 K with 10 hour reaction time. The selectivity of ethylene glycol mono and di acetate as product also has been investigated with different reaction temperature, reactant molar ratio and amount of catalyst. First of all elaborate the selectivity of ethylene glycol mono-acetate (EGMA), which was shown in section 5.2.3. Based on the selectivity graph it was obtained at starting conversion of EG was given maximum selectivity of EGMA, due to at starting reaction stage water formation has been low. The water has formed due to hydrolysis reaction and greatly affects on the reaction system. To avoiding this problem to reach reaction at equilibrium stage, water has been removed with the help of distillation column which reported in many literatures. However the most interesting and valuable product ethylene glycol di-acetate (EGDA) in five component reaction system was investigated as similar manner as EGMA, but most significant factor in the case of EGDA is maximum selectivity about 65 to 66 percentage has been obtained in the amount of 0.5wt% Seralite SRC-120 as a catalyst. Further increasing of catalyst loading and reaction temperature have no much effect on the selectivity of EGDA, because of as increasing the temperature Lewis acid sites are formed but Bronsted acid sites are removed, and Bronsted acid sites are more crucial factor in the catalysis esterification reaction. Hence, if increases the reaction temperature the Bronsted acid sites were reduced and decreases the activity of catalyst. In the part of simulation work, this has been done by non linear least square method and Arrhenius law with the help of Matlab software. It was obtained the equilibrium rate constant increases as increase the reaction temperature and catalyst loading hence increase the rate of reaction because of when liquids are heated the particles gain kinetic energy and move faster increasing the chance of collision between reactant molecules and therefore the increased chance of a fruitful collision, this effectively means the activation energy. The lowest activation energy about 31.99KJ/mol has been obtained with 1.5wt% amount of catalyst loading. .

CHAPTER 7

CONCLUSION

CONCLUSION

Esterification of ethylene glycol with acetic acid in the presence of acid catalysts as Seralite SRC-120 and Molecular Sieve 13x(as Zeolite) has been carried out generally in two consecutive steps. First ethylene glycol with acetic acid to produced ethylene glycol mono acetate then consecutive step form ethylene mono-acetate with acetic acid to ethylene glycol di-acetate. However the most significant result was obtained from experiment as well as simulation data. The highest ethylene glycol conversion was obtained 91.21% in 5 hour and mostly it was converted complete in 10 hours over seralite SRC-120 and 1.5wt% catalyst loading with temperature at 353 K. Similarly the conversion of acetic acid was found to be 46.12 %. About 65 to 66 percentage selectivity of EGDA has been achieved with amount of 0.5wt% Seralite SRC-120 as a catalyst. However the previous work has been reported the 54 to 56 percentage of EGDA selectivity. From figure 5.3.7 was shown the lowest activation energy about 31.99KJ/mol which is better for fastest esterification reaction. Due to low activation energy hydrolysis reaction can be controlled well. The experimental data and calculated data was well matched this means diminishes the chance of error. Molecular Sieve 13X was not given better results, because it has low active surface area and required more activation energy. In the case of molecular sieve 13X, ethylene glycol conversion was achieved to78.67%. The most appropriate reaction temperature for esterification of ethylene glycol with acetic acid was achieved at 353K. The Selectivity of EGMA was reduced with increases of reaction time due to excess water has formed by hydrolysis backward reversible reaction. It was obtained the equilibrium rate constant increases as increase the reaction temperature and catalysts loading hence increase the rate of reaction.

Proposed Future Work

1. Esterification ethylene glycol with acetic acid is well emerging area in the field of research and produces value added product. Which is widely used in many applications such solvent, perfumery, paint, ink, anti-freezant etc. therefore essential research required.
2. Ethylene glycol with acetic acid can be treated with different acid catalyst and investigate the different reaction parameters.
3. Since ethylene glycol is obtain from glycerol, which is available in excess amount in the current market. So esterification of glycerol with acetic acid can be considered as another reaction system. Biofuel as product has been obtained from glycerol, which can been attracted toward research.
4. Ethylene glycol can also be treated with different acids and analyzed which is better reaction system.

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