Kinetics of Esterification of Ethylene Glycol with Acetic Acid Using Cation Exchange Resin Catalyst

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The esterification of ethylene glycol with acetic acid was investigated in a batch reactor in presence of a strongly acidic cation exchange resin, seralite SRC-120, as catalyst in the temperature range of 333 to 363 K. The detailed kinetic study was performed to understand the effect of various process variables such as catalyst loading, ethylene glycol to acetic acid mole ratio, and temperature on conversion of reactants and selectivity to products. Further, two different kinetic models, empirical and kinetic model based on Langmuir-Hinshelwood-Hougen-Watson (LHHW) approach, were developed to correlate the experimental concentration versus time data. The kinetic parameters of the developed models were then estimated at different temperatures using non-linear regression technique based on modified Levenberg-Marquardt algorithm. The calculated results based on the estimated kinetic and equilibrium constants at different temperatures were then compared with the experimental values and LHHW-based model was found to fit the experimental data reasonably better compared to empirical kinetic model. The estimated rate constants at different temperatures of LHHW-based model were then used to estimate the activation energy and frequency factor of the rate constants.

Key words:
Reaction kinetics, modeling, ethylene glycol, ethylene glycol di-acetate, cation exchange resin

Introduction

The growing international energy crisis coupled with rising oil prices and increasing awareness of the environment and pollution has intensified the research on renewable fuels derived from biomass. The bio-oil produced by the process of biomass pyrolysis is nowadays an emerging technology for the production of renewable fuels and value-added chemicals. The bio-oil was first separated into aqueous and non-aqueous fractions by the addition of water. The aqueous fraction of bio-oils containing sugars, anhydrosugars, acetic acid, hydroxyacetone, furfural, and small amounts of guaiacols is a potential source of alkanes (ranging from C_1 to C_6) and polyols (ethylene glycol, 1,2-propanediol, 1,4-butanediol etc.).[1] The ethylene glycol obtained from bio-oil fraction can be utilized to produce ethylene glycol mono- and di-acetate suitable for application as solvent for coating, paints, and oxygenated diesel fuel additives.[2]

The esterification process is widely used in industry to produce esters for a wide range of applications such as plasticizers, solvent, perfumery, flavor chemicals, precursors for pharmaceuticals, agrochemicals, and other fine chemicals.[3–4] In recent times, several esterification reactions with different alcohols and carboxylic acids have been reported in open literature using different types of solid acid catalysts such as zeolites (HB, HY, ZSM-5) and cation exchange resin (Amberlyst 15, Amberlyst 36, Amberlite IRA-120).[5–11]

The esterification reactions are known to be catalyzed by a variety of Lewis or Bronsted acid catalysts. The homogeneous mineral acids such as H_2SO_4 and *p*-toluenesulphuric acid are however highly corrosive to process equipment and difficult to separate from the reaction mixture.[11–13] Moreover, there is an increasing tendency to develop processes that should meet the requirement of generation of nearly zero waste. Thus, it would be preferable to use a safer and simpler catalyst possibly in solid state, such as cation exchange resin. The various types of processes including isomerization, dehydration, etherification,

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acetylation, and esterification have been intensified by solid acid catalysts.[14–17]

The study of esterification of ethylene glycol with acetic acid is however limited in open literature.[18] Schmid *et al.*[19] studied the reaction using acidic cation-exchange resin, Amberlyst 36, as catalyst, and pseudo-homogeneous kinetic model based on activity was then developed using the measured thermodynamic properties of ethylene glycol–acetic acid reactive system.[20] Suman *et al.* studied the entrainer-based reactive distillation of ethylene glycol–acetic acid system using 1,2-dichloroethane (EDC) as an entrainer to enhance the conversion of reactants and selectivity to ethylene glycol di-acetate.[2] Considering the importance of the reaction, the present work was undertaken to study the kinetics of esterification of ethylene glycol with acetic acid in presence of a commercial cation-exchange resin catalyst and to develop suitable kinetic models for its application in design and simulation of reactive distillation column.

Experimental

Chemicals

Ethylene glycol and acetic acid (≥99 % purity) (aldehyde free) were purchased from Merck Specialities Private Limited, Mumbai, India. The strongly acidic (hydrogen form) cation-exchange resin, seralite SRC-120 (mesh number = 20–50, ion-exchange capacity = minimum 4.5 meq g^{-1} dry resin, and pH range = 0–14) was procured from Sisco Research Laboratories Private Limited, Mumbai, India.

Experimental set-up

All kinetic experiments were carried out in batch mode in a 6.5 cm i.d. fully baffled, mechanically agitated glass reactor with a volume of 250 cm^3. A six-blade glass disk turbine impeller with 2.0 cm diameter was used for stirring the reaction mixture. The impeller was kept at a height of 1.5 cm from reactor bottom. The reactor was kept in a constant temperature water bath whose temperature was controlled within ±1 K. The reaction mixture was well agitated with the help of a mechanical stirrer. To avoid the vaporization loss of reaction mixture, reactor setup was equipped with a condenser.

Experimental procedure

In a typical experimental run, about 75 cm^3 of acetic acid with known amount of catalyst (say 1 g) was charged into the reactor and kept well stirred until steady-state temperature was reached. Then the measured volume of ethylene glycol (25 cm^3), kept separately at reaction temperature, was charged into the reactor and the reaction started. Samples were withdrawn from reaction mixture at regular intervals after stopping the stirring and allowing the catalyst to settle. The detailed study of the reaction was performed in wide range of temperature (333–363 K), catalyst loading (0.5 to 1.5 % (w/v)), and acetic acid to ethylene glycol mole ratio (0.66 to 3.13).

Product analysis

The reaction product containing acetic acid, ethylene glycol, ethylene glycol mono-acetate (EGMA), and ethylene glycol di-acetate (EGDA) were analyzed by gas-liquid chromatography (Chemito GC 8610) using carbowax column. The GC equipped with a flame ionization detector (FID) was used for analysis. The column temperature was programmed with an initial temperature of 333 K for one minute, increased at a rate of 20 K min^{-1} up to 473 K, and maintained at 473 K for 2 min. The nitrogen (99.99 % purity) was used as carrier gas. An FID detector was used at a temperature of 523 K. An injector temperature of 523 K was used during the analysis. The moles of water formed in the reaction were obtained from the overall mole balance. Each sample was analyzed three times and average value was taken for further calculation.

Results and discussion

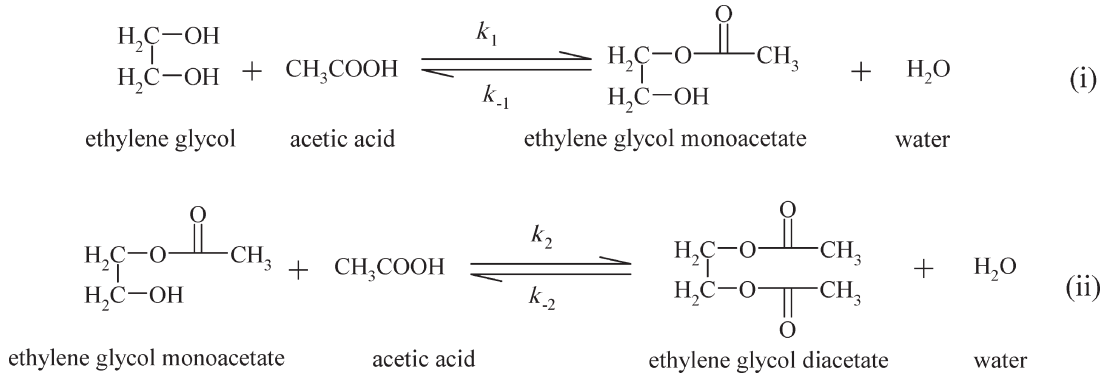
The reaction of ethylene glycol with acetic acid in presence of cation-exchange resin proceeds in two consecutive reversible steps as shown in Scheme 1. In the first step, ethylene glycol reacts with acetic acid to produce EGMA and water. The EGMA formed in the first step reacts further with acetic acid resulting in the formation of EGDA and water. The term selectivity (S) of the two products, EGMA and EGDA, used throughout the present article was defined as follows.

$$S_{EGMA}(\%) = 100 \cdot \frac{moles\ of\ \ EGMA\ \ formed}{mole\ of\ \ AA\ reacted}$$

$$S_{EGDA}(\%) = 100 \cdot \frac{2 \times moles\ of\ \ EGDA\ \ formed}{mole\ of\ \ AA\ reacted}$$

Effect of stirring speed

To determine the role of mass transfer resistances, the effect of agitation speed on the conversion of ethylene glycol was studied. The stirring speed was varied in the range of 1000–2000 rev min^{-1}. The strongly acidic cation-exchange resin (seralite



Scheme 1.

SRC-120) of 1.5 % (w/v) was used in each test. The variation of conversion of ethylene glycol was found to be negligible with speed of agitation as shown in Fig. 1. The external mass transfer resistance factors were therefore unimportant. Therefore, all other experiments were performed at a safe stirring speed of 1500 rev min^{-1}.

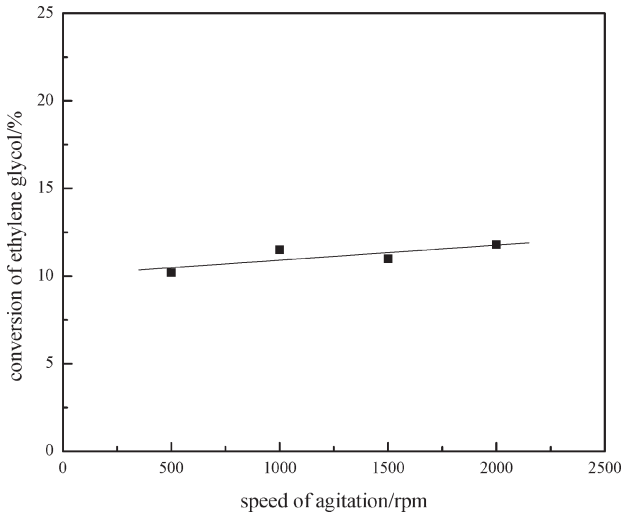


Fig. 1 – *Effect of speed of agitation on conversion of ethylene glycol. Conditions: Acetic acid to ethylene glycol mole ratio = 3.13; temperature = 333 K; catalyst loading = 1.5 % (w/v); matching reaction time = 5 min.*

Effect of temperature

The effect of temperature on conversion of ethylene glycol and selectivity of products was studied in the temperature range of 333–363 K. The effect of temperature on conversion of ethylene glycol is shown in Fig. 2. The conversion of ethylene glycol was found to increase with increase in temperature. The effect of temperature on the selectivity to EGDA is shown in Table 1. It is observed from the table that the selectivity to EGDA is not affected significantly by temperature especially, at high reaction time when the reaction reached close to equilibrium. This is because the standard enthalpy of reaction is relatively small which results in insignificant temperature dependency on the chemical equilibrium.[2,14,15,17] As a result, almost similar equilibrium composition was obtained in the temperature range studied.

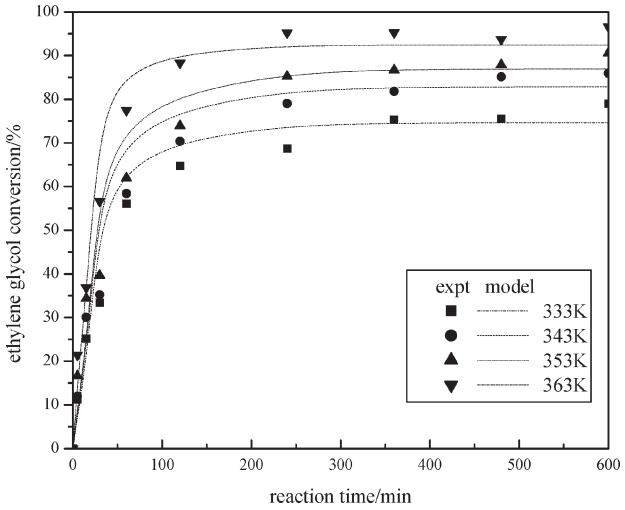


Fig. 2 – *Effect of temperature on conversion of ethylene glycol. Conditions: catalyst loading = 1.5 % (w/v); acetic acid to ethylene glycol mole ratio = 3.13; stirring speed = 1500 rpm.*

Table 1 – *Effect of temperature on selectivity to EGDA*[a]

Temperature/K	Selectivity/% to EGDA at different reaction time		
	30 min	60 min	120 min
333	42.7	48.8	56.2
343	57.8	59.1	58.5
353	56.9	59.9	58.9
363	51.3	54.6	54.8

[a]Conditions: Catalyst loading = 1.5 % (w/v); acetic acid to ethylene glycol mole ratio = 3.13; stirring speed = 1500 rpm.

The initial rates were calculated at different temperatures and Arrhenius plot of ln (initial rate) against $1/T$ was made and is shown in Fig. 3. The apparent activation energy was calculated from the slope of the best-fitted straight line as 39 kJ mol^{-1}. The high value of apparent activation energy further confirms that the reaction system is kinetically controlled. Schmid *et al.* reported the activation energy of 40 kJ mol^{-1} for this reaction.[19]

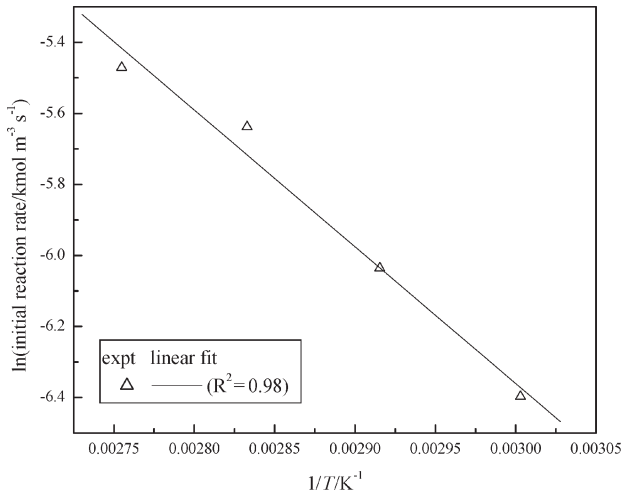


Fig. 3 – *Arrhenius plot of ln(initial rate) against 1/T. Conditions: All conditions are same as in Fig. 2.*

Effect of catalyst loading

The effect of catalyst loading was studied at three different catalyst loadings in the range of 0.5 to 1.5 % (w/v) of catalyst. The conversion of ethylene glycol increases with increase in catalyst loading as shown in Fig. 4. The effect of catalyst loading on selectivity to EGDA is shown in Table 2. The selectivity to EGDA was found to increase with increased reaction time as expected. However, the selectivity to EGDA was found to be almost unaffected by the catalyst loading. From these results, it may be concluded that with increase in catalyst loading, the rate of both esterification and hydrolysis reaction increases equally keeping the selectivity to the products unaffected.

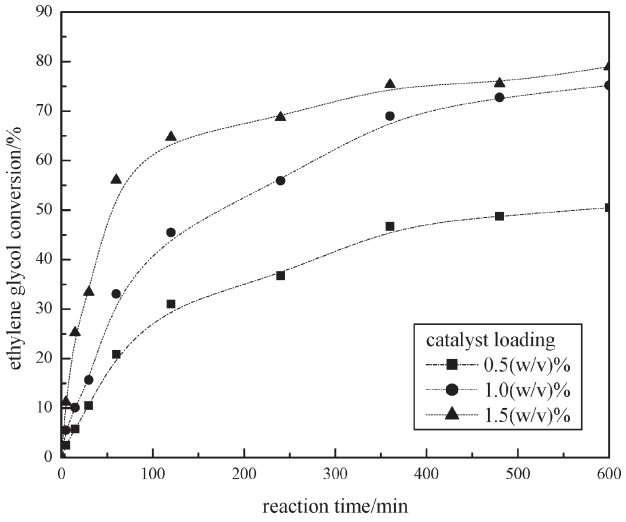


Fig. 4 – *The effect of catalyst loading on conversion of ethylene glycol. Conditions: temperature = 333 K; acetic acid to ethylene glycol mole ratio = 3.13; stirring speed = 1500 rpm.*

Table 2 – *Effect of catalyst loading on selectivity of EGDA*[a]

Catalyst loading/% (w/v)	Selectivity/% to EGDA at different reaction times			
	30 min	60 min	120 min	300 min
0.5	54.9	57.1	60.1	64.6
1.0	58.3	60.6	62.9	63.0
1.5	52.7	55.8	56.1	60.2

[a]Conditions: Acetic acid to ethylene glycol mole ratio = 3.13; temperature at 333 K; stirring speed = 1500 rpm.

Effect of acetic acid to ethylene glycol mole ratio

The effect of acetic acid to ethylene glycol mole ratio was studied at three different mole ratios of 0.66, 1.48, and 3.13, respectively, under identical experimental conditions. The acetic acid to ethylene glycol mole ratio was varied by varying the relative proportions of acetic acid and ethylene glycol keeping the total volume of the mixture constant. With increase in acetic acid to ethylene glycol mole ratio, the conversion of ethylene glycol was increased as shown in Fig. 5a. This is because of the depletion of ethylene glycol relative to acetic acid with increase in acetic acid to ethylene glycol mole ratio. The effect of acetic acid to ethylene glycol mole ratio on EGDA selectivity is shown in Fig. 5b. For fixed conversion of ethylene glycol, selectivity to EGDA was increased with increase in acetic acid to ethylene glycol mole ratio as shown in Fig. 5b. With increase in acetic acid to ethylene glycol mole ratio, the concentration of acetic acid relative to ethylene glycol was increased which in turn enhanced the reaction of EGMA with acetic acid. As a result, the selectivity to EGDA was increased. Similar results have been reported by Suman *et al.*[2] The maximum EGDA selectivity of 70 % was observed at 80 % conversion of ethylene glycol at acetic acid to ethylene glycol mole ratio of 3.13.

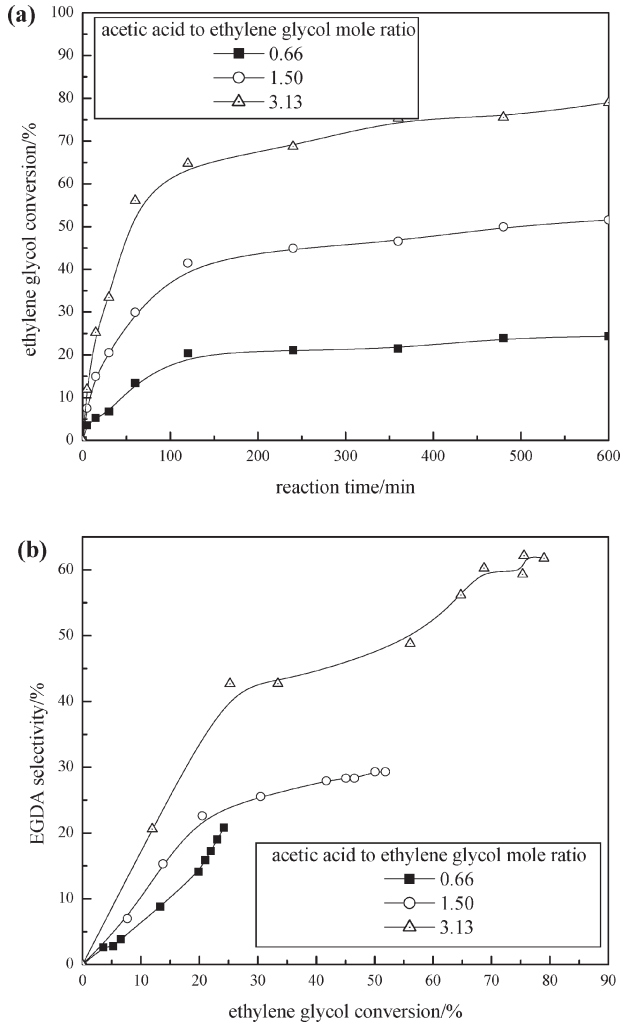


Fig. 5 – *Effect of acetic acid to ethylene glycol mole ratio on (a) ethylene glycol conversion and (b) EGDA selectivity. Conditions: temperature = 333 K; catalyst loading = 1.5 % (w/v); stirring speed = 1500 rpm.*

Modeling

The experimental measurements were used to develop suitable kinetic models for the reaction of ethylene glycol with acetic acid in presence of a strongly acidic cation-exchange resin. In the present work, the two different kinetic models, empirical and kinetic model based on Langmuir-Hinshelwood-Hougen-Watson (LHHW) approach were developed. It was found experimentally that the reaction was free from external mass transfer resistance. The kinetic parameters presented here, however, include intraphase diffusional effects, if any.

Empirical kinetic model

The esterification of ethylene glycol with acetic acid and hydrolysis as reverse reaction are SN^2 type reactions (Scheme 1) and hence, the reactions were considered as second order in the developed empirical model. The rates of formation of five different components involved in the reaction were therefore represented by the following five ordinary differential equations (eqs.1–5).

$$\frac{dc_{EG}}{dt} = -k_1 c_{EG} c_{AA} + k_{-1} c_{EGMA} c_W \quad (1)$$

$$\frac{dc_{AA}}{dt} = -k_1 c_{EG} c_{AA} + k_{-1} c_{EGMA} c_W - k_2 c_{EGMA} c_{AA} + k_{-2} c_{EGDA} c_W \quad (2)$$

$$\frac{dc_{EGMA}}{dt} = -k_2 c_{EGMA} c_{AA} + k_{-2} c_{EGMA} c_W + k_1 c_{EG} c_{AA} - k_{-1} c_{EGMA} c_W \quad (3)$$

$$\frac{dc_{EGDA}}{dt} = k_2 c_{EGMA} c_{AA} - k_{-2} c_{EGMA} c_W \quad (4)$$

$$\frac{dc_W}{dt} = k_1 c_{EG} c_{AA} - k_{-1} c_{EGMA} c_W + k_2 c_{EGMA} c_{AA} - k_{-2} c_{EGDA} c_W \quad (5)$$

Eqs. 1–5 constituted the developed empirical kinetic model involving the four rate constants.

Kinetic model based on Langmuir-Hinshelwood-Hougen-Watson approach

The kinetic models were also formulated following the LHHW approach assuming ethylene glycol, acetic acid, EGMA, and EGDA were adsorbed on surface. Since the reaction was found to be controlled by the kinetics only, the adsorption and desorption resistance was not considered and the model was developed based on surface reaction controlling only. According to this model, the rates of formation of the five components were given by the following five ordinary differential equations (eqs. 6–10).

$$\frac{dc_{EG}}{dt} = -k_1 \theta_{EG} \theta_{AA} + k_{-1} \theta_{EGMA} c_W \quad (6)$$

$$\frac{dc_{AA}}{dt} = -k_1 \theta_{EG} \theta_{AA} + k_{-1} \theta_{EGMA} c_W - k_2 \theta_{EGMA} \theta_{AA} + k_{-2} \theta_{EGDA} c_W \quad (7)$$

$$\frac{dc_{EGMA}}{dt} = -k_2 \theta_{EGMA} \theta_{AA} + k_{-2} \theta_{EGMA} c_W + k_1 \theta_{EG} \theta_{AA} - k_{-1} \theta_{EGMA} c_W \quad (8)$$

$$\frac{dc_{EGDA}}{dt} = k_2 \theta_{EGMA} \theta_{AA} - k_{-2} \theta_{EGMA} c_W \quad (9)$$

$$\frac{dc_W}{dt} = k_1 \theta_{EG} \theta_{AA} - k_{-1} \theta_{EGMA} c_W + k_2 \theta_{EGMA} \theta_{AA} - k_{-2} \theta_{EGDA} c_W \quad (10)$$

where θ_{AA}, θ_{EG}, θ_{EGMA}, θ_{EGDA} represent the fraction of surface covered by acetic acid, ethylene glycol, EGMA, and EGDA, respectively, and are given by the following equations.

$$\theta_{AA} = \frac{K_{AA} c_{AA}}{1 + K_{EG} c_{EG} + K_{AA} c_{AA} + K_{EGMA} c_{EGMA} + K_{EGDA} c_{EGDA}} \quad (11)$$

$$\theta_{EG} = \frac{K_{EG} c_{EG}}{1 + K_{EG} c_{EG} + K_{AA} c_{AA} + K_{EGMA} c_{EGMA} + K_{EGDA} c_{EGDA}} \quad (12)$$

$$\theta_{EGMA} = \frac{K_{EGMA} c_{EGMA}}{1 + K_{EG} c_{EG} + K_{AA} c_{AA} + K_{EGMA} c_{EGMA} + K_{EGDA} c_{EGDA}} \quad (13)$$

$$\theta_{EGDA} = \frac{K_{EGDA} c_{EGDA}}{1 + K_{EG} c_{EG} + K_{AA} c_{AA} + K_{EGMA} c_{EGMA} + K_{EGDA} c_{EGDA}} \quad (14)$$

The developed kinetic model involves four rate constants, k_1, k_2, k_{-1}, and k_{-2} and four adsorption equilibrium constants, K_{AA}, K_{EG}, K_{EGMA}, and K_{EGDA}.

Regression analysis and parameter estimation

The kinetic and equilibrium constants of the developed models were estimated using the experimental data at four different temperatures, 333, 343, 353, and 363 K, by non-linear regression algorithm based on modified Levenberg–Marquardt. The ordinary differential equations of the developed models were integrated using fourth-order Runge-Kutta method with initial guess values of kinetic and/ equilibrium constants. The objective function (F) to be minimized was then calculated based on calculated and experimental concentrations of five different components. The new guess values of the kinetic and/ equilibrium constants were then estimated following modified Levenberg-Marquardt algorithm. This process was repeated to minimize the objective function, F, of eq. 15.

$$F = \sum_{i=1}^{N} \left(\frac{c_{EG,i}^{expt} - c_{EG,i}^{model}}{c_{EG}^{expt}} \right)^2 + \sum_{i=1}^{N} \left(\frac{c_{AA,i}^{expt} - c_{AA,i}^{model}}{c_{AA}^{expt}} \right)^2 + \sum_{i=1}^{N} \left(\frac{c_{EGMA,i}^{expt} - c_{EGMA,i}^{model}}{c_{EGMA}^{expt}} \right)^2 + \sum_{i=1}^{N} \left(\frac{c_{EGDA,i}^{expt} - c_{EGDA,i}^{model}}{c_{EGDA}^{expt}} \right)^2 + \sum_{i=1}^{N} \left(\frac{c_{W,i}^{expt} - c_{W,i}^{model}}{c_{W}^{expt}} \right)^2 \quad (15)$$

The estimated optimized rate constants /equilibrium constants at different temperatures are shown in Table 3 and Table 4 for empirical and LHHW-based models respectively. It was observed from the table that with increasing temperature, the value of the rate constants increased as expected. The value of adsorption equilibrium constants of the developed LHHW-based model was found to decrease with increasing temperature. This is obvious as the adsorption is an exothermic process. The

Table 3 – *Kinetic constants of the empirical kinetic model*[a]

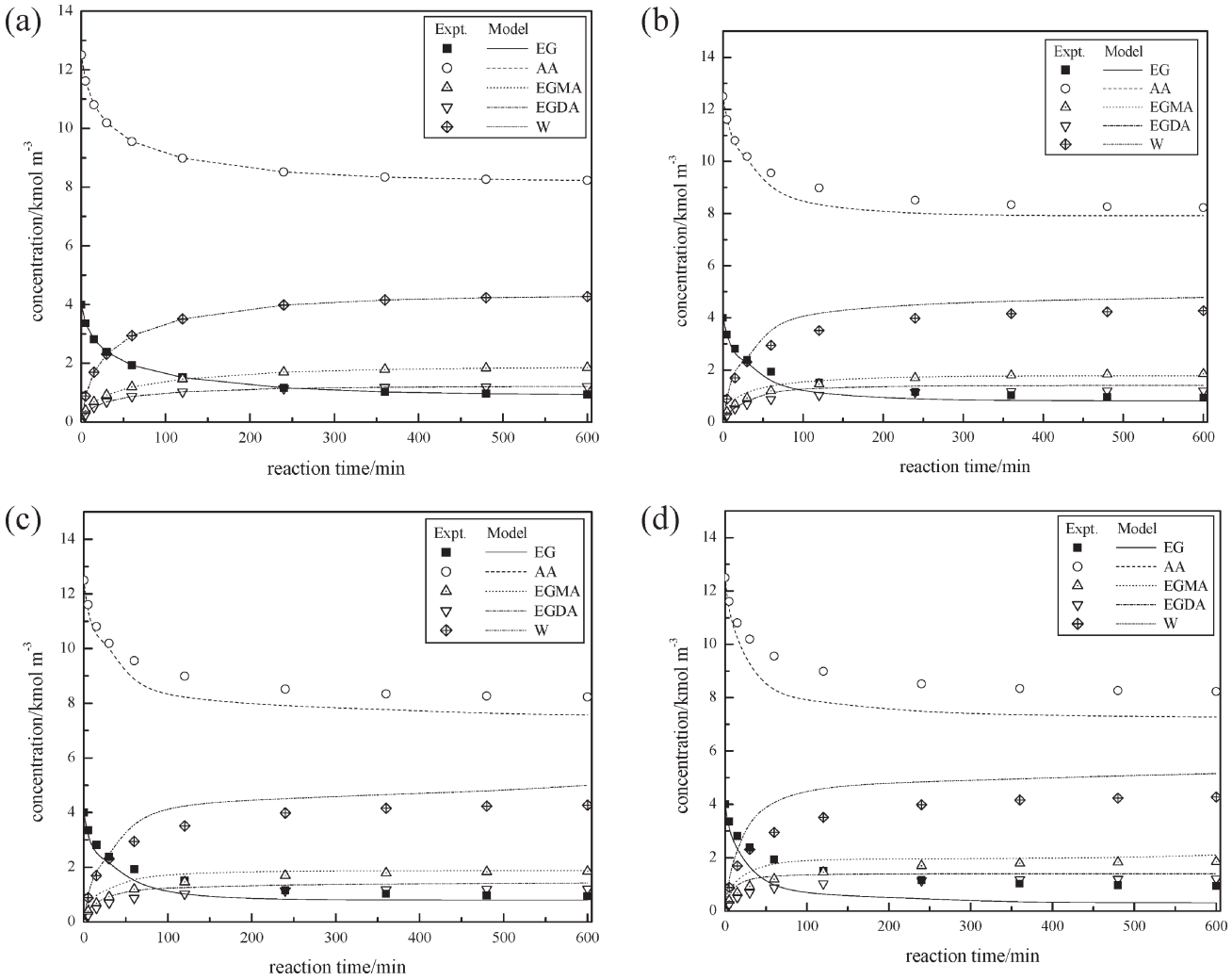
Temperature/K	Rate constants/(kmol m^{-3})$^{-1}$s^{-1}				Objective function (F)
	k_1	k_{-1}	k_2	k_{-2}	
333	$9.70 \cdot 10^{-04}$	$7.91 \cdot 10^{-04}$	$3.17 \cdot 10^{-03}$	$6.82 \cdot 10^{-03}$	11.4
343	$1.19 \cdot 10^{-03}$	$8.39 \cdot 10^{-04}$	$3.26 \cdot 10^{-03}$	$7.42 \cdot 10^{-03}$	13.7
353	$1.69 \cdot 10^{-03}$	$1.04 \cdot 10^{-03}$	$6.07 \cdot 10^{-03}$	$1.27 \cdot 10^{-02}$	7.3
363	$3.49 \cdot 10^{-03}$	$1.34 \cdot 10^{-03}$	$9.07 \cdot 10^{-03}$	$2.27 \cdot 10^{-02}$	2.8

[a]Conditions: Acetic acid to ethylene glycol mole ratio = 3; catalyst loading = 1.5 % (w/v).

Table 4 – *Kinetic and equilibrium adsorption constants of the LHHW-based kinetic model*[a]

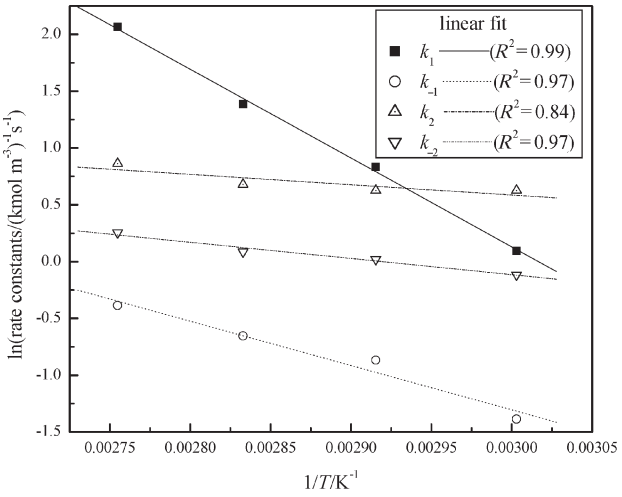
Temperature/K	Rate constants/(kmol m^{-3})$^{-1}$ s^{-1}				Adsorption equilibrium constants/(kmol m^{-3})$^{-1}$				Objective function (F)
	k_1	k_2	k_{-1}	k_{-2}	K_{EG}	K_{AA}	K_{EGMA}	K_{EGDA}	
333	1.10	0.25	1.87	0.89	1.01	0.424	7.51	9.54	6.5
343	2.30	0.42	1.87	8.09	0.98	0.415	8.09	7.05	3.1
353	4.00	0.52	1.97	1.09	0.76	0.390	7.69	6.70	4.5
363	7.90	0.68	2.37	1.29	0.67	0.382	7.62	6.28	7.1

[a]Conditions: Acetic acid to ethylene glycol mole ratio = 3.13; catalyst loading = 1.5 % (w/v).



F i g . 6 – *Experimental versus calculated concentration profiles at different temperatures. Conditions: catalyst loading = 1.5 % (w/v); acetic acid to ethylene glycol mole ratio = 3.13; stirring speed = 1500 rpm; (a) 333 K; (b)343 K; (c) 353 K; (d) 363 K.*

concentrations of ethylene glycol, acetic acid, EGMA, EGDA, and water were then calculated at various reaction times using the estimated rate constants at different temperatures and average relative deviation was calculated for both models. The average relative deviation of 9.2 % and 8.1 % was observed for empirical and LHHW-based model respectively. Therefore, LHHW-based model fits the experimental data better than empirical model. The concentration profile obtained from LHHW-based model at different temperatures was compared with that of experimental data as shown in Fig. 6. The experimental and calculated conversion of ethylene glycol based on LHHW-based model at different temperatures were also compared as shown in Fig. 2 and quite a good agreement was observed between calculated and experimental results. The Arrhenius plot of ln(rate constants) against $1/T$ was then made using the estimated rate constants of the LHHW-based model at different temperatures as shown in Fig. 7. The activation energy and pre-exponential factor were obtained from the slope and intercept of the Arrhenius plot as shown in Table 5.



F i g . 7 – *The Arrhenius plot of ln(rate constants) versus 1/T*

Table 5 – *Activation energy (E) and pre-exponential factor (A) of the kinetic constants of the LHHW-based model*

Rate constants	E, kJ mol^{-1}	A, units are consistent with rate constant
k_1	64.94	$1.75 \cdot 10^{10}$
k_{-1}	32.41	$3.29 \cdot 10^{04}$
k_2	7.55	27.47
k_{-2}	11.82	63.79

Conclusions

In the present work, the detailed kinetics of the esterification of ethylene glycol with acetic acid has been investigated in presence of a strongly acidic cation-exchange resin, seralite SRC-120 as catalyst. The acetic acid to ethylene glycol mole ratio was found to have enormous effect on the product selectivity where higher mole ratio favors selective formation of EGDA. The increase in temperature and catalyst loading has been found to enhance the reaction rate without significantly affecting the product selectivity. The two different kinetic models, empirical and kinetic model based on LHHW approach were also developed to correlate the experimental data. The rate constants and equilibrium constants of the developed kinetic models were estimated using the experimental data at different temperatures using non-linear least square techniques based on Levenberg-Marquardt algorithm. The concentration of different components calculated based on estimated parameters were then compared with experimental data and LHHW-based model was found to fit the experimental data better than empirical model. The activation energies and frequency factors of the rate constants of the LHHW-based model were then determined from the intercept and slope of the Arrhenius plot of ln(rate constants) versus 1/*T*.

ACKNOWLEDGMENTS

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Nomenclature

A – pre-exponential factor
c – concentration, kmol m^{-3}
E – activation energy, kJ mol^{-1}
F – objective function
k – rate constant, (kmol m^{-3})$^{-1}$ s^{-1}
K – adsorption equilibrium constant, (kmol m^{-3})$^{-1}$
T – reaction temperature, K
N – total number of experimental data

Greek Letters

θ – fraction of surface covered by a particular component

Subscripts

1 – forward reaction of eq. i of scheme 1
–1 – reverse reaction of eq. i of scheme 1
2 – forward reaction of eq. ii of scheme 1
–2 – reverse reaction of eq. ii of scheme 1
AA – acetic acid
EG – ethylene glycol
EGDA – ethylene glycol di-acetate
EGMA – ethylene glycol mono-acetate
W – water

Superscripts

Expt – experimental
Model – model

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