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# Kinetics of Alkylation of Benzene with Isopropyl Alcohol over Ce-Exchanged NaX Zeolite

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Alkylation of benzene was carried out in the vapor phase with isopropyl alcohol as an alkylating agent over cerium-exchanged NaX zeolite. The influences of various process parameters such as temperature, space-time, and the feed ratio of benzene to isopropyl alcohol on benzene conversion and cumene selectivity were studied. The experiments were carried out to choose the zone in which the mass transfer effects were negligible. On the basis of product distribution, a mechanism of the cumene synthesis reaction over the catalyst was proposed along with a rate expression for the limiting reactant. The kinetic and adsorption constants of the rate equations were estimated by best fit. From the estimated kinetic constants, the activation energies and frequency factors for various reactions were determined. The activation energy values compare well with those reported by other investigators for same reactions over similar catalysts.

## Introduction

Alkylation reactions are of great interests in petrochemical industry as they lead to several commercially important alkyl aromatics. Cumene is one such alkyl aromatic produced by isopropylation of benzene. The commercial importance of cumene is felt by the world's growing phenol demand, 90% of which is met by cumene. Several zeolite-based catalytic processes have been developed for the production of cumene by the alkylation of benzene with propylene.<sup>1–8</sup> In recent years, a lot of interest is being generated on the production of cumene with isopropyl alcohol as the alkylating agent. This is due to some advantages of using isopropyl alcohol instead of propylene as the alkylating agent. The olefin is the major source of carbonaceous deposits on alkylation catalysts; therefore, a long stable life of the catalysts is observed when alcohol rather than olefin is used as the alkylating agent. Besides, propylene tends to polymerize in the presence of acidic catalysts. To prevent this, a large excess of other reactant needs to be used so as to maintain a low concentration for the olefin. The present work is, therefore, concerned with the alkylation of benzene with isopropyl alcohol over Ce-exchanged NaX zeolite.

Numerous studies dealing with the industrially important alkylation reactions have been reported with various catalysts. The traditional Friedel–Crafts reactions employ mineral acids such as HF and H<sub>2</sub>SO<sub>4</sub> or Lewis acid such as AlCl<sub>3</sub> and BF<sub>3</sub>. The use of these substances involves technological and environmental problems due to their corrosive nature and the difficulty of recycling and separation from the product. The present tendency is to replace these conventional catalysts by solid acids, which are less corrosive. In recent years, much interest has been generated for the use of large pore zeolites.

Several researchers have studied the alkylation of benzene with propylene/isopropyl alcohol for the synthesis of cumene. The effects of various process param-

eters in benzene isopropylation on  $\beta$  zeolite have been studied, and the performance of the catalyst has been compared with that of other catalysts.<sup>9–11</sup> Cumene synthesis over various modifications of  $\beta$  zeolite has also been reported in the literature.<sup>11–14</sup> Corma et al.<sup>15</sup> have reported liquid-phase alkylation of benzene with propylene over zeolites MCM-22, ZSM-5, and  $\beta$ . Detailed kinetic study on MCM-22 led them to conclude that the reaction follows an Eley–Rideal mechanism in which benzene competes for the active site, but its coverage is much lower than that of propylene. Recently, Sridevi et al.<sup>16</sup> have studied the kinetics of benzene isopropylation over H-form of  $\beta$  zeolite. They have reported a simple stoichiometric model with a proposed reaction mechanism. There is, however, no information in the literature on the use of more versatile zeolite X for cumene synthesis. Moreover, replacement of Na ions of synthetic zeolites (e.g., X and Y) with polyvalent cations from rare earth metals (La, Ce, etc.) has been reported to give materials of superior catalytic activity.<sup>17–20</sup> It was, therefore, thought desirable to investigate the kinetics of this commercially important reaction over zeolite NaX modified by exchanging sodium ions with cerium ions. A further objective of this study was to develop a suitable kinetic model and to estimate the unknown parameters of the kinetic model to obtain an intrinsic rate equation.

## Experimental Section

**Materials.** The NaX zeolite used in the present study was obtained from S. D. Fine Chemicals Pvt. Ltd., India. It was in the form of 1.5 mm extrude. Isopropyl alcohol (IPA) and benzene used in this study were of analytical reagent grade. Isopropyl alcohol was obtained from Qualigens Fine Chemicals, Mumbai, India; benzene was from E. Merck (India) Ltd., Mumbai, India.

**Catalyst Preparation.**<sup>21,22</sup> The NaX zeolite was first calcined at 623 K for 3 h and kept ready for cation exchange. The catalyst particles were first heated with 2% NH<sub>4</sub>NO<sub>3</sub> solution at 363  $\pm$  10 K for 6 h, for three times, each time with a fresh 2% NH<sub>4</sub>NO<sub>3</sub> solution with subsequent calcining of the particles at 623 K in between. The catalyst particles thus obtained after a

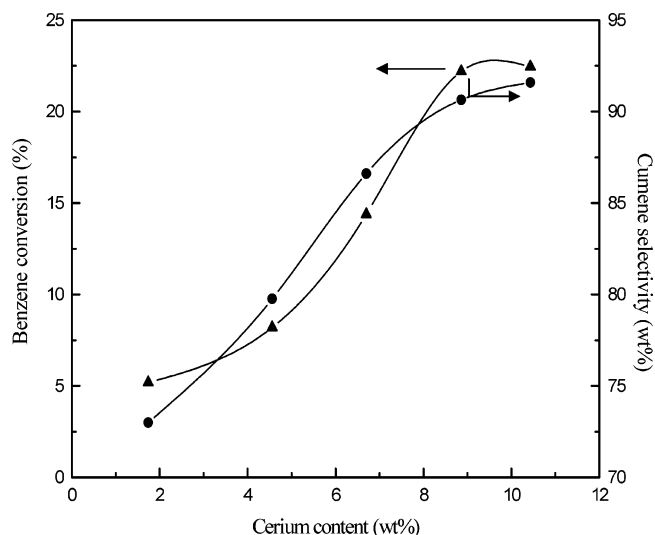
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total of 18 h heating and containing about 5–6% of Na (determined by flame photometer) were refluxed with a required percentage of cerium ammonium nitrate solution for about 16 h, thereby modifying the HX zeolite. This was then dried and calcined at 623 K and ready for use in the reactor. The X-ray diffraction pattern of the Ce-exchanged NaX zeolite exactly matched with that of the virgin NaX zeolite, indicating no structural change during ion exchange. Catalysts treated with 2%, 5%, 7%, 10%, and 12% cerium ammonium nitrate solutions were designated as CeX<sub>2</sub>, CeX<sub>5</sub>, CeX<sub>7</sub>, CeX<sub>10</sub>, and CeX<sub>12</sub>, respectively.

**Determination of Cerium Exchanged on the Catalysts.**<sup>23</sup> Accurately 2 g of freshly calcined catalyst containing cerium was taken in a conical flask and digested with concentrated HCl for about 1 h. The digested material was then diluted with distilled water and filtered through filter paper. The filtrate containing the cerium in solution was transferred to a 500 mL beaker, and its volume was raised to about 250 mL by adding distilled water. To this solution, 50 mL of saturated oxalic acid solution was added, which gave rise to a white precipitate of cerium oxalate. The precipitate was filtered through a Whatman no. 40 ashless filter paper and thoroughly washed with distilled water. The white precipitate along with the filter paper was then ignited over a previously weighed silica crucible at  $1173 \pm 10$  K to a constant weight. On heating, cerium oxalate was converted to Ce<sub>2</sub>O<sub>3</sub>. The percentage of cerium was then calculated from the weight of Ce<sub>2</sub>O<sub>3</sub>.

**Temperature-Programmed Desorption (TPD) of Ammonia.** Ammonia TPD of the modified catalysts was performed in a CHEM-BET 3000 instrument (Quantachrome). In a typical experiment, 0.1 g of the catalyst sample was first degassed at 723 K for 1 h with a nitrogen flow followed by cooling to low temperature ( $\sim 273$  K). A gas mixture of nitrogen and ammonia, consisting of about 1 mol % ammonia and the rest nitrogen, was then passed through the sample for 1 h. The catalyst sample was then heated to 373 K and kept at that temperature until the steady state was attained. The sample was then heated from 373 to 1173 K at a heating rate of 10 K/min. The desorbed ammonia was detected by a TCD analyzer.

**Experimental Procedure and Product Analysis.** The catalytic experiments were carried out in a fixed-bed, continuous down-flow, cylindrical stainless steel (SS 316) reactor (0.025 m i.d. and 0.33 m in length). The reactor was fitted with a preheater in the upstream and a condenser at its outlet. The reactor was heated electrically from outside and properly insulated with asbestos ropes to prevent heat loss. In a typical run, about 0.03 kg of catalyst was loaded into the reactor and supported by inert beads on either side of the bed. The bed temperature was measured by a thermocouple placed in a thermowell extending from the top of the reactor to the center of the bed. The catalyst was activated in situ for 8 h in 1 atm of nitrogen before the experimental runs were started. The aromatic–alcohol mixture was introduced with the help of a metering pump and vaporized in the preheater before contacting the catalyst. The reactant vapors along with nitrogen entered the reactor from the top. The product vapors, along with unreacted reactants, were condensed in the condenser, and the liquid samples collected were analyzed in a gas chromatograph unit fitted with a 4.2 m



**Figure 1.** Effect of Ce content on benzene conversion and cumene selectivity. Conditions: pressure, 1 atm; temperature, 473 K; space-time, 98.11 kg·h/kg-mol; benzene/IPA mole ratio, 4:1; N<sub>2</sub> to feed ratio, 0.44.

**Table 1. Results of Analysis of TPD Profiles of Various Catalysts**

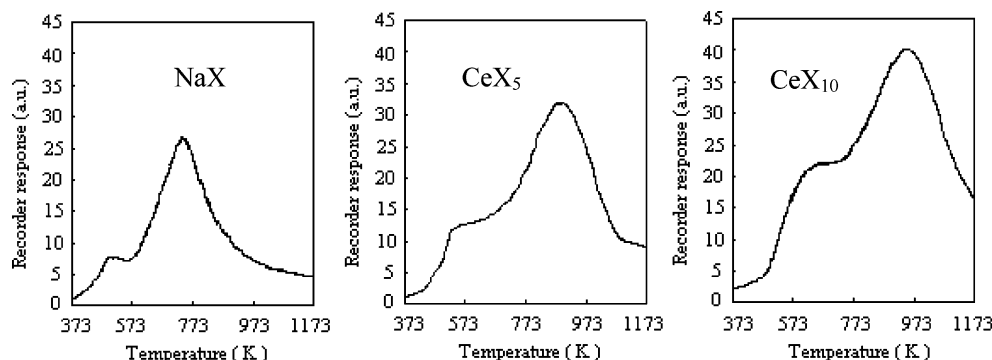
catalyst	Ce content (wt %)	avg temp (K) of		relative area under profile
		peak 1	peak 2	
NaX	0.0	500	750	1.0
CeX <sub>2</sub>	1.74	530	810	1.22
CeX <sub>5</sub>	4.56	570	885	1.58
CeX <sub>7</sub>	6.70	608	910	1.83
CeX <sub>10</sub>	8.86	650	960	2.20
CeX <sub>12</sub>	10.43	680	985	2.45

× 3.2 mm SS column containing Benton 34 and 7% dinonyl phthalate stationary phase on Celite-545 solid support using a flame ionization detector (FID). The material balance was checked, and it was >97%.

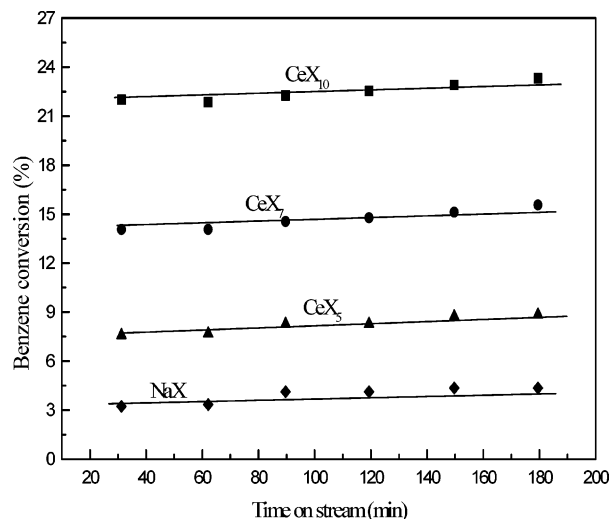
## Results and Discussion

**Effect of Cerium Loading on Catalytic Activity of NaX Zeolite.** NaX zeolite was treated to exchange its sodium ions with cerium ions. As mentioned earlier, the exchange was carried out with cerium nitrate solutions of different concentrations. The cerium content of the exchanged catalyst was estimated by a method described in the Experimental Section and reported in Table 1. Figure 1 shows the plot of cerium concentrations in the catalysts versus benzene conversion and cumene selectivity at a benzene to isopropyl alcohol mole ratio of 4:1 and at a temperature of 473 K. As can be seen from the figure, the benzene conversion and cumene selectivity both increase with an increase in cerium content in the NaX zeolite. This may be due to stronger acid sites generated by the exchange.

TPD of ammonia was studied with NaX as well as Ce-exchanged NaX zeolites, and Figure 2 shows the TPD profiles of three catalysts. The desorption of ammonia corresponding to different peaks is indicative of energy levels at which ammonia is bound to acid sites. The profiles indicate that the catalysts contain mainly two types of acid sites of varying strengths. The strengths of the acid sites increase with Ce exchange as the desorption peaks shift gradually toward the higher temperatures with increasing cerium content of the catalysts. Moreover, the number of acid sites also increases as the peak area increases with Ce exchange.



**Figure 2.** Temperature-programmed desorption profiles for ammonia for various catalysts.



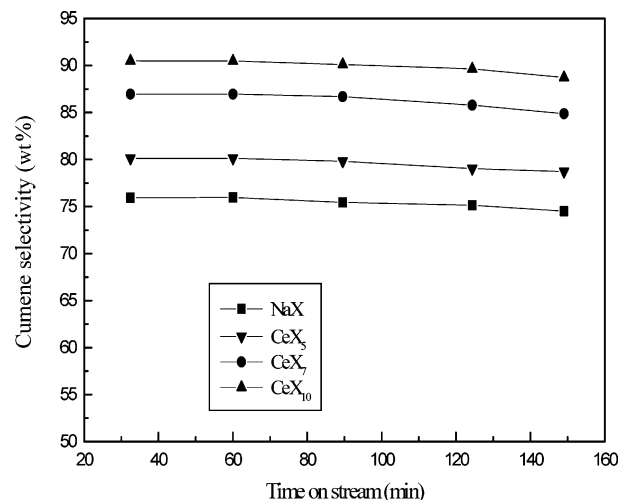
**Figure 3.** Activities of various catalysts in benzene isopropylation. Conditions: pressure, 1 atm; temperature, 473 K; space-time, 98.11 kg·h/kg-mol; benzene to IPA mole ratio, 4:1; N<sub>2</sub> to feed ratio, 0.44.

The increase in catalytic activity is therefore due to the increase in both quantity and strength of the acid sites by cerium exchange.

To support the above conclusion, the TPD profiles of all six catalysts were analyzed for average peak temperatures and areas under the curves as shown in Table 1. It is evident from Table 1 that both the strength and the quantity of acid sites of the catalysts increase as the cerium content of the catalyst increases.

**Effect of Time on Stream on Benzene Conversion and Cumene Selectivity.** The stability of Ce-modified 13X zeolites of different types were tested for about 3 h on stream at 473 K and atmospheric pressure. The benzene conversion remained almost constant during this period as shown in Figure 3. It is also seen from this figure that, among all the catalysts, CeX<sub>10</sub> gives highest conversion. So, the CeX<sub>10</sub> catalyst was used for further study. The effect of time on stream on cumene selectivity is shown in Figure 4. As can be seen from Figure 4, CeX<sub>10</sub> gives negligible variation in cumene selectivity but decreasing trend due to increasing formation of diisopropyl benzenes (DIPBs).

**Mass Transfer Considerations.** For any kinetic study, it is important that the mass transfer resistances be negligible during the reaction. To estimate the external diffusional effects, experiments were carried out at constant space-time and catalyst size, but with varying feed rates. The results shown in Table 2 indicate that the conversions of benzene for both the series at



**Figure 4.** Effect of time on stream on cumene selectivity. Conditions: pressure, 1 atm; temperature, 473 K; space-time, 98.11 kg·h/kg-mol; catalyst, CeX<sub>10</sub>; benzene to IPA mole ratio, 4:1; N<sub>2</sub> to feed ratio, 0.44.

**Table 2. Effect of External Diffusional Resistances on Conversion of Benzene<sup>a</sup>**

space-time (kg·h/kg-mol)	conversion of benzene (%) at	
	<i>b</i>	<i>c</i>
47.96	8.2	8.5
65.41	15.0	15.2
83.02	18.0	18.0

<sup>a</sup> Conditions: temperature, 473 K; benzene to IPA mole ratio, 4:1; *b*, 0.03 kg of CeX<sub>10</sub> catalyst; *c*, 0.05 kg of CeX<sub>10</sub> catalyst.

**Table 3. Effect of Intraparticle Diffusion on Conversion of Benzene<sup>a</sup>**

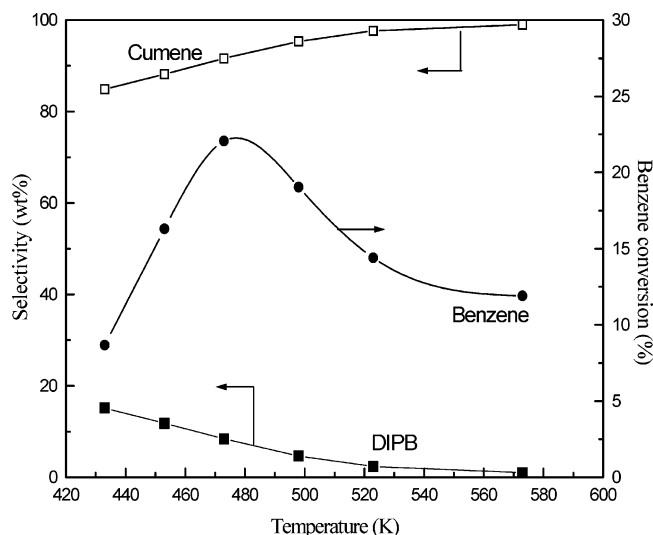
particle size, <i>d<sub>p</sub></i> (mm)	benzene conversion (%) with space-time (kg·h/kg-mol) of		
	47.96	65.41	83.02
0.50	8.3	15.3	18.1
1.00	8.4	15.3	18.1
1.50	8.2	15.0	18.0

<sup>a</sup> Conditions: temperature, 473 K; benzene to IPA mole ratio, 4:1.

constant *W/F* are independent of feed rate. Therefore, the external mass transfer resistance is negligible.

Experiments were also conducted to test the intraparticle diffusional limitations by varying the catalyst particle size while keeping space-time constant. The experimental data obtained are presented in Table 3. The results showed that there was no change in conversion of benzene with catalyst size, indicating negligible intraparticle mass transfer resistance in the particle size





**Figure 5.** Effect of temperature on benzene conversion and product selectivity. Conditions: pressure, 1 atm; space-time, 98.11 kg·h/kg-mol; catalyst, CeX<sub>10</sub>; benzene/IPA mole ratio, 4:1; N<sub>2</sub> to feed ratio, 0.44.

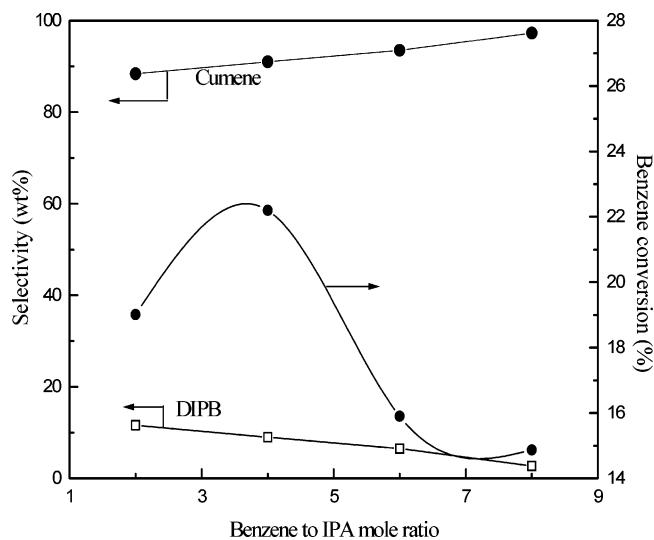
**Table 4. Distribution of Products at Various Temperatures<sup>a</sup>**

reaction temp (K)	product distribution (wt %)			
	cumene	<i>p</i> -DIPB	<i>m</i> -DIPB	oligomers
433	84.0	5.2	9.8	1.0
453	87.2	4.7	7.0	1.1
473	90.5	3.3	5.0	1.2
498	94.0	2.1	2.5	1.4
523	95.7	0.8	1.5	2.0
573	96.2	0.5	0.5	2.8

<sup>a</sup> Conditions: catalyst, CeX<sub>10</sub>; benzene/IPA, 4:1, space-time, 98.11 kg·h/kg-mol.

range studied. The particle sizes employed in the kinetic study were within the intraparticle diffusion-free range. In zeolite-catalyzed reactions, two types of diffusion processes are involved: (a) micropore diffusion inside the zeolite crystal and (b) macropore diffusion between the zeolite crystals within the catalyst pellets. The above experiments for mass transfer resistances confirms only the absence of diffusion in the macropores. The resistance due to micropore could not be evaluated, as it requires a modification of the synthesis conditions of the zeolite that affect the micropore size of the crystals, which would subsequently affect the diffusional characteristics. Hence, the kinetic parameters presented here include these diffusional effects, if any.

**Effect of Temperature on Benzene Conversion and Product Selectivity.** Reactions were carried out at different temperatures in the range of 433–573 K but with same feed composition and space velocity. The product composition was found to change with changing reaction temperature. As can be seen from Figure 5, the conversion of benzene first increases with increase in temperature, reaches a maxima at 473 K, and then decreases. A similar observation was made by Levesque<sup>24</sup> for the reaction of benzene ethylation. The decrease in benzene conversion can be due to (i) reduced availability of alcohol, which goes to side reactions (e.g., oligomerization at higher temperatures) or (ii) dealylation. It is evident from Table 4 that the formation of oligomers increases with increase in temperature, thereby reducing the amount of alcohol available for alkylation. However, the second reason (i.e., dealylation) is more



**Figure 6.** Effect of benzene to IPA mole ratio on benzene conversion and product selectivity. Conditions: pressure, 1 atm; temperature, 473 K; space-time, 98.11 kg·h/kg-mol; catalyst, CeX<sub>10</sub>; N<sub>2</sub> to feed ratio, 0.44.

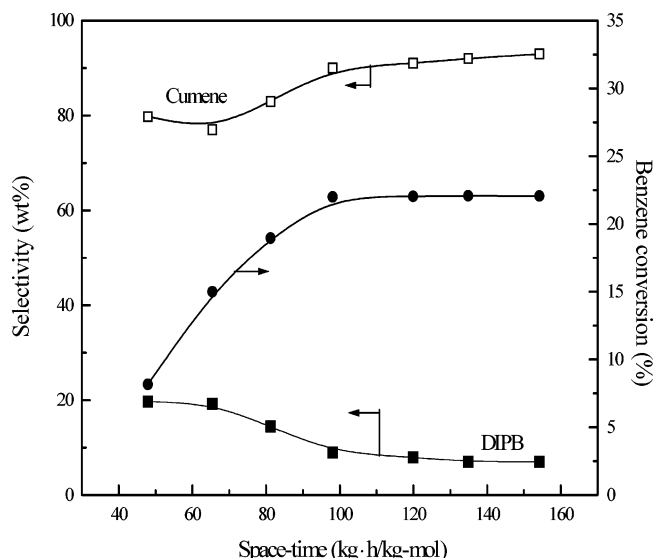
effective in reducing the conversion of benzene. The cumene selectivity increases and that of DIPB decreases with the increase in temperature as shown in Table 4. At higher temperatures, diisopropyl benzene (DIPB) transalkylates to cumene, thereby increasing the selectivity of cumene and decreasing the selectivity of DIPB.

**Effect of Benzene to IPA Mole Ratio.** The reactions were carried out by varying the mole ratio of benzene to isopropyl alcohol from 2 to 8. Benzene conversion was found to increase first and then decreased with an increase in reactant mole ratio. As can be seen from Figure 6, the maximum conversion was obtained at a benzene to IPA mole ratio of 4:1. At mole ratios of benzene and isopropyl alcohol greater than 4, most of the active sites of the catalyst surface are blocked by excess of benzene and lower availability of limiting reactant decreases benzene conversion. With increase in aromatic to alcohol mole ratio, cumene selectivity was found to increase from 88.4% at mole ratio of 2 to 97.3% at mole ratio of 8. The increase in selectivity of cumene is due to the fact that the transalkylation of the product were more favored at higher aromatic to alcohol mole ratios.

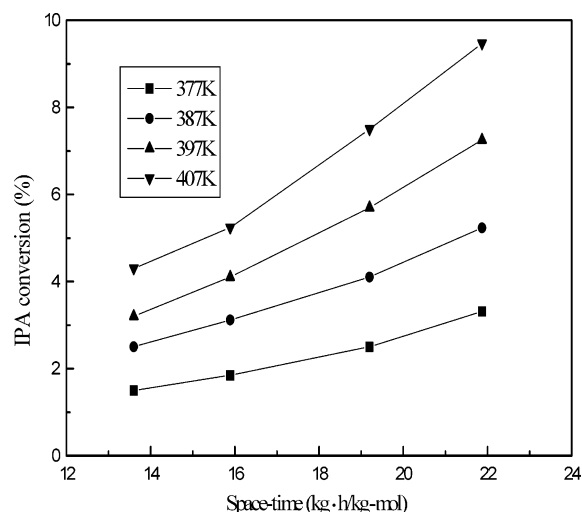
**Effect of Space-Time on Benzene Conversion and Cumene Selectivity.** The effect of space-time was studied in the range of 47.96–98.11 kg·h/kg-mol. As can be seen from Figure 7, the benzene conversion first increases with space-time and then becomes constant, which is quite expected. It is also evident from Figure 7 that the cumene selectivity increases with space-time and becomes constant at space-time values higher than 98.11 kg·h/kg-mol. The exact opposite trend was observed for DIPB selectivity. At higher contact times, transalkylation of DIPB with benzene predominates causing an increase in cumene selectivity and decrease in selectivity of DIPB.

### Kinetic Modeling

The kinetic runs were carried out at four different temperatures (namely, 377, 387, 397, and 407 K). The experiments were carried out to choose the zone in which the mass transfer effects are negligible. Figure 8 presents the effect of space-time on isopropyl alcohol conversion at four different temperatures.



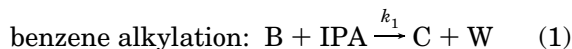
**Figure 7.** Effect of space-time on benzene conversion and product selectivity. Conditions: pressure, 1 atm; temperature, 473 K; catalyst, CeX<sub>10</sub>; benzene/IPA mole ratio, 4:1; N<sub>2</sub> to feed ratio, 0.44.



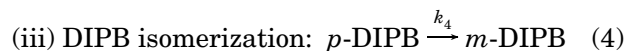
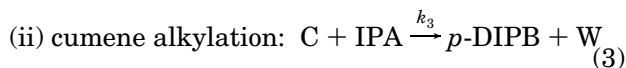
**Figure 8.** Effect of space-time on IPA conversion at various temperatures. Conditions: pressure, 1 atm; temperature, 473 K; catalyst, CeX<sub>10</sub>; benzene/IPA mole ratio, 4:1; N<sub>2</sub> to feed ratio 0.44.

In accordance with the product distribution, the system can be described by the following reactions:

Main reaction:



Secondary reactions:



The ortho isomer of diisopropyl benzene could not be detected in the product and hence does not feature in the system of reactions. Also, cumene cracking has been excluded since it is negligible at the temperatures studied.

**Table 5. Kinetic and Adsorption Parameters of Model Equation 5**

parameters	temperature (K)			
	377	387	397	407
$k_1$ (kg-mol/kg·h·atm <sup>2</sup> )	0.13	0.31	0.8	1.42
$k_2$ (kg-mol/kg·h·atm <sup>2</sup> )	0.006	0.02	0.04	0.1
$k_3$ (kg-mol/kg·h·atm <sup>2</sup> )	1.2	2.7	5.8	9.65
$k_4$ (kg-mol/kg·h·atm <sup>2</sup> )	0.18	0.22	0.3	0.38
$K_A$ (atm <sup>-1</sup> )	17.0	12.6	8.6	5.8
$K_B$ (atm <sup>-1</sup> )	0.04	0.03	0.02	0.01
$K_C$ (atm <sup>-1</sup> )	0.021	0.02	0.014	0.011

For the rate of disappearance of isopropyl alcohol, several models, including the Langmuir–Hinshelwood–Hougen–Watson (L-H-H-W) model, were attempted to fit the kinetic data. The various models tested are as follows:

L-H-H-W models with surface reaction controlling:  
Dual-site mechanism:

$$-r_A = dX_A/d\tau = [k_1 K_A K_B p_A p_B + k_2 K_A^2 p_A^2 + k_3 K_A K_C p_A p_C]/Z^2 \quad (5)$$

where  $Z = 1 + K_A p_A + K_B p_B + K_C p_C$ .

Single site mechanism (with benzene and cumene in gas phase):

$$-r_A = dX_A/d\tau = [k_1 K_A p_A p_B + (k_2/Z) K_A^2 p_A^2 + k_3 K_A p_A p_C]/Z \quad (6)$$

where  $Z = 1 + K_A p_A$ . The adsorption of water and carrier gas has been neglected in the above models.

Stoichiometric model:

$$-r_A = dX_A/d\tau = k_1 p_A p_B + k_2 p_A^2 + k_3 p_A p_C \quad (7)$$

The partial pressures of the various species in the above equations are related to the fractional conversions and the total pressure ( $P$ ) by the following expressions:

$$p_A = (1 - X_A)P/7.2 \quad (8)$$

$$p_B = (4 - X_B)P/7.2 \quad (9)$$

$$p_C = (X_C)P/7.2 \quad (10)$$

$$p_p = (X_p)P/7.2 \quad (11)$$

$$p_m = (X_m)P/7.2 \quad (12)$$

A nonlinear regression algorithm was used for parameter estimation. The optimum values of the parameters were estimated by minimizing the objective function given by

$$f = \sum_{i=1}^n [(X_{\text{pred}})_i - (X_{\text{exp}})_i]^2 \quad (13)$$

The kinetic and adsorption constants evaluated by nonlinear regression are tabulated in Tables 5–7 for model eqs 5–7, respectively.

**Model Discrimination.** By using the values of the constants for model eq 5 as shown in Table 5, the standard error of estimate for the rate of disappearance of IPA was  $\pm 1.35 \times 10^{-5}$ . For model eq 6, with the values of the constants from Table 6, the standard error was  $\pm 2.11 \times 10^{-3}$ . For model eq 7, with the values of

**Table 6. Kinetic and Adsorption Parameters of Model Equation 6**

parameters	temperature (K)			
	377	387	397	407
$k_1$ (kg-mol/kg·h·atm <sup>2</sup> )	0.1	0.14	0.37	0.7
$k_2$ (kg-mol/kg·h·atm <sup>2</sup> )	0.06	0.1	0.13	0.25
$k_3$ (kg-mol/kg·h·atm <sup>2</sup> )	1.15	1.82	2.8	3.77
$K_A$ (atm <sup>-1</sup> )	0.15	0.08	0.03	0.02

**Table 7. Kinetic Parameters of Model Equation 7**

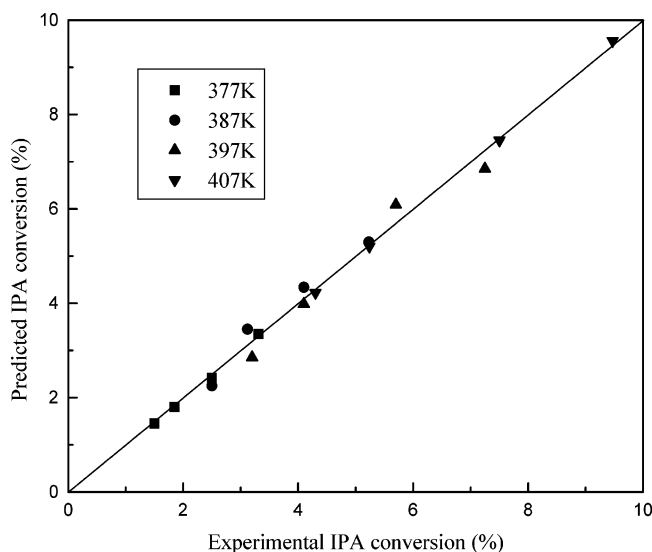
parameters	temperature (K)			
	377	387	397	407
$k_1$ (kg-mol/kg·h·atm <sup>2</sup> )	0.05	0.16	0.31	0.62
$k_2$ (kg-mol/kg·h·atm <sup>2</sup> )	0.003	0.008	0.02	0.04
$k_3$ (kg-mol/kg·h·atm <sup>2</sup> )	1.3	2.64	4.8	9.76

**Table 8. Activation Energies and Pre-exponential Factors of Different Reactions over Ce-Modified NaX (CeX<sub>10</sub>) Zeolite**

reaction	$E_a$ (kJ/mol)	pre-exponential factor (in consistent units)
benzene alkylation	109.8	$2.6 \times 10^{15}$
IPA dehydration to ether	112.0	$2.7 \times 10^{13}$
cumene alkylation to <i>p</i> -DIPB	86.4	$9.5 \times 10^{11}$
<i>p</i> -DIPB isomerization to <i>m</i> -DIPB	32.2	$5.5 \times 10^3$

the constants from Table 7, the standard error was  $\pm 8.12 \times 10^{-5}$ . By comparing the standard errors, model eq 5 was considered to be the best among the three in representing the reaction system under investigation. The experimental and the predicted isopropyl alcohol conversions from eq 5 at four different temperatures were plotted in Figure 9. It shows that the proposed reaction rate expression predicts the IPA conversion values comparable with the experimental ones.

The kinetic constants evaluated and tabulated at various temperatures (Table 5) were used to determine the activation energy and frequency factor using Arrhenius relationships as shown in Table 8. The activation energy values for various reactions compare well with the values of similar reactions on zeolites obtained by other investigators.<sup>25,26</sup> Gentry and Rudham<sup>26</sup> reported an activation energy of 109 kJ/mol in the temperature range of 383–419 K and 110 kJ/mol in the temperature range of 384–425 K for the dehydration

**Figure 9.** Experimental vs predicted IPA conversions.

of isopropyl alcohol on X zeolites. Similar observations were also made by Yue and Olafe<sup>27</sup> over 13X and mordenite and by Rudham and Stockwell<sup>28</sup> over Y zeolite for isopropyl alcohol dehydration.

## Conclusions

Cerium exchanged NaX zeolite was used as catalyst for cumene synthesis by the alkylation of benzene with isopropyl alcohol with good activity and selectivity. No formation of *n*-propylbenzene was observed in the reaction product. A time on stream study showed that the catalyst was quite stable at an operating temperature of 473 K. Based on the product distribution, a reaction mechanism was proposed together with a rate expression for the disappearance of isopropyl alcohol. The kinetic and the adsorption constants of the rate equation were estimated by best fit. The activation energy for the cumene synthesis reaction was determined to be 110 kJ/mol.

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## Nomenclature

A = isopropyl alcohol  
 B = benzene  
 C = cumene  
 DIPB = diisopropyl benzene  
*m*-DIPB = *m*-diisopropyl benzene  
*p*-DIPB = *p*-diisopropyl benzene  
 DIPE = diisopropyl ether  
 $E_a$  = activation energy, kJ/mol  
 $F$  = total feed rate, kg-mol/h  
 IPA = isopropyl alcohol  
 $k_1, k_2, k_3$  = kinetic constant, kg-mol/kg·atm<sup>2</sup>·h  
 $K_B$  = adsorption constant for benzene, atm<sup>-1</sup>  
 $K_A$  = adsorption constant for IPA, atm<sup>-1</sup>  
 $K_C$  = adsorption constant for cumene, atm<sup>-1</sup>  
 $P$  = total pressure, atm  
 $p_A$  = partial pressure of IPA, atm  
 $p_B$  = partial pressure of benzene, atm  
 $p_C$  = partial pressure of cumene, atm  
 $p_m$  = partial pressure of *m*-DIPB, atm  
 $p_p$  = partial pressure of *p*-DIPB, atm  
 $\tau$  = space-time of IPA, kg·h/kg-mol  
 $X_A$  = fractional conversion of IPA  
 $X_B$  = moles of benzene reacted, kg-mol  
 $X_C$  = moles of cumene formed, kg-mol  
 $X_m$  = moles of *m*-DIPB formed, kg-mol  
 $X_p$  = moles of *p*-DIPB formed, kg-mol  
 $X_{\text{expt}}$  = experimental fractional conversion of IPA  
 $X_{\text{pred}}$  = predicted fractional conversion of IPA  
 $W$  = mass of the catalyst, kg  
 $W$  = water

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