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## KINETICS, CATALYSIS, AND REACTION ENGINEERING

## Kinetics of Reductive Isopropylation of Benzene with Acetone over Nano-Copper Chromite-Loaded H-Mordenite

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Alkylation of benzene by acetone was carried out over nano-copper chromite-loaded H-mordenite catalyst in a fixed bed flow reactor with 100% selectivity for the cumene. The catalytic activity of the modified catalyst was found to increase with an increase in copper chromite content in the mordenite. The activity of the catalyst was however found to be dependent on both preactivation temperature and time. Experiments were carried out to find out a mass transfer resistance-free zone by varying different parameters. Kinetic runs were taken in the mass transfer resistance-free zone at constant benzene to acetone molar ratio of 4:1 by varying the space-time under isothermal conditions in the reactor. Various kinetic models were proposed following the Langmuir–Hinshelwood–Hougen–Watson approach. The model parameters were estimated by nonlinear regression analysis. From the estimated kinetic constants of the best model, the activation energy of the reaction was determined to be 120.5 kJ/mol.

## Introduction

Alkylation reactions are of great interest in the 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 through cumene. Several zeolite-based catalytic processes have been developed for the production of cumene by the alkylation of benzene with propylene.<sup>1–9</sup> In recent years, a lot of interest has been generated on the production of cumene with isopropyl alcohol as the alkylating agent due to some advantages of using isopropyl alcohol instead of propylene as the alkylating agent.<sup>10–14</sup>

In the cumene route for the production of phenol, acetone is produced as a low value byproduct. Several researchers have studied the reduction of acetone to produce isopropyl alcohol, which could be used for alkylating benzene.<sup>15–18</sup> Direct use of acetone for isopropylation of benzene could be a viable alternative to the above having high commercial implications as it would reduce the number of chemical transformations necessary for the reuse of the byproduct acetone. With this idea, an attempt has been made in the present work to use acetone itself as the alkylating agent for benzene over an indigenously developed dual-function catalyst containing copper chromite.

Copper chromite has been used extensively for years as a catalyst for various industrial processes such as the partial hydrogenation of vegetable oils and fatty acids, as well as the decomposition or dehydration of alcohols.<sup>19</sup> The utilization of these catalysts in hydrogenation reactions stems from their capability to selectively hydrogenate carbonyl groups while leaving C=C bonds virtually untouched. Several studies have

been devoted to establish the mechanism of copper chromite-catalyzed hydrogenation of acetone to isopropyl alcohol.<sup>15,16,20–24</sup> Copper chromite has also been reported as a catalyst for the reductive N-alkylation of aniline with acetone.<sup>25,26</sup> There is, however, no information in the open literature on the use of copper chromite for reductive alkylation of benzene with acetone. The present investigation, therefore, was aimed at the synthesis of cumene by reductive alkylation of benzene with acetone in the presence of a bifunctional catalyst system comprising a solid acid material, H-mordenite (HM), as alkylation functional and nano-copper chromite as hydrogenation functional. 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 for this commercially important reaction.

## Experimental Section

**Materials.** Acetone and benzene used in this study were of analytical reagent grade. Acetone was obtained from Qualigens Fine Chemicals, Mumbai, India; benzene was from E. Merck (India) Ltd., Mumbai, India. Copper nitrate [Cu(NO<sub>3</sub>)<sub>2</sub>], ammonium dichromate [(NH<sub>4</sub>)<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>], and copper chromite [CuCr<sub>2</sub>O<sub>4</sub>] were also obtained from E. Merck (India) Ltd., Mumbai, India. HM used in the present study was obtained from Süd-Chemie India Pvt. Ltd., Gujarat, India. It was in the form of powder having a SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratio of 4.7 and surface area of 300 m<sup>2</sup>/g.

**Catalyst Preparation.** To prepare nano-copper chromite, equal volumes of 0.1 M Cu(NO<sub>3</sub>)<sub>2</sub> and 0.1 M (NH<sub>4</sub>)<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> solutions were mixed together in a beaker. After addition of triethanolamine (TEA), the mixture was continuously stirred. To avoid precipitation, the pH of the mixture was maintained around 1–2 by adding HNO<sub>3</sub>. Then the solution was heated in

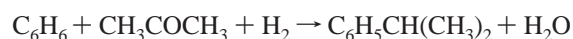
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a heater. At the end of the reaction, the fluffy mass was collected and calcinated at 923 K. The average diameter of the copper chromite was determined with the help of TEM as 31 nm. This nano-copper chromite was then mixed with HM powder in different ratios. Then 20% bentonite powder was mixed with the mixture of copper chromite and HM as a binder. The extrudates were then prepared and dried in an oven overnight at a temperature of 373 K.

**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 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 insulated properly to minimize 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 4 h in 1 atm of nitrogen and then for 5 h in 1 atm of hydrogen before the experimental runs were started. The aromatic–ketone mixture was introduced with the help of a metering pump and vaporized in the preheater before contacting the catalyst. The reactant vapors along with hydrogen 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 × 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). Samples from the gas phase were also analyzed from time to time to ensure no loss of hydrocarbons with the gas phase. The material balance was checked, and it was >97%.

## Results and Discussion

Alkylation of benzene with acetone was carried out in vapor phase over nano-copper chromite-loaded HM. Cumene was detected as the only product of this reductive alkylation reaction. Accordingly, the overall reaction may be represented as

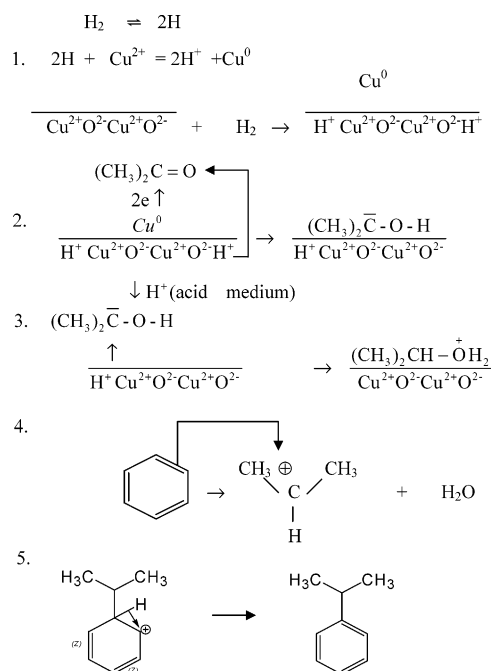


If  $Y_B$ ,  $Y_A$ , and  $Y_{EA}$  are the mole fractions of benzene, acetone, and cumene, respectively, in the product stream, then 1 mol of product will contain  $Y_B$  mol of benzene,  $Y_A$  mol of acetone, and  $Y_C$  mol of cumene. Hence, the amount of acetone converted by alkylation is  $Y_C$  mol.

Total acetone fed into the reactor = acetone in liquid product + acetone converted by alkylation =  $(Y_A + Y_C)$  mol. So, the fractional conversion of acetone,  $X_A$  = mol of acetone converted/mol of acetone fed =  $Y_C/(Y_A + Y_C)$ .

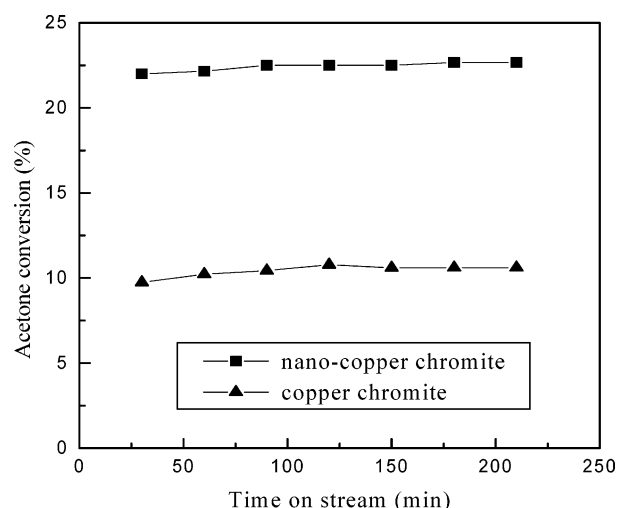
On the basis of the literature information<sup>27–30</sup> and the overall reaction shown above, Scheme 1 can be proposed as a mechanism for hydrogenation of acetone over the catalyst system presently investigated. At the first stage, the reduced state of chromite is formed upon the reversible interaction with hydrogen that results in dissolving protons in the spinel. A corresponding amount of copper as epitaxially bonded flat particles is released at the surface. The second stage is the hydrogenation of acetone. Acetone is adsorbed on  $\text{Cu}^0$  atoms as  $\pi$  complexes, electrons of the metals transfer to antibonding  $\pi$  orbitals of the carbonyl group. Concurrently a proton of the reduced chromite is inserted into an adsorbed acetone molecule. As a result, the organic molecule acquires a negative charge

## Scheme 1. Mechanism of Reductive Isopropylation of Benzene with Acetone

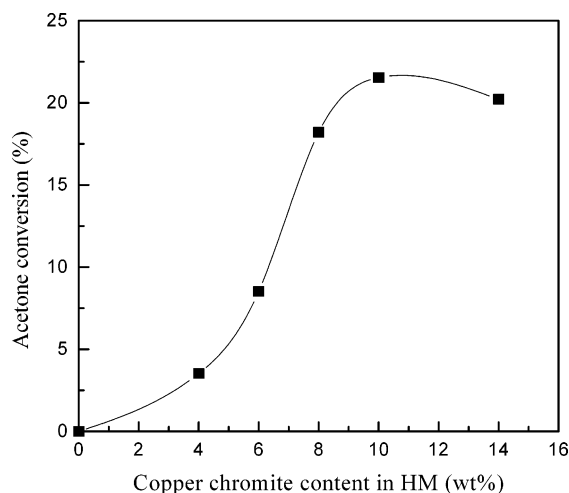


and copper metals are oxidized and occupy the positions in the spinel structure it has left during the reduction. These transformations are followed by insertion of second proton from chromite. Another proton from the acidic medium attracts the OH groups and thereby forms carbonium ions and water. An electrophilic substitution with this ion on benzene forms cumene.

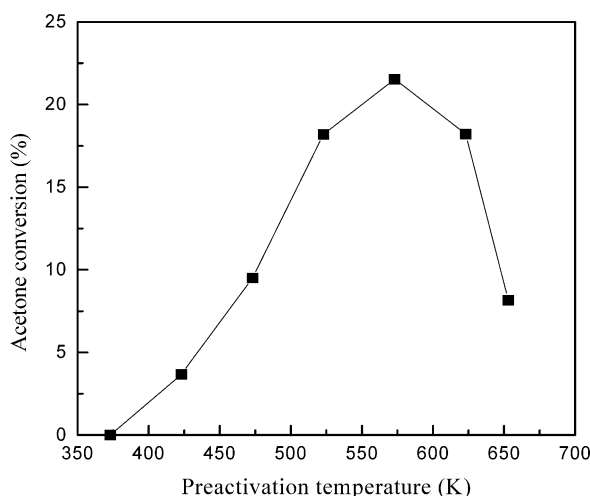
**Catalyst Activity.** The catalytic activity of nano-copper chromite-loaded HM and commercial copper chromite-loaded HM catalyst were tested in 3 h time on stream. As shown in Figure 1, acetone conversion was observed to be higher over nano-copper chromite-loaded HM catalyst than copper chromite-loaded HM catalyst. The cumene selectivity was, however, observed to be 100% over both the catalysts. The higher activity of nano-copper chromite-loaded HM may be due to better dispersion of the hydrogenation functional over the support HM. Further experiments were carried out over nano-copper chromite-loaded HM catalyst.



**Figure 1.** Time on stream behavior of different catalysts. Conditions: benzene/acetone mole ratio, 4:1; temperature, 443 K; space-time, 42.5 kg·h/kgmol; pressure, 1 atm; hydrogen-to-feed ratio, 1.06; catalyst, 10% copper chromite-loaded HM.



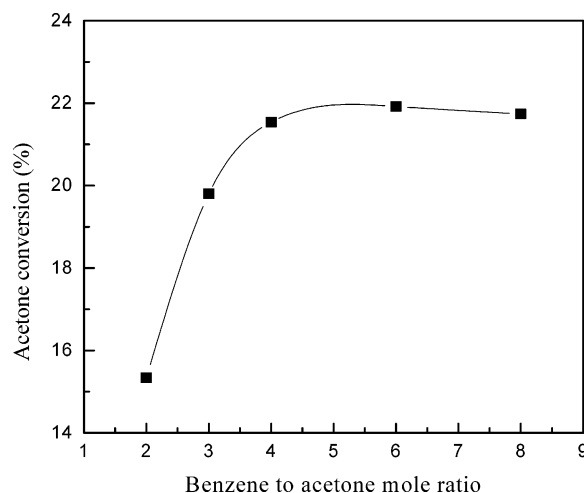
**Figure 2.** Effect of copper chromite content in HM. Conditions: benzene/acetone mole ratio, 4:1; temperature, 443 K; space-time, 42.5 kg·h/kgmol; pressure, 1 atm; hydrogen-to-feed ratio, 1.06.



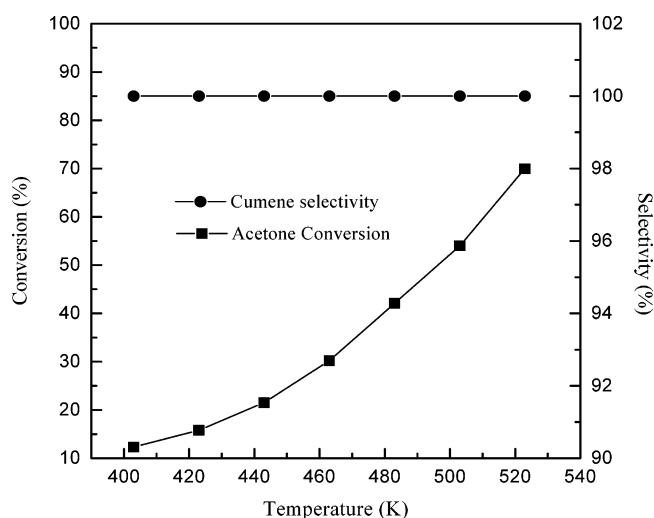
**Figure 3.** Effect of preactivation temperature on conversion of acetone at 443 K. Conditions: benzene/acetone mole ratio, 4:1; space-time, 42.5 kg·h/kgmol; catalyst, 10% nano-copper chromite-loaded HM; pressure, 1 atm; hydrogen-to-feed ratio, 1.06.

**Effect of Copper Chromite Loading on Conversion of Acetone.** Figure 2 shows the effect of nano-copper chromite loading on catalytic activity in terms of acetone conversion. The conversion of acetone was found to increase with an increase in nano-copper chromite content up to 10 wt % and then started to decrease slowly. As the loading of copper chromite increases, the concentration of hydrogenation functional in the catalyst increases, which is responsible for the increase in the reduction (conversion) of acetone with simultaneous formation of cumene. All other reactions were, therefore, carried out with 10% loading of nano-copper chromite in the HM catalyst.

**Effect of Preactivation Temperature.** Typically hydrogenation catalysts are activated by hydrogen before being used. Catalytic activity of nano-copper chromite-loaded HM, preactivated at different temperatures, was studied at 443 K. Figure 3 shows the conversions of benzene obtained at various pretreatment temperatures of the catalyst. At a pretreatment temperature below 423 K, no conversion of acetone was observed. The conversion of acetone was observed to increase with pretreatment temperature, attains a maxima at 573 K, and then decreases. Again at a temperature higher than 683 K, no conversion of acetone was observed. Kinetic studies of the interaction between hydrogen and chromite at temperatures from



**Figure 4.** Effect of feed composition on conversion of acetone. Conditions: temperature, 443 K; space-time, 42.5 kg·h/kgmol; catalyst, 10% nano-copper chromite-loaded HM; pressure, 1 atm; hydrogen-to-feed ratio, 1.06.



**Figure 5.** Effect of temperature on acetone conversion and cumene selectivity. Conditions: benzene/acetone, 4:1; space-time, 42.5 kg·h/kgmol; catalyst, 10% nano-copper chromite-loaded HM; pressure, 1 atm, hydrogen-to-feed ratio, 1.06.

293 K to 573 K demonstrated a dependence of the interaction rate on the extent of reduction of the chromite.<sup>30,31</sup> The rate of interaction of copper ions with the hydrogen in the surface layer increases as the reduction proceeds, reaches a maximum, and then decreases. The maximum rate observed at 573 K corresponds to maximum reduction of copper ions.

**Effect of Feed Mole Ratio on Acetone Conversion.** The effect of feed mole ratio on acetone conversion is shown in Figure 4. As molar ratio of benzene to acetone increases, acetone conversion to cumene also increases. But after a mole ratio of 4, conversion becomes almost constant. At mole ratios of benzene to acetone greater than 4, most of the active sites of the catalyst surface are blocked by an excess of benzene, and the conversion of acetone became constant due to the limited availability of active sites for alkylation.

**Effect of Temperature.** The effect of temperature on conversion of acetone was studied in the temperature range of 403 K to 523 K as shown in Figure 5. The conversion of acetone increases with increase in temperature as expected. It is also evident from Figure 5 that the selectivity for cumene remained 100% even at an acetone conversion of as high as 70%.

**Mass Transfer Considerations.** For kinetic study of any reaction, it should be free from mass transfer resistances. For

**Table 1. Effect of External Diffusional Resistances on Conversion of Acetone<sup>a</sup>**

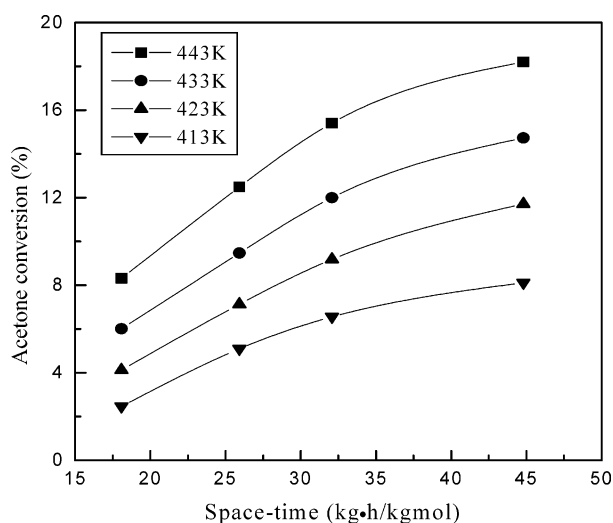
space-time (kg·h/kgmol)	conversion of acetone (%) with	
	0.03 kg of catalyst	0.05 kg of catalyst
18.0	6.0	6.2
26.0	9.5	9.6
32.0	12.0	12.2

<sup>a</sup> Conditions: benzene/acetone mole ratio, 3:1; temperature, 423 K; pressure, 1 atm; hydrogen-to-feed ratio, 1.06; catalyst, 10% nano-copper chromite-loaded HM; average catalyst size, 1 mm.

**Table 2. Effect of Intraparticle Diffusion on Conversion of Acetone<sup>a</sup>**

particle size (mm)	acetone conversion (%) with space-time (kg·h/kgmol) of		
	18.0	26.0	32.0
0.5	6.2	9.6	12.2
1.0	6.0	9.5	12.0
1.5	6.0	9.4	12.0

<sup>a</sup> Conditions: benzene/acetone mole ratio, 3:1; temperature, 423 K; pressure, 1 atm; hydrogen-to-feed ratio, 1.06; catalyst, 10% nano-copper chromite-loaded HM.



**Figure 6.** Effect of space-time on conversion of acetone. Conditions: benzene/acetone, 3:1; catalyst, 10% nano-copper chromite-loaded HM; pressure, 1 atm, hydrogen-to-feed ratio, 1.06.

gas–solid reactions, this resistance can be either external or internal, within the catalyst pellets. 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 1 indicate that the conversions of acetone for both the series at 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 2. The results showed that there was no change in conversion of acetone with catalyst size, indicating negligible intraparticle mass transfer resistance in the particle size 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 confirm only the absence of diffusion in the macropores. The resistance due to micropore could not be

**Table 3. Kinetic and Adsorption Constants of Model Equation 5**

constant	temperature (K)			
	413	423	443	433
$k_s$ , kgmol/kg·h	1.62	3.79	6.85	19.90
$K_A$ , atm <sup>-1</sup>	38.01	34.52	30.20	25.20
$K_B$ , atm <sup>-1</sup>	0.045	0.030	0.025	0.020
$K_C$ , atm <sup>-1</sup>	0.044	0.028	0.017	0.012
$K_H (\times 10^3)$ , atm <sup>-1</sup>	2.01	1.29	0.08	0.05

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.

**Kinetic Modeling.** The kinetic runs were carried out at four different temperatures, namely, 413, 423, 433, and 443 K. The experiments were carried out to choose the zone in which the mass transfer effects are negligible. Figure 6 presents the effect of space-time on acetone conversion at four different temperatures.

Expressions for the rate of reaction of acetone were derived following the Langmuir–Hinshelwood–Hougen–Watson approach. The following assumptions were made in formulating the rate equations:

- The overall rate is governed by the rate of chemical reaction on the surface.
- The adsorption equilibria are maintained during the reaction.
- The hydrogen adsorption is dissociative.
- the adsorption of water does not compete with the adsorption of hydrocarbons.

For the surface reaction-controlled reductive isopropylation of benzene, the rate of reaction of acetone may be expressed as

$$-r_A = k_s C_{AS} C_{BS} C_{HS} \quad (1)$$

If the adsorption rate is large with respect to other steps in the overall conversion process, the concentration of a component on the catalyst surface will be in equilibrium with the concentration of that component in the gas phase. As such, the surface concentrations of various components may be written as

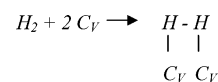
$$C_{AS} = K_A p_A C_V \quad (2)$$

and

$$C_{BS} = K_B p_B C_V \quad (3)$$

where  $C_V$  is the concentration of vacant site on the surface.

For dissociative adsorption of hydrogen



and hence

$$C_{HS} = K_H^{1/2} p_H^{1/2} C_V \quad (4)$$

Substituting the values of  $C_{AS}$ ,  $C_{BS}$ , and  $C_{HS}$  from eqs 2–4 into eq 1, the following kinetic model equations were obtained:

model 1: all three reactants are adsorbed

$$-r_A = \frac{k_s K_A K_B \sqrt{K_H} p_A p_B \sqrt{p_H}}{[1 + K_A p_A + K_B p_B + \sqrt{K_H} \sqrt{p_H} + K_C p_C]^3} \quad (5)$$



**Table 4. Kinetic and Adsorption Constants of Model Equation 6**

constant	temperature (K)			
	413	423	433	443
$k_S$ , kgmol/kg·atm·h	0.0012	0.0261	0.036	0.046
$K_A$ , atm <sup>-1</sup>	36.01	33.52	30.20	26.20
$K_C$ , atm <sup>-1</sup>	0.024	0.018	0.012	0.08
$K_H (\times 10^3)$ , atm <sup>-1</sup>	2.04	1.68	1.42	0.05

**Table 5. Kinetic and Adsorption Constants of Model Equation 7**

constant	temperature (K)			
	413	423	433	443
$k_S$ , kgmol/kg·atm·h	0.035	0.061	0.095	0.125
$K_A$ , atm <sup>-1</sup>	25.01	20.52	18.20	15.20
$K_H (\times 10^3)$ , atm <sup>-1</sup>	2.14	1.88	1.62	0.08

model 2: for benzene in the gas phase

$$-r_A = \frac{k_S K_A \sqrt{K_H} p_A p_B \sqrt{p_H}}{[1 + K_A p_A + \sqrt{K_H} \sqrt{p_H} + K_C p_C]^2} \quad (6)$$

model 3: for both benzene and cumene in the gas phase

$$-r_A = \frac{k_S K_A \sqrt{K_H} p_A p_B \sqrt{p_H}}{[1 + K_A p_A + \sqrt{K_H} \sqrt{p_H}]^2} \quad (7)$$

A mathematical fit for the above rate equations was performed as follows.

For each temperature, the space-time-conversion data were analyzed, and the rates of reaction were obtained by differential analysis of the plug flow reactor equation:

$$-r_{\text{obs}} = \frac{dX_A}{d(W/F_{A0})} \quad (8)$$

The partial pressures in the above equation are related to the conversions and total pressure ( $P$ ) by the relationships:

$$p_A = (1 - X_A)P/8.24 \quad (9)$$

$$p_B = (3 - X_B)P/8.24 \quad (10)$$

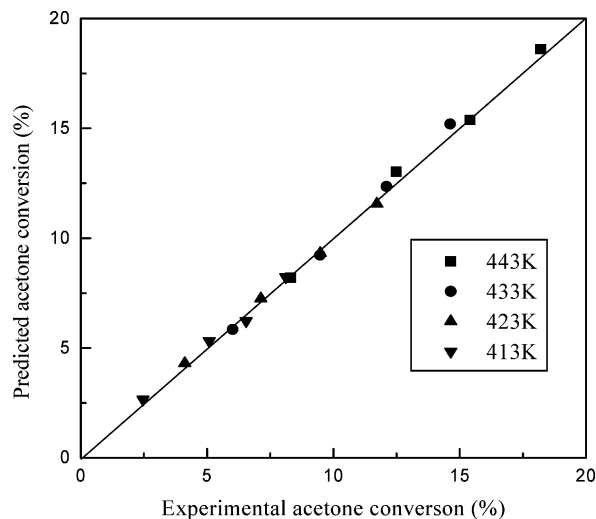
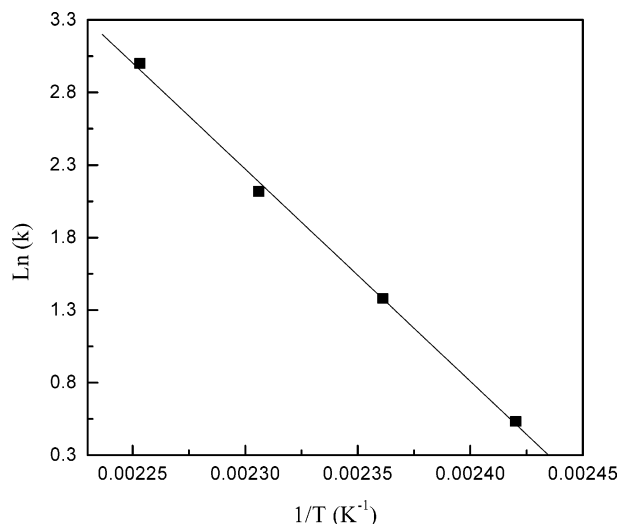
$$p_C = X_C P/8.24 \quad (11)$$

$$p_H = 4.24P/8.24 \quad (12)$$

The rate equation (eq 5) contains five unknown parameters (viz.,  $k_S$ ,  $K_A$ ,  $K_B$ ,  $K_C$ , and  $K_H$ ). These parameters were estimated by treating each temperature data separately. As the rate equation is nonlinear with respect to unknown parameters, a nonlinear regression program based on Marquardt's algorithm<sup>32</sup> was used to obtain a mathematical fit for the above rate equation by minimizing the objective function for the residual sum of squares given by

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

The initial rate estimates of the various constants of the rate expression were made from the composition pattern of the product stream ( $p_A$ ,  $p_B$ , and  $p_C$ ). The kinetic and adsorption constants evaluated by nonlinear regression are tabulated in Tables 3–5 for model eqs 5–7, respectively. It is evident from these tables that with an increase in temperature the kinetic constant increases, which is the right trend for these parameters,

**Figure 7.** Experimental vs predicted acetone conversions.**Figure 8.** Arrhenius plot.

and the adsorption constant shows a decreasing trend with increase in temperature as expected.

**Model Discrimination.** By using the values of the constants for model eq 5 as shown in Table 3, the standard error of estimate for the rate of disappearance of acetone was  $\pm 1.38 \times 10^{-5}$ . For model eq 6, with the values of the constants from Table 4, the standard error was  $\pm 5.23 \times 10^{-3}$ . For model eq 7, with the values of the constants from Table 5, the standard error was  $\pm 8.65 \times 10^{-3}$ . 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 acetone conversions from eq 5 at four different temperatures were plotted in Figure 7. A fairly good correlation is observed between the observed and the predicted acetone conversions. Thus, the proposed kinetic model fits well the experimental data.

The kinetic constants evaluated and reported in Table 3 at various temperatures were used to determine the activation energy and frequency factor using Arrhenius relationship,  $k = k_0 \exp(-E_a/RT)$ . A plot of  $\ln k$  versus  $1/T$  gave a straight line as shown in Figure 8. From the slope and intercept of this straight line, the apparent activation energy was calculated to be 120.5 kJ/mol and the frequency factors  $k_0$  as  $3.94 \times 10^{16}$  kgmol/kg·atm·h. The determined activation energy value com-

pares well with the values of similar reactions on zeolites obtained by other investigators.<sup>13,33</sup> Gentry and Rudham<sup>34</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 of isopropyl alcohol on X zeolites. Similar observations were made by Yue and Olaofe<sup>35</sup> over 13X and mordenite and by Rudham and Stockwell<sup>36</sup> over Y zeolite for isopropyl alcohol dehydration. Activation energy of adsorption of hydrogen is 62.73 kJ/mol. Simentsova et al.<sup>37</sup> also found an activation energy value of 69.74 kJ/mol for hydrogen adsorption over copper chromite.

## Conclusions

The cumene synthesis reaction was studied by reductive alkylation of benzene with acetone in the presence of nano-copper chromite-loaded HM as the catalyst. The 10% copper chromite-loaded HM catalyst showed good activity with 100% selectivity for cumene. The bifunctional catalyst system was also found to be quite stable at an operating temperature of 443 K. A detailed kinetic study of this commercially important reaction was performed, and a reaction mechanism was proposed together with a rate expression for the disappearance of acetone. 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 120.5 kJ/mol.

## Nomenclature

A = acetone  
 B = benzene  
 C = cumene  
 $C_{AS}$  = surface concentration of acetone  
 $C_{BS}$  = surface concentration of benzene  
 $C_{HS}$  = surface concentration of hydrogen  
 $E_a$  = activation energy, kJ/mol  
 $F$  = total feed rate, kgmol/h  
 $F_{Ao}$  = feed rate of acetone, kgmol/h  
 $k_S$  = kinetic constant, in consistent units for eqs 5–7  
 $K_A$  = adsorption constant for acetone, atm<sup>-1</sup>  
 $K_B$  = adsorption constant for benzene, atm<sup>-1</sup>  
 $K_C$  = adsorption constant for cumene, atm<sup>-1</sup>  
 $K_H$  = adsorption constant for hydrogen, atm<sup>-1</sup>  
 $P$  = total pressure, atm  
 $p_A$  = partial pressure of acetone, atm  
 $p_B$  = partial pressure of benzene, atm  
 $p_C$  = partial pressure of cumene, atm  
 $p_H$  = partial pressure of hydrogen, atm  
 $-r_A$  = rate of disappearance of acetone, kgmol/kg·h  
 $-r_{obs}$  = experimentally observed rate of reaction of acetone, kgmol/kg·h  
 $X_A$  = fractional conversion of acetone  
 $X_B$  = moles of benzene reacted, kgmol  
 $X_C$  = moles of cumene formed, kgmol  
 $X_{expt}$  = experimental fractional conversion of acetone  
 $X_{pred}$  = predicted fractional conversion of acetone  
 $W$  = mass of the catalyst, kg

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