

## ALKYLATION OF ETHYL BENZENE BY USING IM-5 CATALYST

Kanchan Pathak, Sarita Chourasia and Asutosh K. Pandey\*

Department of Engineering Chemistry, Rishiraj Institute of technology ( LNCT Group),  
Indore, Madhya Pradesh, India.

### ABSTRACT

Ethylation of ethylbenzene at various WHSV's was investigated on IM-5 catalyst. We have studied the influence of WHSV at 1h<sup>-1</sup>, 3h<sup>-1</sup>, 5h<sup>-1</sup> and 7h<sup>-1</sup> on EB conversion, DEB and p-DEB selectivity at 300°C temperature. The results are illustrated in Fig. 9 and 10 EB conversion decreased with increase in WHSV because of the lower contact time. It decreases with increase in TOS for WHSV 3h<sup>-1</sup>, 5h<sup>-1</sup> and 7h<sup>-1</sup>. But at WHSV 1h<sup>-1</sup>, conversion increased initially and then decreases gradually. DEB Selectivity increased with increase in WHSV, which may be due to suppression of dealkylation and other side reactions. As a result the catalyst is deactivated resulting in the lower yields of DEB as well as p-DEB after few hours on stream, but DEB and p-DEB selectivity is very less at 3:1 mole ratio. Hence, it is better to use EB:EtOH ratio of 2:1 to get optimum yields of DEB and p-DEB.

### INTRODUCTION

The importance of zeolites as catalysts hardly needs to be emphasized. This, to a great extent, can be attributed to their shape selectivity. Zeolites are crystalline microporous aluminosilicates, either of natural or synthetic origin with highly ordered structures<sup>1</sup>. Zeolites are also popularly known as '**molecular sieves**' due to their ability to differentiate between molecules of different shapes and size<sup>2</sup>.

IM-5 and NU-88 are two new, high-silica zeolites that have recently been reported by Benazzi et al.<sup>3,4</sup> and Casci et al.<sup>5</sup>, respectively. Although the framework structures of these synthetic zeolites still remain undetermined, recent results from various catalytic test reactions have suggested that both materials may either contain the twodimensional pore system with two intersecting 10-ring channels or the one-dimensional pore system consisting of 10- ring channels with large internal cavities<sup>4-8</sup>. IM-5 and NU-88, on the other hand, the synthesis of both materials include the use of diquaternary alkylammonium cations with formula (C<sub>5</sub>H<sub>11</sub>)N+(CH<sub>2</sub>)<sub>n</sub>N+(C<sub>5</sub>H<sub>11</sub>) with *n* = 5 and 6, respectively<sup>3,5</sup>, which are formed of two 1-methylpyrrolidinium groups connected by the polymethylene bridging unit. It has been repeatedly shown that the phase selectivity of

zeolite syntheses in the presence of such flexible, linear organic cations as structure-directing agents (SDAs) is sensitive not only to the length of the central alkyl chain and the nature of the groups on the ammonium ion employed but also to the oxide composition of synthesis mixtures<sup>9-14</sup>.

The conversions and product distributions from the catalytic cracking of *n*-octane on H-IM-5 and H-NU-88 with a similar SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratio (25) measured at 500 °C, 2.0 kPa *n*-octane pressure in the feed and 500s on stream. For comparison, the catalytic results from H-ZSM-5, H-EU-1. The *n*-octane conversion (89%) on H-IM-5 is almost the same as that (90%) on H-ZSM-5, serving as a prime example of the uniqueness of medium-pore zeolites in the cracking of linear paraffins<sup>15-17</sup>.

Yashima et al. have reported the result of alkylation of toluene with methanol on HY and HZSM-5 catalyst<sup>18</sup>.

### Characterization

#### Gas liquid chromatography (GC)

GC-analysis of L-lactic acid was done on Perkin Elmer GC Auto System XL-200 by injecting 0.1, 1 and 10 microliter injection volumes of the L-LA 88 % aqueous solution as such to a Perkin-Elmer BP-20 (polyethylene

oxide, terephthalic acid treated) capillary column of 25 meter length by means of on-column injection procedure and comparing with the chromatograms of aqueous solutions of 4, 9 and 19 ppm (that is below 5, 10 and 20 ppm, respectively) concentrations each of methanol, ethanol, acetic acid, and pyruvic acid. The split ratio was 1:60, the detector was FID, the carrier gas was nitrogen with a pressure of 7 psi and the fuel for FID was hydrogen. Oven was isothermal at 50 °C for 30 min, followed by heating with a ramp rate of 5 °C/min from 50 °C till another 30 min. The injector and detector were kept at 250 and 280 °C, respectively.

## EXPERIMENTAL

### Synthesis of Template

The divalent 1,5-bis(N-methylpyrrolidinium) pentane (MPP) cation was prepared by reacting 5.745 g of 1,5-dibromopentane (97%, Aldrich) with 4.25 g of 1-methylpyrrolidine (97%, Aldrich) in acetone (80 ml) approx as a solvent with rapid stirring at room temperature overnight. The excess amine was removed by extraction with diethyl ether (Loba) and recrystallizations were performed in methanol–diethyl ether (Thomas Baker) mixtures. 9.62 g of MPP cation formed. Required template was dissolved in about 50 g of distilled water. To this, 9.62 g of fumed silica was added under stirring. When the mixture is viscous, 20 g water was added to it. After complete addition of fumed silica, 4.44 g NaOH dissolved in 10 g distilled water was added dropwise. Following this, 2.03 g of  $\text{Al}(\text{NO}_3)_2$  dissolved in 10 g distilled water was added to the mixture. The remaining amount of water i.e. 15.37 g was added and the mixture was stirred for 24 hours. After stirring at room temperature for 24 h, the synthesis Mixture (pH=12.07) was charged into Teflon-lined 300-mL autoclaves and heated to 160 °C under rotation (100 rpm) for 14 days. The solid products were recovered by filtration, washed repeatedly with water, and then dried overnight at room temperature. As-synthesized zeolites were calcined under flowing air at 550 °C for 8 h to remove the organic SDA occluded. The calcined samples were then refluxed using  $\text{NH}_4\text{NO}_3$  solutions for 6 h followed by calcination at 550 °C for 8h to get proton form of IM-5<sup>19</sup>.

### Apparatus and procedure

The reaction was carried out in a down flow fixed bed reactor of 13mm inner diameter and 35cm length in a continuous flow system. The reactor was heated to the requisite temperature with the help of a tubular furnace controlled by a digital temperature programmer cum indicator. About 2 g of sieved catalyst (20-30 mesh) was sandwiched at the center of the reactor with a thin layer of quartz wool sandwiched between glass beads. It was heated in dry air at a ramp rate of 2 K/min from room temperature to 773 K and kept for 8 h for calcination. Catalyst was cooled down to room temperature and raised to required reaction temperature in hydrogen flow. The alkylation reaction was carried out at different temperatures i.e. 250, 275, 300, 325 and 350°C with molar ratios of ethylbenzene: ethanol of 1:1, 2:1 and 3:1. Pressure was maintained at 10 bar while the feed was pumped at  $\text{WHSV}=3.0 \text{ h}^{-1}$ . The products were passed through a water-cooled condenser attached at the end of the reactor. The liquid products of the first hour were discarded and only products collected 2<sup>nd</sup> hour onwards was analyzed using GC. This is done to ensure the attainment of steady state for the reaction over the catalyst and also to eliminate initial temperature fluctuations. The products were collected at intervals of 1 h. The reaction was carried out for 7-8 hrs at each experimental condition. After each run, the catalyst was heated at 500 °C for regeneration in order to remove the deposited coke.

## RESULT AND DISCUSSION

### Product Analysis

The products were analyzed using Agilent 7890A series GC system employing Flame Ionization Detector (FID) and Zebron capillary column (50 m x 320  $\mu\text{m}$  x 1.05  $\mu\text{m}$ ). The response of an FID is different for different compounds, hence the response factor (RF) is determined from the response of a mixture of known composition – the standard. This standard is first injected into the GC-FID and analyzed. After GC separation of known mixture, the area of each component is related to its actual concentration and the Rf is calculated.

$$\text{Rf} = \text{Area}\% / \text{wt}\%$$

Conversion and selectivity are calculated as follows

$$\% \text{ Conversion of EB} = \frac{(\sum \text{wt\% of alkylated aromatic products}) * 100}{(\sum \text{wt\% of alkylated aromatics} + \text{wt\% of ethylbenzene})}$$

$$\text{DEB selectivity} = \frac{(\sum \text{wt\% of DEB isomers}) * 100}{(\sum \text{wt\% of alkylated aromatics})}$$

$$\text{p-DEB selectivity} = \frac{(\text{wt\% of 1,4-DEB}) * 100}{(\sum \text{wt\% of total DEB isomers})}$$

$$\% \text{ DEB Yield} = \frac{\text{DEB selectivity} * \text{Conversion of Ethylbenzene}}{100}$$

Ethylation of ethylbenzene (EB) was investigated on IM-5 zeolite using ethyl alcohol (EA) as the alkylating agent. The reactions were conducted in a continuous flow fixed bed reactor at 10 bar  $\text{H}_2$ . Effect of various parameters viz. temperature, ethylbenzene: ethanol mole ratio and WHSV (weight hourly space velocity) etc. were investigated to understand their influence on the conversion of EB, DEB selectivity, p-DEB selectivity and yield.

#### Effect of reaction temperature on IM-5 catalyst

Ethylation of EB was investigated at various temperatures on IM-5 catalyst. It may be seen that as the reaction temperature increases, the conversion of ethylbenzene has also increased. Ethylbenzene conversion has increased with time on stream (TOS) for the reaction at 250 (table 1) and 275 °C (table 2), whereas at higher temperatures 300 (table 3), 325 (table 4) and 350 °C (table 5) it has decreased with TOS. It may be due to the formation of higher aromatics as the dealkylation and other side reactions are dominant at higher temperatures, leading to coke formation, which in turn led to deactivation of the catalyst. On the other hand, at lower temperatures, the alkylating agent is utilized for side reactions, particularly at acid

sites with strong acidity. Once, these strong acid sites are neutralized, the alkylating agent is utilized for ethylation reaction. As the temperature increases, DEB selectivity for the ethylation reaction decreases rapidly reaching about 27% at 350 °C temperature. This is as a result of dealkylation and cracking of DEB to produce EB and benzene. When the temperature increases, the ethylation products undergo cracking or dealkylation leading to the formation of benzene. As a result, benzene selectivity is enhanced at the expense of DEB. The DEB selectivity is almost constant at 300 °C with TOS. The selectivity towards 1,4-diethylbenzene (p-DEB) decreases with increase in temperature, whereas, selectivity to 1,2- and 1,3-diethylbenzene increases. IM-5 is a high silica zeolite, it appears to have medium size pores. Hence, when the reaction temperature increases, the diffusion of 1,2-DEB and 1,3-DEB is better facilitated, which in turn led to higher formation of these two DEB isomers as against p-DEB. The yield of DEB is maximum at 300 °C initially which goes on decreasing with TOS, same is the case for 325 °C with slightly less yield, this may be because of high DEB selectivity and considerable conversion at this temperature. So 300 °C can be considered as the optimum temperature for carrying out this reaction.

**Table 1: Ethylation of EB, temperature: 250 deg. C; Feed: Ethyl benzene: Ethanol (1: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time (hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	1.31	1.19	0.78	0.72	0.83	0.99
Ethyl Benzene	66.64	64.71	62.33	60.58	61.20	61.07
Benzene	0.59	0.46	0.32	0.27	0.25	0.30
Toluene	0.00	0.00	0.00	0.00	0.00	0.00
Xylene	0.00	0.00	0.00	0.00	0.00	0.00
Ethyl toluene	0.03	0.02	0.00	0.00	0.00	0.00
1,3-DEB	8.16	8.27	9.24	9.48	9.27	9.20
1,4-DEB	5.86	6.47	7.10	7.45	7.30	7.34
1,2-DEB	5.14	5.23	5.29	5.40	5.18	5.09
1,4 DIPB	7.95	9.33	10.79	11.77	11.59	11.57
1,3,5-TEB	1.26	1.48	1.76	1.96	1.95	1.90
1,2,4 TEB	0.05	0.05	0.05	0.05	0.05	0.05
1,2,3 TEB	0.05	0.06	0.07	0.07	0.07	0.07
Higher Aromatics	2.94	2.72	2.28	2.25	2.31	2.41
<b>%Conversion</b>	<b>32.47</b>	<b>34.51</b>	<b>37.18</b>	<b>38.99</b>	<b>38.29</b>	<b>31.31</b>
p-DEB Selectivity	30.59	32.41	32.81	33.36	33.57	33.92
DEB Sele.	59.82	58.57	58.61	57.69	57.28	57.03
TEB Sele.	4.25	4.66	5.09	5.380	5.455	5.326
%Yield	19.42	20.21	21.79	22.49	21.93	21.85

**Table 2: Ethylation of EB, temperature: 275 deg. C; Feed: Ethyl benzene: Ethanol (1: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time (hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.94	0.79	0.99	1.03	0.81	0.65
Ethyl Benzene	81.58	79.31	76.77	73.62	72.97	72.41
Benzene	0.00	0.21	0.00	0.00	0.00	0.00
Toluene	0.28	0.18	0.33	0.40	0.29	0.15
Xylene	0.00	0.00	0.00	0.00	0.00	0.00
Ethyl toluene	0.00	0.00	0.00	0.00	0.00	0.00
1,3-DEB	6.18	6.35	6.64	7.14	7.99	8.32
1,4-DEB	2.88	3.25	3.84	4.34	4.95	5.39
1,2-DEB	4.32	4.49	4.67	4.93	5.49	5.66
1,4 DIPB	0.16	0.00	0.19	0.21	0.19	0.06
1,3,5-TEB	1.59	2.04	2.76	3.52	4.22	4.84
1,2,4 TEB	0.00	0.00	0.00	0.00	0.00	0.00
1,2,3 TEB	0.00	0.00	0.00	0.00	0.00	0.00
Higher Aromatics	2.07	3.36	3.80	4.81	3.09	2.52
<b>%Conversion</b>	<b>17.64</b>	<b>20.06</b>	<b>22.46</b>	<b>25.61</b>	<b>26.44</b>	<b>27.12</b>
p-DEB Selectivity	21.51	23.07	25.36	26.44	26.87	27.82
DEB Sele.	76.59	70.86	68.12	64.73	70.28	71.88
TEB Sele.	9.087	10.27	12.41	13.90	16.07	17.96
%Yield	13.51	14.21	15.29	16.58	18.58	19.49

**Table 3: Ethylation of EB, temperature: 300 deg. C; Feed: Ethylbenzene: Ethanol (1: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.42	0.27	0.00	0.00	0.00	0.00
Ethyl Benzene	62.15	61.22	62.14	58.99	60.17	45.47
Benzene	0.00	0.76	0.00	0.48	0.46	0.00
Toluene	0.51	0.00	0.34	0.00	0.00	0.00
Xylene	0.00	0.00	0.00	0.00	0.00	0.00
Ethyl toluene	0.34	0.00	0.29	0.00	0.00	0.00
1,3-DEB	16.28	16.89	16.10	16.56	15.92	19.15
1,4-DEB	3.69	4.25	4.57	5.04	5.00	6.27
1,2-DEB	7.62	7.95	7.49	7.69	7.28	8.88
1,4 DIPB	1.20	1.13	0.98	1.00	0.88	1.20
1,3,5-TEB	3.65	4.82	5.65	6.93	6.67	10.08
1,2,4 TEB	0.14	0.00	0.00	0.00	0.22	0.31
1,2,3 TEB	0.20	0.00	0.00	0.00	0.14	0.20
Higher Aromatics	3.81	2.72	2.42	3.31	3.26	8.43
<b>%Conversion</b>	<b>37.59</b>	<b>38.61</b>	<b>37.86</b>	<b>41.01</b>	<b>39.83</b>	<b>54.83</b>
p-DEB Selectivity	13.38	14.60	16.24	17.19	17.72	18.29
DEB Sele.	73.71	75.53	74.40	71.41	70.78	62.91
TEB Sele.	10.64	12.51	14.92	16.89	17.66	19.42
%Yield	27.70	29.16	28.16	29.28	28.191	34.30

**Table 4: Ethylation of EB, temperature: 325 deg. C; Feed: Ethyl benzene: Ethanol (1: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2.**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.50	0.40	0.13	0.17	0.16	0.14
Ethyl Benzene	54.38	62.97	67.33	71.20	72.30	72.26
Benzene	0.80	0.31	0.18	0.13	0.09	0.06
Toluene	0.11	0.00	0.00	0.00	0.00	0.01
Xylene	0.00	0.00	0.00	0.00	0.00	0.00
Ethyl toluene	0.78	0.35	0.18	0.12	0.00	0.08
1,3-DEB	24.64	19.14	16.59	14.30	13.45	13.08
1,4-DEB	3.53	3.47	3.39	3.18	3.15	3.25
1,2-DEB	7.17	6.60	6.31	5.85	5.84	5.99
1,4 DIPB	1.13	0.55	0.58	0.69	0.71	0.87
1,3,5-TEB	2.55	2.37	2.11	1.84	1.77	1.78
1,2,4 TEB	0.51	0.43	0.37	0.32	0.31	0.15
1,2,3 TEB	0.39	0.14	0.30	0.27	0.22	0.14
Higher Aromatics	3.51	3.27	2.53	1.92	1.99	2.20
<b>%Conversion</b>	<b>45.34</b>	<b>36.78</b>	<b>32.58</b>	<b>28.68</b>	<b>27.58</b>	<b>27.64</b>
p-DEB Selectivity	9.97	11.87	12.91	13.64	14.04	14.55
DEB Sele.	78.31	79.73	80.78	81.48	81.48	80.82
TEB Sele.	7.63	8.037	8.567	8.503	8.34	7.480
%Yield	35.51	29.32	26.32	23.37	22.47	22.34

**Table 5: Ethylation of EB, temperature: 350 OC. C; Feed: Ethyl benzene: Ethanol (1: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	1.03	0.41	1.28	1.62	1.28	1.07
Ethyl Benzene	35.52	35.94	36.08	38.23	37.20	40.36
Benzene	11.19	7.34	6.96	3.44	1.55	1.05
Toluene	3.07	1.13	0.63	0.63	0.32	0.24
Xylene	1.34	4.50	4.98	0.00	0.31	0.23
Ethyl toluene	4.52	3.33	2.15	2.56	1.71	1.22
1,3-DEB	22.59	27.40	23.79	29.58	34.03	34.05
1,4-DEB	2.46	2.58	2.31	3.07	3.52	8.06
1,2-DEB	7.25	7.63	7.24	8.32	8.94	4.08
1,4 DIPB	1.15	0.59	1.33	0.83	1.48	1.39
1,3,5-TEB	2.03	1.84	2.95	1.29	3.63	3.64
1,2,4 TEB	0.37	0.31	0.12	3.35	0.52	0.54
1,2,3 TEB	0.31	0.41	0.37	0.51	0.54	0.53
Higher Aromatics	7.16	6.60	9.82	6.57	4.99	3.54
<b>%Conversion</b>	<b>64.11</b>	<b>63.92</b>	<b>63.46</b>	<b>61.14</b>	<b>62.32</b>	<b>59.2</b>
p-DEB Selectivity	7.612	6.858	6.924	7.501	7.576	17.45
DEB Sele.	50.91	59.07	53.21	68.11	75.55	78.86
TEB Sele.	4.274	4.02	5.5035	8.575	7.618	8.033
%Yield	32.64	37.76	33.76	41.64	47.08	46.68

### Effect of Mole Ratio

Conversion of ethylbenzene decreases with increasing ethanol content in the feed shown in table 6- table 10. Increase in ethanol content in the feed could dilute ethylbenzene in the vapour phase, thus, reducing its reaction with ethyl cation adsorbed on the Brönsted acid sites of the catalysts. The Conversion increases with increase in mole ratio because of the excess amount of ethylbenzene, the disproportionation reaction also takes place to considerable extent along with ethylation reaction. DEB Selectivity is near about same for mole ratios 1:1 and 2:1, at TOS of 3 hours. However, there are some minor changes in DEB selectivity with time on stream, as 1:1

offers slight advantage. p-DEB selectivity is maximum at mole ratio 1:1 and it increased with time on stream, where as p-DEB selectivity decreased with increasing mole ratio. However, with both 1:1 and 2:1 ratios, the p-DEB yield fell with TOS, whereas it was almost constant at mole ratio 3:1. As a result, Yield is lower for 1:1 and 2:1 ratios after few hours on stream. As a result the catalyst is deactivated resulting in the lower yields of DEB as well as p-DEB after few hours on stream, but DEB and p-DEB selectivity is very less at 3:1 mole ratio. Hence, it is better to use EB:EtOH ratio of 2:1 to get optimum yields of DEB and p-DEB.

**Table 6: Ethylation of EB, temperature: 250 deg. C; Feed: Ethyl benzene: Ethanol (2: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.11	0.08	0.24	0.31	0.32	0.32
Ethyl Benzene	87.63	87.50	87.29	86.20	86.01	85.78
Benzene	0.13	0.07	0.29	0.36	0.26	0.23
Toluene	0.77	0.19	0.08	0.04	0.03	0.02
Xylene	0.02	0.00	0.00	0.00	0.00	0.00
Ethyl toluene	0.17	0.02	0.00	0.00	0.00	0.00
1,3-DEB	4.15	4.57	4.48	4.69	4.75	4.83
1,4-DEB	2.12	2.28	2.25	2.55	2.65	3.45
1,2-DEB	3.41	3.57	3.47	3.73	3.81	3.09
1,4 DIPB	0.25	0.19	0.17	0.16	0.15	0.15
1,3,5-TEB	0.61	0.85	0.89	1.07	1.13	1.23
1,2,4 TEB	0.06	0.11	0.09	0.11	0.11	0.12
1,2,3 TEB	0.07	0.08	0.08	0.07	0.06	0.06
Higher Aromatics	0.49	0.49	0.68	0.72	0.72	0.71
<b>%Conversion</b>	<b>12.28</b>	<b>12.42</b>	<b>12.49</b>	<b>13.54</b>	<b>13.71</b>	<b>13.95</b>
p-DEB Selectivity	21.8	21.92	22.03	23.22	23.63	30.31
DEB Sele.	79.01	83.95	81.78	81.274	82.01	81.80
TEB Sele.	6.02	8.28	8.450	9.2477	9.544	10.15
%Yield	9.69	10.41	10.21	11.00	11.24	11.40

**Table 7: Ethylation of EB, temperature: 275 deg. C; Feed: Ethyl benzene: Ethanol (2: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.23	0.33	0.23	0.06	0.00	0.19
Ethyl Benzene	50.85	55.81	62.28	63.45	67.29	67.85
Benzene	5.68	3.81	1.82	1.39	1.03	1.18
Toluene	0.12	0.07	0.00	0.00	0.00	0.00
Xylene	0.14	0.00	0.00	0.15	0.00	0.00
Ethyl toluene	0.27	0.39	0.16	0.00	0.00	0.00
1,3-DEB	23.78	20.92	16.96	16.55	14.56	13.98
1,4-DEB	2.51	2.81	3.37	3.50	3.54	3.56
1,2-DEB	10.42	9.54	8.11	7.96	7.14	6.90
1,4 DIPB	0.36	0.69	1.04	1.01	0.89	0.83
1,3,5-TEB	1.30	1.06	3.41	3.53	3.49	0.59
1,2,4 TEB	2.41	2.93	0.27	0.13	0.24	3.52
1,2,3 TEB	0.30	0.37	0.44	0.45	0.45	0.43
Higher Aromatics	1.63	1.28	1.89	1.82	1.38	0.99
<b>%Conversion</b>	<b>49.03</b>	<b>44.01</b>	<b>37.57</b>	<b>36.51</b>	<b>32.71</b>	<b>32.03</b>
p-DEB Selectivity	6.827	8.4505	11.861	12.500	14.012	14.567
DEB Sele.	75.045	75.848	75.903	76.757	77.15	76.432
TEB Sele.	8.208	9.9350	11.008	11.251	12.767	14.213
%Yield	36.795	33.377	28.516	28.026	25.236	24.479

**Table 8: Ethylation of EB, temperature: 300 deg. C; Feed: Ethyl benzene: Ethanol (2: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.59	0.24	0.00	0.21	1.97	0.28
Ethyl Benzene	59.72	66.01	68.44	71.91	70.77	75.18
Benzene	2.50	1.01	0.67	0.64	0.33	0.68
Toluene	0.11	0.00	0.00	0.00	0.00	0.00
Xylene	0.00	0.00	0.00	0.00	0.00	0.00
Ethyl toluene	0.57	0.21	0.15	0.00	0.00	0.00
1,3-DEB	20.70	17.32	15.99	13.94	12.73	11.40
1,4-DEB	2.44	2.69	2.81	2.58	2.51	2.65
1,2-DEB	9.43	8.21	7.73	6.90	6.45	6.28
1,4 DIPB	0.59	0.99	0.49	0.96	0.43	0.39
1,3,5-TEB	1.30	1.50	1.64	1.41	1.30	1.33
1,2,4 TEB	0.34	0.29	0.29	0.24	0.17	0.20
1,2,3 TEB	0.18	0.10	0.16	0.12	0.12	0.10
Higher Aromatics	1.53	1.43	1.64	1.09	3.20	1.51
<b>%Conversion</b>	<b>39.92</b>	<b>33.83</b>	<b>31.56</b>	<b>27.94</b>	<b>27.80</b>	<b>24.60</b>
p-DEB Selectivity	7.483	9.536	10.575	11.011	11.551	13.037
DEB Sele.	82.062	83.621	84.05	84.01	79.597	82.88
TEB Sele.	4.5758	5.595	6.694	6.331	5.8403	6.616
%Yield	32.762	28.28	26.530	23.472	22.129	20.392

**Table 9: Ethylation of EB, temperature: 325 deg. C; Feed: Ethyl benzene: Ethanol (2: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.57	0.50	0.52	0.34	0.34	0.39
Ethyl Benzene	45.36	46.74	48.34	51.01	53.03	54.70
Benzene	9.59	8.86	6.54	5.25	4.13	3.22
Toluene	0.55	0.46	0.33	0.27	0.20	0.18
Xylene	0.35	0.34	0.27	0.16	0.00	0.12
Ethyl toluene	1.95	1.76	1.48	1.19	0.99	0.93
1,3-DEB	23.48	24.52	25.27	24.72	24.74	23.83
1,4-DEB	2.65	2.30	2.34	2.31	2.38	2.32
1,2-DEB	11.00	10.42	10.73	10.85	10.66	10.49
1,4 DIPB	0.40	0.55	0.40	0.46	0.47	0.48
1,3,5-TEB	0.78	0.77	0.41	0.98	1.06	1.03
1,2,4 TEB	0.59	0.26	0.97	0.30	0.30	0.32
1,2,3 TEB	0.25	0.17	0.30	0.20	0.21	0.21
Higher Aromatics	2.47	2.34	2.09	1.95	1.48	1.77
<b>%Conversion</b>	<b>54.38</b>	<b>53.02</b>	<b>51.40</b>	<b>48.82</b>	<b>46.78</b>	<b>45.08</b>
p-DEB Selectivity	7.144	6.182	6.102	6.109	6.294	6.335
DEB Sele.	68.66	70.59	74.989	77.88	81.036	81.60
TEB Sele.	3.009	2.271	3.276	3.0604	3.353	3.475
%Yield	37.342	37.4286	38.548	38.020	37.910	36.790



**Table 10: Ethylation of EB, temperature: 350 deg. C; Feed: Ethyl benzene: Ethanol (2: 1) WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	1.30	1.08	1.35	1.19	1.21	0.82
Ethyl Benzene	35.11	37.75	38.99	43.90	41.34	41.65
Benzene	22.11	18.28	16.64	13.80	13.52	12.51
Toluene	4.61	3.33	2.71	2.12	0.00	1.53
Xylene	1.97	1.41	1.21	1.02	0.97	0.87
Ethyl toluene	6.46	6.00	5.31	4.54	4.44	3.99
1,3-DEB	10.59	14.11	15.35	15.99	19.24	20.12
1,4-DEB	1.63	1.80	1.86	1.85	2.18	2.22
1,2-DEB	5.06	6.21	6.80	7.25	8.44	8.75
1,4 DIPB	0.73	0.76	0.74	0.66	0.70	0.67
1,3,5-TEB	0.93	0.82	0.70	0.61	0.68	0.95
1,2,4 TEB	0.95	0.98	0.91	0.86	0.99	0.29
1,2,3 TEB	0.22	0.29	0.29	0.27	0.30	0.28
Higher Aromatics	8.31	7.19	7.13	5.93	6.00	5.35
<b>%Conversion</b>	<b>64.42</b>	<b>61.84</b>	<b>60.47</b>	<b>55.57</b>	<b>58.15</b>	<b>58.01</b>
p-DEB Selectivity	9.43	8.147	7.75	7.377	7.29	7.129
DEB Sele.	27.18	36.15	40.2	45.712	51.96	54.031
TEB Sele.	3.307	3.402	3.18	3.1681	3.433	2.657
%Yield	17.5	22.35	24.34	25.402	30.219	31.341

### Effect of WHSV

Ethylation of ethylbenzene at various WHSV's was investigated on IM-5 catalyst shown in table 11 to table 20 . We have studied the influence of WHSV at  $1\text{h}^{-1}$ ,  $3\text{h}^{-1}$ ,  $5\text{h}^{-1}$  and  $7\text{h}^{-1}$  on EB conversion, DEB and p-DEB selectivity at  $300\text{ }^{\circ}\text{C}$  temperature. The results are illustrated in Fig. 9 and 10 EB conversion decreased with increase in WHSV because of the lower contact time. It decreases with increase in TOS for WHSV  $3\text{h}^{-1}$ ,  $5\text{h}^{-1}$  and  $7\text{h}^{-1}$ . But at WHSV  $1\text{h}^{-1}$ , conversion increased initially and then decreases gradually. DEB Selectivity increased with increase in WHSV,

which may be due to suppression of dealkylation and other side reactions. At WHSV  $=1\text{h}^{-1}$ , DEB selectivity increased rapidly with increase in TOS, whereas in other cases it increases very slightly. p-DEB selectivity increased with increase in WHSV and also with TOS . It has increases rapidly for WHSV  $3\text{h}^{-1}$  and reached maximum at TOS 7. But p-DEB Selectivity is low when WHSV is  $1\text{h}^{-1}$ . This may be due to isomerization of p-DEB into m-isomers because of increase in contact time. Yield of DEB is maximum at WHSV  $1\text{h}^{-1}$ , at WHSV  $3\text{h}^{-1}$  it has decreasing with TOS. It is more or less same for WHSV  $5\text{h}^{-1}$  and WHSV.

**Table 11: Ethylation of EB, temperature: 250 deg. C; Feed: Ethyl benzene: Ethanol (3: 1)  
WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	1.29	0.85	0.79	0.74	0.76	0.72
Ethyl Benzene	76.40	78.49	78.24	77.53	77.63	77.61
Benzene	0.64	0.09	0.00	0.00	0.00	0.02
Toluene	0.05	0.01	0.00	0.00	0.00	0.00
Xylene	0.00	0.02	0.02	0.01	0.02	0.00
Ethyl toluene	0.13	0.07	0.07	0.08	0.09	0.00
1,3-DEB	6.75	7.36	7.71	8.02	7.88	7.88
1,4-DEB	3.70	3.23	3.26	3.47	3.53	3.53
1,2-DEB	4.65	4.97	5.02	5.15	5.15	5.15
1,4 DIPB	0.24	0.27	0.27	0.26	0.24	0.24
1,3,5-TEB	3.20	2.62	2.69	2.87	2.96	2.95
1,2,4 TEB	0.14	0.08	0.08	0.08	0.09	0.09
1,2,3 TEB	0.55	0.38	0.38	0.38	0.39	0.39
Higher Aromatics	2.25	1.55	1.48	1.41	1.29	1.42
<b>%Conversion</b>	<b>22.60</b>	<b>20.84</b>	<b>21.14</b>	<b>21.89</b>	<b>21.78</b>	<b>21.82</b>
DEB Sele.	24.50	20.774	20.397	20.86	21.315	21.314
TEB Sele.	67.70	75.283	76.249	76.562	76.605	76.401
%Yield	17.432	14.93	15.0158	15.341	15.884	15.841
p-DEB Selectivity	15.30	15.68	16.116	16.759	16.681	16.671

**Table 12: Ethylation of EB, temperature: 275 deg. C; Feed: Ethyl benzene: Ethanol (1: 1)  
WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.49	1.19	0.10	0.22	0.30	0.25
Ethyl Benzene	46.70	64.71	53.73	55.25	57.61	59.38
Benzene	10.23	0.46	7.27	6.08	6.40	5.18
Toluene	0.13	0.00	0.07	0.10	0.08	0.08
Xylene	0.62	0.00	0.16	0.45	0.36	0.49
Ethyl toluene	0.18	0.02	0.41	0.43	0.15	0.17
1,3-DEB	27.11	8.27	24.22	22.88	21.91	20.42
1,4-DEB	2.18	6.47	2.17	2.28	6.34	2.11
1,2-DEB	7.72	5.23	7.53	7.40	2.47	6.75
1,4 DIPB	0.42	9.33	0.37	0.50	0.56	0.44
1,3,5-TEB	2.13	1.48	2.34	2.85	2.43	2.64
1,2,4 TEB	0.23	0.05	0.14	0.20	0.12	0.18
1,2,3 TEB	0.10	0.06	0.27	0.51	0.25	0.48
Higher Aromatics	1.76	2.72	1.22	0.85	1.02	1.43
<b>%Conversion</b>	<b>53.07</b>	<b>52.28</b>	<b>46.22</b>	<b>44.62</b>	<b>42.61</b>	<b>40.47</b>
p-DEB Selectivity	5.901	5.987	6.397	6.993	7.033	7.202
DEB Sele.	70.082	71.576	73.459	73.108	73.321	72.516
TEB Sele.	4.6583	5.8170	5.9538	8.0017	6.5719	8.1754
%Yield	37.195	37.420	33.951	32.622	31.172	29.347

**Table 13: Ethylation of EB, temperature: 300 deg. C; Feed: Ethyl benzene: Ethanol (1: 1)  
WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.70	0.36	0.54	0.48	0.41	0.39
Ethyl Benzene	46.09	46.66	48.27	49.42	50.08	51.82
Benzene	11.46	9.91	9.15	8.55	7.72	7.20
Toluene	0.41	0.28	0.22	0.19	0.17	0.15
Xylene	0.28	0.19	0.18	0.06	0.06	0.24
Ethyl toluene	0.12	1.06	0.89	0.82	0.89	0.73
1,3-DEB	26.45	26.90	26.52	26.08	26.06	24.98
1,4-DEB	2.11	2.19	2.13	2.13	2.15	2.09
1,2-DEB	7.50	7.85	7.38	7.67	7.58	7.46
1,4 DIPB	0.83	0.35	0.73	0.73	0.30	0.71
1,3,5-TEB	1.39	1.76	1.94	2.08	2.22	2.22
1,2,4 TEB	0.15	0.18	0.18	0.28	0.28	0.27
1,2,3 TEB	0.13	0.13	0.15	0.11	0.11	0.11
Higher Aromatics	0.70	2.18	1.71	1.41	1.96	1.62
<b>%Conversion</b>	<b>53.58</b>	<b>53.17</b>	<b>51.47</b>	<b>50.35</b>	<b>49.72</b>	<b>47.97</b>
p-DEB Selectivity	5.853	5.936	5.91	5.938	6.0037	6.0631
DEB Sele.	67.77	69.724	70.38	71.59	72.281	72.268
TEB Sele.	3.144	3.904	4.445	4.939	5.289	5.4392
%Yield	36.31	37.0	36.226	36.048	35.93	34.670

**Table 14: Ethylation of EB, temperature: 325 deg. C; Feed: Ethyl benzene: Ethanol (1: 1)  
WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	1.14	1.07	0.93	0.86	0.77	0.76
Ethyl Benzene	42.16	42.13	44.50	43.80	43.88	43.83
Benzene	15.75	14.04	1.35	12.62	12.26	12.06
Toluene	1.35	1.06	0.96	0.84	0.78	0.77
Xylene	0.19	0.31	0.30	0.28	0.27	0.27
Ethyl toluene	3.08	3.19	2.95	2.64	2.22	2.53
1,3-DEB	20.70	22.84	23.62	24.04	24.60	24.55
1,4-DEB	2.02	2.18	2.24	2.19	2.20	2.20
1,2-DEB	6.64	6.94	7.40	7.24	7.37	7.29
1,4 DIPB	0.36	0.90	0.90	0.87	0.38	0.87
1,3,5-TEB	1.04	1.28	1.44	1.49	1.56	1.56
1,2,4 TEB	0.12	0.20	0.21	0.29	0.22	0.45
1,2,3 TEB	0.19	0.25	0.20	0.17	0.16	0.18
Higher Aromatics	5.28	3.64	13.00	2.68	3.33	2.68
<b>%Conversion</b>	<b>57.36</b>	<b>57.42</b>	<b>55.08</b>	<b>55.82</b>	<b>55.78</b>	<b>55.83</b>
p-DEB Selectivity	6.887	6.810	6.741	6.533	6.450	6.451
DEB Sele.	51.7744	56.254	60.94	60.465	61.738	61.41
TEB Sele.	2.3637	3.03	3.386	3.5243	3.5037	3.9469
%Yield	29.69	32.298	33.56	33.750	34.435	34.292

**Table 15: Ethylation of EB, temperature: 350 deg. C; Feed: Ethyl benzene: Ethanol (1: 1)  
WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	1.89	1.72	1.33	1.44	0.93	0.36
Ethyl Benzene	40.12	36.54	40.77	40.23	43.64	42.31
Benzene	21.27	18.25	17.58	18.57	15.27	16.63
Toluene	3.85	2.84	2.37	2.64	2.16	2.98
Xylene	0.63	0.55	0.55	0.56	0.28	0.70
Ethyl toluene	5.91	5.48	5.37	5.53	4.96	5.41
1,3-DEB	12.51	12.86	17.55	16.01	17.85	16.81
1,4-DEB	1.41	1.66	2.09	1.99	2.04	1.92
1,2-DEB	5.00	4.96	5.83	5.76	6.16	6.15
1,4 DIPB	0.78	0.75	0.94	0.81	0.92	0.95
1,3,5-TEB	0.77	0.93	1.23	1.15	1.23	1.20
1,2,4 TEB	0.65	0.44	0.35	0.32	0.32	0.40
1,2,3 TEB	0.67	0.25	0.50	0.40	0.46	0.51
Higher Aromatics	4.54	12.79	3.55	4.59	3.77	3.67
<b>%Conversion</b>	<b>59.11</b>	<b>62.82</b>	<b>58.68</b>	<b>59.18</b>	<b>55.95</b>	<b>57.54</b>
p-DEB Selectivity	7.461	8.513	8.19	8.360	7.824	7.723
DEB Sele.	32.624	31.541	43.98	40.738	46.991	43.389
TEB Sele.	3.6020	2.6194	3.5876	3.197	3.633	3.6838
%Yield	19.284	19.815	25.808	24.108	26.293	24.965

**Table 16: Ethylation of EB, temperature:: 275 deg. C; Feed: Ethyl benzene: Ethanol (2: 1)  
WHSV: 1.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.00	0.00	0.00	0.00	0.00	0.00
Aliphatic	0.45	0.61	0.46	0.41	0.37	0.38
Ethyl Benzene	49.96	45.53	45.28	46.75	47.37	49.74
Benzene	9.26	8.26	7.21	6.61	5.48	5.08
Toluene	1.10	0.67	0.51	0.45	0.40	0.35
Xylene	0.10	0.19	0.20	0.13	0.09	0.19
Ethyl toluene	2.11	2.06	1.88	1.74	1.71	1.58
1,3-DEB	19.14	26.14	27.95	27.80	28.04	27.01
1,4-DEB	2.38	2.19	2.27	2.21	2.38	2.23
1,2-DEB	7.05	7.59	7.95	7.90	8.00	8.03
1,4 DIPB	1.44	1.54	0.48	0.45	0.46	0.46
1,3,5-TEB	2.69	1.98	1.96	1.84	1.88	2.00
1,2,4 TEB	0.72	0.35	0.25	0.27	0.43	0.17
1,2,3 TEB	0.26	0.21	0.30	0.26	0.36	0.30
Higher Aromatics	3.33	2.68	0.00	3.19	3.00	2.49
<b>%Conversion</b>	<b>49.81</b>	<b>54.19</b>	<b>54.51</b>	<b>53.05</b>	<b>52.45</b>	<b>50.07</b>
p-DEB Selectivity	8.323	6.089	5.95	5.83	6.206	5.974
DEB Sele.	57.61	66.68	70.3	71.75	73.51	74.694
TEB Sele.	7.398	4.7125	4.628	4.478	5.1211	4.958
%Yield	28.696	36.136	38.34	38.07	38.56	37.402

**Table 17: Ethylation of EB, temperature: 275 deg. C; Feed: Ethyl benzene: Ethanol (2: 1)  
WHSV: 3.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.18	0.24	0.21	0.20	0.21	0.16
Aliphatic	0.23	0.33	0.23	0.06	0.00	0.19
Ethyl Benzene	50.85	55.81	62.28	63.45	67.29	67.85
Benzene	5.68	3.81	1.82	1.39	1.03	1.18
Toluene	0.12	0.07	0.00	0.00	0.00	0.00
Xylene	0.14	0.00	0.00	0.15	0.00	0.00
Ethyl toluene	0.27	0.39	0.16	0.00	0.00	0.00
1,3-DEB	23.78	20.92	16.96	16.55	14.56	13.98
1,4-DEB	2.51	2.81	3.37	3.50	3.54	3.56
1,2-DEB	10.42	9.54	8.11	7.96	7.14	6.90
1,4 DIPB	0.36	0.69	1.04	1.01	0.89	0.83
1,3,5-TEB	1.30	1.06	3.41	3.53	3.49	0.59
1,2,4 TEB	2.41	2.93	0.27	0.13	0.24	3.52
1,2,3 TEB	0.30	0.37	0.44	0.45	0.45	0.43
Higher Aromatics	1.63	1.28	1.89	1.82	1.38	0.99
<b>%Conversion</b>	<b>49.03</b>	<b>44.01</b>	<b>37.57</b>	<b>36.51</b>	<b>32.71</b>	<b>32.03</b>
p-DEB Selectivity	6.827	8.4505	11.861	12.500	14.012	14.567
DEB Sele.	75.045	75.848	75.903	76.757	77.15	76.432
TEB Sele.	8.208	9.9350	11.008	11.251	12.767	14.213
%Yield	36.795	33.377	28.516	28.026	25.236	24.479

**Table 18: Ethylation of EB, temperature: 275 deg. C; Feed: Ethyl benzene: Ethanol (2: 1)  
WHSV: 5.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.00	0.00	0.00	0.00	0.00	0.00
Aliphatic	0.48	0.30	0.37	0.35	0.25	0.24
Ethyl Benzene	61.83	61.57	63.03	64.18	64.71	64.96
Benzene	3.38	2.05	1.91	1.67	1.65	1.69
Toluene	0.06	0.00	0.00	0.47	0.02	0.02
Xylene	0.13	0.09	0.06	0.14	1.18	0.09
Ethyl toluene	0.35	0.17	0.07	0.14	0.19	0.05
1,3-DEB	18.23	18.65	17.43	16.20	16.33	16.15
1,4-DEB	2.84	3.30	3.28	3.26	3.37	3.43
1,2-DEB	7.12	6.70	6.44	6.14	6.13	6.18
1,4 DIPB	0.87	1.02	0.90	0.78	0.74	0.70
1,3,5-TEB	2.26	3.82	4.05	4.14	4.33	4.44
1,2,4 TEB	0.29	0.36	0.13	0.13	0.14	0.15
1,2,3 TEB	0.26	0.22	0.08	0.64	0.68	0.70
Higher Aromatics	1.90	1.74	2.24	1.76	0.28	1.19
<b>%Conversion</b>	<b>37.87</b>	<b>38.24</b>	<b>36.73</b>	<b>35.59</b>	<b>35.13</b>	<b>34.88</b>
p-DEB Selectivity	10.08	11.52	12.071	12.73	13.05	13.29
DEB Sele.	74.79	75.142	74.200	72.18	73.733	74.03
TEB Sele.	7.4597	11.551	11.63	13.834	14.695	15.183
%Yield	28.327	28.735	27.255	25.690	25.901	25.82

**Table 19: Ethylation of EB, temperature: 275 deg. C; Feed: Ethyl benzene: Ethanol (2: 1) WHSV: 7.0 per hr.; Press: 10 bar (H2), H2/HC=2**

Product Component (Wt %)	Time ( hours)					
	2	3	4	5	6	7
Ethanol	0.00	0.00	0.00	0.00	0.00	0.00
Aliphatic	0.69	0.45	0.33	0.25	0.23	0.18
Ethyl Benzene	49.62	55.70	58.41	60.05	60.28	61.05
Benzene	5.77	2.81	1.91	1.64	1.51	1.30
Toluene	0.17	0.05	0.00	0.00	0.00	0.00
Xylene	0.07	0.06	0.04	0.04	0.00	0.00
Ethyl toluene	0.75	0.25	0.16	0.08	0.13	0.12
1,3-DEB	24.24	21.34	19.43	18.38	17.99	17.53
1,4-DEB	3.03	3.24	3.57	3.66	3.79	3.92
1,2-DEB	8.15	7.17	6.71	6.47	6.43	6.25
1,4 DIBP	0.80	0.81	0.90	0.81	0.76	0.72
1,3,5-TEB	3.25	4.81	5.66	5.77	5.93	6.04
1,2,4 TEB	0.13	0.16	0.18	0.18	0.19	0.19
1,2,3 TEB	0.52	0.85	1.02	1.02	1.03	1.03
Higher Aromatics	2.80	2.32	1.68	1.66	1.74	1.66
<b>%Conversion</b>	50.03	<b>44.05</b>	<b>41.39</b>	<b>39.80</b>	<b>39.59</b>	<b>38.84</b>
p-DEB Selectivity	8.563	10.20	12.007	12.83	13.44	14.16
DEB Sele.	71.304	72.393	71.997	71.802	71.423	71.4664
TEB Sele.	7.8437	13.2	16.638	17.563	18.07	18.715
%Yield	35.675	31.89	29.80	28.57	28.272	27.755

## CONCLUSIONS

From the results it can be concluded that the use of higher temperature, higher mole ratio and low WHSV gives good conversion but DEB selectivity decreases so it was found out that at moderate conditions i.e. temperature of 300 °C, mole ratio 2:1 and WHSV=3h<sup>-1</sup>, the conversion of EB and DEB, p-DEB selectivity's and yield are much better. The percent of m-DEB isomers in DEB is more than that of p-DEB, may be because of the acid active sites present on the outer surface zeolite crystals which are not diffusionally constrained. Therefore, they contribute to the isomerization of p-DEB to m-DEB. The isomerization step can generally follow two models: (i) the isomerization of p-diethyl benzene to m-diethyl benzene takes place exclusively on the outer surface, or (ii) the isomerization occurs on the acid sites located both on the outer surface and inside the zeolite channels. Therefore, their elimination of acid sites from the zeolite surface will be helpful for the reaction selectivity with respect to the desired dialkylaromatics. However, if the zeolite modification can be done, not only leading to elimination of the surface sites but also lead to narrowing of the pore opening, like, e.g., with

the surface silylation or deposition of metal oxides, such zeolite modification results increase p- selectivity.

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