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Simulation of an Isothermal Catalytic Membrane Reactor for the Dehydrogenation of ETHYLBENZENE

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Abstract

Mathematical models for predicting the fractional conversion of ethylbenzene and yields of products in a catalytic membrane reactor for the dehydrogenation of ethylbenzene were developed. The mathematical models developed consisted of nonlinear simultaneous differential equations which were solved numerically using the 4th order Runge-kuta algorithm. Prediction by the models of fractional conversion and yields of product compare favorably with outputs of an industrial reactor with maximum deviations of 0.175. The models were subsequently used to simulate the effects of feed inlet temperature, feed molar ratio of steam and ethylbenzene and inlet pressure on the reactor performance.

Keywords: Dehydrogenation of Ethylbenzene, Catalytic membrane reactor, Reactor modeling, Simulation

1. Introduction

Styrene is one of the most important monomers in the petrochemical industry due to its protective, insulative, and synthetic ability when polymerized. The world's production at present is approximately twenty million tons per year (Dennis and Castor, 1992). The styrene process was developed in the nineteen thirties and was used for the production of many different polymeric materials, the most important being poly-styrene, styrene-acrylonitrile, styrene-butadiene latex and acrylonitrile-butadiene styrene resins (ABS). Styrene can be produced by the dehydrogenation of ethyl-benzene in the presence of steam over iron oxide based catalyst, as a by-product in the epoxidation of propene with ethyl-benzene hydro-peroxide and molybdenum complex base catalyst or by the oxidative dehydrogenation of ethyl-benzene (Yee, *et al*., 2003); however the dehydrogenation of ethyl-benzene accounts for over ninety percent of the world's styrene production (Abashar, 2004). The dehydrogenation process is an endothermic reversible reaction and can be operated industrially either adiabatically or isothermally over a fixed bed. The demand for higher conversion of ethylbenzene, high yield and selectivity of the desired reaction products especially styrene had led to new ingenious configuration and design of reactors for the dehydrogenation process. In this regards, multifunctional reactors where reactions combined with separation have received much attention (Collins an Way, (1993); Dixon, (1999) and Devoldere and froment, (1999)). Membrane reactors are one of such type of multi-functional reactors. Recent advances in materials used at high temperatures have allowed the consideration of membranes for integration into reactors for catalytic reactions.

To accomplish this, a membrane that is permeable to a particular reaction product, but impermeable to all other species is placed around the reacting mixture, If reaction is equilibrium limited, the decreased activity of the species being removed permits further conversion to occur beyond that which would be possible if no species were removed. The permeation of gaseous component through the membrane takes place from a higher partial pressure zone to a

lower partial pressure zone for a given component. This can be achieved by either a difference in the total pressure, or by diluting the permeate side with enough inert to lower the mole fraction of the permeating species. Hence the membrane reactor can be used to achieve conversions greater than the original equilibrium value (Ahari *et al*., 2004). The objectives of this study are to develop the mathematical model for the ethylbenzene dehydrogenation and to investigate the effect of operating conditions on an industrial membrane reactor using the developed models.

1.1 *Process Description*

Figure 1a shows a schematic of a typical membrane reactor. The membrane divides the reactor into two zones namely; a reaction zone (tube side) packed with catalyst particles where reactant (ethylbenzene) is introduced and a permeate zone (shell side) where a non-reactive purge gas (steam) is introduced co-currently to the feed in order to send out the permeate gas (hydrogen). Ethylbenzene is first preheated in a heat-exchanger, mixed with superheated steam and sent into the membrane reactor. Hydrogen produced within the reactor permeates out of the tube through the membrane due to pressure difference between the reaction zone (tube) and the permeate zone (shell). The removal of hydrogen reduces side reactions of ethylbenzene with hydrogen. The permeated hydrogen gas is swept out of the reactor using steam. In the reaction zone of the reactor, styrene, other aromatic hydrocarbons such as benzene and toluene, and lean amount of hydrogen found around the reactor tube are collected at the exit or product stream of the reactor.
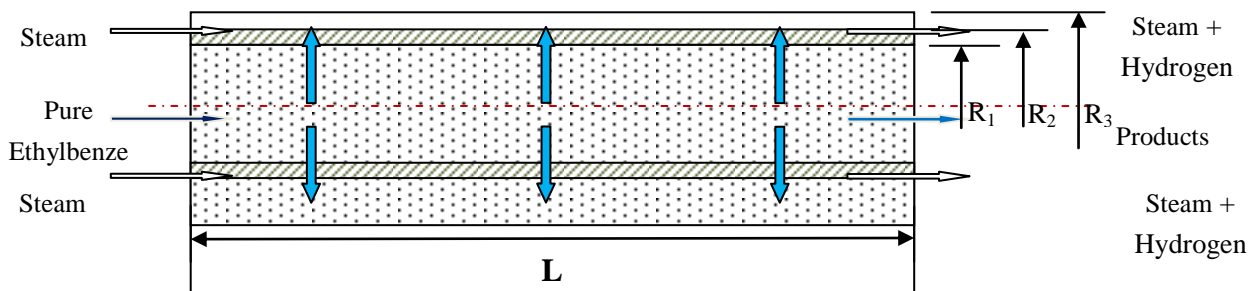

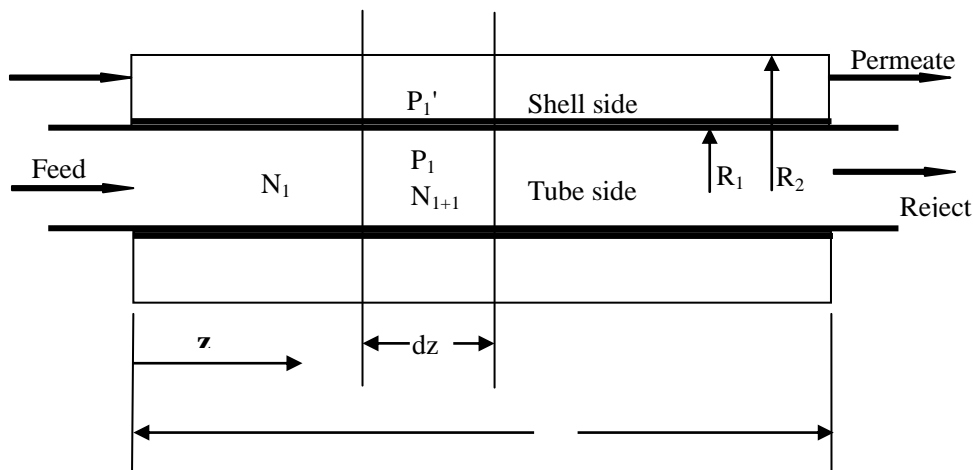Figure 1a: Transverse section of the catalytic packed bed membrane reactor

Figure 1b: Schematic of differential volume of membrane reactor used for material balance.

2. Kinetic Model

Numerous works on the development, type, composition and activity of various catalysts used in the dehydrogenation of ethylbenzene to styrene have been performed: Lee, (1973), Hirano, (1986), Muhler *et al*., (1992) and Wu *et al*., (1993). Various type of reaction mechanism has been postulated to describe the kinetics of ethylbenzene dehydrogenation, a uni-molecular Langmuir-Hinshelwood mechanism, where the reaction rate depends on the adsorption-desorption equilibrium of ethylbenzene and styrene was earlier proposed by Carra and Forni (1965) and Sheel and Crowe, (1969); later supported by Sheppard and Maier, (1986) and Pradeep and Elnashaie, (2004). Others include the works of Clough and Ramirez, (1976), Wu and Liu, (1992), Wu *et al*., (1993), Elnashaie *et al*., (1993). Elnashaie *et al*., (2000) and Ganji, *et al*., (2004) postulated that the kinetic model for the dehydrogenation of ethylbenzene to styrene can be represented by six reversible reactions viz: one main reaction (ethylbenzene to styrene) with five side reactions. Sheppard and Maier, (1986) observed that all side reactions were much slower in comparison to the main reaction and are far from equilibrium at finite time where the main reaction may get completed; therefore all the side reactions could be considered irreversible and the reverse rates excluded from the kinetic model.

The dehydrogenation reaction occurring in the reactor leading to the production of styrene as described by Elnashaie *et al*., (2000) incorporating the conclusions from the observations of Sheppard and Maier (1986) were adapted as the reactions occurring in the reactor. The reaction paths for the dehydrogenation process with their respective reaction rate expressions as follows:

Main reaction:

$$C_6H_5C_2H_5 \quad \xleftarrow{\quad K1 \quad}\rightarrow \quad C_6H_5C_2H_3 + H_2 \qquad (1)$$

$$r_1 = K_1\left(P_{eb} - \frac{P_{st}P_{H_2}}{K_{peb}}\right) \qquad (2)$$

Side reactions:

$$C_6H_5C_2H_5 + H_2 \quad \xrightarrow{\quad K2 \quad} \quad C_6H_5CH_3 + CH_4 \qquad (3)$$

$$r_2 = K_2\left(P_{eb}P_{H_2}\right) \qquad (4)$$

$$C_6H_5C_2H_5 \quad \xrightarrow{\quad K3 \quad} \quad C_6H_6 + C_2H_4 \qquad (5)$$

$$r_3 = K_3(P_{eb}) \qquad (6)$$

$$H_2O + \tfrac{1}{2}C_2H_4 \quad \xrightarrow{\quad K4 \quad} \quad CO + 2H_2 \qquad (7)$$

$$r_4 = K_4\left(P_{H_2O}P_{C_2H_4}^{0.5}\right) \qquad (8)$$

$$H_2O + CH_4 \quad \xrightarrow{\quad K5 \quad} \quad CO + 3H_2 \qquad (9)$$

$$r_5 = K_5\left(P_{H_2O}P_{CH_4}\right) \qquad (10)$$

$$H_2O + CO \quad \xrightarrow{\quad K6 \quad} \quad CO_2 + H_2 \qquad (11)$$
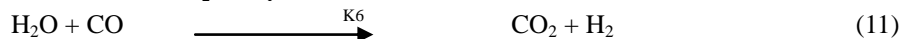
$$r_6 = K_6(P_T/T^2)\left(P_{H_2O}P_{co}\right) \qquad (12)$$

The reaction rate constants in these equations are obtained as:

$$K_j \left(molkg^{-1}s^{-1}bar^{-n}\right) = 10^3 exp\left(A_I - \frac{E_i}{RT}\right) \qquad (13)$$

$$K_{peb} = exp\left(\frac{-\Delta H}{RT}\right) \qquad (14)$$

$$\Delta H = a + bT + cT^2 \qquad (15)$$

a(jmol^{-1})	b(Jmol^{-1}K^{-1})	c(Jmol^{-1}K^{-2})
122725.16	-126.27	-2.19E-03

3. Reactor Model

3.1 *Model Assumption*

The following conditions are imposed on the reactor and process in developing the mathematical model of the reactor.

The mass transfer in radial direction through the membrane is negligible. An axial one-dimensional steady state model was developed; axial diffusion of mass is negligible because the ratio of reactor length to the particle size is large, Radial temperature gradient across the membrane is neglected (adiabatic operation), The catalyst pellet equations are discarded because concentration gradients in catalyst pellet are neglected due to small pellet size (Zeynali, 2010), the catalyst deactivation is minimal, thus, effectiveness factor is equal to unity, The temperature of the fluid phase and the solid phase are the same (Babu and Gujarathi, 2010), The system operates isothermally, the effect of pressure drop on the performance of the reactor is negligible (Wu and Liu, 1992). Hence, isobaric conditions are assumed to prevail in the tube and shell sides, therefore P_{tT} and P_{sT} are constant.

Based on these assumptions a pseudo-homogeneous one-dimensional model was developed for the reacting species by taking a component mole balance of a differential element of the reactor as shown in Figure 1b thus:

TUBE SIDE: Transportation of reacting components and products through the tube:

The mole balance for a reacting component i through reaction path j flowing through the tube is:

$$F_i \frac{dC_{i,j}}{dZ} = -2\pi R_1 J_i \pm \pi R_1^2 \rho r_j \tag{16}$$

In terms of fractional conversion:

$$\frac{dX_{i,j}}{dZ} = \frac{1}{F_i C_i}\left(2\pi R_1 J_i + \pi R_1^2 \rho r_j\right) \tag{17}$$

The basic reactants to be considered for the six reactions are ethylbenzene and steam. These two are not permeating through the membrane, thus the permeate term is zero and equation (17) becomes,

$$\frac{dX_{i,j}}{dZ} = \frac{1}{F_i C_i}\pi R_1^2 \rho r_j \tag{18}$$

Equation (18) was used to write the model equation for each reactant in the six reaction scheme.

For ethylbenzene: i = 1; j = 1, 2, 3

For steam: i = 2   j = 4, 5, 6

Equation (18) is the steady state one-dimensional model equation for the membrane reactor describing the fractional conversion of reactant i along the reactor length.

$$\frac{dX_{1,1}}{dZ} = \frac{1}{F_1 C_1}\pi R_1^2 \rho \left(K_1\left(P_{eb} - \frac{P_{st}P_{H_2}}{K_{peb}}\right)\right) \tag{19}$$

$$\frac{dX_{1,2}}{dZ} = \frac{1}{F_1 C_1}\pi R_1^2 \rho \left(K_2\left(P_{eb}P_{H_2}\right)\right) \tag{20}$$

$$\frac{dX_{1,3}}{dZ} = \frac{1}{F_1 C_1}\pi R_1^2 \rho \left(K_3(P_{eb})\right) \tag{21}$$

$$\frac{dX_{2,4}}{dZ} = \frac{1}{F_2 C_2} \pi R_1^2 \rho \left(K_4 \left(P_{H_2O} P_{C_2H_4}^{0.5} \right) \right) \tag{22}$$

$$\frac{dX_{2,5}}{dZ} = \frac{1}{F_2 C_2} \pi R_1^2 \rho \left(K_5 \left(P_{H_2O} P_{CH_4} \right) \right) \tag{23}$$

$$\frac{dX_{2,6}}{dZ} = \frac{1}{F_2 C_2} \pi R_1^2 \rho \left(K_6 (P_T/T^2) \left(P_{H_2O} P_{co} \right) \right) \tag{24}$$

SHELL SIDE**:** Permeation of hydrogen gas through the membrane and transportation of steam plus hydrogen gas through the shell.

Similarly since no reaction occurs within the shell of the reactor, a non-reactive component mole balance was developed for hydrogen gas as:

$$\frac{dC_{H_2}}{dZ} = \frac{2\pi R_2 J_{H_2}}{F_{H_2}} \tag{25}$$

The permeation flux of hydrogen $\left(J_{H_2} \right)$ through a palladium-palladium alloy composite membrane had been determined by Moustafa and Elnashaie, (2000) as:

$$J_{H_2} = \frac{P_{mH_2}}{\delta} \left(P_{tH_2}^n - P_{sH_2}^n \right) \tag{26}$$

The permeability of hydrogen (P_{mH_2}) as a function of the equilibrium solubility and its diffusivity in palladium is given by the expression of Elnashaie *et al*., (2000) as:

$$\frac{P_{mH_2}}{\delta} = \frac{D_H C_O}{R_2 \sqrt{P_O \ln \frac{R_2}{R_1}}} \tag{27}$$

Substituting equations (26) and (27) into equation (25), the component mole balance of hydrogen through membrane becomes:

$$\frac{dC_{H_2}}{dZ} = \frac{2\pi D_H C_O}{F_{H_2} \sqrt{P_O \ln \frac{R_2}{R_1}}} \left(P_{tH_2}^n - P_{sH_2}^n \right) \tag{28}$$

Where n is a constant; D_H (m²s⁻¹) Fick's diffusion coefficient of hydrogen dissolved in palladium and C_O (mole m⁻³) the solubility or standard concentration of dissolved hydrogen in palladium.

These constants have been determined by Elnashaie *et al*., (2000) as:

$$D_H = 2.3 X 10^{-7} exp \left(\frac{2610}{T} \right) \tag{29}$$

$$C_O = 3.03 X 10^5 T^{-1.0358} \tag{30}$$

P_O is the pressure at permeate side in atm.

4. Methodology

The component partial pressures in the model equations were converted to mole concentrations of the components using the following relationships:

Tube side

$$P_i = Y_i P_t = \left(\frac{N_i}{\sum N_i} \right) P_t \tag{31}$$

Shell side

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$$P_i = Y_i P_s = \left(\frac{N_i}{\sum N_i}\right) P_s \qquad\qquad (32)$$

Where: Yi = mole fraction of component i, Ni = molar concentration of component i

The molar concentrations of each component (N_i) in equations (31) and (32) of the reaction path for the hydrogenation process were obtained using expressions that are functions of the fractional conversion for each reactant as given in Table 2.

If the components are assumed to behave as ideal gases, then the mole fractions of the reactants and products (Y_i) in equations (31) and (32) can be obtained by the expressions given in Table 3 using the molar concentrations obtained from Table 2. The component partial pressures (equations 31, 32) with the component mole fractions given in Table 3 were substituted into the model equations (equations 19 – 24) to obtain model equations in terms of molar concentrations. The fourth order Runge-Kuta algorithm was adopted to develop a visual basic program to solve the final model equations using industrial plant data of Elnashaie and Elshishini, (1994) given in Table 4.

The following boundary conditions apply:

At z = 0: $\quad X_{i,j} = 0$ $\qquad\qquad$ for i = 1, 2; $\qquad$ j = 1, 2,…..,6

$$P_t = P_{ti} \ (pressure\ at\ inlet); \quad P_s = P_{si} \ (pressure\ at\ inlet)$$

The results of the model equations gave the fractional conversions of the reacting components along the reactor length. Substitution of these values into the expressions in Table 2 gave the amount (moles) of reactants and yields of products along the reactor length.

Industrial plant data was used to test the suitability of the models in predicting the conversion of ethylbemzene and yield of the products. The effects of the flowing process variables: Feed Temperature, Feed molar ratio of steam to ethylbenzene (H_2O/EB) and Pressure on the models developed was then investigated.

The major products of this process are styrene, benzene and toluene, therefore only the results for these products are presented.

5. Discussion of Results

5.1 *Model Validation*

The results from the model equations for the yield of the products (styrene, benzene and toluene) and the conversion of ethylbezene as predicted by the model equations in comparison with industrial results of Elnashaie and Elshishini, (1994) are presented in Table 5.

The results showed a reasonable agreement between the model predictions and the industrial plant data. The models predicted the conversion of ethylbenzene and the yield of styrene very accurately. The fractional conversion of ethybenzene and yield of styrene, benzene and toluene along the reactor length as predicted by the models are shown in Figure 2. The fractional conversion of ethylbenzene increased continuously along the reactor length, the yield of styrene rose rapidly initially and gradually reached equilibrium towards the reactor exit, benzene and toluene formation rate are much slower compared to that of styrene, toluene formation is slower than benzene formation because hydrogen produced from subsequent reactions which permeates to the shell side are required for its formation. Selectivity can be expressed as the ratio of product formation to the rate of ethylbenzene consumption. Figure 3 is a plot of the yield of products against conversion of ethylbenzene and shows the relative selectivity of

styrene formation over benzene and toluene formation.

5.2 *Model Simulation*

The effects of temperature of the feed mixture at the reactor inlet, pressure at the entrance to the reactor and feed ratio of steam to ethylbenzene (H_2O/EB) on the models developed were investigated. The effects of varying each of these parameters on the reactor performance are presented.

5.2.1 *Effect of inlet Feed Temperature*

Figure 4 depicts the effect of an increase in feed temperature on conversion of ethylbenzene and yield of styrene, benzene and toluene. Dehydrogenation of ethylbenzene is an endothermic reaction and high temperatures have been reported by Mousavi *et al*., (2012) as necessary for high ethylbenzene conversion because of its thermodynamics. In the temperature range examined, ethylbenzene conversion increased continuously and linearly with corresponding increase in the yields of styrene, benzene and toluene.

Table 6 shows the percentage increase in the conversion of ethylbenzene and the yield of products as the feed temperature was increased. There was a decrease in the percentage increase in the conversion of ethylbenzene and yield of products as the feed temperature was increased in the interval of 850K to 950K. At 950K the conversion of ethylbenzene and yield of styrene were only 6.49% and 0.53% higher than at 925K compared to a 19.02% and 16.11% increase in conversion of ethylbenzene and yield of styrene obtained by increasing feed temperature from 850K to 875K.   Therefore beyond 925K the increase in products yields compared to increase in feed temperature might not be economical.

5.2.2 *Effect of Feed Molar Ratio of Steam to Ethylbenzene (H_2o/Eb)*

Figure 5 shows the effect of the feed molar ratio of steam to ethylbenzene on the conversion of ethylbenzene and the yield of the products. An increase in the steam to ethylbenzene ratio means a decrease in the feed rate (F1) keeping the stem rate (F2) constant, figure 5 shows that when the steam to ethylbenzene ratio was increased, there was a minimal increase in ethylbenzene conversion and a selective increase in styrene yield. This is in agreement with Le chateliar's principle which predicts that the system will attempt to oppose the change affected to the original state of equilibrium, since ethylbenzene dehydrogenation into styrene is a reversible reaction with increasing number of moles, a reduction in ethylbenzene feed rate will shift the equilibrium in the direction of increased concentration, that is the equilibrium shifts to the right. A decrease in the steam to ethylbenzene ratio means an increase in the feed rate (F1) keeping the stem rate (F2) constant. The reverse trend is expected in this case. Simulation results also predicted a reduction in benzene and toluene yields. (Toluene formation requires hydrogen which is selectively withdrawn by the membrane to the shell side of the reactor). Similar trends were also reported in the works of Shuka and Anand, (2011). Figure 5 also indicates a drop in conversion of ethylbemzene and yield of styrene above a steam to ethylbenzene ratio of 7. Minimal amount of steam is recommended in terms of plant economics as the cost of producing steam is reduced.

5.2.3 *Effect of Operating Pressure*

Figure 6 shows the effect of variation of inlet pressure on the conversion of ethylbenzene and the yield of styrene, benzene and toluene. Figure 6 predicted an initial minimal increase then a continuous gradual decrease in the conversion and yield of ethylbenzene and styrene respectively. This trend is correct as the equilibrium conversion of

styrene from the rate equation is inversely proportional to the pressure (p). (The reverse reaction as indicated by rate equation is proportional to p^2, while the forward reaction of styrene formation is proportional to p). Figure 5 also predicts that the yields of benzene and toluene also increased minimally with pressure. This trend Le chateliar's principle also predicts; that an increase in system pressure due to decreasing volume will favor the reaction which involves a reduction in pressure (the reaction will shift to the side with fewer moles of gas). That is to the left, resulting in a decrease in conversion of ethylbenzene as predicted by the simulation results.

6. Conclusion

Mathematical models that can be used to predict the performance of industrial membrane reactors used for the dehydrogenation of ethylbenzene were successfully developed. The accuracy of the developed models was tested using industrial plant data as inputs to solve the model equations. The results of the models (conversion of ethylbenzene and yield of styrene, benzene and toluene) compared favorable with output values from the industrial reactor. Therefore the models could be used to simulate industrial reactors for the dehydrogenation of ethylbenzene. Simulation of the effects of feed inlet temperature, feed molar ratio of steam to ethylbenzene and inlet pressure was performed. The simulation studies have shown possible new operating conditions with improved performance (conversion and yield values). However, final selection of best operating conditions are usually based on the overall process economics.

Nomenclature

D_H Fick's diffusivity coefficient of hydrogen, m^2/sec

P_{mi} Permeability coefficient of component i, $mole.m/m^2.sec.atm$

P Total pressure of gaseous mixture, atm

P_{ti} Partial pressure of component i in tube, atm

P_{si} Partial pressure of component i in shell, atm

P_i Partial pressure of component i, atm

r Radial coordinate, m

R_1 Internal diameter of tube, m

R_2 Outer diameter of tube, m

R_3 Internal diameter of shell, m

r_j Rate of reaction j, mol/sec.kg of catalyst

X_{tij} Fractional conversion of reactant i by reaction j in tube

Z spatial coordinate, m

N_i Permeation rate of component i through membrane, mole/sec

J_i Molar flux of component i through membrane, $mole/sec.m^2$

F_{tio} Molar flow rate of component i in feed to tube side, mole/sec

Ki Rate constant for reaction (i), mole/kg catalyst.sec.atm

K_{eb} Equilibrium constant for reaction (1), atm

C_o Solubility or Standard concentration of dissolved H_2, $mole/m^3$

A_j Dimensionless pre-exponential factor

E_j Activation energy of reaction j, J/mole

Greek Symbols

δ Thickness of membranes, m

ρ Density of catalyst, kg/m^3

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REACTION	KINETIC PARAMETER	
PATH	Ei(J/mol)	Ai
1	83357	0.75
2	100555	0.77
3	188630	12.19
4	103996	0.12
5	65723	-3.21
6	73628	21.24

Table 1: Kinetic Parameters in Rate expression for the six reactions (Elnashaie *et al*., 2001)

Component	Molar concentration (mole/sec)
Ethylbenzene ($C_6H_5C_2H_5$)	$F_1\left(1 - X_{1,1} - X_{1,2} - X_{1,3}\right)$
Styrene ($C_6H_5C_2H_3$)	$F_1 X_{1,1}$
Toluene ($C_6H_5CH_3$)	$F_1 X_{1,2}$
Benzene (C_6H_6)	$F_1 X_{1,3}$
Hydrogen (H_2)	$F_1(X_{1,1} - X_{1,2}) + F_2\left(2X_{2,4} + 3X_{2,5} + X_{2,6}\right)$

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Steam (H_2O)	$F_2(1 - X_{2,4} - X_{2,5} - X_{2,6})$
Ethylene (C_2H_4)	$F_1 X_{1,3} - \frac{1}{2} F_2 X_{2,4}$
Methane (CH_4)	$F_1 X_{1,2} - F_2 X_{2,5}$
Carbon monoxide (CO)	$F_2(X_{2,4} + X_{2,5} - X_{2,6})$
Carbon dioxide (CO_2)	$F_2 X_{2,6}$
Total moles ($\sum N_i$)	$F_2(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})$

Table 2: Table of Molar Concentrations for Reactants and Products

Component	Mole Fraction (Y_i)
Ethylbenzene ($C_6H_5C_2H_5$)	$\dfrac{F_1(1 - X_{1,1} - X_{1,2} - X_{1,3})}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Styrene ($C_6H_5C_2H_3$)	$\dfrac{F_1 X_{1,1}}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Toluene ($C_6H_5CH_3$)	$\dfrac{F_1 X_{1,2}}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Benzene (C_6H_6)	$\dfrac{F_1 X_{1,3}}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Hydrogen (H_2)	$\dfrac{F_1(X_{1,1} - X_{1,2}) + F_2(2 X_{2,4} + 3 X_{2,5} + X_{2,6})}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Steam (H_2O)	$\dfrac{F_2(1 - X_{2,4} - X_{2,5} - X_{2,6})}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Ethylene (C_2H_4)	$\dfrac{F_1 X_{1,3} - \frac{1}{2} F_2 X_{2,4}}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Methane (CH_4)	$\dfrac{F_1 X_{1,2} - F_2 X_{2,5}}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Carbon monoxide (CO)	$\dfrac{F_2(X_{2,4} + X_{2,5} - X_{2,6})}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$
Carbon dioxide (CO_2)	$\dfrac{F_2 X_{2,6}}{F_1(1 + X_{1,1} + X_{1,3}) + F_2(1 + 1.5 X_{2,4} + 2 X_{2,5})}$

Table 3: Table of Mole Fraction for Reactants and Products.

S/N	QUANTITY	NUMERICAL VALUE
1.	Reactor diameter	1.95m
2.	Reactor Length	1.7m
3.	Catalyst bulk density	2146 kg/m^3
4.	Catalyst particle diameter	0.0047m
5.	Bed void fraction	0.445

6.	Catalyst composition	62% Fe_2O_3, 36% K_2CO_3, 2% Cr_2O_3
7.	Inlet pressure	2.4 bar
8.	Inlet temperature	922.59 K
9.	Ethyl benzen in the feed	36.87 kmol/h

Table 4: Operating Conditions for the Industrial reactor (Elnashaie and Elshishini, 1994)

PARAMETER	MODEL PREDICTION	INDUSTRIAL DATA	% DEVIATION
Ethylbenzene Conversion (%)	80.23	82.13	2.37
Yield of Styrene (%)	70.62	71.67	1.54
Yield of Benzene (%)	8.85	9.8	10.73
Yield of Toluene (%)	0.81	0.66	-17.5

Table 5: Comparison of Model Predictions with Industrial Data.

S/No.	Parameters	Temperature (K)				
		850	875	900	925	950
1	Yield of styrene (%)	53.30	61.89	68.37	71.92	72.30
	% Increase		16.11	10.48	5.19	0.53
2	Yield of Benzene (%)	2.34	4.23	7.07	10.96	15.9
	% Increase		80.74	67.17	55.17	45.01
3	Yield of Toluene (%)	0.35	0.53	0.72	0.89	1.02
	% Increase		50.05	35.99	23.97	14.26
4	Conversion of Ethylbenzene (%)	55.99	66.64	76.16	83.78	89.22
	% Increase		19.02	14.28	10.01	6.49

Table 6: Percentage increase in Conversion of Ethylbenzene and Yield of products with Feed Temperature.
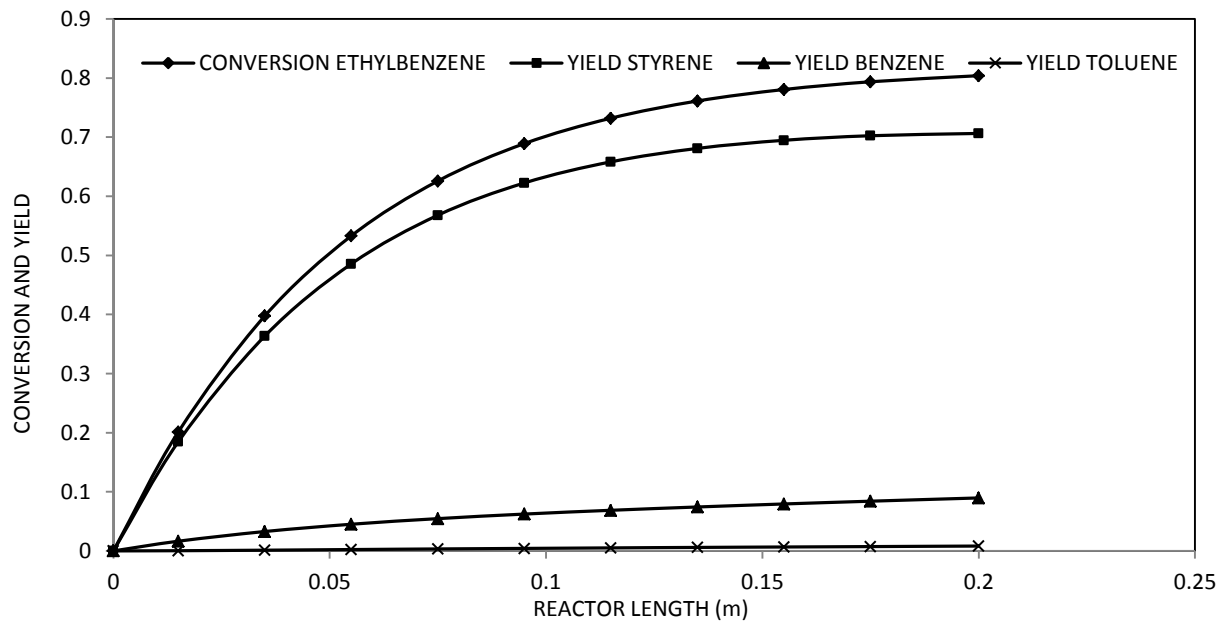
Figure 2: Fractional Conversion of Ethylbenzene and Yield of Styrene, Benzene
and Toluene along Reactor Length.
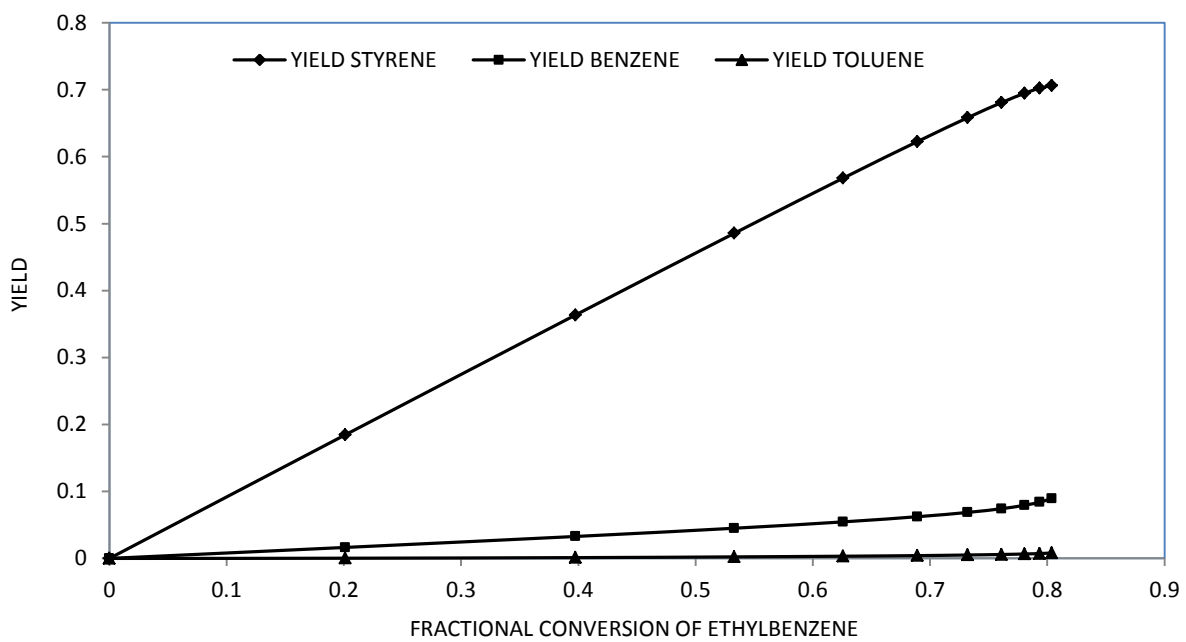
Figure 3: Yield of Styrene, Benzene and Toluene with Fractional Conversion of
Ethylbenzene
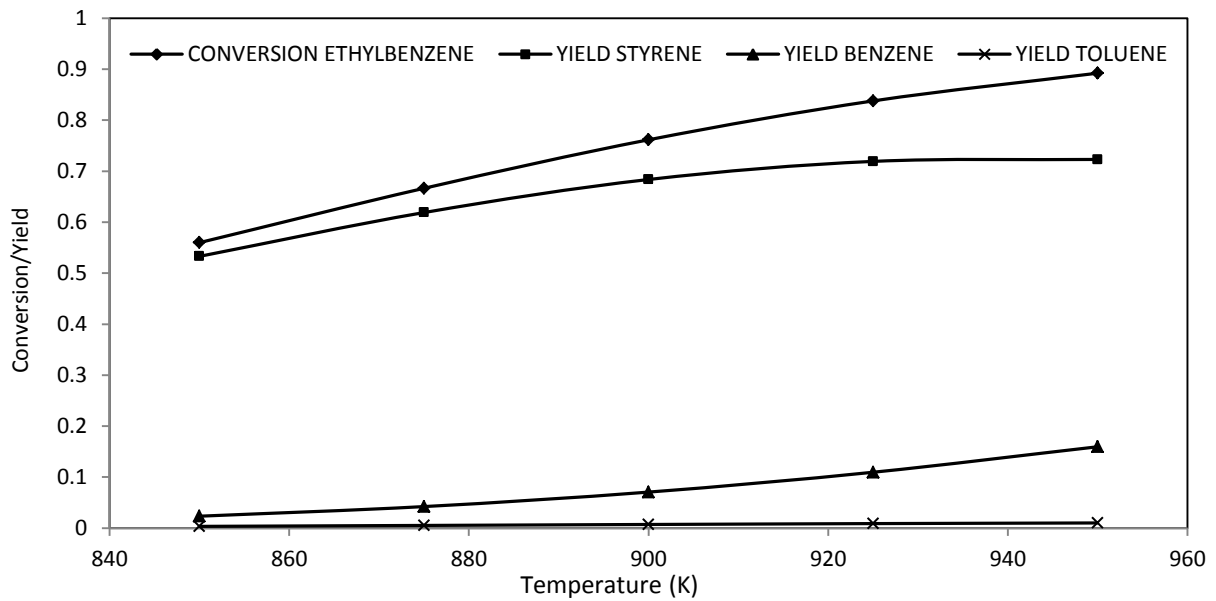
Figure 4: Effect of Feed Temperature on the conversion of Ethylbenzene and yield
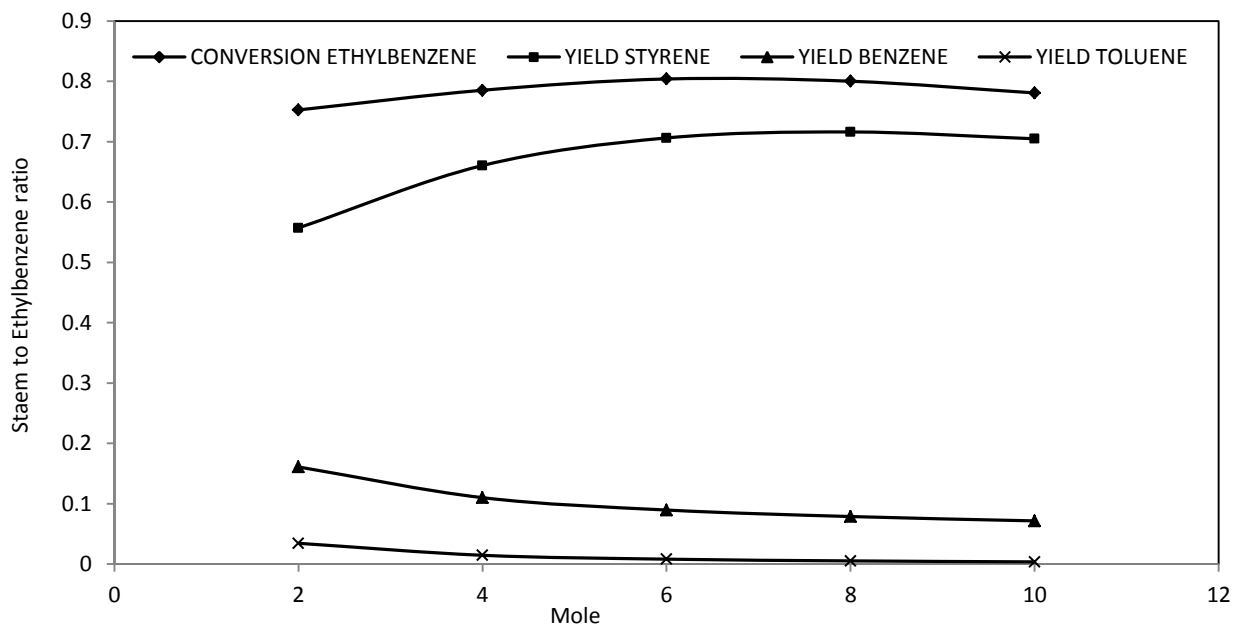of Styrene, Benzene and Toluene

Figure 5: Effect of Steam to Ethylbenzene ratio on Conversion of Ethylbenzene
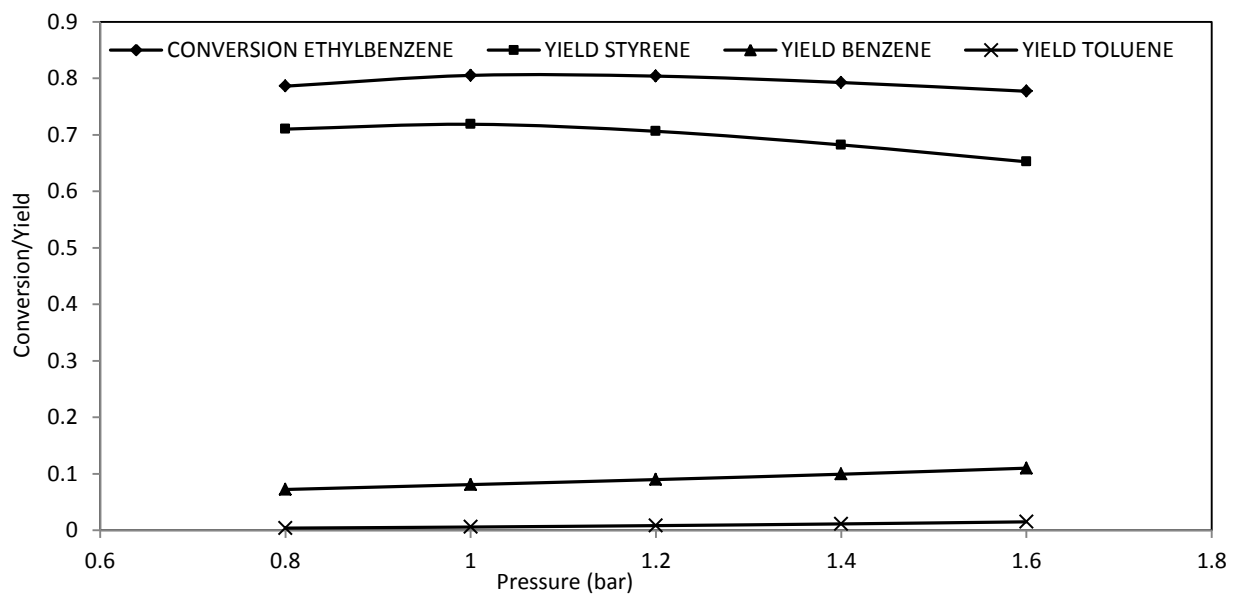and Yield of Styrene, Benzene and Toluene

Figure 6: Effect of Operating Pressure on the conversion of Ethylbenzene and the yield of Styrene, Benzene and toluene