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ARTICLE *in* INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH · NOVEMBER 1993

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# Simulation of the Industrial Fixed Bed Catalytic Reactor for the Dehydrogenation of Ethylbenzene to Styrene: Heterogeneous Dusty Gas Model

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Despite the industrial importance of the catalytic dehydrogenation of ethylbenzene to styrene, no studies are reported in the literature regarding the development of a kinetic model for the intrinsic rate of this multiple reaction system. Most of the kinetic models available in the literature are extracted from industrial reactor data using pseudohomogeneous reactor models. In the present paper a rigorous heterogeneous model is developed for the reactor based on the dusty gas model (Stefan–Maxwell equations) for diffusion and reaction in the catalyst pellets. This model is used to extract intrinsic kinetic constants from industrial reactor data through a simple iteration technique.

## Introduction

The theory of simultaneous diffusion and chemical reaction in porous catalyst pellets has been dealt with in a large number of publications over the past years (Mason et al., 1967; Aris, 1975; Jackson, 1977; Kaza and Jackson, 1979). Several investigators have treated binary nonisothermal systems and systems which exhibit volume change (Abed and Rinker, 1973; Kehoe and Aris, 1973; Wong et al., 1976); multicomponent systems have also received some attention (Haynes, 1984; Kaza and Jackson, 1980; Hesse and Koder, 1973). When pore sizes are small or the pressure is low, diffusion of reactants and products in porous catalysts is described by simple uncoupled equations of the Fickian type, one for each species. Using this type of diffusion equation, a large number of papers have analyzed the problem of a single chemical reaction in a catalyst pellet (Hugo, 1965; Abed and Rinker, 1973; Wong and Denny, 1975). However, for molecular multicomponent diffusion the use of Fickian type diffusion equation is an oversimplification (Abed and Rinker, 1973; Wong et al., 1976; Elnashaie and Abashar, 1993).

In general, for an accurate simulation of a fixed bed catalytic reactors, the effectiveness factors should be computed at each point along the length of the reactor. This requires the formulation and solution of rigorous diffusion–reaction models for the porous pellets based on the more rigorous Stefan–Maxwell equations for multicomponent diffusion rather than the approximate Fick's law. In this investigation a rigorous heterogeneous model simulating the dehydrogenation of ethylbenzene to styrene in a catalytic reactor at high temperatures ranging between 600 and 650 °C is developed and used to extract intrinsic kinetic parameters from industrial data.

This dehydrogenation reaction is a moderately endothermic reaction, so the reactor must be heated to supply the heat required for the reaction to proceed. Superheated

steam is injected to the reactor at 750 °C to provide the necessary heat for the reaction.

## Development of the Model Equations

In the development of the diffusion–reaction model equations for the catalyst pellets the following assumptions are considered:

1. The porous structure of the catalyst pellet is assumed to be homogeneous.
2. Mass transfer through the catalyst pellet occurs by diffusion, and only ordinary molecular and Knudsen diffusion are considered (Haynes, 1984).
3. The gases diffusing through the pellet obey the ideal gas law (Haynes, 1984).
4. Viscous flow is negligible and conditions are isobaric (Burghardt and Arets, 1988).
5. The concentration profiles are symmetrical around the centre of the pellet (Kaza and Jackson, 1979; Kaza et al., 1980).
6. Mass transfer is described by the dusty gas model equation (Mason and Malinauskas, 1983).
7. The pellets are isothermal.
8. External mass- and heat-transfer resistances are negligible.
9. The system is at steady state.

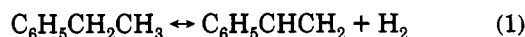
## Rate Expressions

An extensive literature search for intrinsic rates was made; only apparent rates computed from specific industrial reactors, using pseudohomogeneous models, were found (Wenner and Dybdal, 1948; Davidson and Shah, 1965; Sheel and Crowe, 1969; Clough and Ramirez, 1976; Petrov et al., 1984; Sheppard et al., 1986; Bhat, 1988). These industrial rates actually include diffusional limitations and are suitable for the specific reactors used with their specific catalyst particle sizes. Therefore, a rigorous heterogeneous model is developed and used to extract intrinsic rate constants suitable for such heterogeneous models.

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Most literature suggested six independent reactions: the main reaction, i.e., ethylbenzene to styrene, and five side reactions (Sheel and Crowe, 1969; Clough and Ramirez, 1976; Sheppard et al., 1986). These reactions and their reaction rate equations are given as follows (Sheel and Crowe (1969) and the order of the fourth reaction corrected by Crowe (1989)):

main reaction

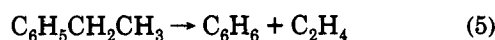


$$r_1 = k_1(P_{\text{EB}} - P_{\text{ST}}P_{\text{H}_2}/K_{\text{EB}}) \quad (2)$$

$$K_{\text{EB}} = \exp(-\Delta F^\circ/RT) \quad (3)$$

$$\Delta F^\circ = a + bT + cT^2 \quad (4)$$

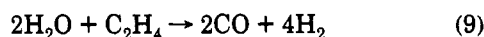
side reactions



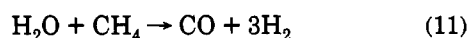
$$r_2 = k_2P_{\text{EB}} \quad (6)$$



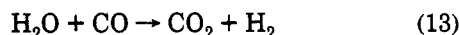
$$r_3 = k_3P_{\text{EB}}P_{\text{H}_2} \quad (8)$$



$$r_4 = k_4P_{\text{H}_2\text{O}}P_{\text{ETH}}^{0.5} \quad (10)$$



$$r_5 = k_5P_{\text{H}_2\text{O}}P_{\text{MET}} \quad (12)$$



$$r_6 = k_6(P_{\text{T}}/T^3)P_{\text{H}_2\text{O}}P_{\text{CO}} \quad (14)$$

### Mass Balance for the Catalyst Pellet

The catalyst packing the reactor is composed of iron oxide ( $\text{Fe}_2\text{O}_3$ ) promoted with potassium carbonate ( $\text{K}_2\text{CO}_3$ ) and chromium oxide ( $\text{Cr}_2\text{O}_3$ ). The catalyst particles are extrudates cylindrical in shape. Since at steady state the problem of simultaneous diffusion and reaction is independent of particle shape (Aris, 1957), an equivalent slab geometry was used for the catalyst pellet, with a characteristic length giving a surface to volume ratio of the slab equal to that of the original shape.

The mass balance equations for component  $i$  are expressed as follows:

$$dN_i/dz = \rho_c R_i \quad (15)$$

Equation 15 is the generalized equation for the flux of component  $i$  diffusing through the catalyst pellet, with the boundary condition at the center:

$$N_i = 0 \quad \text{at} \quad z = 0 \quad (16)$$

where  $R_i$  is the net rate of formation of component  $i$ .

The mass balance equations and the dusty gas model equations as described by Mason and Malinauskas (1983) provide the necessary solution for predicting diffusion through the catalyst pellet. The dusty gas model equations are given by

$$-dC_i/dz = N_i/D_{K_{e,i}} + \sum_{j=1}^n (y_i N_j - y_j N_i)/D_{e,i,j} \quad (17)$$

with the boundary condition at the surface

$$z = z_p \quad C_i(z_p) = C_{i_s} \quad (18)$$

Use of the dusty gas model equation requires finding the fluxes by solving the material balance equations simultaneously with the dusty gas model equations.

While problems of multicomponent diffusion and reaction in porous catalyst generally give rise to pressure gradients within the catalyst pellet, it is possible to neglect the resulting viscous flow contributions to the component flux equations. It was also concluded by many investigators that for realistic parameter values viscous flow does not contribute appreciably to pressure variation and effectiveness factor calculations in porous catalyst pellets (Evans et al., 1961, 1962; Mason et al., 1967; Kehoe and Aris, 1973; Haynes, 1978; Burghardt and Aerts, 1988).

### Algebraic Manipulation of the Pellet Mass Balance Equations

In this investigation 10 flux equations and 10 dusty gas model equations are to be solved. From the number of the stoichiometric equations and the number of the reactants and products, it is clear that the values of the fluxes of four components can be expressed by means of the values of the remaining six components. Simple algebraic manipulation gives the following relations, which are deduced in a straightforward manner from the algebraic manipulation of eq 15 for the different components:

$$N_{\text{EB}} = -N_{\text{ST}} - N_{\text{BZ}} - N_{\text{TOL}} \quad (19)$$

$$N_{\text{H}_2\text{O}} = -N_{\text{CO}} - 2N_{\text{CO}_2} \quad (20)$$

$$N_{\text{MET}} = 2N_{\text{BZ}} + N_{\text{TOL}} - 2N_{\text{ETH}} - N_{\text{CO}} - N_{\text{CO}_2} \quad (21)$$

$$N_{\text{H}_2} = 4N_{\text{CO}_2} + 3N_{\text{CO}} + N_{\text{ETH}} + N_{\text{ST}} - 2N_{\text{BZ}} - N_{\text{TOL}} \quad (22)$$

Therefore only 6 flux equations and 10 dusty gas model equations need to be solved simultaneously to compute the concentration profiles. The performance of the pellet is expressed in terms of the effectiveness factor of each reaction and also the effectiveness factors for the components involved. The components effectiveness factors are computed using the following equation:

$$\eta_j = \frac{1}{r_p R_{j_s}} \int_0^{r_p} R_j dz \quad (23)$$

The global orthogonal collocation technique is used for solving the equations described above.

### The Global Orthogonal Collocation Technique

Villadsen and Stewart (1967) and Villadsen and Michelsen (1978) have provided several methods for the use of the global orthogonal collocation technique to solve two point boundary value differential equations and for evaluating integrals. Goyal et al. (1987) have provided a method of solution of the two point value problem for the nonlinear differential equation using the method of orthogonal collocation, which is a modification to the method of Villadsen and Michelson (1978). The global orthogonal collocation technique described by Villadsen and Michelson (1978) is used in this investigation. The possible improvements in the speed and accuracy of the

solution using the modification of Goyal et al. (1987) are being investigated for another radial flow industrial reactor.

### The Model Equations of the Reactor

Six mass balance differential equations for the six reactions in the reactor were formulated, as well as an energy balance and a pressure drop equation.

The mass balance equations are given by

$$dX_i/dL = \eta_i \rho_B A_B r_i / F_{EB_F} \quad (24)$$

where  $i$  refers to the three reactions of the ethylbenzene (Sheel and Crowe, 1969) and  $X_i$  is the fractional conversion of ethylbenzene in each of the three reactions. Also,

$$dX_j/dL = \eta_j \rho_B A_B r_j / F_{H_2O_F} \quad (25)$$

where  $j$  refers to the reactions of the diluent steam (Sheel and Crowe, 1969) and  $X_j$  is the fractional conversion of the steam in each of the remaining three reactions. The molar flow rates of the 10 components can be computed in terms of these 6 conversions and the feed molar flow rates, using simple mass balance equations.

The Ergun equation (Bird et al., 1960) is used to compute the pressure profiles along the length of the catalyst bed.

$$dP/dL = -1 \times 10^{-5} \frac{(1 - \epsilon_B) G_0}{D_p \epsilon_B^3 \rho_G g_c} \left[ \frac{150(1 - \epsilon_B) \mu_G}{D_p} + 1.75 G_0 \right] \quad (26)$$

The energy balance differential equation is given by

$$dT/dL = \sum_{j=1}^6 (-\Delta H_j) \eta_j r_j \rho_B A_B / \sum_{i=1}^{10} F_i C_{p,i} \quad (27)$$

Solution of the reactor model differential equations (24–27) simulates the molar flow rates, pressure drop, and energy balance of the reactor, while the solution of the catalyst pellet equations (15, 17, and 23) provides the effectiveness factors  $\eta_i$ 's for eqs 24, 25, and 27.

### Solution of the Model Equations

The main objective of the catalyst pellet model is to calculate the effectiveness factors for the six reactions taking place inside the pellet. The effectiveness factors are defined as the ratios of the actual rates taking place in the catalyst pellet to the rates taking place under bulk conditions.

The rate equations obtained from the literature for the calculation of the rates in the pellet and in the bulk are functions of the partial pressures of the components. The partial pressures can be calculated from the mole fractions and the total pressure. The mole fractions of the components in the bulk and at the collocation points in the pellet are thus required, in order to compute the effectiveness factors.

This requires the simultaneous solution of the set of differential equations (15 and 17) together with the flux relations (19–22). The subroutine ZSPOW (IMSL Math/PC-Library) (More et al., 1980) for solving nonlinear algebraic equations was used to solve the algebraic equations resulting from applying the global orthogonal collocation technique to the differential equations of the pellet. The mole fractions obtained were then used to calculate the rates of the reactions. Rates inside the pellet were then divided by rates at the surface to give the effectiveness factors of the reactions. The effectiveness

**Table I. Industrial Reactor Specification, Catalyst Properties, and Feed Conditions (Sheel and Crowe, 1969; Crowe, 1992)**

item	symbol	value	dimension
reactor diameter	$D_R$	1.95	m
catalyst bed depth	$L_B$	1.70	m
catalyst density	$\rho_C$	2146.27	kgcat/m <sup>3</sup>
catalyst diameter	$D_p$	$4.7 \times 10^{-3}$	m
catalyst pore radius	$r_p$	2400	Å
catalyst porosity	$\epsilon$	0.35	
catalyst tortuosity	$\tau$	4.0	
inlet pressure	$P_T$	2.4	bar
inlet temperature	$T^a$	922.59	K
molar feed rate			
ethylbenzene	EB	36.87	kmol of EB/h
styrene	ST	0.67	kmol of ST/h
benzene	BZ	0.11	kmol of BZ/h
toluene	TOL	0.88	kmol of TOL/h
steam	H <sub>2</sub> O	453.10	kmol of H <sub>2</sub> O/h
total molar feed rate	TMF	491.87	kmol/h
total mass flow rate	TMFR	12 238.79	kg/h

<sup>a</sup> Corrected by Crowe (1992).

**Table II. Frequency Factors and Activation Energies of the Apparent Rates of Reactions (Sheel and Crowe, 1969; Crowe, 1989) and the Frequency Factors of the Intrinsic Rates<sup>a</sup>**

reaction	$k_{0i}$ (apparent)	$k_{0i}$ (intrinsic)	$E_i \times 10^{-5}$ (apparent and intrinsic)
1	$3.26 \times 10^3$ <sup>b</sup>	$8.32 \times 10^3$	0.909
2	$2.00 \times 10^9$	$4.29 \times 10^9$	2.080
3	$4.72 \times 10^3$	$6.13 \times 10^3$	0.915
4	$3.26 \times 10^3$	$3.95 \times 10^3$	1.040
5	$1.86 \times 10^2$	$1.42 \times 10^2$	0.657
6	$5.80 \times 10^{12}$	$5.82 \times 10^{12}$	0.736

<sup>a</sup>  $k_i = k_{0i} e^{-E_i/RT}$ , where  $k_{0i}$  is the preexponential factor (units, see Nomenclature) and  $E_i$  is the activation energy (kJ/kmol). <sup>b</sup> Corrected by Crowe (1989).

factors are used to evaluate the actual rates of the reactions in the overall reactor model (eqs 24–27).

The reactor model differential equations (24–27) were integrated. Subroutine DGEAR (ISML Math/PC-Library) (Hindmarsh, 1974) was used for solving these differential equations. DGEAR uses a Runge–Kutta–Verner fifth- and sixth-order method with automatic step size to ensure accuracy.

### Extracting Intrinsic Rate Constants

Pseudohomogeneous models do not account explicitly for the catalyst packing the reactor; however, heterogeneous models account for the catalyst by considering the diffusion of reactants and products through the pores of the catalyst pellet.

In this investigation industrial reactor data from the Polymer Corporation, Sarnia, Ontario, Canada were used (Sheel and Crowe, 1969). The specification of the reactor and the feed conditions to the reactor are given in Table I. These data were obtained from Sheel and Crowe (1969), as were the kinetic data in columns 2 and 4 of Table II. Two corrections in the published values, noted on these tables, were provided by Crowe (1989, 1992). These kinetic constants were effective, not intrinsic, rate constants. These data were used as starting values in an iteration scheme to obtain intrinsic kinetics suitable for heterogeneous models.

The heterogeneous model is used to extract the intrinsic kinetic constants from the industrial data. The rate constants of the pseudohomogeneous model (nonintrinsic rates), given in Table II, were first used as starting values in the heterogeneous model. The results obtained are

**Table III. Results of the Heterogeneous Model with Intrinsic Rate Constants (Last Iteration) As Compared with Those of the Industrial Reactor (Sheel and Crowe, 1969)**

item	industrial reactor		heterogeneous model	
	MFR <sup>a</sup>	conversion, %	MFR	conversion, %
EB	19.45	47.25	19.29	47.45
H <sub>2</sub> O	<sup>b</sup>	<sup>b</sup>	447.32	1.26

item	industrial reactor		heterogeneous model	
	MFR	yield, %	MFR	yield, %
ST	15.57	40.41	15.53	40.17
BZ	1.50	3.77	1.64	4.12
TOL	2.03	3.12	2.07	3.17

$P_E$ , bar	2.32	2.382
$T_E$ , K	850.0	851.10

<sup>a</sup> MFR, molar flow rate (kmol/h);  $P_E$ , outlet pressure (bar);  $T_E$ , outlet temperature (K). <sup>b</sup> Not measured in plant operation.

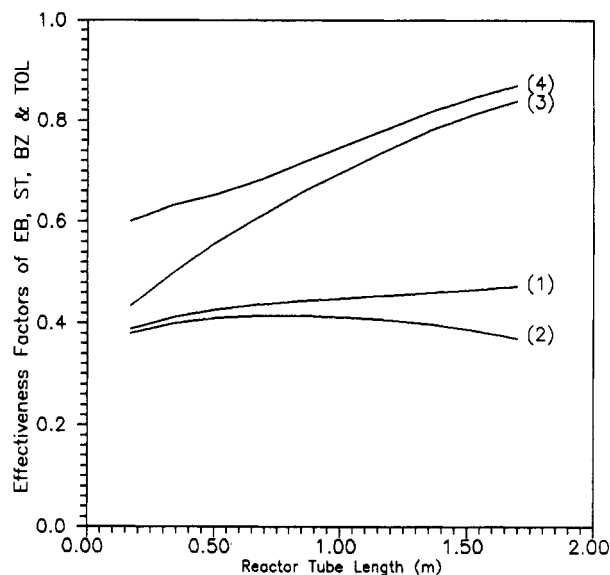
**Table IV. Values of the Effectiveness Factors and of the Apparent and Intrinsic Rates of Consumptions of Components by Individual Reactions and Overall Taken at the End of the Reactor; Last Iteration in the Search of Intrinsic Kinetics**

item	effectiveness factor	apparent rate $\times 10^4$	intrinsic rate $\times 10^4$
reaction 1	0.37	2.89	7.81
reaction 2	0.84	0.55	0.65
reaction 3	0.87	1.23	1.41
reaction 4	0.95	1.25	1.32
reaction 5	1.17	0.81	0.70
reaction 6	1.06	2.07	1.95
ethylbenzene	0.47	4.67	9.88
styrene	0.37	-2.89	-7.81
benzene	0.84	-0.55	-0.65
toluene	0.87	-1.23	-1.41
methane	0.58	-0.42	-0.72
ethylene	1.01	0.08	0.08
hydrogen	0.29	-8.66	-30.08
steam	0.20	4.13	20.96
carbon monoxide	$4.9 \times 10^{-4}$	$8.3 \times 10^{-3}$	17.01
carbon dioxide	1.06	-2.07	-1.95

expected to give low conversions compared to those of the industrial reactor.

The conversions of the six reactions obtained from the industrial reactor were divided by the corresponding ones obtained from the heterogeneous model. Multiplying factors were obtained for the six reactions. The rate equations were then multiplied by the corresponding factors and the program was rerun. The results obtained were again compared with the industrial ones, and new multiplying factors were obtained. The above procedure was iterated until the results obtained were very close to the results of the industrial reactor. The intrinsic frequency factors obtained from this procedure are given in the third column of Table II. The results of using these intrinsic rates in the heterogeneous model are given in Table III, together with the results of the industrial reactor. It is clear that the model and the industrial results match very well. Table IV shows values of the corresponding effectiveness factors, intrinsic rates, and apparent rates of reactions and components at the exit of the reactor.

The effectiveness factors of the components are calculated on the basis of their rates of consumption at the exit of the reactor. For the components which are formed in one single reaction and are not involved in other reactions (i.e., styrene, benzene, toluene, and CO<sub>2</sub>), their effectiveness factors are actually the effectiveness factors of their reactions (i.e., reactions 1, 2, 3, and 6). For most of the reactions (except reactions 5 and 6 with effectiveness

**Figure 1. Effectiveness factor profiles for the three main reactions and components. (1)  $\eta_1 = \eta_{ST}$ ; (2)  $\eta_2 = \eta_{BZ}$ ; (3)  $\eta_2 = \eta_{TOL}$ ; (4)  $\eta_{EB}$ .**

factors slightly greater than unity) the intrinsic rates of the reactions are higher than the apparent rates. Results of Table IV show that the effectiveness factors for the six main reactions are not very far from unity. This justifies the use of the above procedure which is based upon correcting the frequency factors for diffusional limitations, while keeping the activation energies unaltered (Satterfield, 1980).

Figure 1 shows the effectiveness factor profiles for the main reactions and components. The effectiveness factor for the first reaction, which is reversible, shows a weak nonmonotonic behavior along the length of the catalyst bed. The occurrence of such behavior for reversible reactions has been observed earlier by Elnashaie et al. (1988) in connection with the simulation of industrial ammonia converter and was proven rigorously by Elnashaie et al. (1989). The effectiveness factor for this reaction is itself the effectiveness factor for the component styrene production. The effectiveness factor profiles for reactions 2 and 3 (the same for the components benzene and toluene) increase sharply and continuously along the length of the reactor as the rates of these irreversible reactions decrease. The effectiveness factor for ethylbenzene increases slowly along the length of the reactor. Ethylbenzene is consumed in reactions 1, 2, and 3; however, the effectiveness factor is not an additive property as clearly shown in Figure 1 and Table IV.

## Conclusions

A rigorous heterogeneous model was developed and used to separate the effectiveness factors from the apparent rate equations and to extract intrinsic kinetics. An efficient algorithm based on reliable numerical techniques was used. This technique is helpful when no intrinsic kinetics data are available, but it requires availability of sufficient industrial data to be used in the numerical calculations.

Although the use of the effectiveness factors in catalytic modeling taxes the numerical algorithm with extra computation, it is still a very useful tool which represents the complex interaction between diffusion and reaction processes in terms of one number. This leads to better understanding of the effect of the diffusional resistances on reactor performance.

## Nomenclature

$C_i$  = molar concentration of component  $i$ , kmol/m<sup>3</sup>  
 $C_{i_s}$  = molar concentration of component  $i$  at the catalyst surface, kmol/m<sup>3</sup>  
 $C_{p,i}$  = specific heat capacity of component  $i$ , kJ/(kmol·K)  
 $D_{eij}$  = effective molecular diffusivity of component  $i$  binary with  $j$ , m<sup>2</sup>/h  
 $D_{K,i}$  = effective Knudsen diffusivity for component  $i$ , m<sup>2</sup>/h  
 $D_p$  = catalyst particle diameter, m  
 $F_{i_F}$  = molar feed rate of component  $i$ , kmol/h  
 $G_0$  = mass velocity of the gas mixture, kg/(m<sup>2</sup>·h)  
 $g_c$  = proportionality factor, kg·m/(kgf·h<sup>2</sup>)  
 $\Delta H_j$  = heat of reaction  $j$ , kJ/kmol  
 $k_i$  = reaction  $i$  rate constant, kmol·K <sup>$m$</sup> /(kg·h·bar <sup>$n$</sup> ) (for  $k_1$  and  $k_2$ ,  $m = 0$ ,  $n = 1$ ; for  $k_3$  and  $k_5$ ,  $m = 0$ ,  $n = 2$ ; for  $k_4$ ,  $m = 0$ ,  $n = 1.5$ ; for  $k_6$ ,  $m = 3$ ,  $n = 3$ )  
 $k_{oi}$  = reaction  $i$  preexponential factor, kmol·K <sup>$m$</sup> /(kg·h·bar <sup>$n$</sup> ) (for  $k_1$  and  $k_2$ ,  $m = 0$ ,  $n = 1$ ; for  $k_3$  and  $k_5$ ,  $m = 0$ ,  $n = 2$ ; for  $k_4$ ,  $m = 0$ ,  $n = 1.5$ ; for  $k_6$ ,  $m = 3$ ,  $n = 3$ )  
 $L_B$  = catalyst bed length, m  
 $N_i$  = molar flux of component  $i$ , kmol/(m<sup>2</sup>·h)  
 $P_T$  = total pressure of the reactor, bar  
 $R_i$  = intrinsic rate of component  $i$ , kmol/(kg·h)  
 $r_i$  = intrinsic rate of reaction  $i$ , kmol/(kg·h)  
 $R_{i_s}$  = rate of formation of component  $i$  at the catalyst surface, kmol/(kg·h)  
 $r_p$  = half-thickness of the slab, m  
 $T$  = temperature of the reactor, K  
 $X_i$  = conversion of component  $i$  (EB or H<sub>2</sub>O), dimensionless  
 $y_i$  = mole fraction of component  $i$ , dimensionless  
 $z$  = dimensionless thickness of the catalyst pellet

## Greek Letters

$\epsilon_B$  = bed voidage fraction, dimensionless  
 $\eta_i$  = effectiveness factor of reaction or component  $i$ , dimensionless  
 $\mu_G$  = viscosity of the gas mixture, kg/(m·h)  
 $\rho_B$  = bulk density of the catalyst bed, kg/m<sup>3</sup>  
 $\rho_C$  = density of the catalyst particle, kg/m<sup>3</sup>

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Received for review January 5, 1993

Accepted May 18, 1993