An internal-recycle catalytic reactor is described which can be operated under perfectly mixed conditions. The reactor is suitable for evaluating intraparticle mass transfer effects on reaction rate and yield in the consecutive hydrogenation of mesityl oxide over a copper-chromium oxide catalyst. The reactor has the advantages that accurate reaction rates are directly obtained, and that mathematical formulation is simpler than with an integral reactor. Effective diffusivities are determined from conversion data and compared with those calculated by a parallel-pore model and a random-pore model. The effective diffusivities predicted by both models closely agree with each other, and these values are close to those experimentally determined. The tortuosity factors determined from the parallel-pore model range from 1.4 to 3.4. These values fall within the range of previously published values. The calculated conversion and yield show relatively good agreement with the experimental results.

**Introduction**

The overall reaction rate and the selectivity in a catalytic reaction within a porous solid are markedly influenced by the intraparticle mass and heat transfer, and a large number of studies have been published on this problem. Many of these, however, were concerned with rather simplified reaction kinetics. Recently much attention has been paid to the effect of intraparticle diffusion on catalytic reactions in which the kinetics is represented by a rate equation of the Langmuir-Hinshelwood type (L-H type). However, very few papers dealt with the selectivity problems of multiple-reaction systems with the L-H type rate expression.

Integral tubular reactors are often employed for kinetic studies. However, even if isothermal conditions prevail in an integral reactor, the concentration distributions along an axial direction as well as within the catalyst pellet have to be considered. This fact leads to a complicated mathematical formulation. On the other hand, by the use of a catalytic reactor under perfectly mixed conditions the amount of computation is greatly reduced, because the concentration in the bulk fluid phase is uniform throughout the reactor.

Furthermore, this type of reactor has the advantages that point reaction rates of a multiple-reaction system are directly evaluated from large differences in concentration.

**EVALUATION OF MASS TRANSFER EFFECTS ON CONSECUTIVE CATALYTIC REACTION USING AN INTERNAL-RECYCLE CATALYTIC REACTOR**

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tration between the reactor inlet and outlet, and that interphase transport gradients can be minimized by the high circulation rate of gas. Several reactors of this type\textsuperscript{1,2,5,13,20} have recently been developed, and these have proved successful for kinetics studies. However, the reactions tested were limited to rather simple types. These backmixed catalytic reactors would be suitable especially for evaluating effects of intraparticle mass and heat transfer in a multiple-reaction system with a complicated rate expression such as the L-H type.

The purpose of this work is to present an internal-recycle catalytic reactor which behaves as a backmixed reactor, and to reveal both theoretically and experimentally the intraparticle mass transfer effects on a multiple catalytic reaction. The reaction investigated in this paper is a consecutive hydrogenation of mesityl oxide with the L-H type rate expression. Furthermore, the effective diffusivities determined from the data of effectiveness factors are compared with those calculated by both the parallel-pore model and the random-pore model.

1. Experimental

1.1 An internal-recycle reactor

Carberry et al.\textsuperscript{5,20} developed a continuous stirred-tank catalytic reactor in which the catalyst particles were confined in wire gauze baskets attached to a rotating shaft. In this type of reactor, the measurement of catalyst temperature seems to be difficult. When finely divided particles are used, the reacting gas may not flow through the catalysts in the basket but flows mainly outward radially.\textsuperscript{2} To avoid these difficulties, an internal-recycle reactor, shown in Fig. 1, was developed. Recently, Brown and Bennett\textsuperscript{2}, and Livbjerg and Villadsen\textsuperscript{13} also proposed the same type of reactor.

The reactor used here is a stainless steel cylindrical vessel fitted with a draft tube and jacketed with diesel-engine oil. The outer tube is 10.8 cm I.D., 40 cm long; the inner tube is 5.5 cm I.D. The catalyst particles are enclosed in an annular basket made of stainless steel screen. The feed gas is introduced through a ring sparger located at the top of the vessel, and recycled by five six-bladed impellers so that the gas flows down through the catalyst basket and up the inner portion of the draft tube. The temperatures of the catalyst bed at three points and of gas phase were measured. When catalyst pellets were used, the junction points of the thermocouples were embedded in the pellets.\textsuperscript{14} The maximum temperature difference in the bed was within 3°C.

The mixing characteristics of gas in the reactor were determined by both step- and pulse-response method, and it was found that the reactor is always perfectly mixed at impeller speeds above 2000 rpm.

1.2 Hydrogenation of mesityl oxide

The reaction studied is the consecutive hydrogenation of mesityl oxide (designated MSO or \textit{A}) to methyl isobutyl ketone (MIBK or \textit{B}) and to methyl isobutyl carbinol (MIBC or \textit{C}). A commercial copper-chromium oxide catalyst (Nikki, N 202) was used. The reaction scheme and the rates of the two steps have already been studied using a tubular reactor, and are represented as follows\textsuperscript{8}:

\[
\begin{align*}
\text{MSO (A)} & \rightarrow \text{MIBK (B)} \rightarrow \text{MIBC (C)} \\
 r_1 &= \frac{k_1 K_H K_A P_H P_A}{(1 + K_H P_H + K_A P_A + K_B P_B + K_C P_C)^3} \\
 r_2 &= \frac{k_2 K_H K_B (P_H p_B - p_C) / K_{eq}}{(1 + K_H P_H + K_A P_A + K_B P_B + K_C P_C)^3}
\end{align*}
\]

where the \textit{p}'s represent partial pressures. The rate parameters, \textit{k} and \textit{K}, were correlated in terms of Arrhenius equations\textsuperscript{8}.

The interphase heat and mass transfer resistances were found to be negligible above 2000 rpm. To be on the safe side, all runs were carried out at 3000 rpm. The experiments were performed at temperatures of 180, 200 and 220°C. The catalyst was in three sizes, 0.3 mm\textsuperscript{0} (crushed pellets), 3.1 mm\textsuperscript{0} x 3.1 mm (cylindrical pellets) and 5.1 mm\textsuperscript{0} x 4.8 mm. The ratio of the molar flow rate of hydrogen to that of MSO, \textit{m}, was maintained at about 5 for all runs.

1.3 Pore structure of catalyst

Macropore volume distribution of the catalyst pellet (3.1 mm\textsuperscript{0} x 3.1 mm) was obtained by mercury penetration measurement using an Aminco 60,000 psi porosimeter. The nitrogen adsorption isotherm at 77.5°C was measured by an Orr Surface Area-Pore Volume Analyzer, model 2100A, and the micropore volume distribution was determined from the adsorption isotherm by the method of Dollimore and Heal\textsuperscript{7}. In their paper, the amount of surface area of pores greater than 100Å in radius was assumed to be negligibly small compared with that of pores less than 100Å. However, as shown in Fig. 2, a great deal of pore volume is in the range of 100 to 1000Å pore radius. Therefore, the
amount of surface area ($r > 100 \text{Å}$) was calculated from the mercury penetration data using Wheeler's relationship, $\Delta S = 2.2 V_r / r$, to give 12.2 $\text{m}^2/\text{g}$. This fact was taken into account for computing the pore size distribution. The cumulative pore volume distribution curves obtained by both methods were joined at the pore radius of 100 Å. Figure 2 shows a complete pore volume distribution curve obtained by graphical differentiation of the cumulative distribution. This demonstrates that the catalyst has a somewhat broad monodisperse pore size distribution ranging over the transitional diffusion region between the Knudsen diffusion and the bulk diffusion.

The physical properties of the catalyst are summarized in Table 1. The apparent density of the cylindrical pellet, $\rho_p$, was determined from mercury displacement measurements. The true density of the catalyst, $\rho_t$, was measured by an Orr Helium-Air Pycnometer, model 1302. The porosity, $\varepsilon$, was calculated by $\rho_p$ and $\rho_t$. From the pore size distribution, both the cumulative pore volume, $V_g$, and surface area, $S_p$, were evaluated. The BET surface area, $S_{\text{BET}}$, was easily evaluated from the nitrogen adsorption isotherm in the range of relative pressure from 0.05 to 0.35.

### Table 1 Physical properties of catalyst

<table>
<thead>
<tr>
<th>$\rho_p$ [g/cm$^3$]</th>
<th>$\rho_t$ [g/cm$^3$]</th>
<th>$\varepsilon$</th>
<th>$V_g$ [cm$^3$/g]</th>
<th>$S_p$ [m$^2$/g]</th>
<th>$S_{\text{BET}}$ [m$^2$/g]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.15</td>
<td>3.61</td>
<td>0.404</td>
<td>0.187</td>
<td>35.6</td>
<td>35.8</td>
</tr>
</tbody>
</table>

2. Computation of Effectiveness Factor and Yield

The steady-state mass balances for components $A$ and $B$ in the consecutive reaction (1) in a spherical shell give

$$\frac{D_{eA}}{R_k T} \left( \frac{d^2 p_A}{dR^2} + \frac{2}{R} \frac{dp_A}{dR} \right) - \rho_p g_A = 0 \quad (4)$$

$$\frac{D_{eB}}{R_k T} \left( \frac{d^2 p_B}{dR^2} + \frac{2}{R} \frac{dp_B}{dR} \right) - \rho_p (g_1 + r_2) = 0 \quad (5)$$

with boundary conditions

$$p_A = p_{Ar}, \quad p_B = p_{Br}, \quad \text{at} \ R = R_g$$

$$dp_A/dR = dp_B/dR = 0, \quad \text{at} \ R = 0 \quad (6)$$

In deriving these equations, the following assumptions were made: (1) the particle is isothermal, (2) effective diffusivities are constant, and (3) the ideal gas law is applicable.

The maximum temperature rise within the particle may be expressed for the consecutive reaction as

$$\Delta T_{\text{max}} = \frac{1}{k_{\text{es}}} \left[ D_{eA} C_{Ae} (-\Delta H_1 - \Delta H_2) + D_{eB} C_{Be} (-\Delta H_2) \right]$$

(8)

where $k_{\text{es}}$ is effective thermal conductivity of the particle, $\Delta H_1$ and $\Delta H_2$ are heat of reaction of the first and the second step of the reaction, respectively. Assigning the estimated value to each parameter in Eq. (8), the $\Delta T_{\text{max}}$ value was found to be less than 5.5 °C. Thus the assumption (1) may be valid. The effective diffusivity, $D_e$, is generally a function of gas composition in the pore. However, as this effect is not usually strong\(^{(19)}\), the assumption (2) does not lead to serious error.

The reaction rate equations are substituted into Eqs. (4) and (5), and Eqs. (4)–(7) may be rewritten in the dimensionless form

$$\frac{d^2 u_A}{dx^2} + 2 \frac{du_A}{x} - \frac{C_1 u_A u_B}{q^3} = F$$

$$\frac{d^2 u_B}{dx^2} + 2 \frac{du_B}{x} + \frac{C_1 u_A u_B}{q^3} = G$$

(9)

$$u_A = u_{A*}, \quad u_B = u_{B*}, \quad \text{at} \ x = 1$$

(10)

$$du_A/dx = du_B/dx = 0, \quad \text{at} \ x = 0$$

(11)

where

$$x = R/R_0, \quad u_A = p_A / P_t, \quad u_B = p_B / P_t, \quad u_C = p_C / P_t$$

$$q = 1 + \frac{K_A}{1 + K_B}$$

$$K_A = K_A \rho_A, \quad K_B = K_B \rho_B, \quad K_p = K_P \rho_P$$

$$\phi = \frac{R_g}{3} \sqrt{K_A \rho_A R_g T / D_{Ae} P_t^2}$$

$$C_1 = 9 \phi K_A K_B$$

$\phi$ defined in the above equation represents a modified Thiele modulus.

Since the rate terms in Eqs. (9) and (10) contain $u_C$ and $u_B$, these quantities must be represented by $u_A$ and $u_B$. Similar differential equations and boundary conditions may be obtained for components $C$ and $H$. These four differential equations are arranged to eliminate the reaction rate terms, and the two resulting differential equations are integrated twice with the boundary conditions to yield the required relationships,

$$u_C = u_{C*} + r_{A*C} (u_{A*} - u_A) + r_{B*C} (u_{B*} - u_B)$$

(13)

$$u_H = u_{H*} - 2 r_{A*H} (u_{A*} - u_A) - r_{B*H} (u_{B*} - u_B)$$

(14)

where $r_{A*C}$, $r_{B*C}$, $r_{A*H}$ and $r_{B*H}$ represent the ratio of two effective diffusivities, for example, $r_{A*C} = D_{Ae} / D_{Ce}$. These values are approximately calculated by assuming that the effective diffusivity is inversely proportional to the square root of the molecular weight\(^{(19)}\). $u_{C*}$ and $u_{H*}$ denote the dimensionless partial pressure in the bulk, and these are represented as

$$u_{C*} = \frac{1 - (m + 1) u_A - m u_B}{(m - 1)}$$

(15)
Material balances for A and B over the internal-recycle reactor under complete mixing conditions give
\[F_{L}f_{AB} - F_{L}f_{A} + W \phi_{A} = 0 \quad (17)\]
\[F_{L}f_{BB} - F_{L}f_{B} + W \phi_{B} = 0 \quad (18)\]
where \(F_{L}\) is the molar flow rate of the mixture consisting of all organic components, \(W\) is the catalyst weight, \(f\) is the mole fraction based on the mixture of the organic components, and \(\phi\) is the overall rate of formation per unit mass of the catalyst.

The mole fractions, \(f_{A}\) and \(f_{B}\), may be written by means of the relative pressures in the bulk as
\[f_{A} = \left(1 - 2u_{A} - u_{B}\right) \left(m - 2u_{A} + u_{B}\right) \quad (19)\]
\[f_{B} = \left(1 - 2u_{A} - u_{B}\right) \left(m - 2u_{A} + u_{B}\right) \quad (20)\]

The overall rates of formation per unit mass of the catalyst for A and B may be expressed in terms of mass fluxes at the pellet surface.

The differential equations (9) and (10) and the boundary conditions (12), (23) and (24) give a set of nonlinear two-point boundary value problem with nonlinear boundary conditions. Numerical solutions are successfully obtained using a finite difference method combined with the quasilinearization technique presented by Lee. He dealt with cases with linear boundary conditions. However, in this paper, the nonlinear boundary conditions, Eqs.(23) and (24), as well as the nonlinear terms in the differential equations are expanded into linear forms.

A catalytic effectiveness factor, conversion and yield are obtained by substituting the concentration and its gradient at the catalyst surface into the following definitions. The catalytic effectiveness factor for A, \(E_{A}\), is defined as the ratio of the overall rate of disappearance of A at the surface conditions of concentration and temperature, \(r_{1s}\), to the rate of disappearance of A at the experimental conditions. Then \(E_{A}\) is computed by
\[E_{A} = \frac{\phi_{A}}{r_{1s}} = \frac{\left(du_{A}/dx\right)_{x=1}}{3\phi^{2} K'_{A} K'_{H} u_{A} u_{H_{5}}} \quad (25)\]

The conversion of A, \(X_{A}\) and the overall yield of B, \(Y_{B}\), are expressed by
\[X_{A} = 1 - f_{A} = \frac{1 - (m + 1)u_{A} - u_{B}}{1 - 2u_{A} - u_{B}} \quad (26)\]
\[Y_{B} = f_{B} = \frac{1 - (m + 1)u_{B}}{1 - 2u_{A} - u_{B}} \quad (27)\]

On the other hand, when the chemical reaction rate is controlling (\(\phi = 0\)), the overall reaction rates \(\phi_{A}\) and \(\phi_{B}\) in Eqs.(17) and (18) can be replaced by the intrinsic rates \(-r_{1}\) and \((r_{1} - r_{2})\), respectively. Thus Eqs.(17) and (18) are reduced to the simultaneous algebraic equations for \(u_{A}\) and \(u_{B}\), which are solved by the ordinary Newton-Raphson method.

3. Results and Discussion

3.1 Modified Thiele modulus and effective diffusivity

Although effectiveness factors were obtained at various conversions, only the values at 50% conversion are plotted in Fig. 3 for three temperature levels. The variation of the effectiveness factor with conversion was found to be small.

The conversion data are plotted against the time factor \(W/F_{i}\) in Fig. 4. The conversion decreases with increasing particle diameter, which evidently indicates that diffusional resistance within the catalyst particle increases with particle size.

The modified Thiele moduli \(\phi\) corresponding to the experimental runs are directly determined by comparing the reaction rates. Substituting Eq.(25) into Eq.(17) and solving for \(E_{A}\), we obtain
\[E_{A} = \frac{X_{A}}{\left(W/F_{L}\right)_{1s}(X_{A}, Y_{B})} \quad (28)\]

When the values of \(W/F_{L}\) for two sizes are compared at the same conversion (50% conversion is chosen), the ratio of the effectiveness factors is
\[E_{A2}/E_{A1} = \frac{(W/F_{L})_{1s}(X_{A}, Y_{B})}{(W/F_{L})_{1s}(X_{A}, Y_{B})} \quad (29)\]

Since the reaction is consecutive, the yields of the two different catalyst sizes may be generally different, even if the conversions are exactly equal. Thus the two rate terms in Eq.(29) cannot be cancelled. These values can be evaluated from Eq.(2) using the concentrations determined experimentally. From the definition of the modified Thiele modulus, we obtain...
The modified Thiele moduli and the effective diffusivities can be evaluated by the following trial and error procedure. In Eqs. (29) and (30), suffix 1 refers to the smallest catalyst particle, (60×80 mesh, average diameter 0.3 mm), whereas suffix 2 refers to any other.

1. A value of the effectiveness factor for the catalyst size 1, \( E_{A1} \), at 50% conversion is first assumed, and then \( E_{A2} \) for the catalyst size 2 is computed from Eq. (29).
2. The value of the modified Thiele modulus \( \phi_2 \) corresponding to \( E_{A2} \) is obtained from Fig. 3.
3. The value of \( \phi_1 \) can be computed by Eq. (30), and (4) a revised value of \( E_{A1} \) may be evaluated from Fig. 3. The calculation is continued until the assumed and calculated values of \( E_{A1} \) agree.

As \( R_o \), \( k_1 \), and \( \rho_p \) included in the modified Thiele modulus are known, the effective diffusivity \( D_{eA} \) may be computed from \( \phi \). The values of \( \phi \) and \( D_{eA} \) determined for each particle size are listed in Table 2.

### 3.2 Estimation of effective diffusivities

A number of methods have been presented for predicting the effective diffusivity in porous solids. Recent advances in this field were extensively reviewed by Satterfield (17) and Youngquist (21). These predicting methods may be grouped into parallel pore-models and random pore-models. Johnson and Stewart (9) presented a parallel pore-model which utilizes the pore-volume distribution. Although they considered the variation of the diffusivity with gas composition, this effect is considered to be not strong (19). Therefore, the following simplified equation neglecting the effect of composition was used to predict the effective diffusivity:

\[
D_{eA} = \frac{1}{\tau} \sum_{r} \frac{\rho_p \cdot \Delta V_g(r)}{1[D_A + 1]D_eA(r)}
\]

Here \( \tau \) is a tortuosity factor. \( \rho_p \) is the apparent density of the particle, \( \Delta V_g(r) \) is the incremental pore volume. The product, \( \rho_p \cdot \Delta V_g(r) \), gives the void fraction of pores with radii between \( r \) and \( r + dr \). \( D_A \) is the pseudo-binary molecular diffusivity for MSO (A) in the reaction mixture. As the mole fraction of hydrogen is high, \( D_A \) is approximately equal to the binary molecular diffusivity of MSO in hydrogen. The value of \( D_A \) may be calculated by the Chapman-Enskog formula. The Knudsen diffusivity of A, \( D_{KA} \), is given by

\[
D_{KA} = 9.7 \times 10^{-3} \frac{r(T \cdot MA)^{1/2}}{(\text{A})}
\]

where \( r \) is the pore radius in \( \text{Å} \), \( T \) temperature in °K and \( MA \) molecular weight of A.

The tortuosity factor is an adjustable parameter, and the values are observed to vary from less than unity to more than 6. Johnson and Stewart, and Brown et al. (3) recommended using a tortuosity factor of 3, whereas Satterfield and Cadle (18) adopted a factor of 4. In the present study, effective diffusivities at three temperature levels were calculated from Eq. (31) where \( \tau \) was taken 3. Furthermore, tortuosity factors were calculated by substituting the value of effective diffusivity.
determined experimentally into Eq. (31). The values of $D_{eA}$ and $\tau$ are listed in Table 2. These values of $\tau$ range from 1.4 to 3.4 and are less than the recommended values of 3 or 4. However, they are in the acceptable range.

The random-pore model presented by Wakao and Smith was originally developed for bidisperse pore systems, but it can also be applied to monodisperse systems. The effective diffusivity may be calculated by

$$D_{eA} = \frac{\bar{D}_{KA}}{1/D_A + 1/D_{KA}}$$

(33)

where $\bar{D}_{KA}$ is Knudsen diffusivity at the mean pore radius $\bar{r}$, which can be calculated from the pore volume distribution

$$\bar{r} = \int_0^\infty r^2 dV_g(r) / V_g$$

(34)

The predicted effective diffusivities are also listed in Table 2.

As shown in Table 2, the effective diffusivities calculated by both models are in close agreement.

3.3 Comparison of experimental and calculated results for conversion and yield

Since the values of the modified Thiele moduli corresponding to experimental runs are already determined, the theoretical relationships of conversion vs. time factor and yield vs. conversion can be computed.

As shown in Fig. 4, the computed conversions represented by the dotted lines are slightly higher than the experimental data points, but the agreement seems to be acceptable.

Fig. 5 shows the computed yields against conversion $X_A$ for various values of the modified Thiele modulus $\phi$. The solid lines represent the calculated yields for some integral values of $\phi$ ($\phi=3,5,10,20,50$) and the dotted lines are the computed yields corresponding to the values of $\phi$ which were determined by the procedure stated in section 3.1. The yield of the intermediate product $B$, $Y_B$, decreases with increasing particle diameter. Figure 5 indicates that the experimental results are in relatively good agreement with the yields predicted by the model.

Conclusions

An internal-recycle catalytic reactor described in this paper was demonstrated to be useful for evaluating the effects of intraparticle mass transfer on the rate and selectivity of multiple reaction which have complicated rate expression. The use of the internal-recycle catalytic reactor reduces considerably the computation time compared with that for an integral reactor.

By comparing the experimental data of conversion vs. time factor with the theoretical value, the effective diffusivities were determined. The effective diffusivities estimated by the parallel-pore model of Johnson and Stewart show close agreement with those by the random-pore model of Wakao and Smith. The tortuosity factors were evaluated by combining the effective diffusivity and the parallel pore-model. The numerical values range from 1.4 to 3.4, and fall within the range of previously reported values.

The calculated conversion and yield show relatively good agreement with the experimental results.

Acknowledgment

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Nomenclature

$A$ = mesityl oxide (MSO)
$B$ = methyl isobutyl ketone (MIBK)
$C$ = methyl isobutyl carbinol (MIBC)
$D_A$, $D_{AB}$ = effective diffusivity of component $A$, of $B$ [cm$^2$/sec]
$D_{KA}$ = Knudsen diffusivity of $A$ [cm$^2$/sec]
$d_p$ = equivalent particle diameter
$(\text{pellet volume})/(\text{pellet surface area})$ [mm]
$E_A$ = effectiveness factor of $A$ [-]
$F_L$ = molar flow rate of all organic components [gmol/hr]
$F_c$ = total molar flow rate $= F_L (1+m)$ [gmol/hr]
$f$ = mole fraction based on the mixture of MSO, MIBK and MIBC [-]
$H$ = hydrogen
$M_H$ = heat of reaction [kcal/gmol]
$K$ = adsorption equilibrium constant [1/atm]
$K_{eq}$ = thermodynamic equilibrium constant [1/atm]
$K'$ = dimensionless equilibrium constant, $K' = K P_t$
$k_{es}$ = effective thermal conductivity of porous solid [kcal/m-hr-°C]
$k_1$, $k_2$ = rate constant [gmol/hr]
$M_A$ = molecular weight of $A$ [g/gmol]
$m$ = ratio of molar flow rate of MSO to that of hydrogen [-]
$p$ = partial pressure [atm]
$P_T$ = total pressure [atm]
$R$ = radial coordinate [mm]
$R_0$ = radius of spherical pellet [mm]
$r$ = pore radius [Å]
$r_1$, $r_2$ = reaction rate of first, second reaction step [-]
$R_g$ = gas constant, 82.1 [atm-cm$^3$/gmol-°K]
$R_{A1}$, $R_{B1}$, ..., $R_{A15}$, $R_{B15}$ = overall rate of formation of $A$, of $B$ [gmol/g-hr]
$r_{A1}$, $r_{B1}$, ..., $r_{A15}$, $r_{B15}$ = total pressure [atm]
$S_{BET}$ = BET pore surface area [m$^2$/g]
$S_P$ = cumulative pore surface area [m$^2$/g]
$T$ = temperature [°C], [°K]
$\Delta T_{max}$ = maximum temperature rise in catalyst particle [°C]
$u$ = dimensionless pressure, $p_r P_t$ [-]
$V_s$ = cumulative pore volume [cm$^3$/g]
$W$ = catalyst weight charged in reactor [g]
$X_A$ = conversion of $A$ [-]
$x$ = dimensionless radial coordinate [-]
$Y_B$ = yield of $B$ [-]
$z$ = porosity [-]
$\theta$ = dimensionless time, $k_1 W/F_L$ [-]
$p_p$ = apparent density of catalyst particle [g/cm$^3$]
$p_c$ = true density of catalyst [g/cm$^3$]
$\tau$ = tortuosity factor
$\phi$ = modified Thiele modulus [$= (R_0/3)k_3 p_p R_T D_{KA} P_t$]

<Subscripts>
$A$ = mesityl oxide
$B$ = methyl isobutyl ketone
$C$ = methyl isobutyl carbinol
$H$ = hydrogen
$s$ = pellet surface
0 = reactor inlet
1 = first step of reaction
2 = second step of reaction

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