Spatial Patterns for Selective Conversion in Catalytic Reactors

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Steady-state multiplicity in individual catalyst particles can be exploited to produce concentration patterns in a catalytic reactor. Thus, stable, steady-state, spatial patterns can be created in a packed bed reactor by providing for an initial pattern using multiple feeds at different points along the length of the reactor as a start-up strategy. It is shown that the formation of such patterns when properly selected can remarkably improve selectivity and conversion in reaction systems. Computational demonstrations are made with a reaction system in which the desired product must be obtained by reacting two different intermediate products formed by a single primary reactant under different reaction conditions. The patterns that produce high selectivity are those that alternately produce the intermediates in quick succession, so that the main product can be produced promptly without loss of reactor space in the flowing reaction mixture.

Introduction

A novel way of operating catalytic packed bed reactors to improve selectivity and conversion is demonstrated; namely, deliberately creating spatial patterns in the catalyst phase concentration. The patterns specifically arise from catalyst particles, assuming widely different steady states, due to nonlinear multiplicity behavior. The basic underlying notion of reactor operation in this work is that of navigating the fluid reaction mixture through a train of coordinately orchestrated steady states in the catalyst phase so that selective conversion of desired products is accomplished. For such steady-state patterns to prevail, it is necessary that they are dynamically stable.

Patterns have also been of interest to Sheintuch and co-workers (Sheintuch and Shvartsman, 1996). Their focus has been on spatiotemporal patterns produced in reactions in which perturbations from steady state at any location in the reactor cause the appearance of moving fronts until restoration to the original steady state. These studies must be distinguished from our earlier (Trinh and Ramkrishna, 1996, 1997) and present studies, where the focus has been on identifying steady-state patterns that can provide for somewhat diverse reactor performances. In this paper we raise the possibility of improving selective conversion of a desired product in a specific reaction system through the use of spatially created patterns. Such patterns can be produced only following the establishment of symmetry breaking. We expect that the type of investigations by Sheintuch and Adjaye (1990) and Barto and Sheintuch (1994) to be not only theoretically interesting but also practically significant in elucidating the dynamic behavior of perturbations from steady-state patterns considered in this work. Furthermore, the control of patterned steady states will invariably rest on dynamic studies such as those of Sheintuch and co-workers.

Multiple steady states occur in catalyst particles because of nonlinearities associated with the dependence of reaction rates on concentration and/or temperature. The exothermicity of chemical reactions behooves one to include the effects of nonisothermality in the analysis of catalytic reactors. However, mathematical investigation of heterogeneous reactor models for such pattern formation under the most general conditions is difficult and requires guidelines obtained from analysis of simpler situations. We therefore choose to consider isothermal reactor operation in which patterns may be caused by concentration-driven catalyst particle multiplicity. Furthermore, diffusion in catalyst particles is neglected in favor of a mass transfer resistance lumped at the particle surface. These assumptions help us arrive at a heterogeneous packed bed reactor model that can be analyzed rigorously for the appearance of patterns, for their dynamic stability properties, and the manner in which they may be brought about from suitable startup conditions. Although such models are not sufficiently realistic, their study can be used (i) to assess whether there are any advantages to be had by instituting patterns, and (ii) to obtain guidelines for the analysis of more realistic but mathematically complex heterogeneous models.

For a single reaction satisfying Langmuir–Hinshelwood kinetics with substrate inhibition (eq 6), we (Trinh and Ramkrishna, 1996, 1997) have theoretically shown that spatial patterns are asymptotically stable and have established conditions under which specific spatial patterns can be created in a packed bed catalytic reactor. We have further shown (Trinh and Ramkrishna, 1997) that it is more meaningful to seek patterned operation among a class of patterns for which the reactor output is virtually the same or stays within some prescribed limits.

We shall be concerned with the following specific reaction system.

\[ A_1 + A_2 \rightarrow 2A_3 \]
In this reaction system, A₃ is the desired product. To maintain a high level of production of A₃, equal amounts of A₁ and A₂ must be produced. Because A₁ and A₂ both come from A₀, as A₁ increases, A₂ must decrease, which in turn limits the production of A₃.

**Reactor Model**

To demonstrate promotion of the production of A₃ in the reaction system just discussed using patterns, the heterogeneous model for a packed bed reactor is used. Although the reactor model assumptions are the same as those in the works cited, we shall briefly review them here. The fluid phase mixing is described by plug flow with axial dispersion, and transport resistance in the catalyst phase is limited to the particle surfaces. Isothermality is also assumed to simplify the numerical treatment. Relaxing this assumption will not invalidate the present idea but will introduce needless complications in the demonstration.

Let fᵢ and sᵢ be the concentrations of Aᵢ in the fluid phase and in the catalyst phase, respectively. The mass balances in the reactor are given by the following partial differential equations and accompanying boundary and initial conditions.

\[
\frac{\partial f_i}{\partial t} = D \frac{\partial^2 f_i}{\partial x^2} - F \frac{\partial f_i}{\partial x} - k_i a_i (f_i - s_i) \quad (1)
\]

\[
\frac{\partial s_i}{\partial t} = k_i a_i (f_i - s_i) + \sum_{j=1}^{3} v_{ij} R'_j \quad (2)
\]

\[x' = 0, \quad \frac{\partial f_i}{\partial x} = F \frac{\partial f_i}{\partial t} \quad (3)
\]

\[x = L, \quad \frac{\partial f_i}{\partial x} = 0 \quad (4)
\]

\[f_i(x,0) = f_{i,0}(x), \quad s_i(x,0) = s_{i,0}(x) \quad (5)
\]

where \(c^0 = c^0_{i,0,0}\) the Kronecker delta is used to represent the fact that only A₀ is fed to the reactor at concentration \(c^0\), and \(v_{ij}\) are the stoichiometric coefficients for the reaction system already considered with the following values:

\[v_{0,3} = v_{1,2} = v_{2,1} = v_{3,1} = v_{3,2} = 0, v_{0,1} = v_{0,2} = v_{1,3} = v_{2,3} = -1, v_{1,1} = v_{2,2} = 1, v_{3,3} = 2 \quad (6)
\]

For interpretation of the other symbols in eqs 1 and 2, the reader is referred to the Nomenclature section. The rates of reactions producing A₁, A₂, and A₃ are assumed to be respectively, \(R_1 = k_{1} s_1 (1 + v_{1,0} s_0)\), \(R_2 = k_{2} s_2 (1 + v_{2,0} s_0)^2\), and \(R_3 = k_{3} s_3 s_2\). The first of these is Langmuir–Hinshelwood saturation kinetics and the second is Langmuir–Hinshelwood kinetics with substrate inhibition. The latter shows multiple steady states for a catalyst particle exposed to a fluid of fixed concentration of A₀ within a suitable range (see Trinh and Ramkrishna, 1996). The kinetics for the reaction producing A₃ is bilinear in A₁ and A₂.

Defining the following dimensionless variables and parameters, \(x = x/L, \; t = \tau V/F, \; u_i = f_{i,0}/c_0, \; s_i = s_{i,0}/c_0, \; P_e = LF/DA, \; \alpha_i = k_i V a_i / \beta_i = k_i V a_i / F, \; D_{a_1} = k_{1,0} V F, \; D_{a_2} = k_{2,0} V F, \; D_{a_3} = k_{3,0} V a_i F\), the following dimensionless differential equations are obtained.

\[
\frac{\partial u}{\partial t} = P^{-1} \frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial x} - A(u - v) \quad (7)
\]

\[
\frac{\partial v}{\partial t} = B(u - v) - R(v) \quad (8)
\]

\[x = 0, \quad \frac{\partial u}{\partial x} = P(u - u_i), \quad x = 1, \quad \frac{\partial u}{\partial x} = 0 \quad (9)
\]

\[u(x,0) = u^0(x), \quad v(x,0) = v^0(x) \quad (10)
\]

where

\[
\begin{bmatrix}
  u_0 \\
  u_1 \\
  u_2 \\
  u_3 \\
\end{bmatrix} = \begin{bmatrix}
  v_0 \\
  v_1 \\
  v_2 \\
  v_3 \\
\end{bmatrix} \quad (11)
\]

\[
\frac{\partial u}{\partial x} = u_0 \quad (12)
\]

\[
\frac{\partial v}{\partial x} = v_0 \quad (13)
\]

\[
R(v) = \begin{bmatrix}
  -R_1(v_0) & -R_2(v_0) & R_3(v_0) & R_4(v_0) & R_5(v_0) & R_6(v_0) & R_7(v_0) & R_8(v_0) & R_9(v_0) & R_{10}(v_0) \\
\end{bmatrix} \quad (14)
\]

and the matrices \(P\), \(A\), and \(B\) are defined as follows:

\[
P = \begin{bmatrix}
  P_{00} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  P_{10} & P_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  P_{20} & P_{21} & P_{22} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  P_{30} & P_{31} & P_{32} & P_{33} & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix} \quad (15)
\]

\[
A = \begin{bmatrix}
  \alpha_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  \alpha_1 & \beta_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  \alpha_2 & 0 & \beta_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  \alpha_3 & 0 & 0 & \beta_2 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix} \quad (16)
\]

\[
B = \begin{bmatrix}
  \beta_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  \beta_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  \beta_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
  \beta_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix} \quad (17)
\]

The dimensionless kinetics are

\[
R_1(v_0) = D_{a_1} v_0 (1 + \alpha_1 v_0) \quad (18)
\]

\[
R_2(v_0) = D_{a_2} v_0 (1 + \alpha_1 v_0)^2 \quad (19)
\]

\[
R_3(v_1 v_2) = D_{a_3} v_1 v_2 \quad (20)
\]

Figure 1 shows the kinetics for the first two reactions \(R_1 \text{ and } R_2\). These two kinetics show distinct different behaviors with respect to the reactant concentration, \(v_0\). The rate of production of A₃ dominates at high reactant concentration and that of A₂ dominates at low reactant concentration. The production of A₁ is maximized when equal amounts of A₁ and A₂ are produced. Because only the reactant A₀ is fed into the reactor, to obtain equal amounts of A₁ and A₂, the reactant A₀ in the catalyst phase should alternate between states of high and low concentration. Patterns will help to achieve this goal.

**Steady-State Patterns**

The steady states of the reactors is described by the following equations:

\[
P^{-1} \frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial x} - A(u - v) = 0 \quad (21)
\]

\[
B(u - v) - R(v) = 0 \quad (22)
\]
Equations 8 and 9 are subject to the following boundary conditions:

\[ x = 0, \frac{du}{dx} = P(u - u_i); \quad x = 1, \frac{du}{dx} = 0 \]  

(10)

Because the solution of \((u_0(x), v_0(x))\) is independent of \((u_i(x), v_i(x)), i > 0\), only the equations governing the reactant concentration \((u_0, v_0)\) are needed to determine the conditions for existence of steady-state patterns. These conditions can be found in Trinh and Ramkrishna (1996, 1997). The solution to the system, eqs 8 and 9, can be conveniently cast into a system of integral equations and solved by fixed-point iteration.

\[ u(x) = H(x) + PA \int_0^1 G(x, \xi) v[\xi]e^{-\xi} d\xi \]  

(11)

\[ u = v + B^{-1}R(v) \]  

(12)

where

\[ u(x) = \begin{bmatrix} u_0(x) \\ u_1(x) \\ u_2(x) \\ u_3(x) \end{bmatrix}, \quad H(x) = h_0(x) \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \]  

(13)

with

\[ h_0(x) = \exp\left(\frac{Pe_0}{2}x\right)[A \cosh(q_0x) + B \sinh(q_0x)] \]

\[ q_i = \sqrt{\frac{Pe_i^2}{4} + \alpha_i Pe} \]

and the constants

\[ A = \frac{2Pe_0[2q_0 \cosh(q_0) + Pe_0 \sinh(q_0)]}{4Pe_0 q_0 \cosh(q_0) + Pe_0^2 \sinh(q_0) + 4q_0^2 \sinh(q_0)} \]

\[ B = \frac{-2Pe_0[Pe_0 \cosh(q_0) + 2q_0 \sinh(q_0)]}{4Pe_0 q_0 \cosh(q_0) + Pe_0^2 \sinh(q_0) + 4q_0^2 \sinh(q_0)} \]

The dimensionless parameters appearing in the packed bed equations (eqs 3 and 4) depend on the residence time of the reactor, which can be varied by changing the flow rate into the reactor. Using the parameters in Table 1, Figure 2 shows the so-called upper steady-state solution (which corresponds to low consumption of \(A_0\)) and displays the concentration profiles for \(A_0\) and \(A_3\) in the reactor. The production of \(A_3\), as expected for this
steady state, is quite low. Figure 3 shows the concentration profiles of what is known as the lower steady-state solution. Much of the reactant $A_0$ in this case has been consumed not to produce $A_3$, which is the desirable product, but to produce more of the intermediate products, $A_1$ and $A_2$. Consequently, the production of $A_3$ is also low for this steady state.

Figure 4 exhibits a patterned steady state. The patterned steady state results from discontinuities in the catalyst concentration profile of $A_0$. The discontinuities occur when the catalyst concentrations abruptly move from the upper steady state to the lower steady state. At the upper steady state, the reactant concentration, $A_0$, is high and $A_1$ is produced in a larger quantity. On the other hand, at the lower steady state, $A_2$ is produced in a larger quantity. By appropriately alternating between the upper and lower steady states, it is possible to maintain the equal amounts of $A_1$ and $A_2$ required to promote production of $A_3$, the desirable product. Consequently, the production of $A_3$ for the patterned steady state has been promoted. The relatively high production of $A_3$ is not significantly affected by operating the reactor at a different patterned state, as shown in Figure 5.

Stability of Spatial Patterns

We have just shown that spatial patterns can promote production of $A_3$ in the reaction system considered. From the practical point of view, the patterns must be able to at least withstand small perturbations. For infinitesimal perturbations, linear stability analysis is commonly used to determine whether the reactor will eventually return to the patterned state.

To determine the stability of spatial patterns, the system of eqs 3 and 4 is linearized about the spatial patterns to obtain the following:

$$\frac{\partial u}{\partial t} = Pe^{-1}\frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial x} - \alpha(u - v)$$

$$\frac{\partial v}{\partial t} = \beta(u - v) + \frac{dR_1}{dv}(v_0)$$

$$\frac{\partial u_0}{\partial x}(0,t) = Pe \times u$$

$$\frac{\partial u_0}{\partial x}(1,t) = 0$$

It can be shown that the stability of spatial patterns is in fact determined by the $(u_0,v_0)$ component of eqs 15 and 16; that is:

$$\frac{\partial u_0}{\partial t} = \frac{1}{Pe_0}\frac{\partial^2 u_0}{\partial x^2} - \frac{\partial u_0}{\partial x} - \alpha_0(u_0 - v_0)$$

$$\frac{\partial u_0}{\partial x}(0,t) = Pe_0 u_0$$

$$\frac{\partial u_0}{\partial x}(1,t) = 0$$

$$u_0(x,0) = u_0^0(x) \quad v_0(x,0) = v_0^0(x)$$

The stability of spatial patterns is determined by the spectrum of $L$ given by...
To determine the spectrum of \( \mathbf{L} \) is difficult. A simple indicator is developed (Trinh and Ramkrishna, 1997) to test whether, given a spatial pattern \((u_0,v_0)\), the spectrum of \( \mathbf{L} \) is negative. The indicator involves solving the following initial value problem:

\[
\begin{align*}
\frac{1}{\mathbf{Pe}_0} \frac{d}{dx} \left( \exp(-\mathbf{Pe}_0 x) \frac{d}{dx} \right) r(x) &= \alpha_0 u_0(x) - \alpha_0 v_0(x) \\
\frac{\partial \mathbf{R}_1}{\partial v_0}(v_0) + \frac{\partial \mathbf{R}_2}{\partial v_0}(v_0) &= 0
\end{align*}
\]

If \( r(x) > 0 \) for \( 0 \leq x \leq 1 \) and \( r'(1) > 0 \), then \((u_0(x),v_0(x))\) is asymptotically stable.

Asymptotic stability requires a sufficiently small perturbation for the reactor to return to the patterned state. This requirement seems quite stringent for the purpose of promoting the production of \( A_3 \). The topology used in the analysis of asymptotic stability can only accommodate infinitesimal perturbations. A different topology that allows finite perturbation is used for the stability analysis of patterns. The latter topology is used to formulate an \( \epsilon \)-neighborhood of the patterned state that allows functions to deviate by more than \( \epsilon \) over intervals of length less than \( \epsilon^2 \). In this topology, perturbations of magnitude more than \( \epsilon \) are permissible provided they occur only in intervals with cumulative length of \( \epsilon^2 \). The following stability theorem is presented in the foregoing topology.

**Stability Theorem.** If the spectrum of the linearized operator \( \mathbf{L} \) about the patterned state is negative, then there exists a sufficiently small \( \epsilon \)-neighborhood of the patterned state such that the reactor will always remain in this neighborhood if it is initially in this neighborhood.

The theorem ensures a given level of conversion in the reactor provided the reactor is operated in the \( \epsilon \)-neighborhood of the patterns. It may be possible to use the stability theorem just mentioned to address the class of patterns for which the product \( A_3 \) may vary within stipulated limits in a manner similar to that discussed by Trinh and Ramkrishna (1997) for a single reaction. However, this has not been accomplished in this paper.

**Dynamic Analysis**

We show the dynamics of the reactor described by the system of eqs 3 and 4. The procedure for solving the reactor equations for a single reaction can be extended to reaction systems without undue difficulty. The solution procedure for a single reaction is discussed in detail in our previous papers.

To demonstrate the possibility of attaining a patterned steady state from a dynamic viewpoint, the initial catalyst profile for the reactant, \( A_0 \), is expected to possess spatial oscillations. The generation of these spatial oscillations may be difficult to achieve in reality.

A more realistic approach to create an initial profile in the reactor so that patterns may be attained is discussed in the next section.

Figure 6 shows the transient profile of \( A_0 \) at \( t = 1 \), starting with initial condition \( u(0) = 0 \), \( v(0) = \sin^2(40x) \), and \( v(0) = \sin(40x) \) for \( j = 0, 1, 2, \) and \( 3 \). The reactor quickly reaches a patterned steady state at \( t = 10 \) (Figure 7).

**Startup Strategies for Spatial Patterns**

To take advantage of spatial patterns, special effort is required to implement initial patterns. It is shown the spatial patterns can be reach dynamically by providing spatial oscillation in the catalyst phase. It is somewhat artificial and difficult to have such profiles in the catalyst phase. A more realistic and simpler alternative to generate spatial patterns is by instituting multiple feeds (Figure 8). The locations of these feeds should coincide with the locations of discontinuities.

To create an initial patterned state with \( n \) discontinuities, we need to implement \( n \) side feeds. The reactor with \( n \) side feeds is divided into \( n + 1 \) separate sections. With the assumption that there is no dispersion in the fluid preceding the entrance and following the exit of
each section, each section of the packed bed reactor is governed by the following equations

\[
\frac{\partial u_l}{\partial x} = \frac{1}{Pe_l} \frac{\partial^2 u_l}{\partial x^2} - \alpha_l (u_l - v_l) \tag{21}
\]

\[
\frac{\partial v_i}{\partial t} = \beta_i^k (u_l - v_l) + \sum_{j=1}^{3} v_{ij} R_j \quad i = 0, 1, 2, 3 \tag{22}
\]

The auxiliary boundary and initial conditions are

\[
\frac{\partial u_l}{\partial x} = Pe_l (u_l - u_l^0), \quad x = x_k; \quad \frac{\partial u_l}{\partial x} = 0, \quad x = x_{k+1} \tag{23}
\]

\[
\sum_{l=0}^{k-1} F_l^i (x_k, t) + F_k^i c_i^k = \frac{\sum_{l=0}^{k-1} F_l^i c_0^l}{F_k^i} \tag{24}
\]

\[
u_i(x,0) = v_i(x,0) = 0, \quad \text{for } x \in (x_k, x_{k+1}), \quad k = 0, 1, \ldots, n \tag{25}
\]

where \(F^k\) is the \(k\)th side feed of the reactant into the reactor; \(V^k\) is the volume of the reactor between the \(k\)th and \((k+1)\)st feeds; \(c_i^k\) is the concentration of the \(i\)th species at the \(k\)th side feed; and \(x_0 = 0, x_n+1 = 1\).

\[
\alpha_l^k = \frac{k_l a^i V^k}{\sum_{l=0}^{k-1} F_l^i}, \quad \beta_i^k = \frac{k_l a_p V^k}{\sum_{l=0}^{k-1} F_l^i}, \quad \sigma_i^k = \sigma_i^k u^k \tag{26}
\]

In the aforementioned equations, it is assumed that \(\sum_{l=0}^{k-1} F_l^i = 0, F_0^0 = F_0, \text{ and } V_0^0 = V_0\).

To demonstrate the idea, we solve the reactor eqs 21–25 with discontinuities taking place at the axial coordinate of (0.487, 0.517, 0.735). The values of \(F^k\) and \(c_0^k\) are adjusted so that the reactor reaches a steady state with discontinuities at the desired locations. Figure 9 shows the steady state of the reactor with multiple side feeds instituted with the values of the parameters shown in Table 2. No product is fed into the reactor. Shown in Figure 10 is the pattern reached after the removal of the side feeds.

**Conclusions**

The use of pattern formation in packed bed reactor to promote the conversion of the reactant to desirable product is demonstrated in a specific reaction system. The conversion with patterns is more than doubled in the cited case. This increase in conversion is sustained for a class of patterns and is not critical to a specific pattern.

Numerical simulations of the packed bed reactor show that it is possible to achieve discontinuous spatial patterns from uniform feed into the reactor by instigating continuous spatial oscillations in the initial concentration in the catalyst phase. Attempts to establish such a spatial oscillation through an interim temporally oscillating feed were not a success (Trinh, 1997). However, this issue is one that deserves considerable further investigation. The patterns in the reactor are achieved with the use of multiple side feeds.

The reaction system in this work was chosen to demonstrate the structure of reaction systems for which
selective conversion can be improved with patterns. More generally, the potential of patterns to enhance selective conversion exists in reaction systems where persisting with steady states along a single branch can result in the loss of space time for either side reactions or other effects that harm the main reaction, whereas switching to another branch has a positive effect. However, the reaction systems must have the proper mathematical steady-state multiplicity structure for patterns to be of value. Introducing heat effects due to chemical reactions and temperature dependence of reaction rates may broaden the use of patterns in promoting reactor performance or controlling highly exothermic reactions.

Nomenclature

- $A = \text{cross-sectional area of the reactor}, \text{m}^2$
- $a_p = \text{surface area per unit volume of particle}, \text{m}^{-1}$
- $a_v = \text{surface area per unit volume of bed}, \text{m}^{-1}$
- $c_i^{k0} = \text{concentration of } A_i \text{ in the feed}, \text{mol/m}^3$
- $c_i^k = \text{concentration of } A_i \text{ in the } k\text{ th side feed} (c_i^k = 0 \text{ for } i = 0), \text{mol/m}^3$
- $D_i = \text{dispersion coefficient of species } i, \text{m}^2/\text{s}$
- $D_{ai} = \text{Damkohler number of the } i\text{ th reaction}, D_{ai} = K_iV/F$
- $Da_{ik} = \text{Damkohler number of the } i\text{ th reaction in the reactor between the } k\text{ th and } (k+1)\text{st side feeds}, \text{defined by eq } 26$
- $F = \text{volumetric flow rate}, \text{m}^3/\text{s}$
- $F^k = \text{volumetric flow rate of the } k\text{ th side feed}, \text{m}^3/\text{s}$
- $f_i = \text{concentration of species } i \text{ in the fluid phase}, \text{mol/m}^3$
- $f_{i0} = \text{initial concentration of species } i \text{ in the fluid phase}, \text{mol/m}^3$
- $k_i = \text{mass transfer coefficient of species } i, \text{m/s}$
- $K_i = \text{reaction rate constant of reaction number } 1, \text{s}^{-1}$
- $K_2 = \text{reaction rate constant of reaction number } 2, \text{s}^{-1}$
- $K_3 = \text{reaction rate constant of reaction number } 3, \text{m}^3(\text{mol/s})$
- $u = \text{dimensionless concentration vector in the fluid phase}$
- $v = \text{dimensionless concentration vector in the catalyst phase}$
- $L = \text{length of the reactor}, \text{m}$
- $Pe = \text{Peclet number for species } i, Pe = FL/(D_iA)$
- $Pe^k = \text{Peclet number for species } i \text{ in the reactor between the } k\text{ th and } (k+1)\text{st side feeds}, \text{defined by eq } 26$
- $s_i = \text{concentration of species } i \text{ in the catalyst phase}, \text{mol/m}^3$
- $s_{i0} = \text{initial concentration of species } i \text{ in the catalyst phase}, \text{mol/m}^3$
- $R_i^k = \text{the kinetic of the reaction producing } A_i, \text{mol/(m}^3\text{/s)}$
- $R_i^1 = \text{the dimensionless kinetic of the reaction producing } A_i$
- $V = \text{volume of the reactor}, \text{m}^3$
- $V^k = \text{volume of the reactor between the } k\text{ th and } (k+1)\text{st side feeds}, \text{m}^3$
- $x = \text{axial coordinate of the reactor}, \text{m}$
- $x^* = \text{dimensionless axial coordinate of the reactor}$
- $x^k = \text{dimensionless axial coordinate of the } k\text{ th side feed}$
- $t = \text{time}, \text{s}$
- $t^* = \text{dimensionless time, nondimensionalized with respect to resident time of the reactor}$

Greek Letters

- $\alpha_i = \text{dimensionless mass transfer coefficient of species } i, \alpha_i = k_i\varphi/V/F$
- $\alpha_k^i = \text{dimensionless mass transfer coefficient of species } i \text{ in the } k\text{ th and } (k+1)\text{st feeds of the reactor, defined in eq } 26$
- $\beta_i = \text{dimensionless mass transfer coefficient of species } i, \beta_i = k_i\varphi/V/F$
- $\beta_k^i = \text{dimensionless mass transfer coefficient of species } i \text{ in the } k\text{ th and } (k+1)\text{st feeds of the reactor, defined in eq } 26$
- $\epsilon = \text{the magnitude of perturbations from steady state}$
- $\delta_{ij} = \text{Kronecker delta}, \delta_{ij} = 1, \text{if } i = j, \text{otherwise}, \delta_{ij} = 0$
- $v_{ij} = \text{the stoichiometric coefficients of the reaction system}$
- $\alpha_{ij} = \text{adsorption desorption equilibrium constant of species } i, \text{m}^3/\text{mol}$
- $\alpha_i = \text{modified adsorption desorption equilibrium constant of species } i, \alpha_i = \alpha_{ij}$
- $\alpha_i^k = \text{modified adsorption desorption equilibrium constant of species } i \text{ in the } k\text{ th and } (k+1)\text{st feeds, defined in eq } 26$

Subscripts

- $i = \text{property associated with species } A_i$
- $k = \text{properties associated with the reactor in the } k\text{ th and } (k+1)\text{st side feeds}$

Literature Cited


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