



THE EFFECT OF MICROMIXING ON STEADY-STATE MULTIPLICITY FOR AUTOCATALYTIC REACTIONS IN A NONIDEAL MIXING OF CSTR

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Abstract—The effect of micromixing on steady-state multiplicity is not displayed by the universal reaction model (URM) since this URM has considered any chemical species having the same mixing time constant. The modified universal reaction model (MURM) is derived for overcoming the above limitation. The design equations are first derived. Furthermore, the MURM is employed for studying the effect of micromixing on the multiplicity for autocatalytic, isothermal reactions of the type $A + B \rightarrow (\eta + 1)B + \text{product}$ with the overall rate expression being $-\gamma_a = k C_a^p C_b^q$ in a CSTR. The effects of micromixing on necessary and sufficient conditions for multiplicity are presented.

1. INTRODUCTION

Predicting a priority has become quite important for the design and the control of a chemical reactor since steady-state multiplicity occurred. The use of the continuous-flow stirred tank reactor (CSTR) has had an impact on the study of various bifurcation phenomena occurring in chemical reacting systems. Uppal *et al.* (1976) and Balakotaiah and Luss (1983) studied a nonequilibrium chemistry in a CSTR with single inflow and showed that bifurcation phenomena occurred under nonisothermal conditions. As to isothermal conditions, many autocatalytic reactions are known to exhibit multiple states in a CSTR. Gray and Scott (1983) studied an isothermal CSTR and showed that, in addition to the usual bistability behavior, there existed a second hysteresis region. Recently, Kay *et al.* (1989) applied the techniques of singularity theory, which is a very powerful tool for obtaining analytical results for regions of multiple steady-state responses in the parameter space. However, most studies have concentrated on the ideal mixing in a CSTR. The above findings can therefore not be applied in a nonideal mixing CSTR.

Lo and Cholette (1983) and Liou and Chien (1990a, b, 1991) recently discussed the effect of macromixing on the multiplicity in a CSTR via Chollette's model. As to the effect of micromixing, Dudukovic (1977a, b) employed three distinct one-parameter models to study multiplicity in a CSTR with the rate expressed as $-\gamma_a = kC_a/(1 + KC_a)^2$. Marconi and Vastistas (1980) and Vastistas and Marconi (1985)

utilized the random coalescence model, the generalized recycled model and the IEM (interaction by exchange with the mean) model to discuss multiplicity under various chemical reaction systems. Puhl and Nicolis (1986) applied Zwietering's model (1984) towards discussing the micromixing effect on the complex chemical reaction systems. The reactor performance was indicated from all these results to be considerably affected by the micromixing. Hannon and Horsthemke (1986) used a coalescence–dispersion model of the CSTR to study the effect of premixed and unpremixed reactant feeds. They showed that the region of bistability is smaller for segregated feed streams than for a fully premixed feed stream. However, the complex mathematical treatment in the calculation steps is a limitation in previous papers.

The steady-state IEM model of micromixing with singular perturbation has recently been utilized by Fox (1989) for analyzing the steady-state multiplicity of the Nicolis–Puhl reaction. Furthermore, Fox and Villiermaux (1990a, b), Fox *et al.* (1990) and Fox (1991) utilized the unsteady-state IEM model for exploring the dynamic behavior by the perturbation method and numerical simulation. Recently, the study of the effect of micromixing on the chlorite reaction using the unsteady-state IEM model has been presented by Fox *et al.* (1994). They showed that the above reactions are quite sensitive to relatively small changes in the micromixing parameter and derived a polynomial expansion of the IEM model to investigate the dynamic behavior of the system using bifurcation

theory. Based on the above results, the solution of the IEM model still needs an initial guess of mean concentration.

These flaws can be overcome by the universal reaction model (URM) which was developed by Miyawaki *et al.* (1975). The merits of the URM include its corresponding physical meaning, ease of use and no loss of accuracy. Liou *et al.* (1983) discussed how the nonideal mixing effects conversion in several types of chemical reactors. Furthermore, Liou and Shei (1984) demonstrated that the mass exchange coefficients are not a constant according to the experiment of Takao *et al.* (1978). However, the shortcoming lies in the fact that in previous papers each chemical species has the same mixing time constant. Therefore, the URM cannot be applied towards understanding the phenomenon of steady-state multiplicity with micromixing.

Here, the modified universal reaction model (MURM) is proposed. Each of the chemical species is considered to have its own mixing time constant. The MURM can also be simplified to the URM once the values of the mixing time constant become the same. Furthermore, the MURM is employed to investigate the effect of micromixing on multiplicity for autocatalytic, isothermal reactions of the type $A + B \rightarrow (\eta + 1)B + \text{product}$ with the overall rate expression being $-\gamma_a = kC_a^p C_b^q$ in a CSTR. The necessary and sufficient conditions for multiplicity in nonideal mixing indeed differ from those in ideal mixing, as demonstrated from the observed results.

2. MICROMIXING MODELS

The case is first considered in which two miscible solutions containing chemical species (labelled A and B, respectively) are mixed by turbulence and simultaneously react with each other. The two solutions are divided into several lumps of a small scale. These lumps are twisted and divided into a much smaller scale by turbulence, with the solutions finally being mixed to a molecular scale and then reacted with each other.

A distribution concentration-volume in a lump of the MURM is shown in Fig. 1. The MURM, as well as the URM, is assumed to be the same volume for every cell in an isotropic stirred vessel. Unpremixed chemical species A and B feed in the completely segregated regions A_2 and B_2 . A partial fraction of chemical species A and B, which are located in segregated regions, directly flow out of the reactor simultaneously, and the others diffuse into the molecular-mixed regions A_1 and B_1 , respectively. The reaction is assumed to occur only in the molecular-mixed region. The outlet flow is composed of flow coming from the molecular-mixed region and the segregated region.

The degree of micromixing, α_m , is defined as the relative volume ratio of the summation of the $A_1 V_a$ and $B_1 V_b$ to the total mixing system. This definition is true in the light of the fact that the molecular-mixed regions are homogeneous. In an isotropic stirred

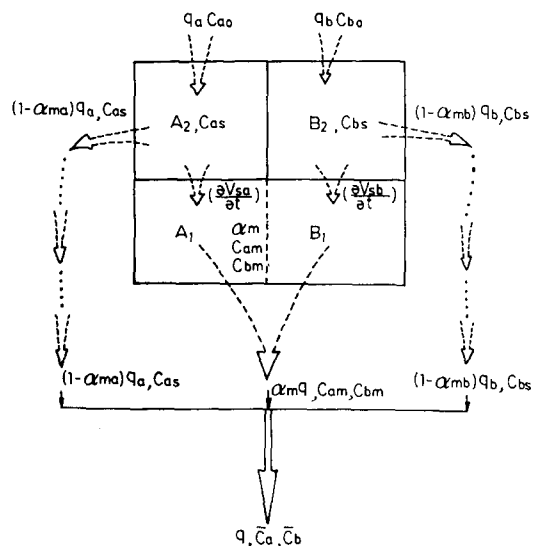


Fig. 1. Schematic representation of the modified universal reaction model.

vessel, α_m is assumed to have a constant value throughout the vessel and to change with time.

The magnitude of the diffusion rate from the segregated region to the molecular-mixed region can be determined for chemical species A and B, $(\partial V_{sa}/\partial t)$ and $(\partial V_{sb}/\partial t)$, by eqs (1a) and 1(b), respectively:

$$\partial V_{sa}/\partial t = -K_a A_2 V_a \quad (1a)$$

$$\partial V_{sb}/\partial t = -K_b B_2 V_b \quad (1b)$$

where K_a and K_b are the inversion of the mixing time constants for A and B components. The diffusion rates are different for chemical species A and B since each of the species has its own mixing time constant and volume of the completely segregated region. This concept and the definition of α_m are the primary differences between the URM and the MURM.

The following equations under the above assumptions are derived;

$$A_1 = \alpha_{ma}, \quad A_2 = 1 - \alpha_{ma} \quad (2)$$

$$B_1 = \alpha_{mb}, \quad B_2 = 1 - \alpha_{mb}$$

and

$$\alpha_m V = A_1 V_a + B_1 V_b = \alpha_{ma} V_a + \alpha_{mb} V_b$$

where V is the volume of a lump, V_a and V_b are the volumes of chemical components A and B in a lump, and α_{ma} and α_{mb} are the degrees of micromixing for chemical species A and B, respectively.

By taking the volume balance in the $A_2 V_a$ region (the density is assumed to be constant),

$$\frac{dA_2 V_a}{dt} = q_a + (\partial V_{sa}/\partial t) - A_2 q_a \quad (3)$$

At the steady state,

$$A_2 = (1 - \alpha_{ma}) = 1/(1 + K_a \tau_a) \quad (4)$$

where $\tau_a = V_a/q_a$.

By taking the volume balance in the B_2V_b region,

$$\frac{dB_2V_b}{dt} = q_b + (\partial V_{sb}/\partial t) - B_2q_b \quad (5)$$

Derived at the steady state,

$$B_2 = (1 - \alpha_{mb}) = 1/(1 + K_b\tau_b) \quad (6)$$

where $\tau_b = V_b/q_b$.

By taking the total mass balance in the $\alpha_m V$ region,

$$\frac{d\alpha_m V}{dt} = -(\partial V_{sa}/\partial t) - (\partial V_{sb}/\partial t) - \alpha_m V \quad (7)$$

Substituting eqs (3) and (5) into eq. (7) at the steady-state produces

$$0 = (q_a - A_2q_a) + (q_b - B_2q_b) - \alpha_m q \quad (8)$$

Furthermore, eqs (4) and (6) are substituted into eq. (8),

$$\alpha_m = \frac{q_a}{q} \alpha_{ma} + \frac{q_b}{q} \alpha_{mb} \quad (9)$$

From eq. (9), α_m is contributed by components A and B. Additionally, the quantity of contribution for each component A and B is dependent on both the product of the magnitude of the molecular-mixed region and the ratio of the flow rate for the component to the overall flow rate.

The relations of $V_a/V = q_a/q$ and $V_b/V = q_b/q$ are observed from eqs (2) and (9). Thus,

$$\tau_a = \tau_b = V/q = \tau \quad (10)$$

can be obtained.

By taking the component A balance in the A_2V_a region

$$\frac{dA_2V_aC_{as}}{dt} = q_aC_{a0} + (\partial V_{sa}/\partial t)C_{as} - A_2q_aC_{as} \quad (11)$$

At the steady state, eqs (3) and (11) can be derived as

$$C_{as} = C_{a0} \quad (12)$$

The concentration in the completely segregated region is inferred from this equation to be equal to the feed concentration for chemical species A, and the chemical reaction does not take place in this region. Following similar treatment, the component B balance in the B_2V_b region is

$$\frac{dB_2V_bC_{bs}}{dt} = q_bC_{b0} + (\partial V_{sb}/\partial t)C_{bs} - B_2q_bC_{bs} \quad (13)$$

At the steady state, eqs (5) and (13) are combined to get

$$C_{bs} = C_{b0} \quad (14)$$

By taking the component A balance in the $\alpha_m V$ region,

$$\frac{d\alpha_m VC_{am}}{dt} = -\left(\frac{\partial V_{sa}}{\partial t}\right)C_{as} - \alpha_m q C_{am} + \alpha_m V \gamma_a \quad (15)$$

Substituting eqs (7) and (12) into eq. (15) yields

$$\alpha_m V \frac{dC_{am}}{dt} = \left(\frac{\partial V_{sa}}{\partial t} + \frac{\partial V_{sb}}{\partial t}\right)C_{am} - \left(\frac{\partial V_{sa}}{\partial t}\right)C_{a0} + \alpha_m V \gamma_a \quad (16)$$

From eqs (3) and (5) at the steady state, we have

$$\frac{\partial V_{sa}}{\partial t} = A_2q_a - q_a = -\alpha_{ma}q_a \quad (17)$$

$$\frac{\partial V_{sb}}{\partial t} = B_2q_b - q_b = -\alpha_{mb}q_b \quad (18)$$

Furthermore, eqs (17) and (18) are substituted into eq. (16),

$$\frac{dC_{am}}{dt} = \frac{1}{\tau}(\delta_a C_{a0} - C_{am}) + \gamma_a \quad (19)$$

where

$$\delta_a = \frac{\alpha_{ma}q_a}{\alpha_m q}$$

Following the above procedures, the component B balance in the $\alpha_m V$ region is

$$\frac{dC_{bm}}{dt} = \frac{1}{\tau}(\delta_b C_{b0} - C_{bm}) + \gamma_a \quad (20)$$

where

$$\delta_b = \frac{\alpha_{mb}q_b}{\alpha_m q} = 1 - \delta_a$$

Thus, eqs (19) and (20) are the design equations of micromixing in the CSTR. The remaining problem is how to determine δ_a , i.e. α_{ma} and α_m . From eqs (4), (6) and (9), we have

$$\alpha_{ma} = \frac{K_a\tau}{1 + K_a\tau} \quad (21)$$

$$\alpha_m = \frac{K_a\tau}{1 + K_a\tau} \frac{q_a}{q} + \frac{K_b\tau}{1 + K_b\tau} \frac{q_b}{q} \quad (22)$$

Then,

$$\delta_a = \left[1 + \frac{K_b\tau(1 + K_a\tau)q_b}{K_a\tau(1 + K_b\tau)q_a}\right]^{-1} \quad (23)$$

The parameters of K_a and K_b are the inversion of the mixing time constants for components A and B ($t_{m,a}$ and $t_{m,b}$) which were previously obtained by Corrisson (1957).

$$t_{m,a} = \frac{1}{2} [3(5/\pi)^{2/3}(L_s^2/\varepsilon)^{1/3} + (v_a/\varepsilon)^{1/2} \ln N_{sc,a}] \quad (24)$$

and

$$t_{m,b} = \frac{1}{2} [3(5/\pi)^{2/3}(L_s^2/\varepsilon)^{1/3} + (v_b/\varepsilon)^{1/2} \ln N_{sc,b}] \quad (25)$$

where L_s is the length scale of segregation, ε is the rate of turbulent energy dissipation per unit of mass, v is

the kinematic viscosity and N_{sc} is the Schmidt number.

In eqs (24) and (25), the first term on the right-hand side is the turbulent mixing time, and the second term is the molecular mixing time for each component. Hence the mass diffusion rate in the segregated region for each component is different. The mixing time constants for components A and B are consequently different from each other.

It is important to note that δ_a depends not only on $K_a\tau$ and $K_b\tau$ but also on q_b/q_a . For the case that $K_a = K_b$, then the MURM is reduced to the URM. It is implied that the diffusion rate from the completely segregated region to the molecular-mixed region for chemical species A and B cannot be discriminated. In the MURM, the above constraint does not exist. So the MURM can be used to study the effect of micro-mixing on multiplicity.

3. APPLICATION TO AUTOCATALYTIC REACTIONS

The reaction system is considered as $A + B \rightarrow (\eta + 1)B + \text{product}$, and the reaction rate is $-\gamma_a = kC_a^p C_b^r$, where η is a stoichiometric coefficient. Once the feed contains two unpremixed feeds A and B, the steady-state performance in the molecular-mixed region becomes

$$0 = \frac{1}{\tau} (\delta_a C_{a0} - C_{am}) - k C_{am}^p C_{bm}^r \quad (26)$$

and

$$0 = \frac{1}{\tau} [(1 - \delta_a) C_{b0} - C_{bm}] + \eta k C_{am}^p C_{bm}^r. \quad (27)$$

The relation of C_{am} and C_{bm} can be written as

$$C_{bm} = (1 - \delta_a) C_{b0} + \eta (\delta_a C_{a0} - C_{am}). \quad (28)$$

Define Y_m to be the conversion in the molecular-mixed region for component A as

$$Y_m = \frac{-(\partial V_{sa}/\partial t) C_{a0} - q \alpha_m C_{am}}{-(\partial V_{sa}/\partial t) C_{a0}} \\ = 1 - \frac{1}{\delta_a} \frac{C_{am}}{C_{a0}}$$

or

$$C_{am} = \delta_a C_{a0} (1 - Y_m). \quad (29)$$

Additionally, the conversion for the component A of the overall system is

$$Y_a = \frac{q_a C_{a0} - q_a C_{a0} (1 - \alpha_{ma}) - q C_{am} \alpha_m}{q_a C_{a0}}.$$

The relation of Y_a and Y_m is

$$Y_a = Y_m \alpha_{ma}. \quad (30)$$

Substituting eqs (28) and (29) into eq. (26) yields

$$\frac{Y_m}{\bar{\theta}} = (1 - Y_m)^p (\lambda \bar{P} + Y_m)^r \quad (31)$$

where

$$\bar{\theta} = (\alpha_{ma}/\alpha_m)^{p+r-1} \theta \\ \theta = (kV/q) \eta^r (q_a C_{a0}/q)^{p+r-1} \\ \bar{P} = (1/\eta) (q_b C_{b0}/q_a C_{a0}) \quad (32)$$

and

$$\lambda = \alpha_{mb}/\alpha_{ma}. \quad (33)$$

4. CONDITIONS FOR MULTIPLE STEADY STATES

The stationary-state condition can be written, from eq. (31), as

$$F = (1 - Y_m)^p (\lambda \bar{P} + Y_m)^r - Y_m/\bar{\theta} = 0. \quad (34)$$

Since $dF/d\bar{\theta}$ does not vanish, when applying the singularity theory, it violates the condition for the appearance of isola and growth to mushroom, so isola and mushroom patterns are not possible. The conditions for the appearance of a hysteresis loop can be written as $F = 0$ and $dF/dY_m = 0$. Differentiating F with respect to Y_m yields

$$(1 - Y_m)^{p-1} (\lambda \bar{P} + Y_m)^{r-1} [r - \lambda \bar{P} p - (p+r) Y_m] \\ - 1/\bar{\theta} = 0. \quad (35)$$

Eliminating $\bar{\theta}$ from eqs (34) and (35) obtains

$$(p+r-1) Y_m^2 + [1 + \lambda \bar{P} (p-1) - r] Y_m + \lambda \bar{P} = 0. \quad (36)$$

The roots of eq. (36), denoted as \bar{Y} , are

$$\bar{Y} = \frac{-[1 + \lambda \bar{P} (p-1) - r] \pm \{[1 - r + \lambda \bar{P} (p-1)]^2 - 4\lambda \bar{P} (p+r-1)\}^{0.5}}{2(p+r-1)}. \quad (37)$$

Since \bar{Y} must be real and $0 < \bar{Y} < 1$, the necessary conditions for \bar{Y} to exist are

$$p+r-1 - \lambda \bar{P} > 0 \\ r-1 - \lambda \bar{P} (p-1) > 0 \quad (38)$$

and

$$[1 - r + \lambda \bar{P} (p-1)]^2 - 4\lambda \bar{P} (p+r-1) > 0.$$

In order to find the boundaries of $\bar{\theta}$, denoted as $\bar{\theta}_1$ and $\bar{\theta}_2$, eq. (37) is substituted into eq. (34),

$$\bar{\theta}_1, \bar{\theta}_2 = \frac{\bar{Y}}{(1 - \bar{Y})^p (\lambda \bar{P} + \bar{Y})^r}. \quad (39)$$

Therefore, the sufficient condition for multiplicity is

$$\bar{\theta}_1 < \bar{\theta} < \bar{\theta}_2. \quad (40)$$

The necessary and sufficient conditions for the system to have multiplicity are obviously a combination of conditions (38) and (40). The violation of any of the

conditions in conditions (38) and (40) would guarantee the uniqueness of the system.

easily obtained. On the other hand, if α and λ are given ($\lambda \neq 1$), then the corresponding $K_a\tau$ and $K_b\tau$ can be computed by

5. NUMERICAL CALCULATION AND GRAPHICAL REPRESENTATION

The parameters α and λ are defined here for the sake of convenience. Define

$$\alpha = K_b\tau / K_a\tau \tag{41}$$

and

$$\lambda = \alpha_{mb} / \alpha_{ma} = \frac{K_b\tau(1 + K_a\tau)}{K_a\tau(1 + K_b\tau)} \tag{42}$$

Note that, once $K_a\tau$ and $K_b\tau$ are given, α and λ can be

$$K_a\tau = \frac{\alpha - \lambda}{\alpha(\lambda - 1)} \tag{43}$$

and

$$K_b\tau = \frac{\alpha - \lambda}{\lambda - 1} \tag{44}$$

A system with a particular set of $(p, r, \bar{P}, \bar{\theta})$ can be easily verified for its multiplicity or uniqueness by examining the criteria. Figures 2 and 3 show the effect of α and λ on the bifurcation curve in the (r, \bar{P}) plane when $p = 1$, and the (r, p) plane when $\bar{P} = 0.1$, respec-

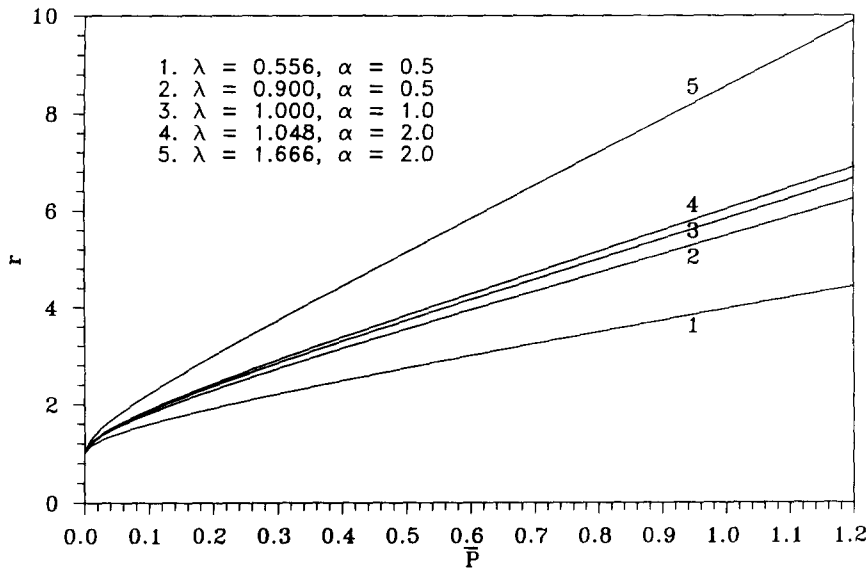


Fig. 2. The effect of λ on the bifurcation curves in the (r, \bar{P}) plane while $p = 1$.

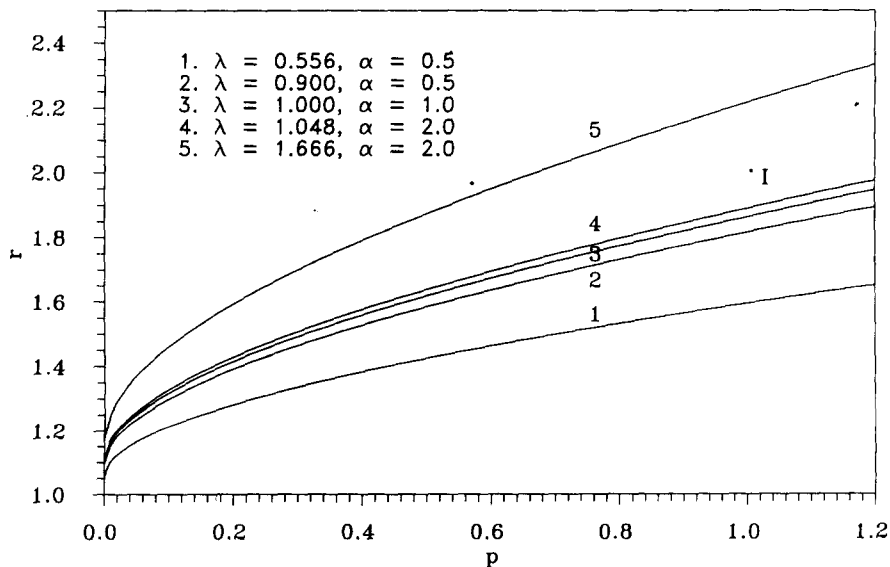


Fig. 3. The effect of λ on the multiplicity region in the (p, r) plane while $\bar{P} = 0.1$.

tively. The multiple steady states occur in the regions above the bifurcation curve. On the other hand, the unique steady state arises in the region below the bifurcation curve. From Figs 2 and 3, when λ is increasing (decreasing), the region of multiplicity is decreasing (increasing). Additionally, the region of multiplicity for $\alpha > 1$ ($\alpha < 1$) is always smaller (larger) than that of the ideal mixing.

Figure 4 indicates the effect of λ on Y_m as a function of θ for the reaction system $(p, r) = (1, 2)$ once $\alpha = 2$, $\bar{P} = 0.1$ and $q_b/q_a = 1$. Multiplicity occurs once $\lambda < 1.048$. And the unique steady state occurs when $\lambda = 1.5$ and $\lambda = 1.666$. This situation can also be confirmed by Fig. 3. Figure 4 corresponds to the system operating at point I in Fig. 3. Point I is situated above the bifurcation curve for $\lambda = 1.05$ and below the bifur-

cation curve for $\lambda = 1.5$ (the bifurcation curve for $\lambda = 1.5$ is omitted in Fig. 3). Multiplicity apparently occurs once $\lambda < 1.05$, and uniqueness occurs once $\lambda > 1.5$.

Figure 5 shows the case where $(p, r) = (1, 1.86)$ when $\alpha = 0.9$, $\bar{P} = 0.1$, and $q_b/q_a = 1$ ($K_a\tau$ is variable). The multiple steady state occurs for $\lambda < 0.931$ ($K_a\tau < 0.5$) and the unique steady state occurs for $\lambda > 0.99$ ($K_a\tau > 10$). Under the conditions that $K_a\tau = 10$, $\bar{P} = 0.1$, and $q_b/q_a = 1$ (α is variable), as shown in Fig. 6, the multiple steady state occurs for $\lambda < 0.917$ ($\alpha < 0.5$), and the unique steady state occurs for $\lambda > 1$ ($\alpha > 1$). Figure 7 shows the exact multiplicity regions in the (θ, r) plane with $p = 1$, $\bar{P} = 0.1$ and $q_b/q_a = 1$. The multiplicity region is observed to have shifted to the right (left) once λ increases (decreases).

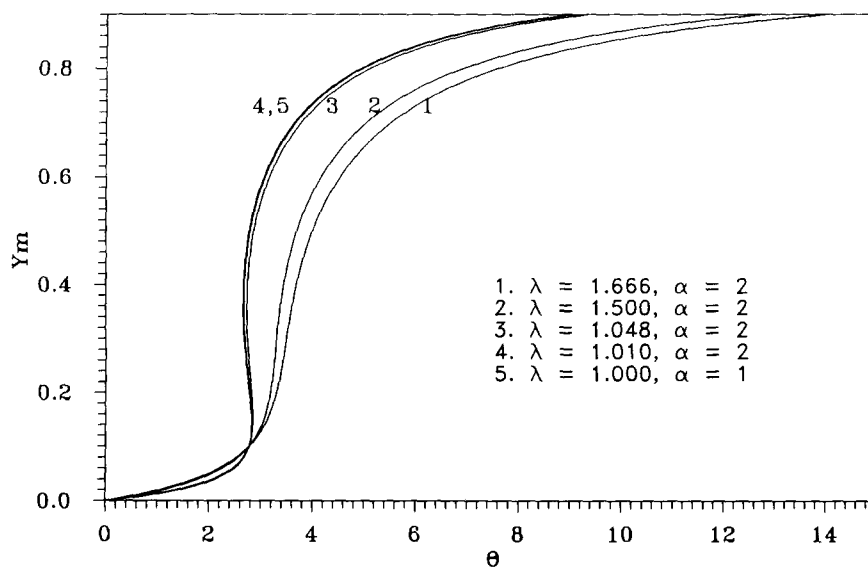


Fig. 4. The effect of λ on Y_m as a function of θ , while $p = 1$, $r = 2$, $\bar{P} = 0.1$, $\alpha = 2$ and $q_b/q_a = 1$.

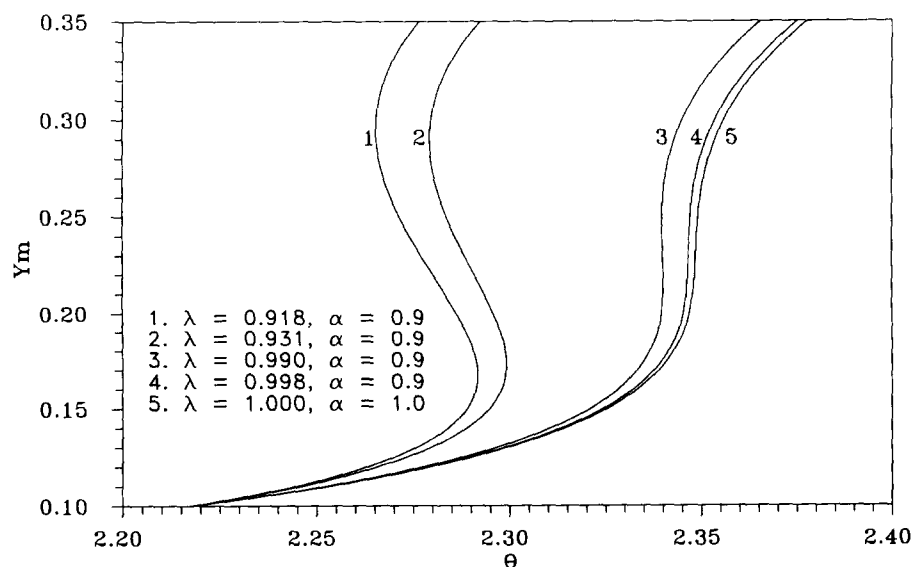


Fig. 5. The effect of λ on Y_m as a function of θ ($K_a\tau$ is variable), while $p = 1$, $r = 1.86$, $\bar{P} = 0.1$, $\alpha = 0.9$ and $q_b/q_a = 1$.

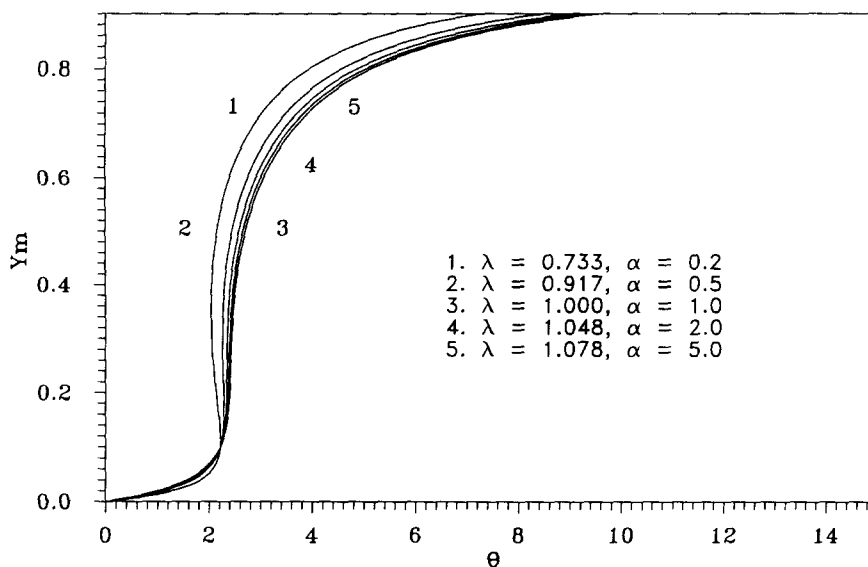


Fig. 6. The effect of λ on Y_m as a function of θ (α is variable), while $p = 1$, $r = 1.86$, $\bar{P} = 0.1$, $K_a\tau = 10$ and $q_b/q_a = 1$.

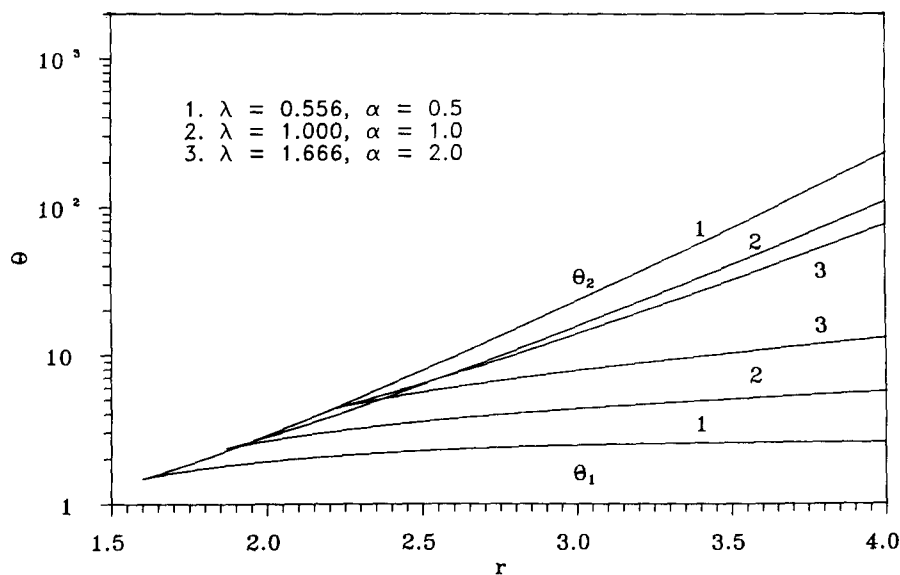


Fig. 7. The effect of λ on the lower boundary θ_1 and upper boundary θ_2 for θ to have multiplicity, while $p = 1$, $\bar{P} = 0.1$, $K_a\tau = 0.2$ and $q_b/q_a = 1$.

6. CONCLUSION

The model of the MURM was derived in the present study. The MURM could be easily employed for solving the problem of steady-state multiplicity in a nonideal CSTR. The original URM could not solve the above problem. On the other hand, the other micromixing models require much more computation time and mathematical treatment. Additionally, the analytic results could not be obtained from other micromixing models. An ideal mixing situation could not be achieved in a CSTR in terms of real application; therefore, these observed results could be used in a chemical reactor design.

From the above analysis, the conditions for multiplicity show no discrepancy between an ideal mixing and a nonideal mixing once $\lambda = 1$. However, the necessary and sufficient conditions are different from each other once λ is not equal to 1. The value λ becomes larger (smaller) than 1 as a response to the multiplicity region's decrease (increase). The magnitude of feed species B entering the maximum-mixed region becomes more (less) than that of feed species A whenever λ becomes larger (smaller) than 1. This autocatalytic reaction indicates that the effect on multiplicity is more decreased (increased) than that of ideal mixing. In the URM, λ is equal to 1, and the

effect of micromixing on the steady-state multiplicity is not displayed since this URM has considered every chemical species as having the same mixing time constant.

NOTATION

A	chemical species for A
B	chemical species for B
C	concentrations, mol/m ³
k	reaction rate constant, (mol/m ³) ^{1-p-r} /s
K_a	inversion of the mixing time constant of chemical species A, s ⁻¹
K_b	inversion of the mixing time constant of chemical species B, s ⁻¹
L_s	length scale of segregation
m	fraction of the total volume in the perfect mixing
N_{sc}	Schmidt number
p	reaction order
\bar{P}	defined in eq. (32)
q	flow rate, m ³ /s
r	reaction order
V	volume, m ³
Y	conversion

Greek letters

α	defined in eq. (41)
α_m	degree of complete mixing
α_{ma}	degree of micromixing for A
α_{mb}	degree of micromixing for B
$-\gamma_a$	reaction rate per unit of reactor volume in the active space
δ	defined in eq. (19)
ε	rate of turbulent energy dissipation per unit mass, m ² /s ³
η	stoichiometric coefficient
θ	defined in eq. (32)
$\bar{\theta}$	defined in eq. (32)
λ	defined in eq. (42)
ν	kinematic viscosity, m ² /s
τ	defined in eq. (10)

Subscripts

0	feed concentration
1	completely segregated region
2	maximum mixedness region
a	chemical species A
b	chemical species B
m	in maximum mixedness region
s	in completely segregated region

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