

The Effect of Micromixing on the Start-up Problem for an Autocatalytical Reaction of CSTR

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Abstract

This paper has analyzed the effect of micromixing of the Modified Universal Reaction Model (**MURM**) on the start-up problem for an autocatalytical reaction, $A + B \rightarrow (h + 1)B + \text{products}$, with an overall rate expression given by $-g_a = KC_a^p C_b^r (p > 0, r > 0)$ in a continuous-flow stirred tank reactor (CSTR) with two unpremixed feeds of autocatalytical species. Using the method of twice roots of discriminator, we obtain the necessary and sufficient conditions for multiplicity and uniqueness and an operated strategy of a high conversion and unique steady state. Furthermore, we have discussed that the effect of micromixing on the start-up parameter and mixing parameter.

1. Introduction

The exact multiplicity criteria for autocatalytical reactions in a perfectly mixed CSTR had been published [3,4]. However, these criteria can only be applied toward the situation in which CSTR is perfect mixing. Recently, the effect of macromixing and micromixing of two unpremixed feeds on the necessary and sufficient conditions for multiplicity in a CSTR have been studied by Chien and Liou [1] and Liou and Chien [5].

The original idea of **MURM** from **URM** (the Universal Reaction Model) that was developed by Miyawaki et al. [14]. The merits of **URM** include the corresponding with physical meaning, ease of use and no loss of accuracy, furthermore, using **URM** does not need an initial guess of mean concentration by using the mixing model of **IEM** (Interaction by exchange with the mean [15]). However, the shortcoming of **URM** lies in the fact that it considers each chemical species has the same mixing time constant, therefore, the **URM** cannot be applied towards understanding the phenomena of steady-state multiplicity with micromixing. **MURM** considers that each of the chemical species has 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 [5].

Recently, Liou and Chien [6] studied the effect of macromixing on the start-up problem of an isothermal autocatalytical reaction by using the modified Cholette model. In this note, we employ **MURM** to discuss the effect of micromixing on the start-up problem of the above reaction system.

2. Review MURM

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.

In Fig. 1, a distribution concentration-volume in a lump of the **MURM** as well as the **URM**, is assumed to be the same volume for each cell in an isotropic stirred vessel. Unpremixed chemical species **A** and **B** feed in 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 other diffuse into the molecular 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, \mathbf{a}_m , is defined as the relative volume ratio of the summation of $A_1 V_a$ and $B_1 V_b$ to the total volume system. This definition is true in the light of the fact that the molecular-mixed regions are homogeneous. In an isotropic stirred vessel, \mathbf{a}_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**, dV_{sa}/dt and dV_{sb}/dt , by Eqs. (1a) and 1(b), respectively:

$$dV_{sa}/dt = -K_a A_2 V_a \quad (1a)$$

$$dV_{sb}/dt = -K_b B_2 V_b \quad (1b)$$

where K_a and K_b are the inversion of the mixing time constant 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 \mathbf{a}_m are the primary difference between the **URM** and **MURM**.

The following equations under the above assumptions are derived;

$$\begin{aligned} A_1 &= \mathbf{a}_{ma}, \\ A_2 &= 1 - \mathbf{a}_{ma}, \\ B_1 &= \mathbf{a}_{mb}, \\ B_2 &= 1 - \mathbf{a}_{mb} \end{aligned} \quad (2)$$

and

$$\mathbf{a}_m V = A_1 V_a + B_1 V_b = \mathbf{a}_{ma} V_a + \mathbf{a}_{mb} V_b$$

where V is the volume of a lump, V_a and V_b are the volumes of each components **A** and **B** in a lump, and \mathbf{a}_{ma} and \mathbf{a}_{mb} are the degree of micromixing for chemical species, **A** and **B**, respectively.

By taking the mass balances in $A_2 V_a$ and $B_2 V_b$ at the steady state (the density is assumed to be constant), respectively we obtain

$$A_2 = 1 - \mathbf{a}_{ma} = 1/(1 + K_a t_a) \quad (3a)$$

$$\text{and } B_2 = 1 - \mathbf{a}_{mb} = 1/(1 + K_b t_b) \quad (3b)$$

where $t_a = V_a / q_a$ and $t_b = V_b / q_b$. By using Eqs. (2), (3) and (4) and taking the total mass balance in the $\mathbf{a}_m V$ region at the steady state, we obtain

$$\mathbf{a}_m q = \mathbf{a}_{ma} q_a + \mathbf{a}_{mb} q_b \quad (4)$$

The relations of $V_a / V = q_a / q$ and $V_b / V = q_b / q$ are observed from Eqs. (2) and (4). Thus,

$$t_a = t_b = t = V / q \quad (5)$$

can be obtained. By taking the component balances for **A** and **B** in the $A_2 V_a$ and $B_2 V_b$ regions at the steady state, respectively we obtain

$$C_{as} = C_{a0} \quad (6a)$$

and

$$C_{bs} = C_{b0} \quad (6b)$$

Remark 1

K_a and K_b are the inversion of the mixing time constant for **A** and **B** (t_{ma} and t_{mb}) component,. Furthermore, t_{ma} and t_{mb} which were previously obtained [2].

$$t_{ma} = \frac{1}{2} \left[3(5/p)^{2/3} (L_s^2 / \epsilon)^{1/3} + (\mathbf{n}_a / \epsilon)^{1/2} \ln N_{sc,a} \right] \quad (7a)$$

and

$$t_{mb} = \frac{1}{2} \left[3(5/p)^{2/3} (L_s^2 / \epsilon)^{1/3} + (\mathbf{n}_b / \epsilon)^{1/2} \ln N_{sc,b} \right] \quad (7b)$$

where L_s is the length scale of the segregation, ϵ is the rate of turbulent energy dissipation per unit mass, \mathbf{n} is the kinematic viscosity, and N_{sc} is the Schmidt number. In Eqs. (7a) and (7b), 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.

The **MURM** considers that each of the chemical species has its own mixing time constant, therefore, the **MURM** can be applied to understanding the effect of the micromixing on the steady-state multiplicity under the

situation of two separate reactant feed streams.

Remark 2

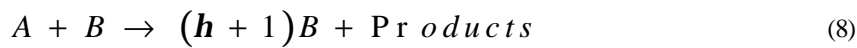
Mehta and Tarbell [12.13] considered that the molecular mixing time for each component is the same in the second term of the right hand in Eqs 7(a) and 7(b). They also discussed that the relations of the inversion of the mixing time constant, K , in the **URM** [14] and the parameters of the other micromixing models exist as follows:

$$\begin{aligned} K &= R_s \text{ (} R_s \text{ is the mass transfer coefficient in the Four Environment} \\ &\quad \text{Model of Mehta and Tarbell [12.13].} \\ &= 1/t_m \text{ (} t_m \text{ is the mixing time constant in turbulent theory} \\ &\quad \text{of Corrsin [2])} \\ &= 1/(2 t_m) \text{ (} t_m \text{ is the micromixing parameter of the IEM model} \\ &\quad \text{in Plasari et al. [16]).} \end{aligned}$$

Therefore, if the mixing conditions (L_s , e , n_a , n_b , $N_{sc,a}$ and $N_{sc,b}$) were known we can decide K_a and K_b from Eqs. 7(a) and 7(b), respectively. Thus, the parameters a_{ma} , a_{mb} or a_m can be determined from Eqs. (2), (3) and (4), respectively.

3. Mathematical model

An autocatalytic reaction of the type is considered as



with the overall rate expression given by

$$-g_a = k C_a^p C_b^r \quad (p > 0, g > 0) \quad (9)$$

occurring in an isothermal CSTR. h is stoichiometric coefficient and k is reaction rate constant. p and g are apparent reaction orders.

The mass balance equations for components **A** and **B** in the molecular-mixed region by using **MURM** at the steady state can be written as

$$0 = \frac{1}{t} (d_a C_{a0} - C_{am}) - k C_{am}^p C_{bm}^r \quad (10)$$

and

$$0 = \frac{1}{t} (d_b C_{b0} - C_{bm}) - k C_{am}^p C_{bm}^r \quad (11)$$

respectively where

$$d_a = (a_{ma} q_a / a_m q) = \left[1 + \frac{K_b t (1 + K_a t) q_b}{K_a t (1 + K_b t) q_a} \right]^{-1} \quad (12)$$

and

$$\mathbf{d}_b = (\mathbf{a}_{mb}q_b / \mathbf{a}_m q) = 1 - \mathbf{d}_a. \quad (13)$$

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

$$C_{bm} = (1 - \mathbf{d}_a)C_{b0} + \mathbf{h}(\mathbf{d}_a C_{a0} - C_{am}) \quad (14)$$

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

$$X_m = 1 - \frac{1}{\mathbf{d}_a} \frac{C_{am}}{C_{a0}}$$

or

$$C_{am} = \mathbf{d}_a C_{a0} (1 - X_m) \quad (15)$$

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

$$X_a = [q_a C_{a0} - q_a C_{a0} (1 - \mathbf{a}_{am}) - q C_{am} \mathbf{a}_m] / (q_a C_{a0}) \quad (16)$$

The relation of X_a and X_m is

$$X_a = X_m \mathbf{a}_{ma} \quad (17)$$

Note $0 \leq X_a \leq X_{ma} \leq 1$ exists.

Substituting Eqs. (11) to (15) into Eq. (10), we can obtain

$$\frac{X}{Aq} = (1 - X)^p (T + X)^r \quad (18)$$

where

$$T = (\mathbf{a}_{mb} / \mathbf{a}_{ma}) (1/h) (q_b C_{b0} / q_a C_{a0}) \quad (19)$$

$$q = (kV / q) \mathbf{h}^r C_{a0}^{p+r-1} \quad (20)$$

$$A = (\mathbf{a}_{ma} / \mathbf{a}_m)^{p+r-1} \quad (21)$$

The left-hand side of Eq. (18) can be regarded as the dimensionless net input of **A** into the reactor by the liquid flow, while the right hand side as the dimensionless consumption rate of **A** by the chemical reaction. From Eq. (18), Damkohler number (q) of the ideal mixing is modified to modified Damkohler number (Aq) of the micromixing.

Thus, we use the method of twice roots of discriminator (Liou and Chien, 1996) to explore the conditions for uniqueness and multiplicity as follows: (the detail deriviation is omitted)

Necessary conditions for uniqueness in terms of T

The uniqueness conditions in terms of the parameter T as follows:

- (a) all T for $a = 0$
- (b) $T \geq -c^2 / (4a)$ for $a < 0$ and $b = 0$ (22)
- (c) $T^- \leq T \leq T^+$ for $a < 0$ and $b = 0$

Necessary conditions for multiplicity in terms of T

- (a) all T for $a > 0$

$$(b) \quad T < -c^2/(4a) \quad \text{for } a < 0 \text{ and } b = 0 \quad (23)$$

$$(c) \quad T < T^- \text{ or } T > T^+ \quad \text{for } a < 0 \text{ and } b = 0$$

where

$$T = (r-1)^2/4r \quad \text{When } p = 1 \quad (24)$$

$$T^+ \text{ and } T^- = \left[\left(\sqrt{rp} \pm \sqrt{r+p-1} \right) / (1-p) \right]^2 \quad \text{When } p \neq 1 \quad (25)$$

and

$$a = 1 - p - r \quad (26a)$$

$$b = 1 - p \quad (26b)$$

$$c = r - 1 \quad (26c)$$

Sufficient condition for multiplicity in terms of q

$$q_1/A = S_1 / \left[(1-S_1)^p (T+S_1)^r \right] \quad (27a)$$

$$q_2/A = S_2 / \left[(1-S_2)^p (T+S_2)^r \right] \quad (27b)$$

Note $S_1 < S_2$ and $q_1 > q_2$. Therefore, the sufficient condition for multiplicity is

$$q_2/A < q < q_1/A \quad (28)$$

Sufficient condition for uniqueness in terms of q

$$q \geq q_1/A \text{ and } q \leq q_2/A \quad (29)$$

Necessary and Sufficient Conditions for Uniqueness and Multiplicity

The necessary and sufficient conditions for the system to have multiplicity are obviously the combination of conditions (23) and (28). The violation of any of the conditions in condition (23) and (28) would guarantee the uniqueness of the system.

Start-up Strategy for a high conversion and uniqueness

From the above results, when the reaction orders and stoichiometric coefficients (p , r and h) are known, a , b and c can be determined. Thus, we can use $T = (\mathbf{a}_{mb}/\mathbf{a}_{ma})(1/h)(q_b C_{b0}/q_a C_{a0})$ in terms of the operation parameters to satisfied conditions in Eq. (23) and avoid multiplicity. Thus, we can follow the operated strategy of Liou and Chien (1996) to obtain a high conversion and uniqueness. The analyzed result of Liou and Chien (1996) also applied to here as the macromixing parameters are replaced by the micromixing parameters in Table 1.

The parameters for $A = (\mathbf{a}_{ma}/\mathbf{a}_m)^{p+r-1}$ and $T = (\mathbf{a}_{mb}/\mathbf{a}_{ma})(1/h)(q_b C_{b0}/q_a C_{a0})$ of a micromixing and $A(=1)$ and $T [= q_b C_{b0}/(h q_a C_{a0})]$ of an ideal mixing are shown in Table 1 under the situation of the two unpremixed feeds. Note that the parameter T does not only depend on

$C_{b0}/(hC_{a0})$ but also depend on $(\mathbf{a}_{mb}/\mathbf{a}_{ma})$ and q_b/q_a .

4. Discussion and conclusion

(A)The mixing parameter \mathbf{a}_m effects on conversion X_a

Since $X_a = X_m \mathbf{a}_{ma}$ and $X_a < \mathbf{a}_{ma}$ at the fixed value of \mathbf{A} , a high conversion will be obtained at the high value of \mathbf{a}_m . For example, the conversion $X_a = 0.8$ ($\mathbf{a}_{ma} = \mathbf{a}_{mb} = \mathbf{a}_m = 0.8$) is larger than that of $X_a = 0.4$ ($\mathbf{a}_{ma} = \mathbf{a}_{mb} = \mathbf{a}_m = 0.4$). This result can be useful in the start-up strategy for a high conversion.

(B)The parameters of K_a and K_b effect on $\mathbf{a}_{mb}/\mathbf{a}_{ma}$ of the start-up parameter \mathbf{T}

From Eqs. 3(a) and (3b), we obtain

$$\mathbf{a}_{mb}/\mathbf{a}_{ma} = \frac{K_b \mathbf{t}}{1 + K_b \mathbf{t}} \bigg/ \frac{K_a \mathbf{t}}{1 + K_a \mathbf{t}}$$

Case (i) $K_a \mathbf{t}, K_b \mathbf{t} \rightarrow \infty$ ($t_{ma}, t_{mb} \rightarrow 0$)

In this case, an ideal mixing exists and $\mathbf{a}_{mb}/\mathbf{a}_{ma} = 1$ does not effect on the start-up parameter \mathbf{T} .

Case (ii) $K_a = K_b$ ($t_{ma} = t_{mb}$)

In this case, a nonideal mixing exists but $\mathbf{a}_{mb}/\mathbf{a}_{ma} = 1$ does not effect on the start-up parameter \mathbf{T} .

Case (iii) $K_a \mathbf{t}, K_b \mathbf{t} \ll 1$ ($t_{ma}, t_{mb} \gg 1$)

In this case, $\mathbf{a}_{mb}/\mathbf{a}_{ma} \rightarrow K_a/K_b$ exists and \mathbf{T} depends on the values of K_a and K_b .

From the above analysis results, the microimixing parameter, $\mathbf{a}_{mb}/\mathbf{a}_{ma}$, effects on the necessary conditions for multiplicity can be discussed as follows:

In Table 1, the parameter \mathbf{T} depends on the micromixing parameter $\mathbf{a}_{mb}/\mathbf{a}_{ma}$ in situation of a nonideal mixing. Additionally, it is shown that the parameter \mathbf{T} is significant on the cases (b) and (c) in condition (23) for multiplicity, i.e., $\mathbf{T} < -c^2/(4a)$ and $\mathbf{T} < \mathbf{T}^-$ or $\mathbf{T} > \mathbf{T}^+$, respectively. Therefore, if the effective feed of \mathbf{B} is more larger than the effective feed of \mathbf{A} , $\mathbf{a}_{mb}/\mathbf{a}_{ma} > 1$, it may change the uniqueness ($\mathbf{T}^- \leq \mathbf{T} \leq \mathbf{T}^+$) in an ideal mixing into multiplicity ($\mathbf{T} > \mathbf{T}^+$) in a nonideal mixing. On the other hand, when the effective feed of \mathbf{B} is smaller than the effective feed of \mathbf{A} , $\mathbf{a}_{mb}/\mathbf{a}_{ma} < 1$, this result may change the uniqueness of a system ($\mathbf{T} \geq -c^2/(4a)$ or $\mathbf{T}^- \leq \mathbf{T} \leq \mathbf{T}^+$) in an ideal mixing into a system of multiplicity ($\mathbf{T} < -c^2/(4a)$ or $\mathbf{T} < \mathbf{T}^-$) in a nonideal mixing. When $\mathbf{a}_{mb}/\mathbf{a}_{ma} = 1$, the start-up problem for \mathbf{T} is not different between $\mathbf{a}_{mb} = \mathbf{a}_{ma} = 1$ of the ideal mixing and $\mathbf{a}_{mb} = \mathbf{a}_{ma} \neq 1$ of the nonideal mixing.

(C) The micromixing parameter $\mathbf{a}_{mb}/\mathbf{a}_{ma}$ effects on the sufficient condition for multiplicity

From Eq. (21), we obtain

$$A = (\mathbf{a}_{ma} q_a / \mathbf{a}_m q)^{p+r-1} = [\mathbf{a}_{ma} / (\mathbf{a}_{ma} (q_a / q) + \mathbf{a}_{mb} (q_b / q))]^{p+r-1}$$

It can be classified into the three cases (i) $A < 1$ (ii) $A = 1$ and (iii) $A > 1$.

case (i) $A < 1$ ($\mathbf{a}_{ma} < \mathbf{a}_m$)

The parameter A in an ideal mixing ($A=1$) changes uniqueness ($Aq > q_1$) to multiplicity ($Aq \leq q_1$) in a nonideal mixing ($A < 1$).

case (ii) $A = 1$ ($\mathbf{a}_{ma} = \mathbf{a}_{mb} = \mathbf{a}_m \neq 1$)

The sufficient condition for uniqueness of start-up problem does not depend on A in a non-ideal mixing.

case (iii) $A > 1$ ($\mathbf{a}_{ma} > \mathbf{a}_m$)

The parameter A in an ideal mixing ($A=1$) changes uniqueness when $Aq < q_2$ to multiplicity when $Aq \geq q_2$ in a nonideal mixing ($A > 1$).

Remark 3

The operation conditions, $q_a = q_b = q/2$ and $p+r-1 > 0$ is usually encountered. We obtain $A > 1$, $A = 1$ or $A < 1$ under $\mathbf{a}_{mb}/\mathbf{a}_{ma} = 1$, $\mathbf{a}_{mb}/\mathbf{a}_{ma} = 1$ or $\mathbf{a}_{mb}/\mathbf{a}_{ma} > 1$, respectively since

$$A = \left[\frac{1}{(q_a / q) + (\mathbf{a}_{mb}/\mathbf{a}_{ma})(q_b / q)} \right]^{p+r-1}$$

In this paper, we employ **MURM** to study the effect of the micromixing on an operated strategy of a high conversion and unique steady-state for an autocatalytical reaction, $A + B \rightarrow (h+1)B$ + products with an overall rate expression given by $-g_a = KC_a^p C_b^r$ ($p > 0, r > 0$) in a CSTR with two unpremixed feeds of autocatalytical species. Generalized correlation for these parameters are needed and the model needs to be validated against experimental data relating chemical reaction to mixing conditions. Such data are not readily available in the literature. To author's knowledge, only Horak, et al. (1971), Lintz and Weber, (1980), and Lintz and Weber (1983b) discussed with the experimental of micromixing the multiplicity of the autocatalytical reactions in a CSTR. It is hoped that the mathematical presented here will encourage work in this direction.

Nomenclature

A the mixing parameter

C_{a0}, C_{b0}	feed concentrations of A and B (mol/l)
C_{am}, C_{bm}	the concentrations for component A and B in the molecular-mixed region
C_{as}, C_{bs}	the concentrations for component A and B in the segregated region
K_A, K_B	the inversion of the mixing time constant for components A and B
k	reaction rate constant
L_s	length scale of segregation
N_{sc}	Schmidt number
ρ	reaction orders of A
q	flow rate of the reacting stream of A
r	reaction orders of B
T	the start-up parameter
t_{ma}, t_{mb}	mixng time constant for component A and B
V	reactor volume
X	the conversion of the active space

Greek Letters

α_m	degree of complete mixing
q	Damkohler number
t	residence time
$-g_a$	reaction rate per unit of reactive volume
e	rate of turbulent energy dissipation per unit mass
	stoichemetric coefficients
ν	the kinematics viscosity

Subscripts

a	reactant species A
b	reactant species B
sa, sb	reactant species A and B in complete segregated region
0	initial concentration
1	molecular-mixed region
2	complete segregated region

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Table 1. A comparison of the parameter of two unpremixed feeds for ideal mixing and micromixing

Mixing	θ	A	\bar{T}
ideal mixing	$(kV/q)\mathbf{h}^r(q_a C_{a0}/q)^{p+r-1}$	1	$q_a C_{b0}/\mathbf{h}q_b C_{a0}$
micromixing	$(kV/q)\mathbf{h}^r(q_a C_{a0}/q)^{p+r-1}$	$(\mathbf{a}_{ma}/\mathbf{a}_m)^{p+r-1}$	$\mathbf{a}_{mb}q_b C_{b0}/(\mathbf{h}\mathbf{a}_{ma}q_a C_{a0})$

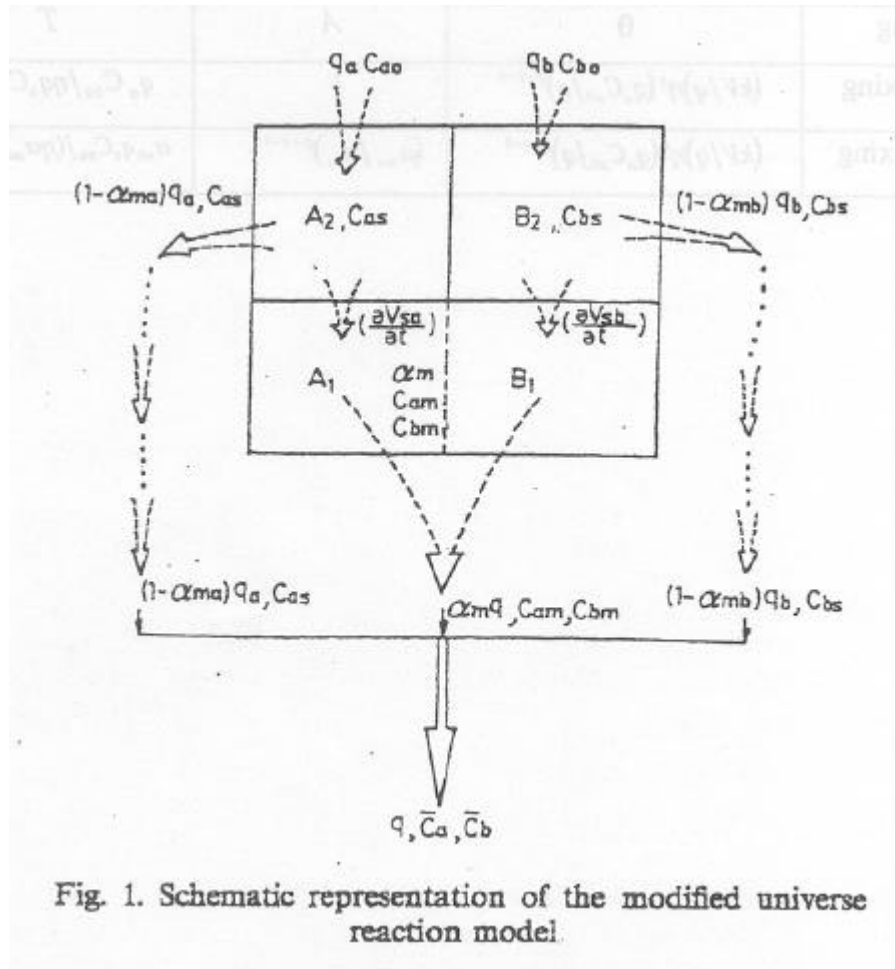


Fig. 1. Schematic representation of the modified universe reaction model.

微觀混合對自身催化反應在 CSTR 之起動-操作問題之影響

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摘 要

在本篇文章，我們使用修正單一反應模式(MURM)之微觀混合探討其對系統具有兩個非預先混合進料之CSTR，其反應型式為 $A + B \rightarrow (h+1)B + \text{產物}$ ，反應速率表示式為 $-g_a = KC_a^p C_b^r (p > 0, r > 0)$ 之起動-操作問題之影響。使用兩次的根判別式方法，我們可得到產生多重穩態與單一穩態之必要與充分條件，以及如何求得高轉化率與單一穩態之操作策略。更進一步本文也討論微觀混合對起動-操作參數與混合參數之影響。