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Dynamical Analysis of a Tubular Biochemical Reactor Infinite-Dimensional Nonlinear Model

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Abstract— **The existence and uniqueness of the state trajectories (limiting substrate and living biomass) are analyzed for a tubular biochemical reactor nonlinear model. It is reported that the trajectories exist on the whole (nonnegative real) time axis and the set of all physically feasible state values is invariant under the dynamics equations. This set takes into account the positivity of the state variables as well as a saturation condition on the substrate. Conditions which guarantee the existence of at least one nontrivial equilibrium profile are reported.**

Index Terms— **Fixed bed tubular reactor, axial dispersion biochemical reactor, equilibrium profiles, positive C_0-semigroup, invariance, nonlinear infinite dimensional systems, fixed point.**

I. INTRODUCTION

Typically axial dispersion fixed bed reactor models are derived by using mass balance principles and consist of nonlinear partial differential equations with e.g. Danckwerts type boundary conditions, see e.g. [7] , [4], [17] and references cited therein. Here we consider a tubular biochemical reactor nonlinear model. The main nonlinearity in the model originates from the substrate inhibition term in the model equations, and is a specific rational function of the state components. The dynamical model used in the present paper describes adequately a large class of bioprocesses in tubular reactors, e.g. in wastewater treatment [15] [1] or in water treatment [2] [3].

The existence and uniqueness of the state trajectories (limiting substrate and living biomass) are analyzed for this model. It is reported that the trajectories exist on the whole (nonnegative real) time axis and the set of all physically feasible state values is invariant under the dynamics equations. This set takes into account the positivity of the state variables as well as a saturation condition on the substrate.

In addition the existence of equilibrium profiles is analyzed. A trivial equilibrium profile is shown to be the one corresponding to the reactor wash-out, i.e. a constant substrate (equal to the inlet substrate) and no biomass in the reactor. Conditions which guarantee the existence of at least one non trivial equilibrium profile are reported.

The analysis essentially uses Lipschitz and dissipativity properties of the nonlinear operator involved in the dynamics, the concept of state trajectory positivity and a specific fixed point result, see [12], [8]. The tools which are used here are similar to those used for the analysis of (plug flow or axial dispersion) nonisothermal chemical tubular reactors: see [9], [10], [11].
This approach is expected to be useful for the feedback control of such biochemical reactor models around equilibrium profiles of interest.

II. BIOCHEMICAL REACTOR DYNAMICAL MODEL

The following nonlinear model of biochemical fixed bed tubular reactor with axial dispersion is considered

$$\frac{\partial S}{\partial \tau} = D\frac{\partial^2 S}{\partial \zeta^2} - v\frac{\partial S}{\partial \zeta} - k\mu(S,X)X \tag{1}$$

$$\frac{\partial X}{\partial \tau} = -k_d X + \mu(S,X)X, \tag{2}$$

with the boundary conditions: for all $\tau \geq 0$,

$$\begin{aligned} D\frac{\partial S}{\partial \zeta}(0,\tau) - vS(0,\tau) + vS_{in} = 0 \\ \text{and} \quad \frac{\partial S}{\partial \zeta}(L,\tau) = 0. \end{aligned} \tag{3}$$

These partial differential equations (PDE's) are obtained by applying balance principles to the limiting substrate concentration $S(\zeta,\tau)$ and the living biomass concentration $X(\zeta,\tau)$ respectively. The substrate inhibition is expressed via the following law:

$$\mu(S,X) = \mu_0 \frac{S}{K_S X + S + \frac{1}{K_i}S^2}\ . \tag{4}$$

In the equations above, $D, k, k_d, K_S, K_i, S_{in}, v$ and μ_0 are positive parameters. In particular, D, v and k_d denote the axial dispersion coefficient, the superficial fluid velocity and the kinetic constant, respectively. On the other hand

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the constants k and K_S are dimensionless, whereas K_i has the dimension of a concentration. In addition the specific growth rate $\mu(S,X)$ has the dimension of the inverse of a time. Finally $\zeta \in [0,L]$ and $\tau \geq 0$ denote the spatial and time variables respectively, and L denotes the length of the reactor.

Observe that the reaction considered here is autocatalytic, i.e. the biomass is not only a product of the reaction, but also a catalyst of that reaction. This feature is modelled by the last term in the right-hand sides (RHS) of equations (1) and (2). In addition the two first terms of the RHS of equation (1) are diffusion and convection terms respectively. The removal-mortality phenomenon for the biomass is modelled by the first term of the RHS of equation (2). This corresponds to the observation that biomass aggregates reach a maximum size beyond which solid particles leave the reactor: this happens notably because of shear forces between the fluid (substrate) going through the reactor and the solid (biomass).

From a physical point of view, it is expected that the following saturation condition holds:

$$0 \quad \leq \quad S \quad \leq S_{in} \ , \tag{5}$$

where S_{in} is the inlet limiting substrate concentration. One of the contributions of this paper is to report that inequalities (5) hold for the biochemical reactor model introduced above. As usual the dynamical analysis of this model will be performed on an equivalent dimensionless infinite dimensional system description. By using the new state components

$$x_1 := \frac{S_{in} - S}{S_{in}} \quad \text{and} \quad x_2 := \frac{X}{S_{in}} \ ,$$

(where x_1 is indeed the conversion and x_2 a standardized biomass with respect to the available reacting matter S_{in}), and the new spatial and time variables

$$z := \frac{\zeta}{L} \quad \text{and} \quad t := \frac{v}{L}\,\tau \ ,$$

respectively, the model (1)-(2) can be rewritten as the following two PDE's:

$$\frac{\partial x_1}{\partial t} = \frac{1}{Pe}\,\frac{\partial^2 x_1}{\partial z^2} - \frac{\partial x_1}{\partial z} + k\tilde{\mu}(x_1,x_2)x_2 \tag{6}$$

$$\frac{\partial x_2}{\partial t} = -\gamma\, x_2 + \tilde{\mu}(x_1,x_2)x_2, \tag{7}$$

with Danckwerts boundary conditions [5]: for all $t \geq 0$,

$$\begin{aligned} &\frac{1}{Pe}\,\frac{\partial x_1}{\partial z}(0,t) - x_1(0,t) = 0 \\ &\text{and} \quad \frac{\partial x_1}{\partial z}(1,t) = 0, \ , \end{aligned} \tag{8}$$

where the modified substrate inhibition law $\tilde{\mu}(x_1,x_2)$ is given by

$$\tilde{\mu} = \beta\,\frac{(1-x_1)}{K_S\,x_2 + (1-x_1) + \alpha(1-x_1)^2} \ , \tag{9}$$

and where the constants α , β , γ and Pe (Peclet number) are given respectively by $\alpha := \dfrac{S_{in}}{K_i}$, $\beta := \dfrac{L}{v}\,\mu_0$, $\gamma := \dfrac{L}{v}\,k_d$ and $Pe := \dfrac{vL}{D}$.

Now the dimensionless model (6)–(9) can be given an infinite dimensional state space description as follows. In the real Hilbert space $L_2[0,1]$, define the linear operator:

$$\begin{aligned} A_1 : D(A_1) \quad &\rightarrow \quad L_2[0,1] \\ x_1 \quad &\mapsto \quad \frac{1}{Pe}\,\frac{d^2x_1}{dz^2} - \frac{dx_1}{dz} \end{aligned}$$

on its domain:

$D(A_1) = \Big\{x_1 \in L_2[0,1] : x_1, \dfrac{dx_1}{dz}$ are absolutely continuous such that $x_1, \dfrac{dx_1}{dz}, \dfrac{d^2x_1}{dz^2} \in L_2[0,1]$ and $\frac{1}{Pe}\,\frac{dx_1}{dz}(0) - x_1(0) = 0 = \frac{dx_1}{dz}(1)\Big\}$.

Consider also the bounded linear operator $A_2 = -\gamma I$ where I is the identity operator on $L_2[0,1]$. Therefore equations (6)–(9) can be rewritten as follows: for all $t \geq 0$,

$$\dot{x}(t) \quad = \quad Ax(t) + N(x(t)) \ , \tag{10}$$

where $x := (x_1,x_2)^T$ is a vector of the real Hilbert space $H := L_2[0,1] \oplus L_2[0,1]$ endowed by the natural induced norm and inner product, $A := \mathrm{diag}(A_1,A_2)$ is defined on its domain $D(A) = D(A_1) \oplus L_2[0,1]$ and N is the nonlinear functional defined on H by $N(x) := (N_1(x),N_2(x))$ where

$$N_1 = kN_2 \quad \text{and} \quad N_2(x_1,x_2) =$$

$$\beta\,\frac{(1-x_1)x_2}{K_S\,x_2 + (1-x_1) + \alpha(1-x_1)^2} \ . \tag{11}$$

In [17], [9], it is shown that the operator A_1 is the generator of an exponentially stable C_0-semigroup of bounded linear operators $T_1(t)$ on $L_2[0,1]$. It is easy to see that A_2 is the generator of an exponentially stable C_0- semigroup of bounded linear operators $T_2(t) = e^{-\gamma t}I$ on $L_2[0,1]$. Therefore A is the generator of an exponentially stable C_0-semigroup of bounded linear operators $T(t)$ on H given by $T(t) = \mathrm{diag}(T_1(t),T_2(t))$.

III. STATE TRAJECTORIES

The well-posedness and invariance properties of the state trajectories of the biochemical reactor dimensionless model (6)–(9) are now studied by using the description (10)–(11), i.e. a semilinear Cauchy Problem of the following form:

$$\left.\begin{array}{rcl} \dot{x}(t) & = & Ax(t) + N(x(t)) \\ x(0) & = & x_0 \in \Omega. \end{array}\right\} \tag{12}$$

where Ω, motivated by (5), is the physically admissible set given by:

$$\begin{aligned} \Omega := \{\ (x_1, x_2) \in H :\ & 0 \leq x_1 \leq 1, \\ & 0 \leq x_2 \ \text{ a. e. in } [0,1]\ \}. \end{aligned} \tag{13}$$

The main tool used in the analysis of this problem is the following theorem, which is an equivalent version of Theorem 5.1 of [12, p. 355], and which gives sufficient conditions for the existence and the uniqueness of the mild solution of a system like (12) on the whole interval $[0, +\infty)$ and for the invariance of the set Ω under the dynamics equations.

Theorem 3.1: Let $(\mathrm{X}, \|.\|)$ be a real Banach space and $\tilde{T}(t)$ a C_0-semigroup of bounded linear operators such that $\|\tilde{T}(t)\| \leq Me^{\omega t}$, for all $t \geq 0$, for some $\omega \in \mathbb{R}$ and $M \geq 1$. Let $\tilde{A}$ be the infinitesimal generator of $\tilde{T}(t)$ and $\tilde{D}$ be a closed subset of X. Assume also that $\tilde{N}$ is a continuous function from $\tilde{D}$ into X. Let us consider the following initial value problem:

$$\left.\begin{array}{rcl} \dot{x}(t) & = & \tilde{A}x(t) + \tilde{N}(x(t)) \\ x(0) & = & x_0 \in \tilde{D}. \end{array}\right\} \tag{14}$$

Assume that

i) $\tilde{D}$ is $\tilde{T}(t)$-invariant; i.e. $\tilde{T}(t)\tilde{D} \subset \tilde{D}$, for all $t \geq 0$;
ii) for all $x \in \tilde{D}$,

$$\lim_{h \to 0^+} \frac{1}{h} d(x + h\tilde{N}(x); \tilde{D}) = 0\ ;$$

iii) $\tilde{N}$ is continuous on $\tilde{D}$ and there exists $l_{\tilde{N}} \in \mathbb{R}^+$ such that the operator $(\tilde{N} - l_{\tilde{N}} I)$ is dissipative on $\tilde{D}$.

Then, (14) has a unique mild solution $x(t, x_0)$ on $[0, +\infty[$, for all $x_0 \in \tilde{D}$. Moreover, if $\mathrm{T}(t)$ is defined on $\tilde{D}$ by $\mathrm{T}(t)x_0 = x(t, x_0)$, for all $t \geq 0$ and $x_0 \in \tilde{D}$, it is a nonlinear semigroup on $\tilde{D}$, with $(\tilde{A} + \tilde{N})$ as its generator.

Remark 3.1: If $\| \tilde{T}(t) \| \leq e^{\omega t}$, then Theorem 3.1 above and Theorem 5.1 of [12, p. 355] are the same. However, if $\| \tilde{T}(t) \| \leq Me^{\omega t}$, one can define an equivalent norm in X , denoted by $| \ . \ |$, such that $| \tilde{T}(t) | \leq e^{\omega t}$. Indeed recall that the following norm

$$| x | := \sup\{e^{\omega t} \| T(t)x \|:\ \ \forall t \geq 0\}\,,$$

is equivalent to the given norm $\|.\|$ on X and $| \tilde{T}(t) | \leq e^{\omega t}$. For this new norm, $\tilde{N}$ is still continuous and $(\tilde{N} - l_{\tilde{N}} I)$ is dissipative. In addition, for all $x \in \tilde{D}$,

$$\lim_{h \to 0^+} \frac{1}{h} d_{|\,.\,|}(x + h\tilde{N}(x); \tilde{D}) = 0,$$

where $d_{|\,.\,|}$ is the metric associated with $| \ . \ |$. Therefore, Theorem 5.1 of [12, p. 355] is applicable.

It turns out that Theorem 3.1 can be applied to the biochemical reactor state space description (10)–(11) and the set Ω of physically admissible state values which is given by (13).
The following lemma can be proved quite easily by using the positivity of the C_0-semigroup $T(t)$, see [9, Lemmas 5.1 and 5.2]. The latter property may be related to the well-known maximum principle for parabolic partial differential equations with different types of boundary conditions, see e.g. [16, Corollary 2.3, p. 124].

Lemma 3.1: For all $t \geq 0,\ T(t)\Omega \subset \Omega$.

The main result reported here is also a consequence of the following additional auxiliary result.

Lemma 3.2: The function $N : \Omega \to H$ is Lipschitz continuous.

Now let Λ be a closed interval of $\mathbb{R}$ and consider the set: $K(\Lambda, L_2[0,1]) := \{\phi \in L_2[0,1] : \phi(z) \in \Lambda$ for a. a. $z \in [0,1]\}$. The proof of the following technical lemma is similar to that of [9, Proposition 3.1].

Lemma 3.3: Assume that $\Lambda = [a, b]$, $f_c : \Lambda \longrightarrow \mathbb{R}$ is a continuous function, and $f_p : [0,1] \times \Lambda \longrightarrow \mathbb{R}$ is a nonnegative bounded measurable function. If $f_c(a) \geq 0$ and $f_c(b) \leq 0$, then

$$\lim_{h \to 0^+} \frac{1}{h} d(\phi + h\mathcal{B}(\phi), K(\Lambda; L_2[0,1])) = 0\ ,$$

where the substitution operator $\mathcal{B}$ is defined on $K(\Lambda, L_2[0,1])$ by

$$[\mathcal{B}(\phi)](z) := f_p(z, \phi(z)) \cdot f_c(\phi(z))\ ,$$

for all $z \in [0,1]$, for all $\phi \in K(\Lambda, L_2[0,1])$.

The following additional lemma can be proved by using Lemma 3.3 above.

Lemma 3.4: For all $(x_1, x_2) \in \Omega$,

$$\lim_{h \to 0^+} \frac{1}{h} d((x_1, x_2) + hN((x_1, x_2)); \Omega) = 0.$$

The following theorem is one of the main results reported here. It follows from the four lemmas above, by using Theorem 3.1.

Theorem 3.2: For every $x_0 \in \Omega$, equation (10) has a unique mild solution $x(t, x_0)$ on the interval $[0, +\infty[$. Moreover, if one sets $\mathrm{T}(t)x := x(t, x_0)$, then $(\mathrm{T}(t))_{t\geq 0}$ is a strongly continuous nonlinear semigroup on Ω, generated by the operator $A + N$.

Hence the state trajectories of the tubular biochemical reactor nonlinear model given by (1)-(4) are well-defined on the whole time interval $[0, +\infty)$. Moreover the physically feasible set Ω is invariant under this model dynamics, i.e. for all $t \geq 0$, $\mathrm{T}(t)\Omega \subset \Omega$.

IV. EQUILIBRIUM PROFILES

The equilibrium profiles analysis of the biochemical reactor dimensionless model (6)–(9) can be performed by using the following fixed point theorem:

Theorem 4.1: [8] Let X be a Banach space, and let $C \subset X$ be a cone in X. Assume that Ω_1, Ω_2 are open subsets of X such that $0 \in \Omega_1, \overline{\Omega_1} \subset \Omega_2$, and let

$$T : C \cap (\overline{\Omega_2} \setminus \Omega_1) \longrightarrow C$$

be a completely continuous operator such that either

(i) $\| Tu \| \leq \| u \|, u \in C \cap \partial\Omega_1,$ and
$\| Tu \| \geq \| u \|, u \in C \cap \partial\Omega_2;$
or

(ii) $\| Tu \| \geq \| u \|, u \in C \cap \partial\Omega_1,$ and
$\| Tu \| \leq \| u \|, u \in C \cap \partial\Omega_2.$

Then T has a fixed point in $C \cap (\overline{\Omega_2} \setminus \Omega_1)$.

The equilibrium profiles $(x_1, x_2) \in \Omega$, are solutions of the following boundary value problem:

$$\frac{1}{Pe}\frac{d^2x_1}{dz^2} - \frac{dx_1}{dz} + k\tilde{\mu}(x_1, x_2)x_2 = 0 \tag{15}$$

$$-\gamma x_2 + \tilde{\mu}(x_1, x_2)x_2 = 0 \tag{16}$$

$$\frac{1}{Pe}\frac{dx_1}{dz}(0) - x_1(0) = 0 = \frac{dx_1}{dz}(1). \tag{17}$$

Obviously $(x_1, x_2) = (0, 0)$ is an equilibrium profile, i.e. $(S, X) = (S_{in}, 0)$ is an equilibrium profile of the original system (1)–(4). This trivial equilibrium corresponds to the reactor wash-out, i.e. the substrate is constant (equal to the inlet substrate) and there is no biomass in the reactor.

In the sequel we will be interested in conditions which guarantee the existence of nontrivial equilibrium profiles and especially those that satisfy the following condition: $\tilde{\mu}(x_1, x_2) = \gamma$, or equivalently

$$x_2 = \frac{\alpha}{K_S}(1 - x_1)(x_1 - \omega) \tag{18}$$

where $\omega := \dfrac{\alpha\gamma - \beta + \gamma}{\alpha\gamma}$. Equilibrium profiles (x_1, x_2) satisfying condition (18) are such that the production rate of the biomass and its removal rate are identically equal.

In order to study the existence of such equilibrium profiles and also for computational purposes, it suffices to consider the two-point boundary value problem given by the differential equation (15), with the boundary conditions (17).
This problem can be rewritten as an equivalent fixed point equation, viz.

$$x_1 = T(x_1), \quad T := -A_1^{-1}N_1 , \tag{19}$$

where the operators A_1 and N_1 are given as in Section II. Equivalently the operator T defined in (19) is given for any function $x \in C(0, 1)$ and for any $z \in [0, 1]$ by

$$[T(x)](z) = \frac{\alpha k\gamma}{K_S}\int_0^1 g(z, \eta)(1 - x(\eta))(x(\eta) - \omega)d\eta , \tag{20}$$

where the function $g(z, \eta)$ is the Green's function of the linear boundary value problem corresponding to (15), (17), viz.

$$\frac{1}{Pe}\frac{d^2x_1}{dz^2} - \frac{dx_1}{dz} = 0$$
$$\frac{1}{Pe}\frac{dx_1}{dz}(0) - x_1(0) = 0 = \frac{dx_1}{dz}(1).$$

This function is given by

$$g(z, \eta) = \begin{cases} e^{Pe(z-\eta)} & \text{if } 0 \leq z \leq \eta \leq 1 \\ \\ 1 & \text{if } 0 \leq \eta \leq z \leq 1. \end{cases}$$

An elementary analysis of this function leads to the following auxiliary result:

Lemma 4.1: For all $z \in [0, 1]$,

$$\frac{1}{Pe}\left(1 - e^{-Pe}\right) \leq \int_0^1 g(z, \eta)\, d\eta \leq 1 .$$

It turns out that Theorem 4.1 can be applied to the operator T defined by (20) on the Banach space $C(0, 1)$ of real-valued continuous functions on $[0, 1]$, equipped with the uniform norm

$$\|x\|_\infty := \max_{z\in[0,1]} |x(z)|.$$

This can be done by considering the nonnegative cone of that space, viz.

$$C := \{x \in [0, 1] : x(z) \geq 0 \ \text{ on } \ [0, 1]\},$$

and by using open neighborhoods Ω_1 and Ω_2 of the origin, that are open balls centered at the origin, viz. $\Omega_1 := B(0, \delta_1) := \{x \in C[0, 1] : \|x\|_\infty < \delta_1\}$, and

$\Omega_2 := B(0, \delta_2)$, where δ_1 and δ_2 are positive constants which can be chosen such that the conditions of Theorem 4.1 are satisfied. In particular one should have that $0 < \delta_1 < \delta_2$.

For example, when the constant ω is negative, one can choose δ_1 such that

$$\delta_1 \ \leq \ \frac{\alpha k \gamma}{K_S} \cdot \frac{1 - e^{-Pe}}{Pe} \cdot m \ ,$$

where

$$m := \min_{y \in [0, \delta_1]} [(1-y)(y-\omega)] \ ,$$

and δ_2 such that

$$\frac{\alpha k \gamma}{K_S} \cdot \frac{(1-\omega)^2}{4} \ \leq \ \delta_2 = 1.$$

Using Lemma 4.1, it can be shown that, in this case, conditions (ii) of Theorem 4.1 hold. A similar analysis can be done when ω is positive.

Using the definitions of the constants α , β , γ and Pe involved in the adimensional model, in terms of the original system parameters (see Section II), and the fact that $\mu_0 > k_d$, this analysis leads to the following result:

Theorem 4.2: Consider the biochemical reactor model (1)-(2), with the boundary conditions (3), where the substrate inhibition is described by (4).

Assume that either
(i)

$$\frac{k k_d}{4 K_S} \cdot \frac{L}{v} \cdot \left(\frac{\mu_0}{k_d} - 1 \right)^2 K_i \leq S_{in}$$

and

$$S_{in} < \left(\frac{\mu_0}{k_d} - 1 \right) K_i \ ,$$

or **(ii)**

$$\left(\frac{\mu_0}{k_d} - 1 \right) \cdot K_i < S_{in}$$

and

$$S_{in} \leq \ \frac{K_S}{k k_d} \cdot \frac{v}{L} \cdot K_i \ \ ,$$

Then the system (1)-(4) has at least one nontrivial equilibrium profile.

The above result is illustrated in Figure 1 where the following parameter values have been considered :

$$\begin{aligned} \mu_0 &= 0.4\ h^{-1}, k_d = 0.01\ h^{-1}, K_S = 1, K_i = 1\ g/l \\ D &= 10\ m/h^2, v = 1\ m/h, k = 2, S_{in} = 20\ g/l \\ L &= 1\ m \end{aligned}$$

i.e. values that meet the conditions **(i)** in Theorem 4.2.

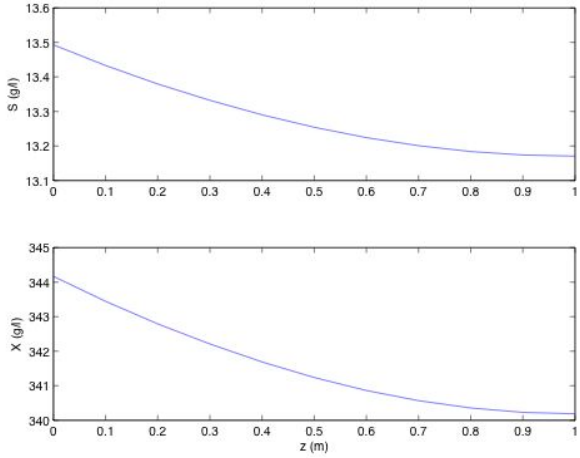

Fig.1 Nontrivial equilibrium profile

V. CONCLUDING REMARKS

Theorem 4.2 shows that the existence of at least two equilibrium profiles is guaranteed under some specific conditions on the system parameters. The existence of the state trajectories on the whole time interval $[0, +\infty)$, reported in Theorem 3.2, together with the latter result, will allow the investigation of asymptotic stability properties of equilibrium profiles for such a model.

Other existence and multiplicity conditions of equilibrium profiles for this model, as well as some numerical aspects, are currently investigated by the authors, with the objective to reach results similar to those which were proved in [11] for nonisothermal chemical reactors.

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