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# Steady thermal regimes of a parallel-plane packed bed reactor with an organized structure

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ABSTRACT

The steady conduction regime of exothermic chemical reactions in a packed bed reactor is investigated analytically. A plane-parallel stratification of the reactive granular material is assumed which modulates the rate of the local volumetric heat generation in the reactor. The approach is based on an exactly solvable nonlinear mathematical model which involves two experimentally accessible control parameters, the *intensity parameter* $\lambda > 0$ and *stratification parameter* $s \geq 0$, respectively. In terms of these parameters, the existence domain of the steady temperature solutions and the occurrence of hot spots are discussed. For a given value of the stratification parameter, an upper bound $\lambda_{max}(s)$ of the intensity parameter has been found, such that above of this maximum value of $\lambda$ the reactor becomes thermally uncontrollable. Below $\lambda_{max}(s)$, unique as well as dual solutions exist. The former ones describe high temperature steady states of the reactor, while the dual solution branches are associated with low and high temperature reaction regimes, respectively. The features of the corresponding temperature distributions are examined in detail.


## 1. Introduction

The present paper is concerned with parallel-plane packed bed reactors having a *stratified structure* in the transversal direction, and an internal *volumetric heat generation* by exothermic reactions. Model calculations are reported which apply to the *steady conduction regime* of such reactors, encountered in the chemical process engineering, in civil engineering, combustion engineering, thermal explosion control and environmental energy engineering. Specific examples in these fields are the ethanol production from cereals in anaerobic fermenters, hardening of the cement paste of massive concrete members, burning of granular fuels, thermal explosion o fine powders, degradation of organic waste materials in aerobic reactors and natural landfills, etc. Since the temperature and heat transfer control belong to the most important factors in all these processes, a special attention is given in the paper to the occurrence of hot spots [1] and to the upper bounds of the existence domain of steady solutions, [2]. The hot spots due to the excessive fermentation heat generation may decelerate the reaction by killing the yeast in the fermenter (see, e.g. [3]). During the hardening of massive concrete slabs, the hot spots due to the hydration heat release may lead to early-age thermal stresses. This may cause cracking, which in turn reduces the durability of highly expensive structures, [4–6]. In rapid-hardening cement-based fiber composites, e.g. adiabatic temperature maxima up to 140 °C have been measured, [7]. In combustion processes of fine granular materials, by contrast, where the overrunning of the *ignition temperature* is a necessary condition of the steady evolution, the occurrence of hot spots is a desired phenomenon. The upper limits of the existence domain of steady solutions represent in these processes the regime above of which the reactor becomes uncontrollable and thermal explosion occurs (see e.g. [8]).

Comparing to the classical literature on the *conduction regime* of parallel-plane packed bed reactors (see, e.g. [8] and [9]), the contribution of the present paper consists of the inclusion in the mathematical model of an *organized structure*, a *stratification* of the reactive granular material, which in turn modulates the rate of the local volumetric heat generation. In a hardening concrete slab, e.g. the plane-parallel stratification implies a gradual variation of the water/cement ratio with the transversal coordinate and, consequently, a variation of the heat released by hydration. The effect of such type of stratification on the possible steady temperature profiles of the packed bed reactors is discussed in the paper in some detail.

## 2. Basic equations and problem formulation

We consider a packed bed reactor with parallel-plane boundaries which are kept at the same constant temperature $T_0$. Be $2L$ the distance between the boundaries. The $x$-axis is perpendicular to

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**Nomenclature**

| | |
|---|---|
| $c$ | specific heat (J/kg K) |
| $E_a$ | activation energy (J) |
| $k$ | thermal conductivity (W/m K) |
| $k_B$ | Botzmann constant ($1.38 \times 10^{-23}$ J/K) |
| $K$ | integration constant |
| $K_*$ | threshold value $e^s$ of $K$ |
| $\tilde{K}_*$ | dual counterpart of $K$ |
| $L$ | half-thickness of packed bed (m) |
| $q$ | dimensionless wall heat flux |
| $Q$ | rate of volumetric heat generation (W/m$^3$) |
| $Q_{tot}$ | dimensionless rate of total heat release |
| $Q_{local}$ | dimensionless rate of local heat release |
| $s$ | stratification parameter |
| $t$ | time variable (s) |
| $T$ | absolute temperature (K) |
| $T_0$ | boundary temperature (K) |
| $W$ | dimensionless function ($W = \theta + sX$) |
| $x$ | dimensional transversal coordinate (m) |
| $X$ | dimensionless transversal coordinate ($X = x/L$) |
| $X_0$ | integration constant |

*Greek symbols*

| | |
|---|---|
| $\alpha$ | constant (K$^{-1}$) $\alpha = E_a/(k_B T_0^2)$ |
| $\lambda$ | intensity parameter |
| $\Lambda$ | dimensionless structure function of stratification ($\Lambda = \lambda\, e^{sX}$) |
| $\rho$ | density (kg/m$^3$) |
| $\theta$ | dimensionless temperature, $\theta = \alpha(T - T_0)$ |

*Subscripts*

| | |
|---|---|
| * | related to threshold value of $K$ |
| *max* | related to maximum value of $\lambda$ |

the boundaries located at $x = -L$ and $x = +L$, respectively (see Fig. 1). The reactor is filled with the mixture of a fine granular material of which composition varies with the $x$-coordinate continuously. We assume that in this *organized structure* an exothermic chemical or biochemical reaction occurs, such that the rate of the volumetric heat generation is a continuous function both of the local temperature $T$ and the coordinate $x$. The temperature field $T = T(x,t)$ in this parallel-plane reactor is governed by the Fourier equation

$$\rho c \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + Q(x, T) \tag{1}$$

where $Q(x,T)$ is the rate of volumetric heat generation by the exothermic reaction and is everywhere positive. We further assume that the density $\rho$, the specific heat $c$ and the thermal conductivity $k$ of the material are slowly varying functions of the coordinate $x$ and of reaction time $t$, such that all of them may be considered as constants.

As it is well known, the heat generated by the exothermic reaction increases in turn the reaction velocity itself, and thus it enhances the rate of heat generation continuously (positive feedback). This phenomenon is described by the Arrhenius law, which implies that the source term $Q(x,T)$ of Eq. (1) has the form

$$Q(x, T) = Q_0(x)\ e^{-(E_a/k_B T)} \tag{2}$$

Here $E_a > 0$ is the activation energy of the reaction and $k_B$ the Boltzmann constant. Assuming that the temperature inside the reactor do not differs substantially from the wall temperature $T_0$, in the exponential of Eq. (2), $1/T$ can be expanded in a Taylor series of the temperature difference $T - T_0$ and, as shown already by Frank-Kamenetzkii [9], the first order approximation $1/T \cong 1/T_0 - (T - T_0)/T_0^2$ may be applied. Thus, Eq. (2) becomes

$$Q(x, T) = \tilde{Q}_0(x)\ e^{\alpha(T - T_0)} \tag{3}$$

where $\tilde{Q}_0(x) = Q_0(x) \exp(-E_a/k_B T_0) > 0$ and $\alpha = E_a/(k_B T_0^2) > 0$.

The thermal evolution of the reactor is determined by the balance of the heat generated by the exothermic reaction and the heat extracted through the walls which are kept at the lower temperature $T_0$ (isothermal wall cooling). The latter process depends obviously on the thermal conductivity and the heat storage capacity of the reacting material. When over the heat outflow process the heat generation dominates, the temperature of the reactor increases uncontrollably. Accordingly, in the industrial practice one is interested to reach a time-independent (steady) working regime of the reactor in which between the generated and extracted heat flows an exact balance holds. In our present model, the temperature field $T = T(x)$ of this steady regime is governed by the two-point boundary value problem

$$k \frac{\mathrm{d}^2 T}{\mathrm{d}x^2} + \tilde{Q}_0(x)\ e^{\alpha(T - T_0)} = 0, \quad T(-L) = T(L) = T_0 \tag{4}$$

Now, introducing the dimensionless coordinate $X$ and the dimensionless temperature $\theta$ by the definitions $X = x/L$, $\theta(X) = \alpha(T - T_0)$, Eq. (4) becomes

$$\frac{\mathrm{d}^2 \theta}{\mathrm{d}X^2} + \Lambda(X)\ e^{\theta} = 0, \quad \theta(-1) = \theta(1) = 0 \tag{5}$$

where the notation $\Lambda(X) = \alpha\ L^2\ \tilde{Q}_0(x)/k > 0$ has been used. The dimensionless function $\Lambda(X)$ describes the way in which the structure of the packed bed is organized with respect to local intensity $\tilde{Q}_0(x)$ of the heat generation. In order to be specific, in the present model calculations we assume that the structure exhibits a *plane-parallel stratification* described by the exponential law

$$\Lambda(X) = \lambda\ e^{sX} \tag{6}$$

Here $\lambda$ and $s$ are the *control parameters* of our engineering problem. The *intensity parameter* $\lambda$ is necessarily positive (exothermic reactions), while the parameter $s$ which characterizes the stratification of the reacting material in the packed bed, may be positive, negative or zero. Hence, for a given $\lambda$, the intensity of the volumetric heat

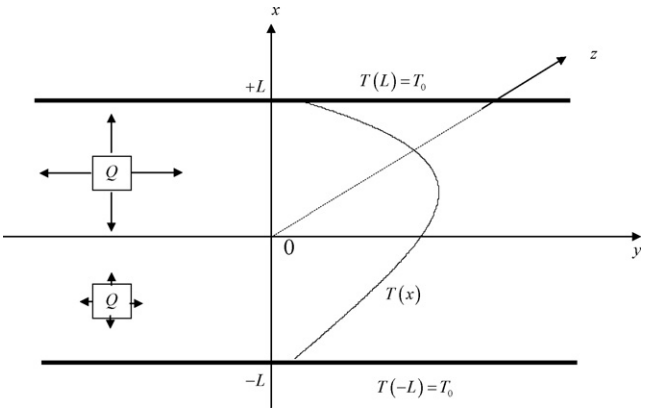


**Fig. 1.** Schematic representation of the parallel-plane reactor with coordinate system, volumetric heat generation $Q(X)$, isothermal boundary conditions $T(\pm L) = T_0$ and a typical asymmetric temperature distribution $T(x)$. Due to the stratified structure of the reactive material in the $x$-direction, the rate of the volumetric heat generation $Q(x)$ depends on the $x$ coordinate explicitly and, in spite of the symmetric boundary conditions $T(\pm L) = T_0$, the temperature profiles $T(x)$ are asymmetric with respect to the midplane of the reactor.