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Onset of convection in a horizontal porous layer driven by catalytic surface reaction on the lower wall

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ABSTRACT

The onset of convection in a horizontal layer filled with a fluid-saturated porous medium is studied in this paper. On the lower wall there is an exothermic surface reaction, described by the Arrhenius kinetics, while the upper wall is subjected to uniform temperature and concentration. The problem, cast in dimensionless form, is governed by three dimensionless parameters pertaining to the exothermic reaction and the Lewis number. Once the basic state is solved, a linearized stability analysis is then performed and the resulting eigenvalue problem is solved using a conventional shooting method. One determines numerically the critical Rayleigh and wave numbers at the onset of convection, for various values of the problem parameters.

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1. Introduction

Literature concerning convective flow in porous media is abundant. Much of the recent work in this area and more specifically to convection in fluid-saturated porous layers may be found in the recent books [1–9].

However, recent years revealed an increased interest about fluid and thermal systems where chemical reactions take place. These chemical reactions may undergo throughout the volume of (porous) region which is analyzed or along interfaces/boundaries of this region. Real-world applications include chemical engineering systems, contaminant transport in groundwater systems, or geothermal processes. The catalytic systems are modeled usually by including the description of the reaction kinetics of the catalytic process and the transport of momentum, heat, and mass coupled to this process. Concerning the transport phenomena, access to the catalyst is determined by the transport of mass and energy in a reactor. In heterogeneous catalysis, the access to the catalyst is maximized through the use of porous structures. Examples of catalytic surface reactions are methane/ammonia and propane oxidation over platinum, see for instance [10,11].

Many papers focusing on chemically reacting flows were devoted in the past to the situation where the reaction occurs in a spatially manner, see the references contained in [12]. But our interest in the present context is related to the chemical reactions which take place along interfaces/boundaries of the flow region.

In clear fluids a number of papers dealing with the effects of catalytic chemical reactions on external convective processes appeared in the last years. In [13] the free-convection boundarylayer flow at a three-dimensional stagnation point of attachment on a curved surface, due to an exothermic catalytic chemical reaction on that surface is considered. It is assumed that the flow is driven purely by heat supplied to the surrounding fluid by an exothermic catalytic chemical reaction on the surface and this reaction can be modeled using single, first-order Arrhenius kinetics. Other two important papers focusing on free-convection stagnation point driven by the same mechanism of catalytic surface reaction are [14,15], while [16,17] are studies in the same area, involving flows along vertical surfaces in viscous fluids.

Models for convective flows on reactive surfaces in porous media have been proposed for external flows by Merkin and Mahmood [18], Mahmood and Merkin [19], Minto et al. [20]. The study by Merkin and Mahmood [18] was extended by Postelnicu [21] for porous media saturated with non-Newtonian fluids. In both [18,21] bifurcation diagrams were presented for various combinations of the problem parameters and hysteresis bifurcation curves were identified, whenever they exist.

We consider in this paper the situation when the convective flow in the porous layer is driven by an exothermic catalytic reaction taking place on the lower surface whereby a reactive species *P* reacts to form an inert product *Q*. On the upper surface usual boundary conditions of uniform temperature and concentration are imposed.

It seems, at the author's best knowledge, that this kind of boundary conditions have been not taken into account till now in the analysis of the onset of convection in horizontal fluid-saturated porous layers. Thus, the aim of the present paper is to find how the critical Rayleigh number is modified by these boundary conditions.

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| Nomenclature | | | | |
|--------------|---|--------------|---|--|
| А, В | dimensionless parameters, defined in (13) | t | time | |
| С | concentration | х, у | co-ordinates along the porous layer and normal to it, | |
| D | thermal diffusion of the porous medium | | respectively | |
| h | depth of the horizontal layer | | | |
| Ε | activation energy | Greek | Freek symbols | |
| k | wave number | β | coefficient of thermal expansion | |
| k_0 | rate constant | 3 | activation energy parameter | |
| k_m | thermal conductivity of the porous medium | φ | dimensionless concentration | |
| k_T | thermal conductivity of the surface | κ | thermal diffusivity of the porous medium | |
| Κ | permeability | θ | dimensionless temperature | |
| Le | Lewis number | ρ | density | |
| Q | heat of reaction | $\dot{\psi}$ | stream function | |
| R^{*} | universal gas constant | | | |
| R | Rayleigh number | Subscr | Subscripts | |
| u, v | components of the Darcian velocity in the x - and y - | b | basic state | |
| | direction | С | critical value | |
| Т | temperature | r | reference conditions | |

2. Analyis

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We consider a horizontal layer, see Fig. 1, of depth h, filled with a fluid-saturated porous medium. The upper wall is subjected to uniform temperature and concentration, while on the lower wall there is an exothermic surface reaction, whereby reactant P is converted to an inert product Q via the following first-order non-isothermal reaction

$$P \to Q + \text{heat}, \text{ rate} = k_0 C \exp\left(-\frac{E}{R^*T}\right)$$
 (1)

known as the Arrhenius kinetics. Here *E* is the activation energy, R^* is the universal gas constant, k_0 is the rate constant, *T* is the temperature and *C* is the concentration of reactant *P* within the convective fluid. This reaction scheme is a realistic one and has been used in the past in modeling of combustion processes, and also for reactive processes in porous media [18–21]. As noted in [18,19], the surface reaction releases heat, which produces a convective flow close to the surface and, in turn, fresh reactant will replace that used up in the reaction. In this way, an interaction will occur between the convective flow, heat transfer and mass transport of the reactant.

Using usual notations, the governing equations which describe the problem at hand are mass conservation, Darcy's law, equation of energy and that of concentration

$$\frac{\partial u}{\partial \bar{x}} + \frac{\partial v}{\partial \bar{y}} = 0 \tag{2}$$

$$\bar{u} = -\frac{K}{\mu} \frac{\partial \bar{p}}{\partial \vec{x}}, \ \bar{v} = -\frac{K}{\mu} \frac{\partial \bar{p}}{\partial \bar{y}} + \frac{\rho g \beta K}{\mu} (T - T_r)$$
(3)

$$\frac{\partial T}{\partial \bar{t}} + \bar{u}\frac{\partial T}{\partial \bar{x}} + \bar{v}\frac{\partial T}{\partial \bar{y}} = \kappa \left(\frac{\partial^2 T}{\partial \bar{x}^2} + \frac{\partial^2 T}{\partial \bar{y}^2}\right) \tag{4}$$

$$\frac{\partial C}{\partial \bar{t}} + \bar{u}\frac{\partial C}{\partial \bar{x}} + \bar{v}\frac{\partial C}{\partial \bar{y}} = D\left(\frac{\partial^2 C}{\partial \bar{x}^2} + \frac{\partial^2 C}{\partial \bar{y}^2}\right)$$
(5)

where T_r is a reference temperature and over-bars refer to dimensional quantities. The \bar{x} and \bar{y} axes are taken along the porous layer and normal to it, respectively, and the lower wall is located at $\bar{y} = 0$. We point out that in writing Eq. (3), the Boussinesq approximation was invoked and differences in reactant concentration (which may induce buoyancy forces) are assumed to be small. The Darcy's model is justifiable when the heat of reaction is small or moderate. Otherwise, when the heat of reaction is large, non-Darcy models must be used, see also [12,22].

The thermal boundary conditions on the lower wall are

$$k_T \frac{\partial T}{\partial \bar{y}} = -Qk_0 C \exp\left(-\frac{E}{R^*T}\right), D \frac{\partial C}{\partial \bar{y}} = k_0 C \exp\left(-\frac{E}{R^*T}\right)$$
(6)

where k_T is the thermal conductivity of the surface, Q is the heat of reaction, which is taken as positive, meaning that heat is taken from the surface into the surrounding fluid-porous medium by conduction. Eliminating the pressure, using the streamfunction ψ and introducing the dimensionless quantities

$$x = \frac{\bar{x}}{h}, y = \frac{\bar{y}}{h}, t = \frac{h^2}{\kappa}\bar{t}, u = \frac{\kappa}{h}\bar{u}, v = \frac{\kappa}{h}\bar{v}, \theta = \frac{E}{R^*T_r^2}(T - T_r), \varphi = \frac{C}{C_r}$$
(7)

Eqs. (1)-(4) become

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = R \frac{\partial \theta}{\partial x} \tag{8}$$

$$\frac{\partial\theta}{\partial t} + u\frac{\partial\theta}{\partial x} + v\frac{\partial\theta}{\partial y} = \frac{\partial^2\theta}{\partial x^2} + \frac{\partial^2\theta}{\partial y^2}$$
(9)

$$\frac{\partial \varphi}{\partial t} + u \frac{\partial \varphi}{\partial x} + v \frac{\partial \varphi}{\partial y} = \frac{1}{Le} \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \right)$$
(10)

where $Le = \kappa/D$ is the Lewis number and *R* is the Rayleigh number defined as

$$R = \frac{\rho g \beta K h}{\mu \kappa} \cdot \frac{R^* T_r^2}{E}$$
(11)



Fig. 1. Geometry of the problem.

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