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ANALYSIS OF DOUBLE-DIFUSSIVE LAMINAR NATURAL CONVECTION IN POROUS MEDIA

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Abstract. This paper presents an analysis of the macroscopic heat and mass transport equations for laminar flow in permeable structures. Two driving mechanisms are considered to contribute to the overall momentum transport, namely temperature driven and concentration driven mass fluxes. Double-diffusive natural convection mechanism is investigated for the fluid phase in laminar regime. Equations are presented based on the double-decomposition concept, which considers both time fluctuations and spatial deviations about mean values. This work intends to demonstrate that additional transport mechanisms are mathematically derived if temperature, concentration and velocity present simultaneously time fluctuations and spatial deviations within the domain of analysis. Stability analysis of mixtures composed of lighter or heavier components under gradients of temperature and concentration is discussed.

Keywords. Double Decomposition, Laminar Flow, Porous Media, Natural Convection

1. Introduction

The study of double-diffusive natural convection in porous media has many environmental and industrial applications, including grain storage and drying, petrochemical processes, oil and gas extraction, contaminant dispersion in underground water reservoirs, electrochemical processes, etc (Mamou et all (1995), Mohamad and Bennacer (2002), Goyeau et all (1996), Nithiarasu et all (1997), Mamou et all (1998), Bennacer et all (2001), Bennacer et all (2003)). In some specific applications, the fluid mixture may become turbulent and difficulties arise in the proper mathematical modeling of the transport processes under both temperature and concentration gradients.

Modeling of macroscopic transport for incompressible flows in rigid porous media has been based on the volume-average methodology for either heat Hsu and Cheng (1990) or mass transfer (Bear (1972), Bear and Bachmat (1967), Whitaker (1966), Whitaker (1967)). If time fluctuations of the flow properties are considered, in addition to spatial deviations, there are two possible methodologies to follow in order to obtain macroscopic equations: a) application of time-average operator followed by volume-averaging (Masuoka and Takatsu (1996), Kuwahara et all (1996), Kuwahara and Nakayama (1998), Nakayama and Kuwahara (1999)), or b) use of volume-averaging before time-averaging is applied (Lee and Howell (1987), Wang and Takle (1995), Antohe and Lage (1997), Getachewa et all (2000)). This work intends to present a set of macroscopic mass transport equations derived under the recently established double decomposition concept (Pedras and de Lemos (2000), Pedras and de Lemos (2001), Pedras and de Lemos (2001b), Pedras and de Lemos (2001c)), through which the connection between the two paths a) and b) above is unveiled. That methodology, initially developed for the flow variables, has been extended to heat transfer in porous media where both time fluctuations and spatial deviations were considered for velocity and temperature Rocamora and de Lemos (2000). Flow about an interface Silva and de Lemos (2003), Silva and de Lemos (2003b), buoyant flows de Lemos and Braga (2003) and mass transfer de Lemos and Mesquita (2003) have also been investigated. Recently, a general classification of all proposed models for turbulent flow and heat transfer in porous media has been published de Lemos and Pedras (2001). Here, double-diffusive laminar natural convection flow in porous media is considered.

2. Local Instantaneous Transport Equation

The steady-state microscopic instantaneous transport equations for an incompressible binary fluid mixture with constant properties are given by:

$$\nabla \cdot \mathbf{u} = 0 \tag{1}$$

$$r \nabla \cdot (\mathbf{uu}) = -\nabla p + m \nabla^2 \mathbf{u} + r\, \mathbf{g} \tag{2}$$

$$(rc_p)\nabla\cdot(\mathbf{u}T) = \nabla\cdot(l\nabla T) \tag{3}$$

$$r\nabla\cdot(\mathbf{u}\,m_\ell + \mathbf{J}_\ell) = r\,R_\ell \tag{4}$$

where $\mathbf{u}$ is the mass-averaged velocity of the mixture, $\mathbf{u} = \sum_\ell m_\ell \mathbf{u}_\ell$, $\mathbf{u}_\ell$ is the velocity of species ℓ, m_ℓ, is the mass fraction of component ℓ, defined as $m_\ell = r_\ell / r$, r_ℓ is the mass density of species ℓ (mass of ℓ over total mixture volume), r is the bulk density of the mixture ($r = \sum_\ell r_\ell$), p is the pressure, m is the fluid mixture viscosity, $\mathbf{g}$ is the gravity acceleration vector, c_p is the specific heat, T is the temperature and l is the fluid thermal conductivity. The generation rate of species ℓ per unit of mixture mass is given in Eq. (4) by R_ℓ.

An alternative way of writing the mass transport equation is using the volumetric molar concentration C_ℓ (mol of ℓ over total mixture volume), the molar weight M_ℓ (g/mol of ℓ) and the molar generation/destruction rate R^*_ℓ (mol of ℓ/total mixture volume), giving:

$$M_\ell\nabla\cdot(\mathbf{u}\,C_\ell + \mathbf{J}_\ell) = M_\ell\,R^*_\ell \tag{5}$$

Further, the mass diffusion flux $\mathbf{J}_\ell$ (mass of ℓ per unit area per unit time) in Eq. (4) or Eq. (5) is due to the velocity slip of species ℓ,

$$\mathbf{J} = r_\ell(\mathbf{u}_\ell - \mathbf{u}) = -r_\ell D_\ell \nabla m_\ell = -M_\ell D_\ell \nabla C_\ell \tag{6}$$

where $\mathbf{D}_\ell$ is the diffusion coefficient of species ℓ into the mixture. The second equality in Eq. (6) is known as Fick's Law, which is a constitutive equation strictly valid for binary mixtures under the absence of any additional driving mechanisms for mass transfer Hsu and Cheng (1990). Therefore, no Soret or Dufour effects are here considered.

Rearranging Eq. (5) for an inert species, dividing it by $\mathbf{M}_\ell$ and dropping the index ℓ for a simple binary mixture, one has,

$$\nabla\cdot(\mathbf{u}\,C) = \nabla\cdot(D\nabla C) \tag{7}$$

If one considers that the density in the last term of Eq. (2) varies with temperature and concentration, for natural convection flow, the Boussinesq hypothesis reads, after renaming this density r_T,

$$r_T \cong r\,[1 - b\,(T - T_{ref}) - b_C\,(C - C_{ref})] \tag{8}$$

where the subscript ref indicates a reference value and b and b_C are the thermal and salute expansion coefficients, respectively, defined by,

$$b = -\frac{1}{r}\frac{\partial r}{\partial T}\bigg|_{p,C}, \qquad b_C = -\frac{1}{r}\frac{\partial r}{\partial C}\bigg|_{p,T} \tag{9}$$

Equation (8) is an approximation of Eq. (9) and shows how density varies with temperature and concentration in the body force term of the momentum equation.

Further, substituting Eq. (8) into Eq. (2), one has,

$$r\nabla\cdot(\mathbf{uu}) = -\nabla p + m\nabla^2\mathbf{u} + r\,\mathbf{g}[1 - b\,(T - T_{ref}) - b\,(C - C_{ref})] \tag{10}$$

Thus, the momentum equation becomes,

$$r\nabla\cdot(\mathbf{uu}) = -(\nabla p)^* + m\nabla^2\mathbf{u} - r\,\mathbf{g}[(b\,(T - T_{ref}) + b_C\,(C - C_{ref})] \tag{11}$$

where $(\nabla p)^* = \nabla p - r\,\mathbf{g}$ is a modified pressure gradient.

As mentioned, there are, in principle, two ways that one can follow in order to treat turbulent flow in porous media. The first method applies a time average operator to the governing Eq. (4) before the volume average procedure is conducted. In the second approach, the order of application of the two average operators is reversed. Both techniques aim at derivation of a suitable macroscopic turbulent mass transport equation.

Volume averaging in a porous medium, described in detail in references (Slattery (1967), Whitaker (1969), Gray and Lee (1977)), makes use of the concept of a Representative Elementary Volume (REV), over which local equations are integrated. After integration, detailed information within the volume is lost and, instead, overall properties referring to a REV are considered. In a similar manner, statistical analysis of turbulent flow leads to time mean properties. Transport equations for statistical values are considered in lieu of instantaneous information on the flow.

Before undertaking the task of developing macroscopic equations, it is convenient to recall the definition of volume average.

2.1. Volume Average Operator

The volume average of φ taken over a Representative Elementary Volume in a porous medium can be written as:

$$\langle j \rangle^v = \frac{1}{\Delta V} \int_{\Delta V} j \, dV \tag{12}$$

The value $\langle j \rangle^v$ is defined for any point x surrounded by a Representative Elementary Volume, of size ΔV. This average is related to the intrinsic average for the fluid phase as:

$$\langle j_f \rangle^v = f \langle j_f \rangle^i \tag{13}$$

where $f = \Delta V_f / \Delta V$ is the medium porosity and ΔV_f is the volume occupied by the fluid in a REV. Furthermore, one can write:

$$j = \langle j \rangle^i + {}^i j \tag{14}$$

with $\langle {}^i j \rangle^i = 0$. In Eq. (14), ${}^i j$ is the spatial deviation of j with respect to the intrinsic average $\langle j \rangle^i$.

Further, the local volume average theorem can be expressed as (Slattery (1967), Whitaker (1969), Gray and Lee (1977)):

$$\begin{aligned}
\langle \nabla j \rangle^v &= \nabla (f \langle j \rangle^i) + \frac{1}{\Delta V} \int_{A_i} \mathbf{n} j \, dS \\
\langle \nabla \cdot \mathrm{j} \rangle^v &= \nabla \cdot (f \langle \mathrm{j} \rangle^i) + \frac{1}{\Delta V} \int_{A_i} \mathbf{n} \cdot \mathrm{j} \, dS \\
\langle \frac{\partial j}{\partial t} \rangle^v &= \frac{\partial}{\partial t} (f \langle j \rangle^i) - \frac{1}{\Delta V} \int_{A_i} \mathbf{n} \cdot (\mathbf{u}_i j) dS
\end{aligned} \tag{15}$$

where $\mathbf{n}$ is the unit vector normal to the fluid-solid interface and A_i is the fluid-solid interface area within the REV. It is important to emphasize that Ai should not be confused with the surface area surrounding volume ΔV.

2.2. Macroscopic Equations For Buoyancy Free Flows

For non-buoyant flows, macroscopic equations considering laminar flow and the mecanism of turbulence have been already derived in detail for momentum Pedras and de Lemos (2001), heat de Lemos and Braga (2003), de Lemos and Rocamora (2002) and mass de Lemos and Mesquita (2003) transfer and for this reason their derivation need not to be repeated here. They read:

Momentum transport

$$r\nabla\cdot\left(\frac{\mathbf{u}_D\mathbf{u}_D}{f}\right)=-\nabla(f\langle p\rangle^i)+m\nabla^2\mathbf{u}_D-\left[\frac{mf}{K}\mathbf{u}_D+\frac{c_F f r|\mathbf{u}_D|\mathbf{u}_D}{\sqrt{K}}\right] \tag{16}$$

Heat transport

$$(r\,c_p)_f\,\nabla\cdot(\mathbf{u}_D\langle T\rangle^i)=\nabla\cdot\{\mathbf{K}_{eff}\cdot\nabla\langle T\rangle^i\} \tag{17}$$

$$\mathbf{K}_{eff}=[f\,l_f+(1-f)\,l_s]\mathbf{I}+\mathbf{K}_{tor}+\mathbf{K}_{disp} \tag{18}$$

The subscripts f and s refer to fluid and solid phases, respectively, and coefficients K's come from the modeling of the following mechanisms:

- Tortuosity: $\left[\frac{1}{\Delta V}\int_{A_i}\mathbf{n}\left(l_f T_f-l_s T_s\right)dS\right]=\mathbf{K}_{tor}\cdot\nabla\langle T\rangle^i$ (19)

- Thermal dispersion: $-(r\,c_p)_f\,f\langle{}^i\mathbf{u}\,{}^iT_f\rangle^i=\mathbf{K}_{disp}\cdot\nabla\langle T\rangle^i$ (20

Mass transport

$$\nabla\cdot(\mathbf{u}_D\langle C\rangle^i)=\nabla\cdot\mathbf{D}_{eff}\cdot\nabla(f\langle C\rangle^i) \tag{21}$$

$$\mathbf{D}_{eff}=\mathbf{D}_{disp}+\mathbf{D}_{diff} \tag{22}$$

$$\mathbf{D}_{diff}=\langle D\rangle^i\mathbf{I}=\frac{1}{r}\frac{m_f}{Sc}\mathbf{I} \tag{23}$$

The coefficient $\mathbf{D}_{disp}$ in Eq. (21) appears due to the nonlinearity of the convection term. It comes from the modeling of the following mechanisms:

- Mass dispersion: $-\langle{}^i\mathbf{u}\;{}^iC\rangle^i=\mathbf{D}_{disp}\cdot\nabla\langle C\rangle^i$ (24

2.3. Macroscopic Double-Diffusion Effects

Mean Flow

Focusing now attention to buoyancy effects only, application of the volume average procedure to the last term of Eq. (11) leads to,

$$\langle r\,\mathbf{g}[b(T-T_{ref})+b_C(C-C_{ref})]\rangle^v=\frac{\Delta V_f}{\Delta V}\frac{1}{\Delta V_f}\int_{\Delta V_f}r\,\mathbf{g}[b(T-T_{ref})+b_C(C-C_{ref})]dV \tag{25}$$

Expanding the left hand side of Eq. (25) in light of Eq. (14), the buoyancy term becomes,

$$\begin{aligned}&\langle r\,\mathbf{g}[b(T-T_{ref})+b_C(C-C_{ref})]\rangle^v\\&=r\,\mathbf{g}f[b_f(\langle T\rangle^i-T_{ref})+b_{C_f}(\langle C\rangle^i-C_{ref})]+\underbrace{r\,\mathbf{g}bf\left\langle{}^iT\right\rangle^i}_{=0}+\underbrace{r\,\mathbf{g}b_Cf\left\langle{}^iC\right\rangle^i}_{=0}\end{aligned} \tag{26}$$

where the third and forth terms on the r.h.s. are null since $\langle {}^{i} j \rangle^{i} = 0$. Here, coefficients b_f and b_{Cf} are the macroscopic thermal and salute expansion coefficients, respectively. Assuming that gravity is constant over the REV, expressions for them based on Eq. (26) are given as,

$$b_f = \frac{\langle r\, b\,(T - T_{ref})\rangle^{v}}{r\, f(\langle T\rangle^{i} - T_{ref})};\; b_{C_f} = \frac{\langle r\, b_C (C - C_{ref})\rangle^{v}}{r\, f(\langle C\rangle^{i} - C_{ref})} \tag{27}$$

Including Eq.(26) into Eq.(16) the macroscopic time-mean Navier-Stokes (NS) equation for an incompressible fluid with constant properties is given as,

$$\begin{aligned} r\nabla\cdot\left(\frac{\mathbf{u}_D\mathbf{u}_D}{f}\right) = &-\nabla(f\langle p\rangle^{i}) + m\nabla^2\mathbf{u}_D + \\ &+ r\,\mathbf{g}f[b_f(\langle T\rangle^{i} - T_{ref}) + b_{C_f}(\langle C\rangle^{i} - C_{ref})] \\ &-\left[\frac{mf}{K}\mathbf{u}_D + \frac{c_F f r|\mathbf{u}_D|\,\mathbf{u}_D}{\sqrt{K}}\right] \end{aligned} \tag{28}$$

Before proceeding, it is interesting to comment on role of coefficients b_f and b_{C_f} on the overall mixture density value. Figure 1 presents the variation of r as a function of temperature or concentration gradients. Here, only fluids that became less dense with increasing temperature are considered (Figure 1a). However, two situation might occurs when increasing $\langle C\rangle^{i}$, namely the mixture might became less dense with the addition of a lighter solute (Figure 1b), or else, a denser fluid may result by mixing a heavier component to it (Figure 1c). Implications of that on the stability of the entire fluid system will be discussed below.

2.3. Hydrodynamic Stability

For a system oriented in the upward direction with gravity acting downward, the hydrodynamic stability of a thermal system will depend on both the thermal and concentration drives acting on a R.E.V., according to Eq.(28). Depending on the direction of the property gradients, both such drives may induce instability leading eventually to turbulent flow. As such, unconditionally **unstable** situations are presented in Figure 2 where hotter fluid (Figure 2a) composed by a less dense mixture is positioned at the bottom of the fluid layer (Figure 2b). For positive b_f and b_{Cf} values, with negative gradients of $\langle T\rangle^{i}$ and $\langle C\rangle^{i}$, both drives expressed by Eq.(28). An initially laminar flow may then undergo transition and become turbulent.

Turbulence, if existing, might decay and the flow may relaminarize. Also in this category is the case of top heated systems with heavier components flowing at the bottom (Figure 2f). Any other combination regarding a heavier or a lighter component flowing in a non-isothermal fluid may be conditionally unstable, depending upon the balance between source and sink terms that might appear as a result of temperature and concentration distribution within the flow.

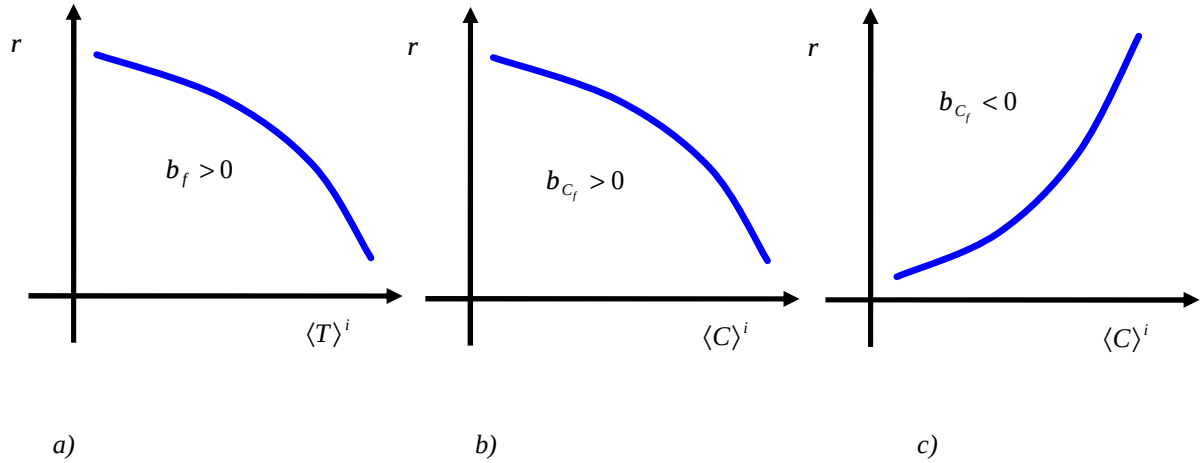

Figure 1 - Behaviour of mixture density: a) Lighter mixture with increasing $\langle T\rangle^{i}$, b) Lighter mixture with increasing $\langle C\rangle^{i}$, c) Heavier mixture with increasing $\langle C\rangle^{i}$.

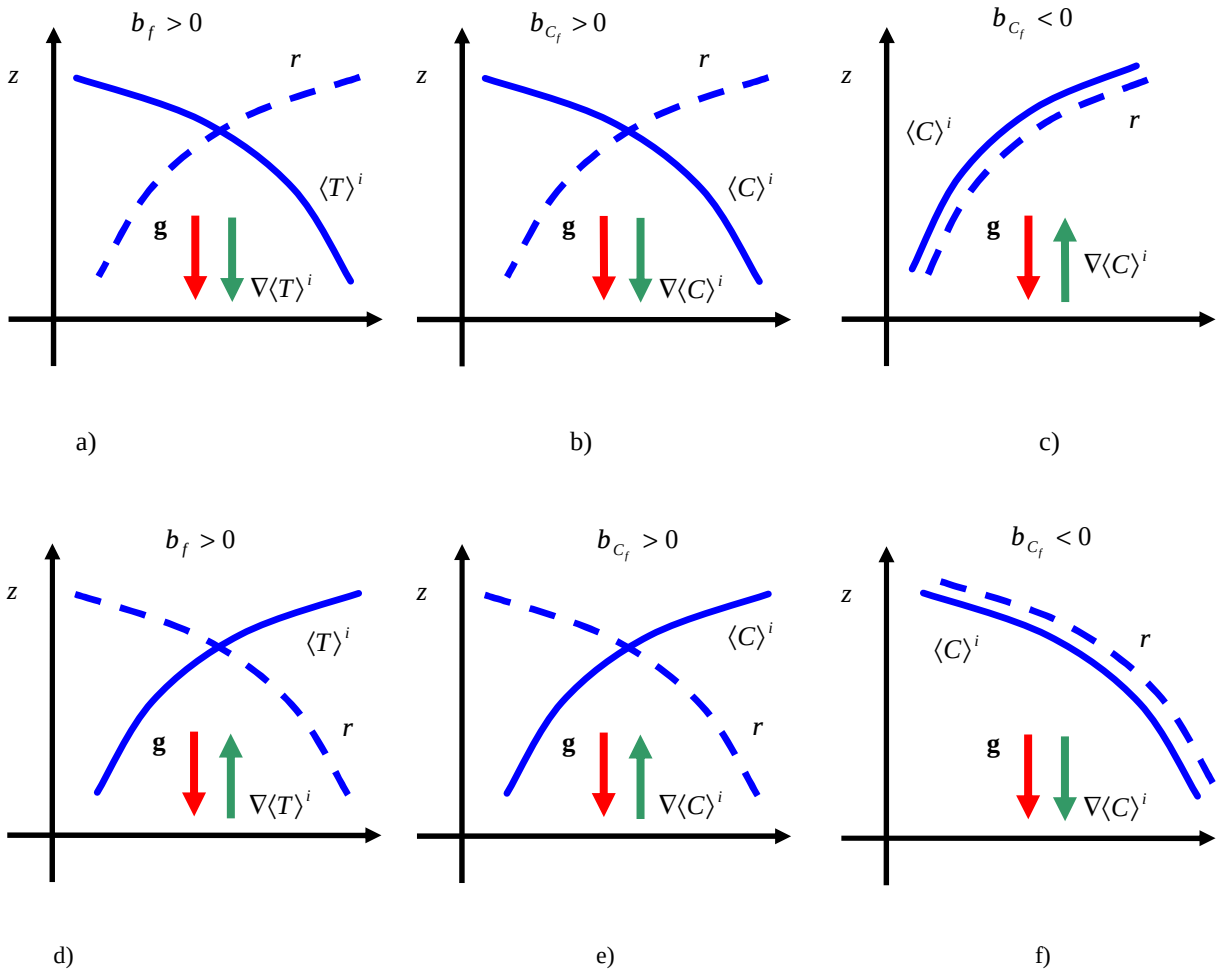

Figure 2 – Stability analysis of a layer of fluid subjected to gradients of temperature and concentration: 1) Unconditionally **unstable** cases: hotter fluid (a) with less dense mixture at the bottom (b)-(c); 2) Unconditionally **stable** cases: colder fluid (d) with more dense mixture at the bottom (e)-(f).

3. Conclusions

In this work, equations were derived for laminar double-diffusive natural convection in porous media. Derivations were carried out under the light of the double decomposition concept (Pedras and de Lemos (2000), Pedras and de Lemos (2001)). Extra terms appearing in the equations needed to be modeled in terms of $\mathbf{u}_D$, $\langle T \rangle$ and $\langle C \rangle$. Hydrodynamically stable flows occur under certain temperature and concentration distributions, which dampen turbulence and eventually lead to a relaminarization process. Unconditionally unstable situations were also reviewed, which will cause disturbances to grow leading to transition and turbulence. Ultimately, it is expected that additional research on this new subject be stimulated by the derivations here presented.

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