Analysis of turbulent double-diffusive free convection in porous media using the two-energy equation model

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ABSTRACT

This paper presents an analysis of macroscopic heat and mass transport for turbulent flow in permeable structures, which is based on the thermal non-equilibrium assumption between the porous matrix and the working fluid. Two driving mechanisms are here considered to contribute to the overall momentum transport, namely fluid-temperature driven and concentration driven mass fluxes. The fluid temperature, however, is also affected by the solid temperature distribution as the two phases exchange heat through their interfacial area. Essentially, here the double-diffusive natural convection mechanism is investigated for the fluid phase in turbulent 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 velocity, fluid temperature and mass concentration simultaneously present time fluctuations and spatial deviations about average values. A modeled form for the entire set of transport equations is presented where turbulent transfer is based on a macroscopic version of the \(k-\varepsilon\) model.

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1. Introduction

Analyses of double-diffusive phenomena in free convection in permeable media has many environmental and industrial applications, such as in oil and gas extraction, movement of gas concentration into the ground, contaminant dispersion in soils, grain storage and drying, petrochemical processes, electrochemical processes, to mention a few [1–9]. In some specific applications, the voids are large enough and the fluid mixture may become turbulent. In such instances, difficulties arise in the proper mathematical modeling of the transport processes under both temperature and concentration gradients.

Usually, modeling of macroscopic transport for incompressible flows in rigid porous media has been based on the volume-average methodology for either heat or mass transfer [10–14]. If fluctuations in time are also of concern due the existence of turbulence in the intra-pore space, a variety of mathematical models have been published in the literature in the last decade. One of such views, which entails simultaneous application of both time and volume averaging operators to all governing equations, has been organized and published in a book [15] that describes, in detail, an idea known in the literature as the double-decomposition concept (see chapter 3, pgs. 27–32 in ref. [15] for details).

In an earlier work [16], double-diffusive effects in porous media have been treated considering thermal equilibrium between the porous matrix and the permeating fluid. Or say, in ref. [16] the fluid temperature was assumed to be the same of that of the solid when analyzing double-diffusive mechanisms. Later [17], buoyancy-free flows were investigated with the so-called two-energy-equation model, or 2EEM for short, which is based on the Local Thermal Non-equilibrium Hypothesis (LTNE) meaning that the average temperature of the fluid is not equal to the average temperature of the solid matrix. However, in ref. [17] no double-diffusion was considered.

Therefore, the purpose of this contribution is to extend the work in ref. [16] on turbulent double-diffusion using only one energy equation, assuming now the thermal non-equilibrium hypotheses in ref. [17], which requires an independent energy balance for each phase. As such, the expectation herein is that, by combining now such two models that were developed on separate, a larger number of physical processes can now be more realistically tackled.

2. Local instantaneous transport equation

The steady-state local (microscopic) instantaneous transport equations for an incompressible binary fluid mixture with constant properties flowing in an inert heterogeneous medium are given in details elsewhere and for that, they will be just repeated here. They read:

within the fluid:

\[
\text{Continuity: } \nabla \cdot \mathbf{u} = 0 \tag{1}
\]

\[
\text{Momentum: } \rho \nabla \cdot (\mathbf{u} \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g} \tag{2}
\]

\[
\text{Energy-fluid phase: } \left( \rho c_p \right) \left( \nabla \cdot (\mathbf{u} T_f) \right) = \nabla \cdot (k_f \nabla T_f) + S_f \tag{3}
\]

\[
\text{Mass concentration: } \rho \nabla \cdot (\mathbf{u} m_r + \mathbf{J}_r) = \rho R_r \tag{4}
\]
within the solid:

\[
\text{Energy-solid phase (porous matrix)}: \nabla \cdot (k_s \nabla T_s) + S_e = 0.
\]

where \( \mathbf{u} \) is the mass-averaged velocity of the mixture, \( \mathbf{u} = \sum m_i \mathbf{u}_i \), \( \mathbf{u}_i \) is the velocity of species \( \ell \), \( m_i \) is the mass fraction of component \( \ell \), defined as \( m_i = \rho_i / \rho, \rho \) is the mass density of species \( \ell \) (mass of \( \ell \) over total mixture volume), \( \rho \) is the bulk density of the mixture \( \left( \rho = \sum \rho_i \right) \), \( p \) is the pressure, \( \mu \) is the fluid viscosity, \( g \) is the gravity acceleration vector, \( c_p \) is the specific heat, \( \gamma \) is the speed of sound, \( \mathbf{S} \) refers to fluid and solid phases, respectively, \( T_j \) and \( T_s \) are the fluid and solid temperature, \( k_f \) and \( k_s \) are the fluid and solid thermal conductivities and \( S \) is the heat generation term. If there is no heat generation either in the solid or in the fluid, one has further \( S_j = S_s = 0 \). The generation rate of species \( \ell \) per unit of mixture mass is given in Eq. (4) by \( R_{\ell} \). Also, as pointed out in ref. [16], an alternative way of writing the mass transport equation is using the volumetric molar concentration \( C_\ell / \rho \) over total mixture volume, the molal weight \( M_\ell \), and the molar generation/destruction rate \( R_{\ell}^\prime \) (mol of \( \ell \) per unit of mixture volume), giving:

\[
M_\ell \nabla \cdot (u \mathbf{C}_\ell + \mathbf{J}_\ell) = M_\ell R_{\ell}^\prime. 
\]

Further, the mass diffusion flux \( \mathbf{J}_\ell \) (mass of \( \ell \) per unit area per unit time) in Eq. (4) or (6) is due to the velocity slip of species \( \ell \),

\[
\mathbf{J}_\ell = \rho_\ell (\mathbf{u}_\ell - \mathbf{u}) = -\rho_\ell \nabla m_\ell = -M_\ell D_\ell \nabla C_\ell,
\]

where \( D_\ell \) is the diffusion coefficient of species \( \ell \) into the mixture. The second equality in Eq. (7) 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 [10]. Therefore, no Soret or Dufour effects are here considered.

Rearranging Eq. (6) for an inert species, dividing it by \( M_\ell \) and dropping the index \( \ell \) for a simple binary mixture, one has,

\[
\nabla \cdot (u C) = \nabla \cdot (D \nabla C).
\]

If one considers that the density in the last term of Eq. (2) varies with the area. Also, Eq. (9) is an approximation of Eq. (10) and shows how the exchange of heat between the two phases across the interstitial volume averaging Eqs. (3) and (5), \( T_j \) is going to be related to \( T_s \) due to the exchange of heat between the two phases across the interstitial area. Also, Eq. (9) is an approximation of Eq. (10) and shows how density varies with the fluid temperature and mass concentration in the body force term of the momentum equation. Substituting now Eq. (9) into Eq. (2), one has,

\[
\rho \nabla \cdot (u \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho g \left[ 1 - \beta \left( T_j - T_{ref} \right) \right] \beta_c \left( C - C_{ref} \right). 
\]

Thus, the momentum equation becomes after some rearrangement,

\[
\rho \nabla \cdot (u \mathbf{u}) = -\nabla p^* + \mu \nabla^2 \mathbf{u} + \rho g \left[ 1 - \beta \left( T_j - T_{ref} \right) \right] \beta_c \left( C - C_{ref} \right). 
\]

where \( \nabla p^* \) is a modified pressure gradient.
3. Time and volume average operators — The double decomposition concept

For the sake of completeness, although the information below has been given in detail in a number of articles and books, including [15] for example, it is convenient to recall the definition of time average and volume average.

The time average of a general quantity \( \varphi \) is defined as:

\[
\bar{\varphi} = \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \varphi \, dt
\]  

(13)

where the time interval \( \Delta t \) is small compared to the fluctuations of the average value, \( \bar{\varphi} \), but large enough to capture turbulent fluctuations of \( \varphi \). Time decomposition can then be written as,

\[
\varphi = \bar{\varphi} + \varphi' \tag{14}
\]

with \( \bar{\varphi} = 0 \). Here, \( \varphi' \) is the time fluctuation of \( \varphi \) around its average \( \bar{\varphi} \).

Further, the volume average of \( \varphi \) taken over a Representative Elementary Volume (REV, Fig. 1) in a porous medium can be written as [18–20]:

\[
\langle \varphi \rangle = \frac{1}{\Delta V} \int \varphi \, dV. \tag{15}
\]

The value \( \langle \varphi \rangle \) is defined for any point \( \mathbf{x} \) surrounded by a REV of size \( \Delta V \). This average is related to the intrinsic average for the fluid phase as:

\[
\langle \varphi \rangle^v = \phi \langle \varphi \rangle^i \tag{16}
\]

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

\[
\varphi = \langle \varphi \rangle^i + \varphi' \tag{17}
\]

with \( \langle \varphi \rangle^i = 0 \). In Eq. (17), \( \varphi' \) is the spatial deviation of \( \varphi \) with respect to the intrinsic average \( \langle \varphi \rangle^i \).

Further, the local volume average theorem can be expressed as [18–20]:

\[
\begin{align*}
\langle \nabla \varphi \rangle^v &= \nabla \langle \varphi \rangle^i + \frac{1}{\Delta V} \int_{\mathcal{A}_i} \mathbf{n} \cdot \varphi \, dS \\
\langle \varphi \varphi \rangle^v &= \langle \varphi \rangle^i \langle \varphi \rangle^i + \frac{1}{\Delta V} \int_{\mathcal{A}_i} \mathbf{n} \cdot \varphi \, dS \\
\langle \frac{\partial \varphi}{\partial t} \rangle^v &= \frac{\partial}{\partial t} \langle \varphi \rangle^i - \frac{1}{\Delta V} \int_{\mathcal{A}_i} \mathbf{n} \cdot (\mathbf{u} \varphi) \, dS
\end{align*}
\]

(18)

where \( \mathbf{n} \) is the unit vector normal to the fluid–solid interface, pointing from the fluid towards the solid phase, \( \mathcal{A}_i \) is the fluid–solid interface area within the REV. It is important to emphasize that \( \mathcal{A}_i \) should not be confused with the surface area surrounding volume \( \Delta V \). In ref. [15] it is shown that for a rigid, homogeneous porous medium saturated with an incompressible fluid, the following relationships apply:

\[
\begin{align*}
\overline{\langle \varphi \rangle} &= \langle \varphi \rangle^i \\
\overline{\langle \varphi \rangle^i} &= \langle \varphi \rangle^i
\end{align*}
\]

(19)

Therefore, a general quantity \( \varphi \) can be expressed by either,

\[
\varphi = \overline{\langle \varphi \rangle} + \langle \varphi \rangle^i + \varphi' \tag{20}
\]

or

\[
\varphi = \langle \varphi \rangle^i + \overline{\langle \varphi \rangle} + \langle \varphi \rangle^i + \varphi'. \tag{21}
\]

Expressions (20) and (21) encompass what is recalled in the literature as the “double decomposition” concept where \( \varphi' \) can be understood as either the time fluctuation of the spatial deviation or the spatial deviation of the time fluctuation. Also, \( \langle \varphi \rangle^i = \overline{\langle \varphi \rangle} = 0 \).

Fig. 1. Representative elementary volume (R.E.V.), intrinsic average; space and time fluctuations (see ref. [15]).
4. Time averaged transport equations

In order to apply the time average operator to Eqs. (1), (3), (5), (8) and (12), one considers,

\[
\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}' \quad T_f = T_f' + T_f, T_s = T_s' + T_s, \quad C = \bar{C} + C', \quad p = \bar{p} + p'.
\]

(22)

Substituting Eq. (22) into the governing equations and considering constant properties for both the fluid and the solid,

\[
\nabla \cdot \mathbf{u} = 0
\]

(23)

\[
\rho \nabla \cdot (\nabla \mathbf{u}) = - (\nabla \mathbf{p})' + \mu \nabla^2 \mathbf{u} + \nabla \cdot \left(- \rho \mathbf{u} \mathbf{u}' \right) - \rho \left[ \beta \left( T_f - T_{ref} \right) + \beta_C (\bar{C} - C_{ref}) \right]
\]

(24)

\[
\left( \rho c_p \right)' \nabla \cdot (\nabla T_f) = \nabla \cdot \left( k \nabla T_f \right) + \nabla \cdot \left( - \rho \bar{c}_p \mathbf{u} T_f \right)
\]

(25)

\[
0 = \nabla \cdot \left( k \nabla T_s \right).
\]

(26)

\[
\nabla \cdot \left( \bar{\mathbf{u}} \bar{\mathbf{C}} \right) = \nabla \cdot \left( D \nabla \bar{C} \right) + \nabla \cdot \left( - \bar{\mathbf{u}} C \right)
\]

(27)

For clear fluid, the use of the eddy-diffusivity concept for expressing the stress–strain rate relationship for the Reynolds stress appearing in Eq. (24) gives,

\[
- \rho \mathbf{u} \mathbf{u}' = \mu_s 2 \mathbf{D} - \frac{2}{3} \rho \mathbf{k}
\]

(28)

where \( \mathbf{D} \) is the mean deformation tensor, \( k = \bar{\mathbf{u}} \cdot \mathbf{u} / 2 \) is the turbulent kinetic energy per unit mass, \( \mu_s \) is the turbulent viscosity and \( \mathbf{k} \) is the unity tensor. Similarly, for the turbulent heat flux on the r.h.s. of Eqs. (25) and (27) the eddy diffusivity concept reads,

\[
- \rho c_p \mathbf{u} T_f = c_p \left( \frac{\mu_t}{\mu} \right)_f \nabla T_f; \quad - \bar{\rho} \bar{c}_p \bar{C} = \left( \frac{\mu_t}{\bar{\mu}} \right)_t \nabla \bar{C}
\]

(29)

where \( \left( \frac{\mu_t}{\mu} \right)_f \) and \( \left( \frac{\mu_t}{\bar{\mu}} \right)_t \) are the Prandtl and Schmidt numbers, respectively.

Further, a transport equation for the turbulent kinetic energy is obtained by multiplying first, by \( \mathbf{u}' \), the difference between the instantaneous and the time-averaged momentum equations. Thus, applying further the time average operator to the resulting product, one has,

\[
\rho \nabla \cdot (\mathbf{u} k) = - \nabla \cdot \left[ \mathbf{u}' \left( \frac{P}{\rho} + q \right) \right] + \mu \nabla^2 k + P + G_T + G_C - \rho \varepsilon
\]

(30)

where \( P = - \rho \mathbf{u} \mathbf{u}' \cdot \nabla \mathbf{u} \) is the generation rate of \( k \) due to gradients of the mean velocity and

\[
G_T = - \rho \beta g \bar{\mathbf{u}} T_f = \beta \frac{\mu_t}{\mu} \mathbf{g} \cdot \nabla T_f
\]

(31)

\[
G_C = - \rho \beta_C \mathbf{g} \cdot \bar{\mathbf{C}} = \beta_C \frac{\mu_t}{\bar{\mu}} \mathbf{g} \cdot \nabla \bar{C}
\]

(32)

are the thermal and concentration generation rates of \( k \) due to temperature and concentration fluctuations, respectively. Also, \( q = \mathbf{u}' \cdot \mathbf{u}' / 2 \) and, on the right of Eqs. (31) and (32), the models in Eq. (29) have been applied.

5. Macroscopic equations for buoyancy free flows

5.1. Mean continuity equation

When the average operators (13)–(15) are simultaneously applied over Eqs. (1)–(2), macroscopic equations for turbulent flow are obtained. Volume integration is performed over a Representative Elementary Volume (REV) shown in Fig. 1 resulting in,

\[
\nabla \cdot \mathbf{u}_0 = 0
\]

(33)

where, \( \mathbf{u}_0 = \phi (\mathbf{u}) ' \) and \( (\mathbf{u}) ' \) identifies the intrinsic (liquid) average of the time-averaged velocity vector \( \mathbf{u} \).

For non-buoyant flows, macroscopic equations considering turbulence have been already derived in detail for momentum, heat, and mass transfer [15] and for this reason their derivation need not to be repeated here. They are read as follows.

6. Mean momentum transport

\[
\rho \nabla \cdot \left[ \mathbf{u}_0 \mathbf{u}_0 \right] = - \nabla \left( \phi \mathbf{p}'' \right) + \mu \nabla^2 \mathbf{u}_0 + \nabla \cdot \left( - \rho \phi (\mathbf{u} \mathbf{u}')'' \right) - \frac{\mu_t}{K} \mathbf{u}_0 + \frac{c_f \phi \rho (\mathbf{u} \mathbf{u}')''}{\sqrt{K}}
\]

(34)

\[
\left( \mathbf{D}'' \right)'' = \frac{1}{2} \left\{ \nabla \left( \phi (\mathbf{u} \mathbf{u}')'' \right) + \left[ \nabla \left( \phi (\mathbf{u} \mathbf{u}')'' \right) \right]' \right\}
\]

(36)

\[
\left( k'' \right)'' = \frac{\left( \mathbf{u} \mathbf{u}' \right)''}{2}
\]

(35)

\[
\mu_v = \rho \bar{c}_u f_v \left( \frac{k''}{\varepsilon} \right)^2
\]

(37)

where \( \bar{c}_u \) is a constant and \( f_v \) is damping function to be presented later.

7. Macroscopic turbulence field

The intrinsic turbulent kinetic energy per unit mass and its dissipation rate are governed by the following equations,

\[
\rho \left[ \frac{\partial}{\partial t} \left( \phi k'' \right) + \nabla \cdot \left( \mathbf{u}_0 \phi k'' \right) \right] = \nabla \cdot \left[ \left( \mu + \frac{\mu_t}{\sigma} \right) \nabla \left( \phi k'' \right) \right] - \rho (\mathbf{u} \mathbf{u}')'' : \nabla \mathbf{u}_0 - c_1 (\mathbf{u} \mathbf{u}')'' : \nabla \mathbf{u}_0
\]

(38)

\[
\rho \left[ \frac{\partial}{\partial t} \left( \phi \varepsilon'' \right) + \nabla \cdot \left( \mathbf{u}_0 \phi \varepsilon'' \right) \right] = \nabla \cdot \left[ \left( \mu + \frac{\mu_t}{\sigma} \right) \nabla \left( \phi \varepsilon'' \right) \right] + c_1 (\mathbf{u} \mathbf{u}')'' : \nabla \mathbf{u}_0 \left( \frac{\varepsilon''}{k''} \right) - c_2 f_v \phi \rho (\mathbf{u} \mathbf{u}')'' : \nabla \mathbf{u}_0 \left( \frac{\varepsilon''}{k''} \right)
\]

(39)

where the \( c_i \)'s are constants and \( f_2 \) is a another damping function. Usually, two forms of the \( k-\varepsilon \) model are employed, namely the High Reynolds (Launher and Spalding [21]) and Low Reynolds number (Abe et al. [22]) turbulence models. The constants and formulae used as damping functions are showed in Table 1.

8. Two-energy equation model (2EEM)

Similarly, macroscopic energy equations are obtained for both fluid and solid phases by applying time and volume average operators to
Eqs. (3) and (5). As in the flow case, volume integration is performed
over a Representative Elementary Volume (REV), resulting in,

\[
\left( \rho c_p \right)_f \frac{\partial}{\partial t} \left( \langle u^T \rangle_i \right) = - \nabla \cdot \left( K_i \nabla \langle T_f \rangle_i \right) + \frac{1}{V} \int \left( \phi \left( \langle u^T \rangle_i \right) \right) + \frac{1}{V} \int \left( \frac{1}{L} \int n_{i f k} \nabla T_f dA \right)
\]

where the expansion,

\[
\langle u^T \rangle_i = \left( \langle u^T \rangle_i \right) + \left( \frac{1}{V} \int \left( \phi \left( \langle u^T \rangle_i \right) \right) \right) + \frac{1}{V} \int \left( \frac{1}{L} \int n_{i f k} \nabla T_f dA \right)
\]

has been used in light of the double decomposition concept given by
Eqs. (19)–(21) (see ref. [15] for details). For the solid phase, one has,

\[
0 = \nabla \cdot \left( K_i \nabla \langle T_s \rangle_i \right) - \frac{1}{V} \int \nabla \cdot \left( n_{i f k} \nabla T_f \right) dA
\]

In Eqs. (40) and (42), \( \langle T_f \rangle_i \) and \( \langle T_s \rangle_i \) denote the intrinsic time-
average temperature of solid and fluid phases, respectively. These equations
are the macroscopic energy balances for the fluid and the porous
matrix (solid), respectively.

Also, in order to use Eqs. (40) and (42), the underscored terms have
to be modeled as a function of \( \langle T_f \rangle_i \) and \( \langle T_s \rangle_i \). To accomplish this, a
gradient type diffusion model is used for all terms not involving the
interfacial heat transfer, in the form,

Turbulent heat flux : \( -\left( \rho c_p \right)_f \left( \phi \left( \langle u^T \rangle_i \right) \right) = K_i \cdot \nabla \langle T_f \rangle_i \) (43)

Thermal dispersion : \( -\left( \rho c_p \right)_f \left( \phi \left( \langle u^T \rangle_i \right) \right) = K_{disp} \cdot \nabla \langle T_f \rangle_i \) (44)

Turbulent thermal dispersion : \( -\left( \rho c_p \right)_f \left( \phi \left( \langle u^T \rangle_i \right) \right) = K_{disp-t} \cdot \nabla \langle T_f \rangle_i \) (45)

Finally, Eqs. (40) and (42) can be rewritten using the concept of
overall effective conduction in the form,

\[
0 = \nabla \cdot \left( K_{eff} \nabla \langle T_s \rangle_i \right) - \frac{1}{V} \int n_{i f k} \nabla T_s dA
\]

where

\[
K_{eff} = \left[ K_i + K_{disp} + K_{disp-t} \right] (49)
\]

The turbulent heat flux and turbulent thermal dispersion terms, \( K_i \) and
and \( K_{disp-t} \) are here modeled through the Eddy diffusivity concept as
[17]:

\[
K_i + K_{disp-t} = \phi \left( \rho c_p \right)_f \frac{v_{t_i}}{\Pr_{t_i}} (51)
\]

where \( \Pr_{t_i} \) is the macroscopic turbulent Prandtl number for the fluid
energy equation.

9. Interfacial heat transfer, \( h_f \)

In Eqs. (40) and (42) the heat transferred between the two phases
can be modeled by means of a film coefficient \( h_f \) such that,

\[
h_f \left( \langle T_s \rangle_i - \langle T_f \rangle_i \right) = \frac{1}{V} \int n_{i f k} \nabla T_s dA = \frac{1}{V} \int n_{i f k} \nabla T_f dA
\]

where \( n_{i f k} = A_i / \Delta V \) is the interfacial area per unit volume. In porous
media, the high values of \( A_i \) make them attractive for transferring
thermal energy via conduction through the solid followed by convection to a fluid stream.

\[
\left( \rho \, c_p \right)_f \nabla \cdot \left( \mathbf{u}_f \left( \nabla \left( T_f \right) \right) \right) = \nabla \cdot \left[ \mathbf{K}_{eff,f} \cdot \nabla \left( T_f \right) \right] + h_f a_l \left( T_s - T_f \right),
\]

(53)

\[
0 = \nabla \cdot \left[ \mathbf{K}_{g,x} \cdot \nabla \left( T_s \right) \right] - h_s a_i \left( T_s - T_f \right).
\]

(54)

Wakao et al. [23] proposed a correlation for \( h_f \) for completely packed bed and compared results with their experimental data. This correlation reads,

\[
\frac{h_f D}{k_f} = 2 + 1.1 \text{Re}_0^{0.8} \text{Pr}^{1/3}.
\]

(55)

Kuwahara et al. [24] also obtained the interfacial convective heat transfer coefficient for laminar flow, as follows,

\[
\frac{h_f D}{k_f} = \left( 1 + \frac{4 \left( 1 - \phi \right)}{\phi} \right) + \frac{1}{2} \left( 1 - \phi \right)^{1/2} \text{Re}_0 \text{Pr}^{1/3}, \text{ valid for } 0.2 < \phi < 0.9.
\]

(56)

Eq. (56) is based on porosity dependency and is valid for packed beds of particle diameter \( D \). Following this same methodology, in which the porous medium is considered an infinite number of solid square rods, Saito and de Lemos [25] proposed a correlation for obtaining the interfacial heat transfer coefficient for turbulent flow as,

\[
\frac{h_f D}{k_f} = 0.08 \left( \frac{\text{Re}_0}{\phi} \right)^{0.8} \text{Pr}^{1/3}, \text{ for } 1.0 \times 10^4 < \frac{\text{Re}_0}{\phi} < 2.0 \times 10^7, \text{ valid for } 0.2 < \phi < 0.9.
\]

(57)

Table 2 shows three variant correlations for the fluid to solid heat transfer coefficient \( h_f \) and the specific surface area of the porous medium \( a_s \), which appears in both energy equations.

10. Mass transport

\[
\nabla \cdot \left( \mathbf{D} \right) = \nabla \cdot \mathbf{D}_{\text{eff}} - \nabla \left( \phi \mathbf{C} \right),
\]

(58)

\[
\mathbf{D}_{\text{eff}} = \mathbf{D}_{\text{disp}} + \mathbf{D}_{\text{diff}} + \mathbf{D}_t + \mathbf{D}_{\text{disp},t}
\]

(59)

\[
\mathbf{D}_{\text{diff}} = \langle \mathbf{D} \rangle \mathbf{I} - \frac{1}{\rho \, \text{Sc}} \mathbf{I}
\]

(60)

\[
\mathbf{D}_t = \mathbf{D}_{\text{disp},t} = \frac{1}{\rho \, \text{Sc}_{\phi}} \mathbf{I}
\]

(61)

where \( \text{Sc}_{\phi} \) is a macroscopic turbulent Schmidt number.

Coefficients \( \mathbf{D}_{\text{disp}}, \mathbf{D}_t \), and \( \mathbf{D}_{\text{disp},t} \) in Eq. (58) appear due to the non-linearity of the convection term. They come from the modeling of the following mechanisms:

- Mass dispersion : \( -\langle \mathbf{u} \mathbf{C} \rangle = \mathbf{D}_{\text{disp}} \cdot \nabla \langle \mathbf{C} \rangle \)

(62)

- Turbulent mass flux : \( -\langle \mathbf{u} \mathbf{C} \rangle = -\langle \mathbf{u} \mathbf{C} \rangle = \mathbf{D}_t \cdot \nabla \langle \mathbf{C} \rangle \)

(63)

- Turbulent mass dispersion: \( -\langle \mathbf{u} \mathbf{C} \rangle = \mathbf{D}_{\text{disp},t} \cdot \nabla \langle \mathbf{C} \rangle \).

(64)

Here also mechanisms (63) and (64) are added up as [16];

\[
-\langle \mathbf{u} \mathbf{C} \rangle = \frac{1}{\rho \, \text{Sc}_{\phi}} \frac{1}{\rho} \mathbf{I} \cdot \nabla \langle \mathbf{C} \rangle = \left( \mathbf{D}_t + \mathbf{D}_{\text{disp},t} \right) \cdot \nabla \langle \mathbf{C} \rangle.
\]

(65)

11. Double-diffusion effects with a two-energy equation model

11.1. Mean flow

Focusing now attention to buoyancy effects only, application of the volume average procedure to the last term of (24) leads to,

\[
\langle \rho g \left[ \beta (T_f - T_{ref}) + \beta_c (C - C_{ref}) \right] \rangle^y
\]

\[
= \frac{\Delta V_f}{\Delta V} \int \rho g \left[ \beta (T_f - T_{ref}) + \beta_c (C - C_{ref}) \right] dV.
\]

(66)

Expanding the left hand side of Eq. (66) in light of Eq. (17), the buoyancy term becomes,

\[
\langle \rho g \left[ \beta (T_f - T_{ref}) + \beta_c (C - C_{ref}) \right] \rangle^y
\]

\[
= \rho g \beta \left( \langle T_f \rangle - T_{ref} \right) + \beta_c \left( \langle C \rangle - C_{ref} \right)
\]

\[
+ \rho g \beta_c \phi \left( \langle T_f \rangle - T_{ref} \right) + \rho g \beta_c \phi \left( \langle C \rangle - C_{ref} \right)
\]

(67)

where the third and fourth terms on the r.h.s. are null since \( \langle \phi \rangle = 0 \). Here, coefficients \( \beta_0 \) and \( \beta_c \) are the macroscopic thermal and salut expansion coefficients, respectively. Assuming that gravity is constant over the REV, expressions for them based on Eq. (67) are given as,

\[
\beta_c = \frac{\rho \beta_c (T_f - T_{ref})^y}{\rho \phi \left( \langle T_f \rangle - T_{ref} \right)}, \quad \beta_{c} = \frac{\rho \beta_c (C - C_{ref})^y}{\rho \phi \left( \langle C \rangle - C_{ref} \right)}.
\]

(68)
Including Eq. (67) into Eq. (34), the macroscopic time-mean Navier–Stokes (NS) equation for an incompressible fluid with constant properties is given as,

\[\rho \nabla \cdot \left( \frac{\mathbf{u}_0 \mathbf{u}_0}{\phi} \right) = -\nabla \left( \phi [p] \right) + \mu \nabla^2 \mathbf{u}_0 + \nabla \cdot \left( -\rho \left( \frac{\mathbf{u}_0 \mathbf{u}_0}{\phi} \right) \right) - \rho \phi \beta_a \left( \left( \mathbf{T}_f \right)^i \right)_a + \beta_{c_a} \left( \left( \mathbf{T} \right)^i - C_{\text{eff}} \right)\]

where the superscript * on the pressure gradient that would appear in Eq. (69) by the volume-average of Eq. (24), has been dropped.

As pointed out by [16], it is interesting to comment on role of coefficients \(\beta_a\) and \(\beta_{c_a}\) on the overall mixture density value. Here, only fluids that became less dense with increasing temperature are considered. However, two situations might occur when increasing \(\mathbf{T}\), namely the mixture might become less dense with the addition of a lighter solute, or else, a denser fluid may result by mixing a heavier component to it. Implications of that on the stability of the entire fluid system were discussed in ref. [16] where more details can be found.

### 11.2. Turbulent field

As mentioned, this work extends and combines earlier developments for turbulent double-diffusion using the thermal equilibrium model [16] with the hypothesis of thermal non-equilibrium [17]. For clear fluid, the buoyancy contribution to the k equation is given by Eqs. (31) and (32).

Volume averaging Eq. (31) in reference [16] has resulted in the term,

\[(G_f)^* = G_f' = \left( \mu \phi \nabla \mathbf{u}_f \right)^* = -\rho \phi \beta_a \phi \mathbf{g} \cdot \nabla \left( \mathbf{T}_f \right)^i\]

where the model in Eq. (29) has been applied. Eq. (70) represents an additional macroscopic generation/destruction rate of \(\langle k^i \rangle\) due to temperature variation in porous media, where \(\beta_a\) is a macroscopic coefficient given by \(\beta_a = \langle \rho \bar{\mathbf{u}} \nabla \mathbf{u} \rangle \). Reference [16], coefficients \(\beta_a\) (Eq. (10)), \(\beta_b\) (Eq. (68)) and \(\beta_a\) (Eq. (70)) were all assumed to be equal, for simplicity. Also, in ref. [16] the temperature used in Eq. (70) was the same regardless of the phase. Here, however, it is the gradient of the intrinsic fluid temperature \(\langle \mathbf{T}_f \rangle\), that is considered to promote the driving mechanism to generate/destroy turbulence.

In order to add the effect of concentration variation within the fluid, one applies the volume average operator to Eq. (32) such that,

\[(G_c)^* = G_c' = \left( \mu \phi \mathbf{g} \cdot \nabla \mathbf{c} \right)^* = -\rho \phi \beta_{c_a} \phi \mathbf{g} \cdot \nabla \langle \mathbf{c} \rangle^i\]

where the coefficient \(\beta_{c_a}\), for a constant value of \(\mathbf{g}\) within the REV, is given by \(\beta_{c_a} = \langle \rho \phi \mathbf{g} \rangle\), which, in turn, is not necessarily equal to \(\beta_{c_a}\) given by Eq. (68). However, for the sake of simplicity and in the absence of better information, one can use a similar argument as in reference [16] and make use of the assumption \(\beta_c = \beta_{c_a} = \beta_{c_a}'\).

Further, expanding the r.h.s. of Eq. (71) in light of Eqs. (17) and (19), one has

\[-\rho \phi \beta_{c_a} \mathbf{g} \cdot \langle \mathbf{c} \rangle^i = -\rho \phi \beta_{c_a} \mathbf{g} \cdot \left( \langle \mathbf{u} \rangle^i + \langle \mathbf{u}' \rangle^i \right)^i = -\rho \phi \beta_{c_a} \mathbf{g} \cdot \left( \langle \mathbf{u} \rangle^i + \langle \mathbf{u}' \rangle^i \right)^i = -\rho \phi \beta_{c_a} \mathbf{g} \cdot \left( \langle \mathbf{u} \rangle^i + \langle \mathbf{u}' \rangle^i \right)^i = -\rho \phi \beta_{c_a} \mathbf{g} \cdot \left( \langle \mathbf{u} \rangle^i + \langle \mathbf{u}' \rangle^i \right)^i (72)\]

The last two terms on the right of Eq. (72) are null since \langle \mathbf{c} \rangle^i = 0 and \langle \mathbf{u} \rangle^i = 0. In addition, the following physical significance can be inferred to the two remaining terms, which were fully commented upon in ref. [16] and for that they will be just listed:

I. Generation/destruction rate of turbulence energy due to macroscopic concentration fluctuations,

II. Generation/destruction rate due to turbulent concentration dispersion.

A model for Eq. (72) is still needed in order to solve an equation for \(\langle k^i \rangle\), which is a necessary information when computing \(\mu_t\) using Eq. (37). Consequently, terms I and II above have to be modeled as a function of average concentration, \(\langle \mathbf{c} \rangle\). To accomplish this, a gradient type diffusion model is used, in the form,

• Buoyancy generation of \(\langle k^i \rangle\) due to turbulent salutation fluctuations:

\[-\rho \phi \beta_{c_a} \mathbf{g} \cdot \langle \mathbf{c} \rangle^i = \rho \phi \beta_{c_a} \mathbf{g} \cdot \left( \mathbf{D}_t \cdot \nabla \langle \mathbf{c} \rangle \right)\]

(73)

• Buoyancy generation of \(\langle k^i \rangle\) due to turbulent salutation dispersion:

\[-\rho \phi \beta_{c_a} \mathbf{g} \cdot \langle \mathbf{c} \rangle^i = \rho \phi \beta_{c_a} \mathbf{g} \cdot \left( \mathbf{D}_{\text{disp}, t} \cdot \nabla \langle \mathbf{c} \rangle \right)\]

(74)

The buoyancy concentration coefficients seen above, namely \(\mathbf{D}_t\) and \(\mathbf{D}_{\text{disp}, t}\), were used before in Eqs. (63) and (64), respectively. Note that the terms given by Eqs. (73) and (74) arise only if the flow is turbulent and if buoyancy is of importance.

Using then Eq. (65) the macroscopic buoyancy generation of \(k\) due to concentration fluctuations can be modeled as,

\[G_{\mu_c} = -\rho \phi \beta_{c_a} \mathbf{g} \cdot \langle \mathbf{c} \rangle^i = \rho \phi \beta_{c_a} \mathbf{g} \cdot \left( \mathbf{D}_t + \mathbf{D}_{\text{disp}, t} \right) \cdot \nabla \langle \mathbf{c} \rangle^i = \rho \phi \beta_{c_a} \frac{\mu_c}{S_{\text{c}}} \mathbf{g} \cdot \nabla \langle \mathbf{c} \rangle^i\]

(75)

where \(\mu_c\), \(S_{\text{c}}\) and the two coefficients \(\mathbf{D}_t\) and \(\mathbf{D}_{\text{disp}, t}\) have been defined before.

Final transport equations for \(\langle k \rangle = \left( \langle \mathbf{u} \rangle^2 - \langle \mathbf{u} \rangle^2 \right) / 2\) and \(\langle c \rangle = \mu \left( \nabla \langle \mathbf{u} \rangle^2 \right) / \rho\), in their so-called High Reynolds number form can now include the buoyancy generation terms due to temperature and concentration fluctuations as,

\[\rho \nabla \cdot \left( \mathbf{u}_c \langle k \rangle^i \right) = \nabla \cdot \left( \mathbf{H}_t \right) + \frac{\rho}{\phi} \left( \mu \phi \beta_{c_a} \mathbf{g} \cdot \langle \mathbf{c} \rangle^i \right)\]

(76)
\[ \rho \nabla \cdot \left( \mathbf{u}_D (\phi i)^j \right) = \nabla \cdot \left[ \left( \mu + \frac{\mu_k}{\sigma_\mu} \right) \nabla \left( \phi (\phi i)^j \right) \right] + \frac{G_i}{k_i} \right] c_1 \phi \phi i^j + c_2 G_i + c_1 \left( G_i^{2f} + G_i^{2h} \right) - c_3 \phi \phi i^j \right] \] (77)

where, \( \alpha_k = 1 \), \( \alpha_t = 1.3 \), \( c_1 = 1.44 \), \( c_2 = 1.92 \), \( \mu_k = 0.09 \) and \( \nu_k = 0.28 \) are non-dimensional constants (see ref. [15]). The production terms have the following physical significance:

1. \( P_i = -\rho \left[ \mathbf{u} \cdot \nabla \mathbf{u} \right] : \nabla \mathbf{u}_D \) is the production rate of \( \langle k_i \rangle \) due to gradients of \( \mathbf{u}_D \);

2. \( G_i = c_3 \rho \frac{\partial \langle k_i \rangle}{\partial x} \) is the generation rate of the intrinsic average of \( \langle k_i \rangle \) due to the action of the porous matrix;

3. \( G_i^j = \beta^j \phi \frac{\partial \langle k_i \rangle}{\partial x} \) \( \cdot \nabla \langle T_f \rangle \) is the generation of \( \langle k_i \rangle \) due to mean temperature variation within the fluid, and

4. \( G_i^{2h} = \beta^h \phi \frac{\partial \langle k_i \rangle}{\partial x} \) \( \cdot \nabla \langle C \rangle \) is the generation of \( \langle k_i \rangle \) due to concentration gradients.

12. Conclusions

In this work, equations were derived for turbulent double-diffusive natural convection in porous media. Derivations were carried out under the light of the double decomposition concept [15]. Extra terms appearing in the equations needed to be modeled in terms of \( \mathbf{u}_D \), \( \langle T_f \rangle \) and \( \langle C \rangle \). Here, two different models were combined in order to broaden the ability to analyze more complex flow systems. The first model dealt with characterizing turbulent double-diffusive mechanism but was limited to situations were the so-called thermal equilibrium between phases applied [16]. In addition, the second description of turbulent flow in porous media made no consideration about buoyancy effects but was able to handle situations where the difference in both the fluid and the solid material was considerable [17]. By combining the two models in one single mathematical characterization, the work herein aims at extending the tool described in detail in ref. [15] to solve an ever-broader range of practical problems in engineering.

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