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Modeling of double-diffusive turbulent natural convection in porous media

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Abstract

This paper presents an analysis of the macroscopic heat and mass transport equations for turbulent 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 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 temperature, concentration and velocity present simultaneously time fluctuations and spatial deviations within the domain of analysis. A modeled form for the final mass transport equation is presented where turbulent transfer is based on a macroscopic version of the k–ε model. Stability analysis of mixtures, composed of lighter or heavier components under gradients of temperature and concentration, is discussed.

Keywords: Double-diffusion; Natural convection; Turbulence modeling; Porous media; Volume-average; Time-average; Mass transport

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. [1–7]. 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 [8] or mass transfer [9–12]. 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 [13–16], or (b) use of volume-averaging before time-averaging is applied [17–20]. This work intends to present a set of macroscopic mass transport equations derived under the recently established double decomposition concept [21–25], 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 [26]. Flow about an interface [27,28], buoyant flows [29] and mass transfer [30] have also been investigated. Recently, a general classification of all proposed models for turbulent flow and heat

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Nomenclature

c_F	Forchheimer coefficient
C_ℓ	volumetric molar concentration
c_p	specific heat
D_ℓ	diffusion coefficient
$\mathbf{D}_{disp}$	mass dispersion
$\mathbf{D}_{disp,t}$	turbulent mass dispersion
$\mathbf{D}_t$	turbulent mass flux
$\mathbf{g}$	gravity acceleration vector
$\mathbf{I}$	unity tensor
$\mathbf{J}_\ell$	mass diffusion coefficient
k	turbulent kinetic energy per unit mass, $k = \overline{\mathbf{u}'\cdot\mathbf{u}'}/2$
$\langle k\rangle^i$	intrinsic (fluid) average of k
K	permeability
ℓ	chemical species
m_ℓ	mass fraction of component ℓ
M_ℓ	molar weight of component ℓ
p	pressure
Pr_t	turbulent Prandtl number
Sc_t	turbulent Schmidt number
T	temperature
$\mathbf{u}$	mass-averaged velocity of the mixture
$\bar{\mathbf{u}}_D$	Darcy velocity vector
$\mathbf{u}_\ell$	velocity of species ℓ

Greek symbols

β	thermal expansion coefficient
β_C	salute expansion coefficient
β_ϕ	macroscopic thermal expansion coefficient
β_{C_ϕ}	macroscopic salute expansion coefficient
λ	fluid thermal conductivity
μ	fluid mixture viscosity
μ_t	turbulent viscosity
μ_{t_ϕ}	macroscopic turbulent viscosity
ε	dissipation rate of k
$\langle\varepsilon\rangle^i$	intrinsic (fluid) average of ε
ρ	bulk density of the mixture
ρ_ℓ	mass density of species ℓ
ϕ	porosity

Subscripts

β	buoyancy
ℓ	chemical species
t	turbulent
ϕ	macroscopic
C	concentration
T	temperature

Superscripts

i	intrinsic (fluid) average
v	volume (fluid + solid) average
k	turbulent kinetic energy

transfer in porous media has been published [31]. Here, double-diffusive turbulent 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

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

$$\rho\nabla\cdot(\mathbf{uu}) = -\nabla p + \mu\nabla^2\mathbf{u} + \rho\mathbf{g} \tag{2}$$

$$(\rho c_p)\nabla\cdot(\mathbf{u}T) = \nabla\cdot(\lambda\nabla T) \tag{3}$$

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

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 $m_\ell = \rho_\ell/\rho$, ρ_ℓ is the mass density of species ℓ (mass of ℓ over total mixture volume), ρ is the bulk density of the mixture ($\rho = \sum_\ell \rho_\ell$), p is the pressure, μ is the fluid mixture viscosity, $\mathbf{g}$ is the gravity acceleration vector, c_p is the specific heat, T is the temperature and λ is the fluid thermal conductivity. The generation rate of species ℓ per unit of mixture mass is given in (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 (4) or (5) is due to the velocity slip of species ℓ,

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

where D_ℓ 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 [8]. Therefore, no *Soret* or *Dufour* effects are here considered.

Rearranging (5) for an inert species, dividing it by M_ℓ 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 (2) varies with temperature and concentration, for natural convection flow, the Boussinesq hypothesis reads, after renaming this density ρ_T,

$$\rho_T \cong \rho[1 - \beta(T - T_{ref}) - \beta_C(C - C_{ref})] \tag{8}$$

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

$$\beta = -\frac{1}{\rho}\frac{\partial \rho}{\partial T}\bigg|_{p,C}, \quad \beta_C = -\frac{1}{\rho}\frac{\partial \rho}{\partial C}\bigg|_{p,T} \tag{9}$$

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

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

$$\rho\nabla \cdot (\mathbf{uu}) = -\nabla p + \mu\nabla^2\mathbf{u} + \rho\mathbf{g}[1 - \beta(T - T_{ref}) - \beta_C(C - C_{ref})] \tag{10}$$

Thus, the momentum equation becomes,

$$\rho\nabla \cdot (\mathbf{uu}) = -(\nabla p)^* + \mu\nabla^2\mathbf{u} - \rho\mathbf{g}[\beta(T - T_{ref}) + \beta_C(C - C_{ref})] \tag{11}$$

where $(\nabla p)^* = \nabla p - \rho\mathbf{g}$ 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 equations 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 Refs. [32–34], 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 time average and volume average.

3. Volume and time average operators—the double decomposition concept

The volume average of φ taken over a representative elementary volume in a porous medium can be written as

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

The value $\langle\varphi\rangle^v$ 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

$$\langle\varphi\rangle^v = \phi\langle\varphi\rangle^i \tag{13}$$

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

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

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

Further, the local volume average theorem can be expressed as [32–34]

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

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 A_i should not be confused with the surface area surrounding volume ΔV.

Further, the time average of a general quantity φ is defined as

$$\bar{\varphi} = \frac{1}{\Delta t}\int_t^{t+\Delta t}\varphi\,dt \tag{16}$$

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

$$\varphi = \bar{\varphi} + \varphi' \tag{17}$$

with $\overline{\varphi'} = 0$. Here, φ' is the *time fluctuation* of φ around its average $\bar{\varphi}$.

Pedras and de Lemos [21,22] showed that for a rigid, homogeneous porous medium saturated with an incompressible fluid, the following relationships apply:

$$\begin{aligned}
&\overline{\langle\varphi\rangle^i} = \langle\bar{\varphi}\rangle^i \\
&{}^i\bar{\varphi} = {}^i\overline{\varphi} \\
&\langle\varphi'\rangle^i = \langle\varphi\rangle^{i'}
\end{aligned} \tag{18}$$

Therefore, a general quantity φ can be expressed by either,

$$\varphi = \overline{\langle\varphi\rangle^i} + \langle\varphi\rangle^{i'} + \overline{{}^i\varphi} + {}^i\varphi' \tag{19}$$

$$\varphi = \langle\bar{\varphi}\rangle^i + {}^i\bar{\varphi} + \langle\varphi'\rangle^i + {}^i\varphi' \tag{20}$$

Expressions (19) and (20) comprise the double decomposition concept where ${}^{\mathrm{i}}\varphi'$ can be understood as either the *time fluctuation of the spatial deviation* or the *spatial deviation of the time fluctuation*. Also, $\langle {}^{\mathrm{i}}\varphi' \rangle^{\mathrm{i}} = \overline{{}^{\mathrm{i}}\varphi'} = 0$.

4. Time averaged transport equations

In order to apply the time average operator to Eqs. (1), (3), (7) and (11), one considers

$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{u}', \quad T = \overline{T} + T', \quad C = \overline{C} + C', \quad p = \bar{p} + p' \tag{21}$$

Substituting (21) into the governing equations and considering constant property flow,

$$\nabla \cdot \bar{\mathbf{u}} = 0 \tag{22}$$

$$\rho \nabla \cdot (\bar{\mathbf{u}}\bar{\mathbf{u}}) = -(\nabla \bar{p})^{*} + \mu \nabla^2 \bar{\mathbf{u}} + \nabla \cdot (-\rho \overline{\mathbf{u}'\mathbf{u}'}) - \rho \mathbf{g}[\beta(\overline{T} - T_{\mathrm{ref}}) + \beta_{\mathrm{C}}(\overline{C} - C_{\mathrm{ref}})] \tag{23}$$

$$(\rho c_p) \nabla \cdot (\bar{\mathbf{u}}\overline{T}) = \nabla \cdot (k \nabla \overline{T}) + \nabla \cdot (-\rho c_p \overline{\mathbf{u}'T'}) \tag{24}$$

$$\nabla \cdot (\mathbf{u}C) = -\nabla \cdot (D \nabla C) + \nabla \cdot (-\overline{\mathbf{u}'C'}) \tag{25}$$

For clear fluid, the use of the eddy-diffusivity concept for expressing the stress–strain rate relationship for the Reynolds stress appearing in (23) gives

$$-\rho \overline{\mathbf{u}'\mathbf{u}'} = \mu_{\mathrm{t}} 2\overline{\mathbf{D}} - \frac{2}{3}\rho k \mathbf{I} \tag{26}$$

where $\overline{\mathbf{D}} = [\nabla \bar{\mathbf{u}} + (\nabla \bar{\mathbf{u}})^{\mathrm{T}}]/\mathbf{2}$ is the mean deformation tensor, $k = \overline{\mathbf{u}' \cdot \mathbf{u}'}/2$ is the turbulent kinetic energy per unit mass, μ_{t} is the turbulent viscosity and $\mathbf{I}$ is the unity tensor. Similarly, for the turbulent heat flux on the R.H.S. of (24) and (25) the eddy diffusivity concept reads

$$-\rho c_p \overline{\mathbf{u}'T'} = c_p \frac{\mu_{\mathrm{t}}}{Pr_{\mathrm{t}}} \nabla \overline{T}; \quad -\rho \overline{\mathbf{u}'C'} = \frac{\mu_{\mathrm{t}}}{Sc_{\mathrm{t}}} \nabla \overline{C} \tag{27}$$

where Pr_{t} and Sc_{t} are known as the turbulent 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

$$\rho \nabla \cdot (\bar{\mathbf{u}} k) = -\rho \nabla \cdot \overline{\left[\mathbf{u}' \left(\frac{p'}{\rho} + q \right) \right]} + \mu \nabla^2 k + P + G_T + G_{\mathrm{C}} - \rho \varepsilon \tag{28}$$

where $P = -\rho \overline{\mathbf{u}'\mathbf{u}'} : \nabla \bar{\mathbf{u}}$ is the generation rate of k due to gradients of the mean velocity and

$$G_{\mathrm{T}} = -\rho \beta \mathbf{g} \cdot \overline{\mathbf{u}'T'} \tag{29}$$

$$G_{\mathrm{C}} = -\rho \beta_C \mathbf{g} \cdot \overline{\mathbf{u}'C'} \tag{30}$$

are the thermal and concentration generation rates of k due to temperature and concentration fluctuations, respectively. Also, $q = \mathbf{u}' \cdot \mathbf{u}'/2$.

5. Macroscopic equations for buoyancy free flows

For non-buoyant flows, macroscopic equations considering turbulence have been already derived in detail for momentum [22], heat [29,35] and mass transfer [30] and for this reason their derivation need not to be repeated here. They read:

Momentum transport

$$\rho \nabla \cdot \left(\frac{\bar{\mathbf{u}}_{\mathrm{D}} \bar{\mathbf{u}}_{\mathrm{D}}}{\phi} \right) = -\nabla(\phi \langle \bar{p} \rangle^{\mathrm{i}}) + \mu \nabla^2 \bar{\mathbf{u}}_{\mathrm{D}} + \nabla \cdot (-\rho \phi \langle \overline{\mathbf{u}'\mathbf{u}'} \rangle^{\mathrm{i}}) - \left[\frac{\mu \phi}{K} \bar{\mathbf{u}}_{\mathrm{D}} + \frac{c_{\mathrm{F}} \phi \rho |\bar{\mathbf{u}}_{\mathrm{D}}| \bar{\mathbf{u}}_{\mathrm{D}}}{\sqrt{K}} \right] \tag{31}$$

$$-\rho \phi \langle \overline{\mathbf{u}'\mathbf{u}'} \rangle^{\mathrm{i}} = \mu_{\mathrm{t}_\phi} 2 \langle \overline{\mathbf{D}} \rangle^{\mathrm{v}} - \frac{2}{3} \phi \rho \langle k \rangle^{\mathrm{i}} \mathbf{I} \tag{32}$$

$$\langle \overline{\mathbf{D}} \rangle^{\mathrm{v}} = \frac{1}{2} \{ \nabla(\phi \langle \bar{\mathbf{u}} \rangle^{\mathrm{i}}) + [\nabla(\phi \langle \bar{\mathbf{u}} \rangle^{\mathrm{i}})]^{\mathrm{T}} \} \tag{33}$$

$$\langle k \rangle^{\mathrm{i}} = \langle \overline{\mathbf{u}' \cdot \mathbf{u}'} \rangle^{\mathrm{i}}/2$$

$$\mu_{\mathrm{t}_\phi} = \rho c_\mu \frac{\langle k \rangle^{\mathrm{i}^2}}{\langle \varepsilon \rangle^{\mathrm{i}}} \tag{34}$$

Heat transport

$$(\rho c_p)_{\mathrm{f}} \nabla \cdot (\mathbf{u}_{\mathrm{D}} \langle \overline{T} \rangle^{\mathrm{i}}) = \nabla \cdot \{ \mathbf{K}_{\mathrm{eff}} \cdot \nabla \langle \overline{T} \rangle^{\mathrm{i}} \} \tag{35}$$

$$\mathbf{K}_{\mathrm{eff}} = [\phi \lambda_{\mathrm{f}} + (1 - \phi)\lambda_{\mathrm{s}}]\mathbf{I} + \mathbf{K}_{\mathrm{tor}} + \mathbf{K}_{\mathrm{t}} + \mathbf{K}_{\mathrm{disp}} + \mathbf{K}_{\mathrm{disp,t}} \tag{36}$$

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

Tortuosity: $$\left[\frac{1}{\Delta V} \int_{A_i} \mathbf{n}(\lambda_{\mathrm{f}} \overline{T_{\mathrm{f}}} - \lambda_{\mathrm{s}} \overline{T_{\mathrm{s}}}) \, \mathrm{d}S \right] = \mathbf{K}_{\mathrm{tor}} \cdot \nabla \langle \overline{T} \rangle^{\mathrm{i}} \tag{37}$$

Thermal dispersion: $$-(\rho c_p)_{\mathrm{f}} \phi \langle {}^{\mathrm{i}}\bar{\mathbf{u}}^{\mathrm{i}} \overline{T_{\mathrm{f}}} \rangle^{\mathrm{i}} = \mathbf{K}_{\mathrm{disp}} \cdot \nabla \langle \overline{T} \rangle^{\mathrm{i}} \tag{38}$$

Turbulent heat flux: $$-(\rho c_p)_{\mathrm{f}} \phi \overline{\langle \mathbf{u}' \rangle^{\mathrm{i}} \langle T_{\mathrm{f}}' \rangle^{\mathrm{i}}} = \mathbf{K}_{\mathrm{t}} \cdot \nabla \langle \overline{T} \rangle^{\mathrm{i}} \tag{39}$$

Turbulent thermal dispersion:

$$-(\rho c_p)_{\mathrm{f}} \phi \langle \overline{{}^{\mathrm{i}}\mathbf{u}'^{\mathrm{i}} T_{\mathrm{f}}'} \rangle^{\mathrm{i}} = \mathbf{K}_{\mathrm{disp,t}} \cdot \nabla \langle \overline{T} \rangle^{\mathrm{i}} \tag{40}$$

Mechanisms (39) and (40) were modeled together in [29,35] by assuming,

$$-(\rho c_p)_{\mathrm{f}}\langle\overline{\mathbf{u}'T'_{\mathrm{f}}}\rangle^{\mathrm{i}} = c_{p_{\mathrm{f}}}\frac{\mu_{\mathrm{t}_\phi}}{Pr_{\mathrm{t}_\phi}}\nabla\langle\overline{T}_{\mathrm{f}}\rangle^{\mathrm{i}} \tag{41}$$

or

$$\mathbf{K}_{\mathrm{t}} + \mathbf{K}_{\mathrm{disp,t}} = \phi c_{p_{\mathrm{f}}}\frac{\mu_{\mathrm{t}_\phi}}{Pr_{\mathrm{t}_\phi}}\mathbf{I} \tag{42}$$

Mass transport

$$\nabla\cdot(\bar{\mathbf{u}}_{\mathrm{D}}\langle\overline{C}\rangle^{\mathrm{i}}) = \nabla\cdot\mathbf{D}_{\mathrm{eff}}\cdot\nabla(\phi\langle\overline{C}\rangle^{\mathrm{i}}) \tag{43}$$

$$\mathbf{D}_{\mathrm{eff}} = \mathbf{D}_{\mathrm{disp}} + \mathbf{D}_{\mathrm{diff}} + \mathbf{D}_{\mathrm{t}} + \mathbf{D}_{\mathrm{disp,t}} \tag{44}$$

$$\mathbf{D}_{\mathrm{diff}} = \langle D\rangle^{\mathrm{i}}\mathbf{I} = \frac{1}{\rho}\frac{\mu_\phi}{Sc}\mathbf{I} \tag{45}$$

$$\mathbf{D}_{\mathrm{t}} + \mathbf{D}_{\mathrm{disp,t}} = \frac{1}{\rho}\frac{\mu_{\mathrm{t}_\phi}}{Sc_{\mathrm{t}}}\mathbf{I} \tag{46}$$

Coefficients $\mathbf{D}_{\mathrm{disp}}$, $\mathbf{D}_{\mathrm{t}}$ and $\mathbf{D}_{\mathrm{disp,t}}$ in (43) appear due to the nonlinearity of the convection term. They come from the modeling of the following mechanisms:

$$\text{Mass dispersion:}\quad -\langle{}^{\mathrm{i}}\bar{\mathbf{u}}^{\mathrm{i}}\overline{C}\rangle^{\mathrm{i}} = \mathbf{D}_{\mathrm{disp}}\cdot\nabla\langle\overline{C}\rangle^{\mathrm{i}} \tag{47}$$

$$\text{Turbulent mass flux:}\quad -\overline{\langle\mathbf{u}'\rangle^{\mathrm{i}}\langle C'\rangle^{\mathrm{i}}} = -\overline{\langle\mathbf{u}\rangle^{\mathrm{i}'}\langle C\rangle^{\mathrm{i}'}} = \mathbf{D}_{\mathrm{t}}\cdot\nabla\langle\overline{C}\rangle^{\mathrm{i}} \tag{48}$$

Turbulent mass dispersion:

$$-\langle\overline{{}^{\mathrm{i}}\mathbf{u}'{}^{\mathrm{i}}C'}\rangle^{\mathrm{i}} = \mathbf{D}_{\mathrm{disp,t}}\cdot\nabla\langle\overline{C}\rangle^{\mathrm{i}} \tag{49}$$

Here also mechanisms (48) and (49) are added up as [30]

$$-\langle\overline{\mathbf{u}'C'}\rangle^{\mathrm{i}} = \frac{1}{\rho}\frac{\mu_{\mathrm{t}_\phi}}{Sc_{\mathrm{t}\phi}}\nabla\langle\overline{C}\rangle^{\mathrm{i}} = \langle D_{\mathrm{t}}\rangle^{\mathrm{i}}\nabla\langle\overline{C}\rangle^{\mathrm{i}} = (\mathbf{D}_{\mathrm{t}} + \mathbf{D}_{\mathrm{disp,t}})\cdot\nabla\langle\overline{C}\rangle^{\mathrm{i}} \tag{50}$$

6. Macroscopic double-diffusion effects

6.1. Mean flow

Focusing now attention to buoyancy effects only, application of the volume average procedure to the last term of (23) leads to

$$\langle\rho\mathbf{g}[\beta(\overline{T}-T_{\mathrm{ref}}) + \beta_{\mathrm{C}}(\overline{C}-C_{\mathrm{ref}})]\rangle^{\mathrm{v}} = \frac{\Delta V_{\mathrm{f}}}{\Delta V}\frac{1}{\Delta V_{\mathrm{f}}}\int_{\Delta V_{\mathrm{f}}}\rho\mathbf{g}[\beta(\overline{T}-T_{\mathrm{ref}}) + \beta_{\mathrm{C}}(\overline{C}-C_{\mathrm{ref}})]\,\mathrm{d}V \tag{51}$$

Expanding the left hand side of (51) in light of (14), the buoyancy term becomes

$$\langle\rho\mathbf{g}[\beta(\overline{T}-T_{\mathrm{ref}}) + \beta_{\mathrm{C}}(\overline{C}-C_{\mathrm{ref}})]\rangle^{\mathrm{v}} = \rho\mathbf{g}\phi[\beta_\phi(\langle\overline{T}\rangle^{\mathrm{i}} - T_{\mathrm{ref}}) + \beta_{C_\phi}(\langle\overline{C}\rangle^{\mathrm{i}} - C_{\mathrm{ref}})] + \underbrace{\rho\mathbf{g}\beta\phi\overline{\langle{}^{\mathrm{i}}T\rangle^{\mathrm{i}}}}_{=0} + \underbrace{\rho\mathbf{g}\beta_{\mathrm{C}}\phi\overline{\langle{}^{\mathrm{i}}C\rangle^{\mathrm{i}}}}_{=0} \tag{52}$$

where the third and forth terms on the R.H.S. are null since $\langle{}^{\mathrm{i}}\varphi\rangle^{\mathrm{i}} = 0$. Here, coefficients β_ϕ and β_{C_ϕ} are the *macroscopic* thermal and salute expansion coefficients, respectively. Assuming that gravity is constant over the REV, expressions for them based on (52) are given as

$$\beta_\phi = \frac{\langle\rho\beta(\overline{T}-T_{\mathrm{ref}})\rangle^{\mathrm{v}}}{\rho\phi(\langle\overline{T}\rangle^{\mathrm{i}} - T_{\mathrm{ref}})},\qquad \beta_{C_\phi} = \frac{\langle\rho\beta_{\mathrm{C}}(\overline{C}-C_{\mathrm{ref}})\rangle^{\mathrm{v}}}{\rho\phi(\langle\overline{C}\rangle^{\mathrm{i}} - C_{\mathrm{ref}})} \tag{53}$$

Including (52) into (31), the macroscopic time-mean Navier–Stokes (NS) equation for an incompressible fluid with constant properties is given as

$$\rho\nabla\cdot\left(\frac{\bar{\mathbf{u}}_{\mathrm{D}}\bar{\mathbf{u}}_{\mathrm{D}}}{\phi}\right) = -\nabla(\phi\langle\bar{p}\rangle^{\mathrm{i}}) + \mu\nabla^2\bar{\mathbf{u}}_{\mathrm{D}} + \nabla\cdot(-\rho\phi\langle\overline{\mathbf{u}'\mathbf{u}'}\rangle^{\mathrm{i}}) - \rho\mathbf{g}\phi[\beta_\phi(\langle\overline{T}\rangle^{\mathrm{i}} - T_{\mathrm{ref}}) + \beta_{C_\phi}(\langle\overline{C}\rangle^{\mathrm{i}} - C_{\mathrm{ref}})] - \left[\frac{\mu\phi}{K}\bar{\mathbf{u}}_{\mathrm{D}} + \frac{c_{\mathrm{F}}\phi\rho|\bar{\mathbf{u}}_{\mathrm{D}}|\bar{\mathbf{u}}_{\mathrm{D}}}{\sqrt{K}}\right] \tag{54}$$

Before proceeding, it is interesting to comment on role of coefficients β_ϕ and β_{C_ϕ} on the overall mixture density value. Fig. 1 presents the variation of ρ as a function of temperature or concentration gradients. Here, only fluids that became less dense with increasing temperature are considered (Fig. 1a). However, two situation might occurs when increasing $\langle\overline{C}\rangle^{\mathrm{i}}$, namely the

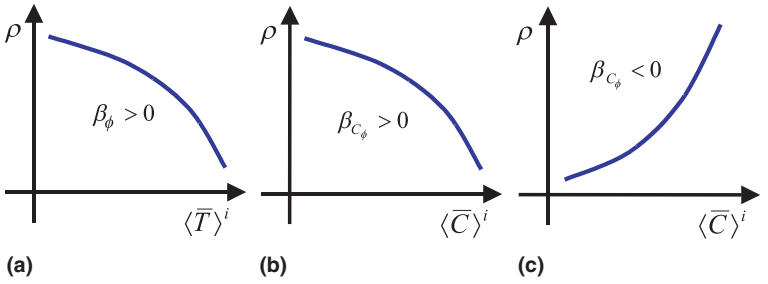

Fig. 1. Behaviour of mixture density: (a) lighter mixture with increasing $\langle\overline{T}\rangle^{\mathrm{i}}$, (b) lighter mixture with increasing $\langle\overline{C}\rangle^{\mathrm{i}}$, (c) heavier mixture with increasing $\langle\overline{C}\rangle^{\mathrm{i}}$.

mixture might became less dense with the addition of a lighter solute (Fig. 1b), or else, a denser fluid may result by mixing a heavier component to it (Fig. 1c). Implications of that on the stability of the entire fluid system will be discussed below.

6.2. Turbulent field

As mentioned, this work extends and combines earlier developments for momentum [22], heat [35] and mass [30] transfer in order to include the buoyancy production terms in the turbulence model equations. For clear fluid, the buoyancy contribution to the k equation is given by Eqs. (29) and (30).

For thermally-driven flows, volume averaging of (30) in Ref. [29] has resulted in the term

$$G_\beta^{\mathrm{i}} = \beta_\phi^k \phi \frac{\mu_{\mathrm{t}_\phi}}{Pr_{\mathrm{t}_\phi}} \mathbf{g} \cdot \nabla \langle \overline{T} \rangle^{\mathrm{i}} \tag{55}$$

as an additional macroscopic generation/destruction rate of $\langle k \rangle^{\mathrm{i}}$ due to temperature variation in porous media, where β_ϕ^k is a macroscopic coefficient. In Ref. [29], coefficients β (Eq. (9)), β_ϕ (Eq. (53)) and β_ϕ^k (Eq. (55)) were all assumed to be equal, for simplicity.

In order to add the effect of concentration variation within the fluid, one applies the volume average operator to (30) such that

$$\langle G_{\mathrm{C}} \rangle^{\mathrm{v}} = G_{\beta_{\mathrm{C}}}^{\mathrm{i}} = \langle -\rho \beta_{\mathrm{C}} \mathbf{g} \cdot \overline{\mathbf{u}' C'} \rangle^{\mathrm{v}} = -\rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot \langle \overline{\mathbf{u}' C'} \rangle^{\mathrm{i}} \tag{56}$$

where the coefficient $\beta_{C_\phi}^k$, for a constant value of $\mathbf{g}$ within the REV, is given by $\beta_{C_\phi}^k = \frac{\langle \beta_{\mathrm{C}} \overline{\mathbf{u}' C'} \rangle^{\mathrm{v}}}{\phi \langle \overline{\mathbf{u}' C'} \rangle^{\mathrm{i}}}$, which, in turn, is not necessarily equal to β_{C_ϕ} given by (53). However, for the sake of simplicity and in the absence of better information, one can use a similar argument as in Ref. [29] and make use of the assumption $\beta_{C_\phi}^k = \beta_{C_\phi} = \beta_{\mathrm{C}}$. Further, expanding the R.H.S. of (56) in light of (14) and (18), one has

$$\begin{aligned}
&-\rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot \langle \overline{\mathbf{u}' C'} \rangle^{\mathrm{i}} \\
&\quad = -\rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot \langle \overline{(\langle \mathbf{u}' \rangle^{\mathrm{i}} + {}^{\mathrm{i}}\mathbf{u}')(\langle C' \rangle^{\mathrm{i}} + {}^{\mathrm{i}}C')} \rangle^{\mathrm{i}} \\
&\quad = -\rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot \Big(\langle \overline{\langle \mathbf{u}' \rangle^{\mathrm{i}} \langle C' \rangle^{\mathrm{i}}} \rangle^{\mathrm{i}} + \langle \overline{{}^{\mathrm{i}}\mathbf{u}' {}^{\mathrm{i}}C'} \rangle^{\mathrm{i}} \\
&\qquad + \langle \overline{\langle \mathbf{u}' \rangle^{\mathrm{i}} {}^{\mathrm{i}}C'} \rangle^{\mathrm{i}} + \langle \overline{{}^{\mathrm{i}}\mathbf{u}' \langle C' \rangle^{\mathrm{i}}} \rangle^{\mathrm{i}} \Big) \\
&\quad = -\rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot \Bigg(\underbrace{\overline{\langle \mathbf{u} \rangle^{i'} \langle C \rangle^{i'}}}_{\mathbf{I}} + \underbrace{\langle \overline{{}^{\mathrm{i}}\mathbf{u}' {}^{\mathrm{i}}C'} \rangle^{\mathrm{i}}}_{\mathbf{II}} \\
&\qquad + \underbrace{\overline{\langle \mathbf{u}' \rangle^{\mathrm{i}} \langle {}^{\mathrm{i}}C' \rangle^{\mathrm{i}}}}_{=0} + \underbrace{\overline{\langle {}^{\mathrm{i}}\mathbf{u}' \rangle^{\mathrm{i}} \langle C' \rangle^{\mathrm{i}}}}_{=0} \Bigg)
\end{aligned} \tag{57}$$

The last two terms on the right of (57) are null since $\langle {}^{\mathrm{i}}C' \rangle^{\mathrm{i}} = 0$ and $\langle {}^{\mathrm{i}}\mathbf{u}' \rangle^{\mathrm{i}} = 0$. In addition, the following physical significance can be inferred to the two remaining terms:

I. *Generation/destruction rate of turbulence energy due to macroscopic concentration fluctuations*: Buoyancy generation/destructions rate of $\langle k \rangle^{\mathrm{i}}$ due to time fluctuations of macroscopic velocity and concentration. This term is also present in turbulent flow in clear (non-obstructed) domains and represents an exchange between the energy associated with the macroscopic turbulent motion and potential energy. In stable stratification, within regions of high concentration of heavier solutes ($\beta_{C_\phi}^k < 0$), this term damps turbulence by being of negative value whereas the potential energy of the system is increased. On the other hand, in unstable stratification, for high concentration regions of lighter mixtures ($\beta_{C_\phi}^k > 0$), it enhances $\langle k \rangle^{\mathrm{i}}$ at the expense of potential energy. A more detailed analysis on the stability of mixture systems is presented below.

II. *Generation/destruction rate due to turbulent concentration dispersion*: Buoyancy generation/destruction rate of $\langle k \rangle^{\mathrm{i}}$ in a porous medium due to time fluctuations and spatial deviations of both microscopic velocity and concentration. This term might be interpreted as an additional source/sink of turbulence kinetic energy due the fact that time fluctuations of local velocities and concentration present a spatial deviation in relation to their macroscopic value. Then, additional exchange between turbulent kinetic energy and potential energy in systems may occur due to the presence of a porous matrix.

A model for (57) is still needed in order to solve an equation for $\langle k \rangle^{\mathrm{i}}$, which is a necessary information when computing μ_{t_ϕ} using (34). Consequently, terms I and II above have to be modeled as a function of average concentration, $\langle \overline{C} \rangle^{\mathrm{i}}$. To accomplish this, a gradient type diffusion model is used, in the form,

- Buoyancy generation of $\langle k \rangle^{\mathrm{i}}$ due to *turbulent salute fluctuations*:

$$-\rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot \overline{\langle \mathbf{u} \rangle^{i'} \langle C \rangle^{i'}} = \rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot (\mathbf{D}_{\mathrm{t}} \cdot \nabla \langle \overline{C} \rangle^{\mathrm{i}}) \tag{58}$$

- Buoyancy generation of $\langle k \rangle^{\mathrm{i}}$ due to *turbulent salute dispersion*:

$$-\rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot \langle {}^{\mathrm{i}}\overline{\mathbf{u}'^{\mathrm{i}} C'} \rangle^{\mathrm{i}} = \rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot (\mathbf{D}_{\mathrm{disp,t}} \cdot \nabla \langle \overline{C} \rangle^{\mathrm{i}}) \tag{59}$$

The buoyancy concentration coefficients seem above, namely $\mathbf{D}_{\mathrm{t}}$ and $\mathbf{D}_{\mathrm{disp,t}}$, were used before in (48) and (49), respectively. It should be noticed that these terms arise only if the flow is turbulent and if buoyancy is of importance.

Using then (50) the macroscopic buoyancy generation of k due to concentration fluctuations can be modeled as

$$\begin{aligned}
G_{\beta_{\mathrm{C}}}^{\mathrm{i}} &= -\rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot \langle \overline{\mathbf{u}' C'} \rangle^{\mathrm{i}} \\
&= \rho \beta_{C_\phi}^k \phi \mathbf{g} \cdot [(\mathbf{D}_{\mathrm{t}} + \mathbf{D}_{\mathrm{disp,t}}) \cdot \nabla \langle \overline{C} \rangle^{\mathrm{i}}] \\
&= \beta_{C_\phi}^k \phi \frac{\mu_{\mathrm{t}_\phi}}{Sc_{\mathrm{t}_\phi}} \mathbf{g} \cdot \nabla \langle \overline{C} \rangle^{\mathrm{i}}
\end{aligned} \tag{60}$$

where μ_{t_ϕ}, Sc_{t_ϕ} and the two coefficients $\mathbf{D}_t$ and $\mathbf{D}_{disp,t}$ have been defined before.

Final transport equations for $\langle k\rangle^i = \langle \overline{\mathbf{u}'\cdot\mathbf{u}'}\rangle^i/2$ and $\langle\varepsilon\rangle^i = \mu\langle\nabla\mathbf{u}' : (\nabla\mathbf{u}')^T\rangle^i/\rho$, in their so-called high Reynolds number form can now include the buoyancy generation terms due to temperature and concentration fluctuations as

$$\rho\nabla\cdot(\bar{\mathbf{u}}_D\langle k\rangle^i) = \nabla\cdot\left[\left(\mu+\frac{\mu_{t_\phi}}{\sigma_k}\right)\nabla(\phi\langle k\rangle^i)\right] + P^i + G^i + G^i_\beta + G^i_{\beta_C} - \rho\phi\langle\varepsilon\rangle^i \quad (61)$$

$$\rho\nabla\cdot\left(\bar{\mathbf{u}}_D\langle\varepsilon\rangle^i\right) = \nabla\cdot\left[\left(\mu+\frac{\mu_{t_\phi}}{\sigma_\varepsilon}\right)\nabla(\phi\langle\varepsilon\rangle^i)\right] + \frac{\langle\varepsilon\rangle^i}{\langle k\rangle^i}\left[c_1P^i + c_2G^i + c_1c_3(G^i_\beta + G^i_{\beta_C}) - c_2\rho\phi\langle\varepsilon\rangle^i\right] \quad (62)$$

where c_1, c_2, c_3 and c_k are constants and the production terms have the following physical significance:

1. $P^i = -\rho\langle\overline{\mathbf{u}'\mathbf{u}'}\rangle^i{:}\nabla\bar{\mathbf{u}}_D$ is the production rate of $\langle k\rangle^i$ due to gradients of $\bar{\mathbf{u}}_D$;
2. $G^i = c_k\rho\frac{\phi\langle k\rangle^i|\bar{\mathbf{u}}_D|}{\sqrt{K}}$ is the generation rate of the intrinsic average of k due to the action of the porous matrix;
3. $G^i_\beta = \beta^k_\phi\phi\frac{\mu_{t_\phi}}{Pr_{t_\phi}}\mathbf{g}\cdot\nabla\langle\overline{T}\rangle^i$ is the generation of $\langle k\rangle^i$ due to mean temperature variation within the fluid, and
4. $G^i_{\beta_C} = \beta^k_{C_\phi}\phi\frac{\mu_{t_\phi}}{Sc_{t_\phi}}\mathbf{g}\cdot\nabla\langle\overline{C}\rangle^i$ is the generation of $\langle k\rangle^i$ due to concentration gradients.

7. 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 REV, according to (54). 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 Fig. 2 where hotter fluid (Fig. 2a) composed by a less dense mixture is positioned at the bottom of the fluid layer (Fig. 2b). For positive β_ϕ and β_{C_ϕ} values, with negative gradients of $\langle\overline{T}\rangle^i$ and $\langle\overline{C}\rangle^i$, both drives expressed by (55) and (60) will give $G^i_\beta > 0$ and $G^i_{\beta_C} > 0$, respectively, causing positive sources term in the $\langle k\rangle^i$-Eq. (61). If a heavier component is positioned at the top of this heated-from-below layer (Fig. 2c), hydrodynamic instability will also occur and a source term will appear in (61). An initially laminar flow may then undergo transition and become turbulent.

On the other hand, for a layer heated from above (Fig. 2d) with lighter components flowing at the top (Fig. 2e), both values of source terms G^i_β and $G^i_{\beta_C}$, in Eq. (61), will be less than zero, leading to an unconditionally stable situation. 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 (Fig. 2f). Any other combination regarding a heavier or a lighter component flowing in a non-isothermal fluid may be conditionally unstable,

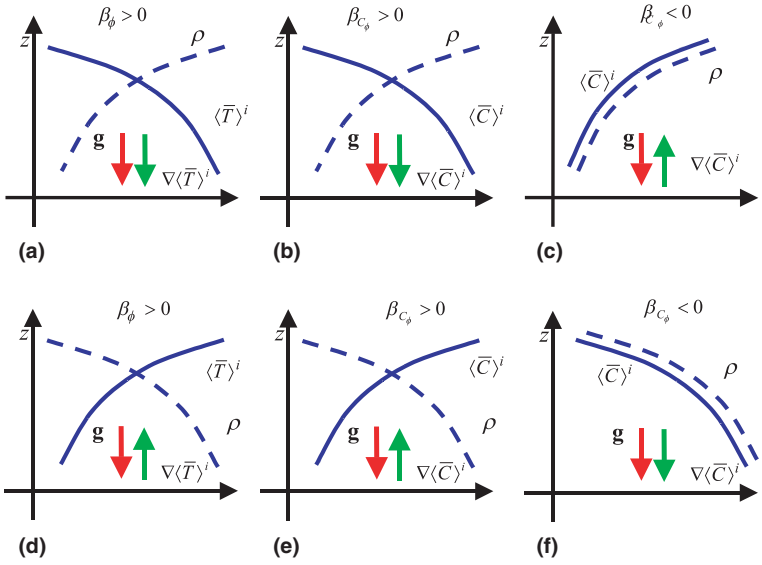

Fig. 2. Stability analysis of a layer of fluid subjected to gradients of temperature and concentration. Unconditionally *unstable* cases: hotter fluid (a) with less dense mixture at the bottom (b)–(c). Unconditionally *stable* cases: colder fluid (d) with denser mixture at the bottom (e)–(f).

depending upon the balance between source and sink terms that might appear as a result of temperature and concentration distributions within the flow.

8. 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 [21,22]. Extra terms appearing in the equations needed to be modeled in terms of $\bar{\mathbf{u}}_D$, $\langle\overline{T}\rangle$ and $\langle\overline{C}\rangle$. 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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