A Model for Complex Heat and Mass Transport Involving Porous Media with Related Applications

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Abstract

Heat and mass transfer involving porous media is prevalent in, for example, air-conditioning, drying, food storage, and chemical processing. Such applications require non-equilibrium heat and mass (or moisture) transfer modeling inside porous media in conjugate fluid/porous/solid framework. Moreover, modeling of turbulence and turbulent heat and mass transfer becomes essential for many applications. A comprehensive literature review shows a scarcity of models having such capabilities. In this respect, the objectives of the present thesis are to: i) develop a formulation that simulates non-equilibrium heat and mass transfer in conjugate fluid/porous/solid framework, ii) demonstrate the capabilities of the developed formulation by simulating complex related problems, and iii) extend the developed model to such class of problems that involve turbulence and turbulent heat and mass transfer. To develop the required formulation, we first specify transport equations for each region. In the fluid region, mass, momentum, energy, and water vapour transport equations are solved to model flow and energy of moist air-vapour mixture. The volume-averaged version of these equations form the model for the fluid-constituent of porous media, while the transport equations of energy and water mass fraction are solved inside the solid-constituent of porous media and solid region. Mathematical conditions are developed at all the interfaces to ensure smooth transport of relevant quantities across the interfaces. The developed formulation is demonstrated and validated by simulating the problems of evaporative cooling and convective drying of wet porous materials. In this respect, each simulated case demonstrates critical aspects of the developed formulation. Moreover, the simulated cases are found to be in excellent agreement with experimental data. The developed formulation is extended to turbulent flow regimes often encountered in heat and mass transfer problems related to food stacks. In this respect, the closure is obtained for the macroscopic turbulence and turbulent non-equilibrium heat and mass transfer model inside porous media composed of randomly packed spheres. The closure is obtained by simulating the problem at the pore-level scale of a bed of randomly-packed spheres. Lastly, the closure results are presented in the form of power law-based correlations to be utilized in the macroscopic model.
Keywords

Heat transfer, mass transfer, porous media, computational fluid dynamics (CFD), conjugate domains, convective drying, turbulence modeling, model closure
Co-Authorship Statement

Chapter two is a journal article published in International Journal of Heat and Mass Transfer. It is co-authored by Khan, F.A., Fischer, C. and Straatman, A.G.

Chapter three is a journal article published in Journal of Food Engineering. It is co-authored by Khan, F.A., and Straatman, A.G.

Chapter four is a journal article submitted to and currently under review in International Journal of Heat and Mass Transfer. It is co-authored by Khan, F.A., and Straatman, A.G.

In all the cases, I conducted the research and analysis under the guidance and supervision of Dr. Straatman.
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<thead>
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<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$A$</td>
<td>area, m$^2$</td>
</tr>
<tr>
<td>$a_{fs}$</td>
<td>interfacial surface area of porous media, m$^2$</td>
</tr>
<tr>
<td>$A_{fs}$</td>
<td>specific interfacial surface area of porous media, m$^{-1}$</td>
</tr>
<tr>
<td>$c_E$</td>
<td>inertia coefficient of porous media</td>
</tr>
<tr>
<td>$c_p$</td>
<td>specific heat at constant pressure in fluid region, J/(kg. K)</td>
</tr>
<tr>
<td>$c_{ps}$</td>
<td>specific heat in solid region, J/(kg. K)</td>
</tr>
<tr>
<td>$C_{1e}, C_{2e}, C_\mu$</td>
<td>turbulence model constants</td>
</tr>
<tr>
<td>$D$</td>
<td>binary diffusivity coefficient, m$^2$/s</td>
</tr>
<tr>
<td>$D$</td>
<td>deformation tensor</td>
</tr>
<tr>
<td>$d_s$</td>
<td>mean sphere diameter, cm</td>
</tr>
<tr>
<td>$f$</td>
<td>body force per unit mass, m/s$^2$</td>
</tr>
<tr>
<td>$h$</td>
<td>specific enthalpy, J/kg</td>
</tr>
<tr>
<td>$H$</td>
<td>channel height, m</td>
</tr>
<tr>
<td>$h_{fg}$</td>
<td>latent heat of evaporation at 0°C in fluid region, J/kg</td>
</tr>
<tr>
<td>$h_{fs}$</td>
<td>interfacial heat transfer coefficient in porous media, W/(m$^2$.K)</td>
</tr>
<tr>
<td>$h_{fs,m}$</td>
<td>interfacial mass transfer coefficient in porous media, m/s</td>
</tr>
<tr>
<td>$k$</td>
<td>thermal conductivity, W/(m.K), turbulent kinetic energy per unit mass, m$^2$/s$^2$ (only for chapter four)</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>$K$</td>
<td>Darcy permeability of porous media, m$^2$</td>
</tr>
<tr>
<td>$L$</td>
<td>REV length, m</td>
</tr>
<tr>
<td>$l_d$</td>
<td>ligament diameter, m</td>
</tr>
<tr>
<td>$m$</td>
<td>mass, kg</td>
</tr>
<tr>
<td>$\dot{m}$</td>
<td>mass flow rate, kg/s</td>
</tr>
<tr>
<td>$n$</td>
<td>outward normal unit vector</td>
</tr>
<tr>
<td>$Nu$</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>$P$</td>
<td>pressure, Pa</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>$R$</td>
<td>gas constant, J/(kg. K)</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>$S$</td>
<td>source in a transport equation</td>
</tr>
<tr>
<td>$Sc$</td>
<td>Schmidt number</td>
</tr>
<tr>
<td>$Sh$</td>
<td>Sherwood number</td>
</tr>
<tr>
<td>$T$</td>
<td>temperature, °C</td>
</tr>
<tr>
<td>$t$</td>
<td>time, s</td>
</tr>
<tr>
<td>$U$</td>
<td>extrinsic velocity, m/s</td>
</tr>
<tr>
<td>$v$</td>
<td>fluid velocity [=($u,v,w$)], m/s</td>
</tr>
<tr>
<td>$V$</td>
<td>volume, m$^3$</td>
</tr>
</tbody>
</table>
\( X \) moisture content, kg \( \text{water} / \text{kg dry matter} \)

\( y \) distance in \( y \)-direction from origin, m

\( Y \) mass fraction

\( \alpha \) volume fraction

\( \mu \) dynamic viscosity, N.s/m\(^2\)

\( \mu_t \) turbulent eddy viscosity, N.s/m\(^2\)

\( \nu_f \) kinematic viscosity, m\(^2\)/s

\( \nu_t \) turbulent kinematic viscosity, m\(^2\)/s

\( \sigma_T \) turbulent Prandtl number for energy equation

\( \sigma_k \) turbulent Prandtl number for \( k \) (only for chapter four)

\( \sigma_\varepsilon \) turbulent Prandtl number for \( \varepsilon \) (only for chapter four)

\( \rho_s \) density of solid, kg/m\(^3\)

\( \rho_f \) density of fluid mixture, kg/m\(^3\)

\( \omega_{\text{spec}} \) specific humidity, kg of H\(_2\)O/ kg of dry air

\( \omega_{\text{rel}} \) relative humidity, %

\( \varepsilon \) porosity, dissipation rate of turbulent kinetic energy, m\(^2\)/s\(^3\) (only for chapter four)

\( \lambda_x \) thermal conductivity of \( x \)-constituent of porous media, W/(m.K) (only for chapter four)

\( \phi \) porosity (only for chapter four)
\( \varphi \)  
a quantity

\( \bar{\varphi} \)  
time-average of \( \varphi \)

\( \langle \varphi \rangle \)  
extrinsic volume-average of \( \varphi \)

\( \langle \varphi \rangle^x \)  
Intrinsic volume-average of \( \varphi \) (\( x \) is fluid or solid constituent of porous media)

\( \langle \bar{\varphi} \rangle \)  
volume-time-average of \( \varphi \)

subscripts and superscripts

\( a \)  
air

\( disp \)  
dispersive

\( e \)  
energy

\( eff \)  
effective property in porous media

\( f \)  
fluid

\( fl \)  
fluid side of interface

\( fs \)  
interfacial

\( o \)  
value at previous time level

\( P \)  
control volume over which the equation is being integrated

\( por \)  
porous side of interface

\( s \)  
solid

\( sol \)  
solid side of interface
$t$  total

$v$  vapour

$w$  water
Chapter 1

1 Introduction

1.1 Motivation and background

Heat and mass transfer involving porous media is prevalent in, for example, air-conditioning, drying, food storage, and chemical processing. Such applications involve porous media of various types and characteristic lengths such as fabrics, desiccants, grains and produce, food stacks, and bricks, etc. These applications also involve heat and mass transfer between solids, fluids and gas-vapor mixtures, and must be treated as conjugate fluid/porous/solid problems for analysis and design. In addition, due to the possible presence of water in its liquid and vapor phases, mass transfer of moisture often occurs due to evaporation and/or condensation. All combined, the conjugate heat and mass transfer that takes place in numerous engineering applications presents several interesting challenges in terms of analysis and design. To this end, analytical solutions are often not possible and numerical modeling is counted on to provide analysis and insight into complex heat and mass transfer problems.

In terms of numerical modeling of porous media, scale of porous media becomes important. If I model a transport process at the pore-level, or microscopic scale, of the porous media then the usual form of the transport equations can be utilized. However, such an approach requires the modeling of each pore inside porous media, which is computationally expensive. An alternate approach is to model the transport processes at the macroscopic scale of the porous media because at this scale porous media can be considered as porous continuum comprised of fluid and solid-constituents (or phases) as shown in Fig. 1.1. In addition, at the macroscopic scale, two approaches can be taken to model heat and mass transfer inside porous media. From the modeling perspective, the simplest approach is to consider thermal and mass equilibrium between the fluid and solid-constituents of the porous media, which yields one solution for temperature and moisture concentration at a given location within the porous media. However, such approach limits the applicability of heat and mass transport models inside porous media
to a certain class of problems. Conversely, to capture the physics of more complex heat and mass transfer problems, a non-equilibrium approach is utilized, which provides a separate solution for each constituent at a given location within porous media. As a result, the modeling of non-equilibrium heat and mass transfer inside a porous media enables the simulation of more complicated problems. In particular, the non-equilibrium heat and mass transfer approach is required to simulate the problems that involve unsteadiness or where the fluid and solid-constituents of porous media have considerably different properties.

An even more diverse class of heat and mass transfer problems can be considered if fluid/porous/solid domain conjugacy is combined with the non-equilibrium approach inside the porous media. Such models can then simulate heat and mass transfer problems related to evaporative cooling, convective drying, chemical processing, food stacks storage and processing, etc. as shown in Fig. 1.2. Although at the microscopic scale, a food stack cannot be considered as a porous media, as described earlier, it can be modeled as porous continuum at the macroscopic scale. However, heat and mass transfer within food stacks generally becomes turbulent due to the comparatively large size of randomly packed produce within the stacks. As a result, in some cases, it is also essential to model macroscopic turbulence and turbulent heat and mass transfer inside porous media.

![Figure 1.1: Porous media modeling at microscopic and macroscopic scales.](image)
The present work is directed at improving the capability of current computational Fluid Dynamics (CFD) modelling and discretization practices to incorporate non-equilibrium heat and mass transfer in a general conjugate framework, which includes interfaces between fluid-porous, fluid-solid and porous-solid regions. Several key issues in current modelling practices are resolved inside the porous region, and in particular, at interfaces between the fluid and porous regions. The result is a general and robust framework for conjugate modelling that can be utilized for many target applications in engineering and industry. Validation of the computational framework is carried out by solving problems in evaporative cooling, drying and fully-turbulent packed beds of spheres.

The remainder of the introductory chapter introduces volume-averaging, which is the key element for up-scaling the transport equations in the porous media, and then describes modelling practices for heat and mass transfer, which provides a context for where the current work fits into engineering analysis. Scope and objectives are given to close the chapter.

Figure 1.2: Heat and mass transfer applications related to a) convective drying; b) produce storage (adapted from Ambaw et al. [1]); c) evaporative cooling.
1.2 Volume-averaging

Before considering current practices in computational modelling, it is essential to discuss the process of volume-averaging, which is necessary in porous regions of the domain. As mentioned earlier, from the computational perspective, modeling of porous media at the macroscopic scale is feasible, however, to utilize this approach, I need to up-scale the transport equations of a process to the macroscopic scale of the porous media. This up-scaling is achieved by performing a volume-averaging operation of the transport equations. The volume-averaging operation produces additional terms that require closure to complete the model.

In volume-averaging, integration of a transport equation is performed over a representative elementary volume (REV) of the porous media. After volume-averaging is performed, there exists a volume-averaged value of a quantity \( \varphi \) at every point in space inside porous media. Mathematically, the volume-averaging of \( \varphi \) is expressed as [2]

\[
\langle \varphi \rangle = \frac{1}{V} \int_{V_f} \varphi \, dV
\]  

(1.1)

where, \( V \) refers to the volume over which the averaging is carried out, \( V_f \) is the fluid volume inside \( V \), and \( \langle \varphi \rangle \) is defined as the extrinsic-average of \( \varphi \). Similarly, an intrinsic-average \( \langle \varphi \rangle^f \) of \( \varphi \) is evaluated as [2]

\[
\langle \varphi \rangle^f = \frac{1}{V_f} \int_{V_f} \varphi \, dV
\]  

(1.2)

The porosity of porous media \( \varepsilon \) is then obtained as [2]

\[
\varepsilon = \frac{\langle \varphi \rangle}{\langle \varphi \rangle^f}
\]  

(1.3)
1.3 Literature survey of heat and mass transfer modelling

1.3.1 Basic modeling

The most basic models utilize simple heat and mass balance equations to model various heat and mass transfer problems. In this respect, an indirect evaporative cooler was modeled by Riffat and Zhu [3] using the resistance circuit analogy and energy balance equations for heat transfer, while mass transfer was modeled using the empirical correlations. In a similar way, the complex problem of dew point evaporative cooling was modeled by Zhao et al. [4] and Zhan et al. [5]. Moreover, Woods and Kozubal [6] modeled the novel system of desiccant-enhanced evaporative air-conditioning, which involves air dehumidification through desiccant drying followed by an indirect evaporative cooling step, using an elaborate set of heat and mass balance equations. Earlier, using the same approach, the problem of desiccant evaporative cooling was also modeled by Feyka and Vafai [7], and Mago et al. [8]. The convective drying of porous materials has also been modeled, in a simple manner, using the correlations that predict moisture content as a function of temperature and other problem parameters (see, for example Akpınar et al. [9], Demir et al. [10], Menges and Ertekin [11], and Seiiedlou et al. [12]).

More sophistication and advancement is achieved by modeling heat and mass transfer problems using the differential transport equations of energy and moisture. In such cases, it is often necessary to model the flow using the conservation of mass-momentum differential equations. Using this approach, Wu et al. [13] utilized the transport equations of energy and moisture to simulate the case of direct evaporative cooling. The group incorporated both the mass of evaporated water and latent heat of water evaporation as source terms in the model. In another study, Martín [14] modeled a semi-indirect evaporative cooling process using a commercial finite-volume package Fluent. The energy of evaporation/condensation was incorporated in the model using the existing heat and mass transfer correlations. Due to the incapability of Fluent to simulate evaporation/condensation as such, its model was included using the user-defined function option. Earlier, Chourasia and Goswami [15] modeled heat and mass transport inside a stack of potatoes as porous media using the transport equations of mass, momentum,
energy, and moisture. For the problem of convective drying of porous materials, diffusion-based transport equations of energy and moisture, comprised of unsteady and diffusive terms, have been utilized. Moreover, these models employ convective boundary conditions at the surface of wet porous materials. In this respect, the required convective heat and mass transfer coefficients are evaluated using Nusselt and Sherwood number correlations (see, for example Golestani et al. [16], Perussello et al. [17], Srikiatden and Roberts [18], and Younsi et al. [19]).

Based on the above discussion I can conclude that energy and moisture transport differential equations are frequently used to model various heat and mass transfer problems. However, such studies mostly utilize a single transport equation of energy and moisture for modeling the inside of the porous media, which inherently incorporates the assumption of equilibrium heat and mass transfer. While, this simplification is valid for many cases, some cases require the modeling of non-equilibrium heat and mass transfer inside porous media. By non-equilibrium heat and mass transfer inside porous media, I refer to a model that has separate energy and moisture transport equations for each of the fluid and solid-constituents. In addition, the review further shows that the conjugate framework problems involving heat and mass transfer can be simplified by segregating the fluid and porous regions and then using convective boundary conditions to link them in an explicit manner. However, in such case, the robustness of the model depends upon the correlations used to calculate the convective coefficients. To avoid this dependence, heat and mass transfer modeling in an implicit conjugate framework is required. The subsequent section is dedicated to the review of studies that consider non-equilibrium approaches and/or a conjugate framework to model heat and mass transfer involving porous media.

1.3.2 Conjugate and non-equilibrium approaches

The existing literature shows that some studies have employed non-equilibrium heat and mass transport inside porous media. In this respect, an early attempt was made by Liu et al. [20] to model non-equilibrium moisture transfer inside a porous media by incorporating separate transport equations for liquid water and water vapour. The formulation was generic, and also included evaporation and condensation of moisture.
However, the group considered thermal equilibrium between liquid and gas phases inside porous media. Similarly, Zhang et al. [21] modeled non-equilibrium heat and mass transfer for a rotary desiccant dehumidifier. However, their model was specifically intended for such class of problems. For the problem of convective drying of porous materials, non-equilibrium mass transfer inside porous media was considered by De Bonis and Ruocco [22]. Their model included conjugate heat and mass transfer between fluid and porous regions, however, they considered thermal equilibrium inside the porous material. In another study, the concept of air-conditioning a space through evaporative cooling of wet porous walls was simulated by Chen [23] using energy and moisture transport equations inside porous region. In this respect, the author used separate transport equations for water and water vapour, but, assumed local thermal equilibrium within porous domain.

Few non-equilibrium modeling studies exist for problems related to heat and mass transfer of food or produce stacks. Recently, Ambaw et al. [1] modeled the distribution of a gas, which is used to control a fruit ripening process, inside conjugate fluid/porous domains. In this respect, the group employed separate concentration transport equations of the gas for each phase of the porous region. However, their model did not consider heat transfer inside the conjugate domains. Conversely, Ferrua and Singh [24] simulated forced air cooling of strawberry packs using thermal non-equilibrium approach. Earlier, Zou et al. [25,26] proposed a comprehensive air flow and heat transfer formulation for the applications related to the ventilation of packed foods. In this respect, they modeled air flow and heat transfer in conjugate fluid/porous/solid domains, and also incorporated non-equilibrium heat transfer inside the porous domain. However, in their work, no description of continuity of flow and heat transfer was provided at fluid-solid, fluid-porous, and porous-solid interfaces. Considering thermal and moisture equilibrium inside porous region, Moureh et al. [27] simulated turbulent airflow inside and around slotted-enclosures filled with spheres (porous domain). The nature of their study warranted consideration of conjugate fluid/porous domains. However, the authors relied on Fluent to deal with the complexities associated with a fluid/porous interface.
For problems related to convective drying of porous materials, few studies have utilized a conjugate-domain approach. Many studies utilized interfacial heat and mass transfer conditions to link the fluid and porous regions (See for example Defraeye et al. [28], Erriguible et al. [29], Murugesan et al. [30], Suresh et al. [31], and Younsi et al. [32]). However, all of these studies considered thermal and moisture equilibrium inside the porous media. Moreover, some of the groups [28,29,32] obtained solutions in the fluid and porous regions separately using different software/codes, but, explicitly linked both regions. In this respect, first the fluid region was solved for one time step then based on the fluid region’s solution heat and mass fluxes were imposed at fluid-porous interfaces to obtain solution inside porous region for the same time step.

1.3.3 Turbulence and turbulent heat and mass transfer

As mentioned earlier, for problems related to, for example, food stacks, heat and mass transfer can be turbulent due to large size of packed produce. In addition, many problems involve conjugate domains as well, which means that from turbulence modeling perspective, I need to model turbulence in the fluid and porous regions and at fluid-porous interfaces. Turbulence modeling in clear fluid regions has been extensively studied, however, the existing literature shows few studies focused on modeling macroscopic turbulence at fluid-porous interfaces. In this respect, Chandesris and Jamet [33], and de Lemos [34] studied turbulence treatment at fluid-porous interfaces using the \( k-\varepsilon \) model.

Turbulent heat and mass transfer inside food or produce stacks is widely modeled at the macroscopic scale of porous media. For example, as described earlier, Moureh et al. [27] modeled turbulent airflow inside and around slotted-enclosures filled with spheres to examine the distribution of airflow. The group modeled turbulence in the fluid and porous regions using the Reynolds stress models (RSM). Similarly, to predict turbulent airflow, temperature, and humidity distributions inside a cold storage room containing boxes loaded with spheres, Delele et al. [35] modeled turbulence using a combination of \( k-\varepsilon \) and \( k-\omega \) models. Moreover, Ambaw et al. [1] simulated turbulence inside conjugate fluid/porous domains, with the porous domain comprised of randomly packed spheres, using SST \( k-\omega \) model. In addition, Alvarez and Flick [36] modeled turbulent airflow to
simulate the cooling process of packed food stacks using the transport equation of turbulent kinetic energy.

For modeling turbulence and turbulent heat and mass transfer at the macroscopic scale of porous media, the transport equations require time-averaging along with volume-averaging. In this respect, the employed time-averaging operation is identical to that used in the clear fluid region. The time-averaging of a quantity \( \varphi \) is expressed as [37]

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

(1.4)

and, in general, the split of \( \varphi \) into its time-averaged component \( \bar{\varphi} \) and temporal deviation \( \varphi' \) is defined as

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

(1.5)

Due to the fact that both time- and volume-averaging operations are performed one after another, one can wonder if the order of averaging operations is critical. To answer this question, Pedras and de Lemos [37] proposed double decomposition concept, which involves time-averaging followed by volume-averaging or vice versa. The group found that the solution is not dependent upon the order of averaging i.e. \( \langle \bar{\varphi} \rangle_f = \langle \bar{\varphi} \rangle^f \).

For turbulence modeling at the macroscopic scale of porous media, the existing literature generally utilizes the \( k-\varepsilon \) model, although turbulence inside the porous media has also been modeled using RSM and Large Eddy Simulation (LES) approaches by Kuwata and Suga [38] and Kuwahara et al. [39], respectively. In addition, in their work, Kuwahara et al. [39] compared the results of LES and \( k-\varepsilon \) model, and found that \( k-\varepsilon \) model is capable of modeling turbulence at the macroscopic scale inside porous media. The existing \( k-\varepsilon \) turbulence models can be classified based on their definition of turbulent kinetic energy \( k \). In this respect, the most popular \( k-\varepsilon \) models were proposed by Nakayama and Kuwahara [40] and Pedras and de Lemos [37], who defined macroscopic turbulence kinetic energy inside porous media as
\[ k_{NK} = \frac{1}{2} \langle \vec{v}' \cdot \vec{v}' \rangle_f \] (1.6)

where, \( \vec{v}' \) represents the microscopic velocity fluctuation in time.

Later, Teruel and Rizwan-uddin [41,42] added a dispersive component of turbulent kinetic energy in Eq. 1.6 to define total macroscopic turbulent kinetic energy as

\[ k_{total} = k_{NK} + \frac{1}{2} \langle \vec{v} \cdot \vec{v} \rangle_f \] (1.7)

where, \( \vec{v} \) refers to the spatial deviation of time-averaged velocity

Based on the above discussion, I can say that macroscopic \( k-\varepsilon \) turbulence models inside porous media already exist. However, as these models are derived using volume- and time-averaging operations, additional terms arise due to averaging that require closure to complete these models. Similarly, time- and volume-averaged heat and mass transfer equations also require closure in order to be utilized in the macroscopic model. In general, the closure is obtained by simulating the problem at the microscopic scale of porous media i.e. inside REV.

Since the present work is focused on macroscopic turbulence and turbulent heat and mass transfer inside randomly packed bed of spheres (treated as porous media), I require turbulence, energy and mass transfer information at the microscopic scale of the considered porous media.

The existing literature shows numerous studies that have incorporated turbulence and heat transfer at the microscopic scale of packed spheres. However, most of the studies utilized a structurally packed bed of spheres, and were focused on different aspects of the problem [43-47]. Very few studies have employed the more realistic random packing of spheres at the microscopic scale. In this respect, previously mentioned work of Ambaw et al. [1] used random packing of spheres to simulate the problem. Similarly, turbulent airflow through randomly packed spheres contained in vented boxes was simulated by Delele et al. [48] to examine turbulent flow inside the domain. In another study, turbulent
flow and heat transfer inside packed beds composed of randomly arranged short circular cylinders, rather than spheres, was simulated by Mathey [49].

From the above discussion, I can state that microscopic simulation studies inside packed beds of spheres, in general, did not focus on the macroscopic model closure. However, the existing literature shows a few such attempts, where simple two- and three-dimensional structurally composed REVs were utilized. When it comes to the closure of the macroscopic $k$-$\varepsilon$ model, closures were obtained for two- and three-dimensional REVs, composed of a structured array of circular and square rods, and flat plates by Nakayama and Kuwahara [40], Pedras and de Lemos [37], Teruel and Rizwan-uddin [41,42], Chandesris et al. [50] and Drouin et al. [51]. For the case of packed spheres, closure of the macroscopic turbulence model was obtained by Alvarez and Flick [36]. However, the group utilized a transport equation of $k$ and an expression for $\varepsilon$ to model the macroscopic turbulence. Recently, Mathey [49] obtained the closure of the macroscopic $k$-$\varepsilon$ model by considering REVs composed of structurally packed spheres. Moreover, the author also included the dispersive effects of turbulence in his work. However, the model closure was obtained for a small range of Reynolds number with packed bed porosity being constant. The existing literature shows very few studies focused on the closure of macroscopic heat and mass transport equations. In this respect, the closures obtained by de Lemos [52] are only limited to two-dimensional REVs composed of structured array of circular, elliptical, and square rods.

1.4 Development of transport equations

The details of the model development capable of simulating non-equilibrium heat and mass transfer in conjugate fluid/porous/solid domains are provided in chapter 2, however, the development of the transport equations is omitted. In this section, I demonstrate how the required form of the transport equations utilized in the fluid and porous regions are obtained. As a brief overview, heat and mass transfer of the moist air (dry air-water vapour mixture) is modeled in the fluid region. In this respect, the air flow is modeled using the mass and momentum conservation equations. The moisture content of the air is quantified by solving the water vapour mass fraction $Y_v$ transport equation. The density
of air-water vapour mixture $\rho_f$ is constantly updated to account for moisture gain or loss. In addition, the present study models the energy of the air-water vapour mixture, which is composed of sensible and latent components, by solving its energy transport equation.

In the porous region, non-equilibrium heat and mass transfer is considered. The moist air forms the fluid-constituent of the porous media, and utilizes the same transport equations proposed in the fluid region. The solid-constituent is considered to be composed of a solid-structure holding water. In such case, the heat and mass transfer of the solid-constituent is modeled by including its energy and water mass fraction $Y_w$ transport equations, respectively.

Since the present work is focused on the development of a model that simulates heat and mass transfer problems over a moderate temperature range from around 0º C to 50ºC, heat transfer due to radiation is not considered. Moreover, due to this reason, most thermophysical properties are also considered constant.

1.4.1 Fluid region

The mass and momentum transport equations, in their usual forms, are expressed as

$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{v}) = 0$$  \hspace{1cm} (1.8)

$$\frac{\partial (\rho_f \mathbf{v})}{\partial t} + \nabla \cdot (\rho_f \mathbf{v} \mathbf{v}) = -\nabla P + \mu_f \nabla^2 \mathbf{v} + \rho_f f$$ \hspace{1cm} (1.9)

The water vapour mass fraction equation is given as [53]

$$\frac{\partial (\rho_f Y_v)}{\partial t} + \nabla \cdot (\rho_f Y_v \mathbf{v}) = \nabla \cdot (\rho_f D_f \nabla Y_v) + S_v$$ \hspace{1cm} (1.10)

In the present work, the energy transport equation takes a different form to account for the entire energy of air-water vapour mixture. To drive the required form of the energy equation, I start with the following expression [54]
\[
\sum_l \frac{\partial (\rho_{f,l} h_l)}{\partial t} + \sum_l \nabla . (\rho_{f,l} h_l \mathbf{v}_l) = -\nabla q + S_e
\] (1.11)

I can decompose the species velocity \( \mathbf{v}_l \) into the average mixture velocity \( \mathbf{v} \) and species diffusion velocity \( \mathbf{v}_{d,l} \), which leads to the following expression

\[
\sum_l \frac{\partial (\rho_{f,l} h_l)}{\partial t} + \sum_l \nabla . (\rho_{f,l} h_l \mathbf{v}_l) = -\nabla q - \sum_l \nabla . (\rho_{f,l} h_l \mathbf{v}_{d,l}) + S_e
\] (1.12)

The relation between species density \( \rho_{f,l} \) and mixture density \( \rho_f \) is given as

\[
\sum_l \rho_{f,l} = \rho_f \sum_l Y_l
\] (1.13)

By incorporating \( \rho_f \), the energy equation takes the following form

\[
\sum_l \frac{\partial (\rho_f Y_l h_l)}{\partial t} + \sum_l \nabla . (\rho_f Y_l h_l \mathbf{v}_l) = -\nabla q - \sum_l \nabla . (\rho_{f,l} h_l \mathbf{v}_{d,l}) + S_e
\] (1.14)

The Fick’s law of diffusion is defined as [53]

\[
\rho_{f,l} \mathbf{v}_{d,l} = -\rho_f D_f \nabla Y_l
\] (1.15)

Using the Fick’s law, I obtain

\[
\sum_l \frac{\partial (\rho_f Y_l h_l)}{\partial t} + \sum_l \nabla . (\rho_f Y_l h_l \mathbf{v}_l) = -\nabla q + \sum_l \nabla . (\rho_f D_f \nabla Y_l h_l) + S_e
\] (1.16)

The total species enthalpy \( h_l \) can be decomposed into sensible and latent components as

\[
h_l = c_{p,l} T + h_{fg,l}
\] (1.17)

By including this decomposition, I arrive at the following form of the energy equation
\[
\sum_{i} \frac{\partial}{\partial t} \left[ \rho_f Y_i (c_{p,i} T + h_{f,g,i}) \right] + \sum_{i} \nabla \cdot \left[ \rho_f Y_i \mathbf{v} (c_{p,i} T + h_{f,g,i}) \right] \\
= -\nabla q + \sum_{i} \nabla \cdot \left[ \rho_f D_f \nabla Y_i (c_{p,i} T + h_{f,g,i}) \right] + S_e
\]  

(1.18)

The Fourier’s law of conduction expresses the conductive heat flux \( q \) as [55]

\[
q = -k_f \nabla T
\]

(1.19)

Lastly, I employ Eq. 1.19 to obtain the required form of the air-water vapour mixture energy equation, which is given as

\[
\sum_{i} c_{p,i} \frac{\partial}{\partial t} (\rho_f Y_i T) + \sum_{i} h_{f,g,i} \frac{\partial}{\partial t} \rho_f Y_i + \sum_{i} \nabla \cdot (\rho_f Y_i \mathbf{v}) + \sum_{i} h_{f,g,i} \nabla \cdot (\rho_f Y_i \mathbf{v}) \\
= k_f \nabla^2 T + \sum_{i} \nabla \cdot \left[ \rho_f D_f \nabla Y_i (c_{p,i} T + h_{f,g,i}) \right] + S_e
\]

(1.20)

1.4.2 Porous Region

During the volume-averaging of a transport equation, I often encounter volume-averaging of spatial derivatives. In such cases, the spatial averaging theorem is utilized, which is defined as [2]

\[
\langle \nabla \varphi \rangle = \nabla \langle \varphi \rangle + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \varphi \, da
\]

(1.21)

where \( a_{fs} \) is the interfacial surface area of the REV, and \( \mathbf{n} \) is the unit vector normal to \( a_{fs} \). In other instances, I need to volume-average the products. In such situations, I decompose a quantity into its intrinsic average and spatial deviation, and consider that the volume-average of spatial deviation equals zero. In the present work, the decomposition of mixture density \( \rho_f \), velocity \( \mathbf{v} \), mass fraction \( Y \), and temperature \( T \) is given as
\[ \rho_f = \langle \rho_f \rangle_f + \tilde{\rho}_f \approx \langle \rho_f \rangle_f \]
\[ \mathbf{v} = \langle \mathbf{v} \rangle_f + \tilde{\mathbf{v}} , \quad \langle \tilde{\mathbf{v}} \rangle = 0 \]  
\[ Y = \langle Y \rangle_f + \tilde{Y} , \quad \langle \tilde{Y} \rangle = 0 \]
\[ T = \langle T \rangle_f + \tilde{T} , \quad \langle \tilde{T} \rangle = 0 \]  
(1.22)

For the present study, I consider the spatial deviation of mixture density \( \tilde{\rho}_f \) to be negligible. This simplification is justified because the mixture density of moist air does not change significantly with moisture gain or loss. In addition, in terms of magnitude, I consider \( \langle Y \rangle_f \gg \tilde{Y}, \langle T \rangle_f \gg \tilde{T} \), and \( \tilde{\mathbf{v}} \) to be of same order as \( \langle \mathbf{v} \rangle_f \)[2]. Moreover, I also consider the porosity of porous media to be constant.

Based on the aforementioned volume-averaging information, I obtain the volume-averaged form of the transport equations proposed for the fluid region. With the simplification of mixture density, the volume-averaging of mass and momentum equations follows the procedure discussed by Whitaker [2], which will not be repeated here for conciseness. The extrinsic form of the closed volume-averaged mass and momentum transport equations are given as [2]

\[ \epsilon \frac{\partial \langle \rho_f \rangle_f}{\partial t} + \nabla . \langle \langle \rho_f \rangle_f \rangle \langle \mathbf{v} \rangle = 0 \]  
(1.23)

\[ \frac{\partial \langle \langle \rho_f \rangle_f \rangle \langle \mathbf{v} \rangle}{\partial t} + \frac{1}{\epsilon} \nabla . \langle \langle \rho_f \rangle_f \rangle \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle \]
\[ = -\epsilon \nabla \langle P \rangle_f + \mu_f \nabla^2 \langle \mathbf{v} \rangle + \epsilon \langle \rho_f \rangle_f \mathbf{f} - \frac{\epsilon \mu_f}{K} \langle \mathbf{v} \rangle - \frac{\epsilon \langle \rho_f \rangle_f c_E}{\sqrt{K}} \langle |\mathbf{v}| \rangle \langle \mathbf{v} \rangle \]  
(1.24)

where the last two terms on the right-hand side of Eq. 1.24 are usually referred as the Darcy and Forchheimer terms, respectively. These terms account for the additional pressure drop that fluid experiences through porous media.

I now focus on volume-averaging of water vapour mass fraction equation (Eq. 1.10)
presented earlier. The volume-averaging of the unsteady term is carried out as

\[
\left\{ \frac{\partial (\rho_f Y_v)}{\partial t}\right\} = \frac{\partial (\rho_f Y_v)}{\partial t} = \frac{\partial (\langle \rho_f \rangle f (Y_{v,f})^f + \bar{Y}_v)}{\partial t} = \varepsilon \frac{\partial (\langle \rho_f \rangle f (Y_{v,f})^f)}{\partial t}
\]  

(1.25)

For the advective term, I use the spatial averaging theorem (Eq. 1.21), which results in

\[
\langle \nabla \cdot (\rho_f Y_v \mathbf{v}) \rangle = \nabla \cdot \langle \rho_f Y_v \mathbf{v} \rangle + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot \rho_f Y_v \mathbf{v} \, da = \nabla \cdot \left( \varepsilon \langle \rho_f \rangle f (Y_{v,f})^f (\mathbf{v})^f + \langle \rho_f \rangle f \bar{Y}_v \mathbf{v} \right)
\]

(1.26)

The second term on the right-hand side of Eq. 1.26 becomes zero with the application of the no-slip hydrodynamic boundary condition at \(a_{fs}\). For the first term on the right-hand side of Eq. 1.26, I split the quantities using Eq. 1.22. The resulting advective term is expressed as

\[
\langle \nabla \cdot (\rho_f Y_v \mathbf{v}) \rangle = \nabla \cdot \left( \langle \rho_f \rangle f (Y_{v,f})^f (\mathbf{v})^f + \langle \rho_f \rangle f \bar{Y}_v \mathbf{v} \right)
\]

(1.27)

Similarly, the diffusive term is expanded as

\[
\langle \nabla \cdot (\rho_f D_f \nabla Y_v) \rangle = \nabla \cdot \langle \rho_f D_f \nabla Y_v \rangle + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot \rho_f D_f \nabla Y_v \, da = \nabla \cdot \langle D_f \rho_f \rangle \langle \nabla Y_v \rangle + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot \rho_f D_f \nabla Y_v \, da = \nabla \cdot \left( D_f \langle \rho_f \rangle \langle \nabla Y_v \rangle \right) + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot \rho_f D_f \nabla Y_v \, da = \nabla \cdot \left( D_f \langle \rho_f \rangle f \left( \varepsilon \nabla (Y_{v,f})^f + \frac{1}{V} \int_{a_{fs}} \mathbf{n} Y_v \, da \right) \right) + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot \rho_f D_f \nabla Y_v \, da
\]

(1.28)

The second term inside the brackets on the right-hand side of Eq. 1.28 can be written as

\[
\frac{1}{V} \int_{a_{fs}} \mathbf{n} Y_v \, da = \frac{1}{V} \int_{a_{fs}} \mathbf{n} \langle Y_v \rangle^f \, da + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \bar{Y}_v \, da
\]

(1.29)

Since, \(\langle Y_v \rangle^f\) remains constant inside the REV, it can be moved out of the integral, which yields
\[
\frac{1}{V} \int_{a_{fs}} n \ Y_v \ da = \left\{ \frac{1}{V} \int_{a_{fs}} n \ da \right\} \langle Y_v \rangle_f + \frac{1}{V} \int_{a_{fs}} n \ Y_v' \ da = - (\nabla \varepsilon) \langle Y_v \rangle_f + \frac{1}{V} \int_{a_{fs}} n \ Y_v' \ da = \frac{1}{V} \int_{a_{fs}} n \ Y_v' \ da \quad (1.30)
\]

Using this simplification, the diffusive term is written as

\[
\langle \nabla \cdot (\rho_f D_f \nabla Y_v) \rangle = \nabla \cdot (\varepsilon D_f \langle \rho_f \rangle_f \nabla \langle Y_{v,f} \rangle_f) + \nabla \cdot \left( D_f \langle \rho_f \rangle_f \frac{1}{V} \int_{a_{fs}} n \ Y_v' \ da \right) + \frac{1}{V} \int_{a_{fs}} n \ \rho_f D_f \nabla Y_v \ da \quad (1.31)
\]

The volume-averaging of the source term \( S_v \) results in \( \varepsilon S_{v,f} \). The resulting volume-averaged water vapour mass fraction equation can be expressed as

\[
\varepsilon \frac{\partial \left( \langle \rho_f \rangle_f \langle Y_{v,f} \rangle_f \right)}{\partial t} + \nabla \cdot (\varepsilon \langle \rho_f \rangle_f \langle Y_{v,f} \rangle_f \langle \psi \rangle_f)

= \nabla \cdot \left( \varepsilon D_f \langle \rho_f \rangle_f \nabla \langle Y_{v,f} \rangle_f + D_f \langle \rho_f \rangle_f \frac{1}{V} \int_{a_{fs}} n \ Y_v' \ da - \langle \rho_f \rangle_f \langle \tilde{Y}_{v,f} \tilde{\psi} \rangle \right) + \frac{1}{V} \int_{a_{fs}} n \ \rho_f D_f \nabla Y_v \ da + \varepsilon S_{v,f} \quad (1.32)
\]

Eq. 1.32 in its current form cannot be utilized because it includes the additional terms that require closure. In this respect, the second and third terms inside the brackets on the right-hand side of Eq. 1.32 are closed using a gradient-diffusion type model. The second term on the right-hand side of Eq. 1.32 represents interfacial moisture transfer between the fluid and solid-constituents of porous media. This term is closed using a gradient-convection type model. Consequently, the extrinsic form of closed volume-averaged water vapour transport equation is expressed as
\[
\frac{\varepsilon}{\partial t} \frac{\partial (\rho_f Y_{v,f})}{\partial t} + \nabla \cdot (\rho_f Y_{v,f} \mathbf{v}) = \nabla \cdot (\rho_f D_{eff,f} \nabla (Y_{v,f})^f) + \varepsilon S_{v,f} + \langle \dot{m}_{fs} \rangle
\]

The volume-averaging of solid-constituent’s water mass fraction equation also follows the same steps. The resulting closed form of the volume-averaged water transport equation is given as

\[
(1 - \varepsilon) \frac{\partial (\rho_s Y_{w,s})}{\partial t} = \nabla \cdot (\rho_s D_{eff,s} \nabla (Y_{w,s})^s) + (1 - \varepsilon) S_{w,s} - \langle \dot{m}_{fs} \rangle
\]

Using the same process, I now volume-average the air-water vapour mixture energy equation (Eq. 1.20). The unsteady terms are volume-averaged as

\[
\left[ \sum_i c_{p,i} \frac{\partial (\rho_f Y_{i,f} T_f)}{\partial t} \right] + \left[ \sum_i h_{fg,i} \frac{\partial (\rho_f Y_i)}{\partial t} \right]
\]

\[
= \sum_i c_{p,i} \frac{\partial (\rho_f Y_{i,f} T_f)}{\partial t} + \sum_i h_{fg,i} \frac{\partial (\rho_f Y_i)}{\partial t}
\]

\[
= \sum_i c_{p,i} \frac{\partial ((\rho_f Y_{i,f}^f + \bar{Y}_{i,f}) (T_f^f + \bar{T}_f))}{\partial t}
\]

\[
+ \sum_i h_{fg,i} \frac{\partial ((\rho_f Y_{i,f}^f + \bar{Y}_{i,f}))}{\partial t}
\]

\[
= \sum_i \varepsilon c_{p,i} \frac{\partial ((\rho_f Y_{i,f}^f (T_f)^f)}{\partial t} + \sum_i \varepsilon h_{fg,i} \frac{\partial ((\rho_f Y_{i,f}^f)}{\partial t}
\]

Using the steps described earlier, the volume-averaging of the sensible and latent advective terms is carried out as
\[
\left\langle \sum_{i} c_{p,i} \nabla (\rho f Y_i T_f \mathbf{v}) \right\rangle = \sum_{i} c_{p,i} \left\langle \nabla (\rho f Y_i T_f \mathbf{v}) \right\rangle \\
= \sum_{i} c_{p,i} \nabla (\rho f Y_i T_f \mathbf{v}) + \sum_{i} c_{p,i} \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot \rho f Y_i T_f \mathbf{v} \, da \\
= \sum_{i} c_{p,i} \nabla (\rho f)^f (\langle Y_i,f \rangle^f + \bar{Y}_{i,f}) (\langle T_f \rangle^f + \bar{T}_f) (\langle \mathbf{v} \rangle^f + \bar{\mathbf{v}}) \\
= \sum_{i} c_{p,i} \nabla (\rho f)^f (\langle Y_i,f \rangle^f (\langle T_f \rangle^f + (\langle \mathbf{v} \rangle^f + \bar{\mathbf{v}}))\\n+ (\rho f)^f (\langle T_f \rangle^f (\bar{\mathbf{v}} \bar{Y}_{i,f})) \\
\] (1.36)

\[
\left\langle \sum_{i} h_{fg,i} \nabla (\rho f Y_i \mathbf{v}) \right\rangle = \sum_{i} h_{fg,i} \left\langle \nabla (\rho f Y_i \mathbf{v}) \right\rangle \\
= \sum_{i} h_{fg,i} \nabla (\rho f Y_i \mathbf{v}) + \sum_{i} h_{fg,i} \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot \rho f Y_i \mathbf{v} \, da \\
= \sum_{i} h_{fg,i} \nabla (\rho f)^f (\langle Y_i,f \rangle^f + \bar{Y}_{i,f}) (\langle \mathbf{v} \rangle^f + \bar{\mathbf{v}}) \\
= \sum_{i} h_{fg,i} \nabla (\rho f)^f (\langle Y_i,f \rangle^f (\langle \mathbf{v} \rangle^f + \bar{\mathbf{v}}))\\n+ (\rho f)^f (\langle \mathbf{v} \rangle^f (\bar{\mathbf{v}} \bar{Y}_{i,f})) \\
\] (1.37)

The diffusive term of the energy equation is volume-averaged as

\[
\langle k_f \nabla^2 T \rangle = \left\langle \nabla (k_f \nabla T_f) \right\rangle = \nabla (\langle k_f \nabla T_f \rangle) + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot k_f \nabla T_f \, da \\
= k_f \nabla \left( \nabla \langle T_f \rangle + \frac{1}{V} \int_{a_{fs}} \mathbf{n} T_f \, da \right) + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot k_f \nabla T_f \, da \\
= \nabla \left( \epsilon k_f \nabla \langle T_f \rangle^f + k_f \frac{1}{V} \int_{a_{fs}} \mathbf{n} \bar{T}_f \, da \right) + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot k_f \nabla T_f \, da \\
\] (1.38)

In the similar manner, the volume-averaging of the species diffusion energy transport term is conducted as
\[
\left( \sum_i \nabla \left[ \rho_f D_f \nabla Y_i (c_{p,i} T_f + h_{f,g,i}) \right] \right) \\
= \sum_i \nabla \left( \rho_f D_f \nabla Y_i (c_{p,i} T_f + h_{f,g,i}) \right) \\
+ \sum_i \frac{1}{V} \int_{a_{fs}} \mathbf{n} \cdot \rho_f D_f \nabla Y_i (c_{p,i} T_f + h_{f,g,i}) \, da
\]  

(1.39)

The first term on the right-hand side of Eq. 1.39 is further expanded as
\[
\sum_i \nabla \left( \rho_f D_f \nabla Y_i (c_{p,i} T_f + h_{f,g,i}) \right) \\
= \sum_i \nabla c_{p,i} D_f \left( \rho_f T_f \nabla Y_i \right) + \sum_i \nabla h_{f,g,i} D_f \left( \rho_f \nabla Y_i \right) \\
= \sum_i \nabla c_{p,i} D_f \left( \langle \rho_f \rangle^f \langle T_f \rangle^f + \bar{T}_f \right) \nabla Y_i + \sum_i \nabla h_{f,g,i} D_f \left( \langle \rho_f \rangle^f \nabla Y_i \right) \\
= \sum_i \nabla c_{p,i} D_f \left( \langle \rho_f \rangle^f \langle T_f \rangle^f \right) \nabla Y_i + \sum_i \nabla h_{f,g,i} D_f \langle \rho_f \rangle^f \nabla Y_i + \sum_i \nabla c_{p,i} D_f \left( \langle \rho_f \rangle^f \bar{T}_f \nabla Y_i \right) + \sum_i \nabla h_{f,g,i} D_f \langle \rho_f \rangle^f \langle \bar{T}_f \nabla Y_i \rangle + \sum_i \nabla h_{f,g,i} D_f \langle \rho_f \rangle^f \left( \epsilon \nabla \langle Y_{i,f} \rangle^f + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \tilde{Y}_{i,f} \, da \right) \\
+ \sum_i \nabla h_{f,g,i} D_f \langle \rho_f \rangle^f \left( \epsilon \nabla \langle Y_{i,f} \rangle^f + \frac{1}{V} \int_{a_{fs}} \mathbf{n} \tilde{Y}_{i,f} \, da \right) \\
\]  

(1.40)

The entire volume-averaged air-water vapour mixture energy transport equation can be written as
The closure for the energy equation is also obtained using the gradient-type models as explained earlier. The last term on the right-hand side of Eq. 1.41 may represent interfacial energy transfer due to mass transfer, which also accounts for the latent energy of water vapor evaporation. However, in the present model, the latent energy of water vapor evaporation is already accounted by fluid-constituent by tracking the entire air-vapor mixture energy i.e. when moist air gains or losses moisture it uses its energy to account for that moisture exchange. Therefore, including this last term in the model will add the latent energy of water vapor evaporation to the fluid-constituent, which will negate the effects of evaporative cooling. Consequently, the last term on the right-hand side of Eq. 1.41 is neglected in the present work. The resulting extrinsic form of the closed volume-averaged energy transport equation for the air-water vapour mixture is
expressed as

\[
\sum_{i} \varepsilon c_{p,i} \frac{\partial (\langle \rho_f \rangle f (Y_{i,f}) f (T_f)^f)}{\partial t} + \sum_{i} \varepsilon h_{f,g,i} \frac{\partial (\langle \rho_f \rangle f (Y_{i,f}) f)}{\partial t} \\
+ \sum_{i} c_{p,i} \nabla . (\langle \rho_f \rangle f (Y_{i,f}) f (T_f)^f (v)) + \sum_{i} h_{f,g,i} \nabla . (\langle \rho_f \rangle f (Y_{i,f}) f (v)) \\
= k_{eff,f} \nabla^2 (T_f)^f \\
+ \sum_{i} \nabla . [\langle \rho_f \rangle f D_{eff,f} \nabla (Y_{i,f}) f (c_{p,i} (T_f)^f + h_{f,g,i})] + \varepsilon S_{e,f} \\
+ h_{fs} A_{fs} (\langle T_s \rangle^s - \langle T_f \rangle^f)
\]

The volume-averaging of the solid-constituent’s energy equation also follows the same procedure, which will not be repeated here. The resulting closed form of the volume-averaged solid-constituent’s energy transport equation is given as

\[
\sum_{i} (1 - \varepsilon) c_{ps,i} \frac{\partial (\langle \rho_s \rangle s (Y_{i,s}) f (T_s)^s)}{\partial t} \\
= k_{eff,s} \nabla^2 (T_s)^s + \sum_{i} \nabla . [\langle \rho_s \rangle s D_{eff,s} \nabla (Y_{i,s})^s (c_{ps,i} (T_s)^s)] \\
+ (1 - \varepsilon) S_{e,s} - h_{fs} A_{fs} (\langle T_s \rangle^s - \langle T_f \rangle^f)
\]

\[1.42\]

\[1.43\]

1.5 Thesis motivation and objectives

The literature review presented in the section 1.3 describes the capabilities of different heat and mass transfer models from various aspects. In terms of non-equilibrium heat and mass transfer inside porous media, some numerical models [20,22,23] incorporated non-equilibrium mass transfer, while others included non-equilibrium heat transfer [24-26]. In addition, most of these models utilized a non-equilibrium approach specifically designed for the particular case under study.

Similarly, heat and mass transfer in a conjugate framework has been specifically modeled as well [1,22,24-26], however, all such studies considered thermal and/or moisture equilibrium inside the porous media. For the problems related to convective drying, as
Chapter 1

mentioned earlier, some groups [28,29,32] maintained conjugacy by explicitly linking the fluid and porous region solutions obtained using different software/codes, which highlights their lack of a generic conjugate framework. In addition, the work of Moureh et al. [27] relied on Fluent to formulate the fluid-porous interface. None of these studies required the solid region to be included in the conjugate framework, which is essential for some heat and mass transfer problems discussed earlier. In this respect, only Zou et al. [25,26] proposed a conjugate fluid/porous/solid framework. However, no description of interface treatment was provided, and their model did not include mass transfer.

The existing literature on macroscopic turbulence and turbulent heat and mass transfer inside porous media shows the availability of such models, however, the models require closure for the considered porous media. With respect to the closure for randomly packed bed of spheres, efforts were only made by Alvarez and Flick [36], and Mathey [49], however, both studies utilized structurally packed bed of spheres rather than more realistic randomly packed bed of spheres.

It can be concluded based on the above discussion that no study, as yet, has proposed a generic formulation that simulates non-equilibrium heat and mass transfer in a conjugate fluid/porous/solid framework. In addition, to the authors’ knowledge, closure for a macroscopic model that simulates turbulence and non-equilibrium turbulent heat and mass transfer inside porous media composed of randomly packed bed of spheres still does not exist in the existing literature. Therefore, there is a need of a model that fulfills all of these requirements, and accurately simulates various related heat and mass transfer problems discussed earlier. In addition, the model must be generic and capable of being modified to the problem requirements.

Based on this discussion, the overall objective of the present work is to develop a formulation that simulates various heat and mass transport problems in complex domains involving porous media over wide range of Reynolds numbers. This overall objective can be achieved by fulfilling the following specific objectives:

1. The first objective is focused on developing a model that incorporates non-equilibrium heat and mass transport in conjugate fluid/porous/solid framework.
2. The second objective is focused on the demonstration of the developed formulation by simulating the problems that essentially require non-equilibrium heat and mass transfer capabilities in conjugate framework.

3. The third objective is to extend the applicability of the developed model to such class of problems that essentially involve turbulence and non-equilibrium turbulent heat and mass transport.

1.6 Thesis outline

The remaining chapters of the thesis are focused on achieving the objectives mentioned earlier. A brief aim and overview of each chapter is given as:

- Chapter 2: The development of a formulation that simulates non-equilibrium heat and mass transport in conjugate fluid/porous/solid framework is presented. In this respect, the required transport equations for each region are presented, which is followed by a novel interfacial formulation. For ease, the discretization and implementation of the developed formulation is also included. For the purpose of model demonstration and validation, the problems of direct and indirect evaporative cooling and drying of a wet porous block are simulated. In addition, each selected case demonstrates a core capability of the developed formulation. The overall aim of this chapter is to develop the required generic formulation and to demonstrate that it is adaptable to different types of heat and mass transfer problems, and yet capable of providing physically realistic solutions. Consequently, this chapter forms the base of the thesis, from where the developed model is further utilized/extended to achieve the remaining proposed goals.

- Chapter 3: The convective drying of a wet porous material using conjugate framework is presented. Although, drying process of a wet porous block is already covered in chapter 2, that case utilizes an internal drying airflow through moist permeable wood wool. Moreover, that case serves as a simple demonstration of the developed model to simulate such class of problems. In
chapter 3, convective drying of an apple slice as wet porous material along with the surrounding airflow region is modeled using the conjugate framework and verified using highly cited experimental data. The modeling of such a complex simultaneous heat and mass transfer problem provides a comprehensive and critical assessment of the developed formulation. It further demonstrates the capability of the developed model to accurately predict heat and mass exchange within the porous region and at fluid-porous interfaces under varying airflow conditions. In this respect, the mass exchange conditions at a fluid-porous interface are comprehensively discussed and modified to meet the problem requirements. In addition, the detailed modeling of apple flesh as a porous material is also carried out to show the intricate modeling capabilities of the developed model. Lastly, this chapter serves as an intermediate step towards the extension of the developed model, where implicit dynamic coupling of porous material phases is essential for the applications related to food storage and processing industries.

- Chapter 4: This chapter extends the capability of the developed formulation to model such class of problems that involve turbulence and turbulent heat and mass transfer inside porous media. In this respect, this chapter focuses on closure of the available macroscopic turbulence and non-equilibrium turbulent heat and mass transfer models inside a porous media composed of a randomly packed bed of spheres. The closure is obtained by simulating the problem at the microscopic scale of the porous media. In addition, the applicability of the closure is extend by including the parametric variation of different geometric and flow parameters.

- The last chapter covers the overall summary of the thesis, and also highlights the novel contributions made and the future recommendations.
References


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Chapter 2

2 Numerical model for non-equilibrium heat and mass transfer in conjugate framework*

2.1 Introduction

Fluid flow and heat transfer problems involving conjugate fluid/porous/solid regions have many applications in thermal management, drying, curing, filtration, etc. Thus, there is a need for robust numerical models capable of simulating such classes of problems. The developed formulation must be capable of modeling fluid flow, and sensible and latent heat exchange in conjugate fluid/porous/solid regions, and be accurate and robust at interfaces between these regions where sudden changes can occur in flow characteristics.

With respect to numerically modeling of fluid flow and heat transfer in conjugate domains, a significant amount of work has been reported (see reference [1] for comprehensive literature review). Costa et al. [2] proposed a finite-element approach to simulate flows in conjugate fluid/porous domains. Their approach considered local thermal equilibrium in the porous region, which assumes that the total energy of a porous continuum comprised of fluid and solid can be characterized by a single temperature. While this is reasonable for solid materials of low conductivity, it is not appropriate for highly conductive metals, or for cases where the temperature of the fluid (or solid) is important for determining physical thresholds, such as in evaporative cooling. In addition, because of the discretization approach used at the interfaces between fluid-solid regions, their model was restricted to very low Reynolds numbers (< 10). The most comprehensive recent work in conjugate domain modelling of heat and fluid flow was carried out by Betchen et al. [1]. Their work describes a conjugate domain model, based upon the finite-volume approach that accounts for fluid flow and non-equilibrium (sensible) heat transfer in porous regions. One key contribution of their work was interface treatment between regions of the conjugate domain. Robust mathematical conditions were developed and discretized that enable stable, smooth transitions across

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fluid-porous interfaces over a wide range of Reynolds numbers (up to 1000) in the laminar regime.

A new class of diverse problems such as drying, fluidized bed reactors, chemical reactors, evaporative cooling, produce refrigeration, etc. can be numerically modeled if, in addition to flow and heat transfer, mass transfer is considered in the conjugate fluid/porous/solid framework. A significant amount of work has been reported focused on the numerical modelling of the problems involving heat and mass transfer. In this respect, simple heat and mass balance equations have been proposed to model different heat and mass transfer problems, such as dehumidification of air through desiccant drying, indirect evaporative cooling, and Maisotsenko cycle cooling [3-7]. A novel desiccant evaporative cooling system (DES) capable of providing conditioned-air by utilizing low grade thermal energy [8], which involves dehumidification of air through desiccant drying followed by evaporative cooling process to lower its temperature, has also been modeled previously using mass and energy balance equations [9-12].

More sophisticated finite-volume and finite-difference numerical formulations have been proposed to model different types of heat and mass transfer problems inside porous media. However, most of these studies have considered local thermal-equilibrium to model heat transfer [13-19]. For the problems related to produce refrigeration, only a few studies have considered the thermal non-equilibrium approach to model heat transfer [20, 21]. Moreover, few studies have proposed specifically formulated non-equilibrium heat and mass transfer models to study desiccant drying process [22, 23]. Very few studies have proposed air flow and heat transfer numerical models in conjugate fluid/porous domains. In this respect, Moureh et al. [24, 25] focused solely on air flow modeling, and relied on a commercial Computational Fluid Dynamics (CFD) package to deal with the complexities associated with the fluid/porous interface. Zou et al. [26, 27] presented an air and heat transfer numerical model in conjugate fluid/porous/solid domains for the problem of produce packaging. However, no information pertaining to the interface treatment was provided.
It can be concluded from the above literature that no study, as yet, has proposed a non-equilibrium heat and mass transfer numerical formulation for porous materials. Moreover, no study, as yet, has considered such a formulation in a conjugate fluid/solid/porous domain framework. The aim of the present work is to develop a numerical formulation capable of modeling fluid flow, heat and mass transfer in conjugate fluid/solid/porous domains. The key objective of this work is to extend the work of Betchen et al. [1] by incorporating latent heat and mass transfer in the existing formulation. In this regard, special attention will be given to ensure that heat and mass transfer occurs smoothly across all the interfaces. Moreover, to accurately capture the physics of the heat and mass transfer problems, non-equilibrium heat and moisture transport equations will be introduced. To achieve the present objective, an in-house CFD code will be described. The assessment of the developed formulation will be made by simulating problems related to evaporative cooling. In this respect, direct and indirect evaporative cooling simulation results will be validated against available experimental results to comprehensively test the different features of the developed formulation. In addition, a transient problem of drying of a porous material initially saturated with water will also be simulated to further assess the formulation.

Another novel feature of the present study is the manner in which the latent energy of the moist air flow is accounted in the transport equation of energy. Previously, studies focused on modeling the phenomenon of evaporative cooling in porous media have accounted for the latent heat of evaporation of water in energy equation by utilizing a source term [15-17]. In the present formulation, a more general approach has been taken to account for this latent energy in the energy equation. Further discussion regarding this approach will be made later in the section describing the numerical formulation.

2.2 Model formulation

This section presents the transport equations required to simulate the thermal non-equilibrium heat and mass transfer in conjugate fluid/porous/solid domains, wherein moist air is the working fluid. In general, atmospheric air is a mixture of nitrogen, oxygen, argon, carbon dioxide, water vapour, and other contaminants such as dust, whereas dry air refers only to the gas components when all contaminants and water
vapour have been removed. Since the variation of trace gases in the atmosphere is small, it is convenient to treat atmospheric air solely as a mixture of dry air, which comprises all of the gas components, and water vapour. This approach is used frequently for non-reacting mixtures and has an error of less than 0.2% [28]. By this approach, the air water vapour mixture is characterized using mixture properties, and the local vapour content can be quantified by the introduction of one additional transport equation to the conventional conservation of mass-Navier-Stokes formulation. In the present work, a transport equation for the water vapour mass fraction ($Y_v$) transport is introduced to account for the local vapour content, and the mass exchange between constituents in the porous region.

The two most common ways of specifying the amount of water vapour in air is through the specific humidity ($\omega_{spec}$) and the relative humidity ($\omega_{rel}$) as shown below [28]

$$\omega_{spec} = \frac{m_v}{m_a} = \frac{(R_a/R_v)p_v}{P_a}$$

(2.1)

$$\omega_{rel} = \frac{P_v}{P_g}$$

(2.2)

where $m_v$ is the mass of water vapour, $m_a$ is the dry air mass, $P_a$ is the dry air partial pressure, $P_v$ is water vapour partial pressure, $P_g$ is the saturation pressure of water at that temperature, and $R_a$ and $R_v$ are the gas constants for air and water vapour, respectively. The sum of $P_a$ and $P_v$ is the total air mixture pressure ($P_t$) available from the solution of mass and momentum transport equations. The saturation pressure ($P_g$) at a given temperature is found using Antoine equation for water vapour requiring temperature [29]. The temperature of the air-vapour mixture ($T$) is obtained by solving the energy transport equation for the dry air-water vapour mixture. The relation between the vapour mass fraction ($Y_v$) and specific humidity can be expressed as

$$Y_v = \frac{\omega_{spec}}{1 + \omega_{spec}}$$

(2.3)
The vapour mass fraction ($Y_v$) along with the moist air total pressure ($P_t$) can then be used to calculate the vapour pressure ($P_v$) by the following expression

$$P_v = \frac{Y_v R_v P_t}{R_a + Y_v (R_v - R_a)} \quad (2.4)$$

The mixture density ($\rho_f$) can then be calculated as

$$\rho_f = \rho_a + \rho_v = \frac{P_a}{R_a T} + \frac{P_v}{R_v T} \quad (2.5)$$

### 2.2.1 Fluid region

The conservation of mass and momentum equations of the air-water vapour mixture in the pure fluid region take their conventional forms

$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{v}) = 0 \quad (2.6)$$

$$\frac{\partial (\rho_f \mathbf{v})}{\partial t} + \nabla \cdot (\rho_f \mathbf{v} \mathbf{v}) = -\nabla P + \mu_f \nabla^2 \mathbf{v} + \rho_f \mathbf{f} \quad (2.7)$$

Since it is the mixture density ($\rho_f$) that is used in the transport equations, no additional source terms are required in Eq. 2.6. The transient term in Eq. 2.6 accounts for density changes due to mass transfer during a given time interval, an amount which is also reflected exactly in the advective imbalance. In this regard, the proposed method takes advantage of the fact that the discretization approach to be used includes transient effects. In fact, virtually all modern solvers include transient effects and many use the time step as a method of controlling the diagonal dominance of the coefficient matrix in the linear solver. An additional benefit of using the mixture density approach is that the discrete mass equation, multiplied by a reference value, can be subtracted from all other transport equations to remove the necessity to account for temporal changes in fluid density within a time step. This will be discussed further in section 2.4.
The water vapour transport equation is expressed as [30]

\[
\frac{\partial (\rho_f Y_v)}{\partial t} + \nabla \cdot (\rho_f Y_v \mathbf{v}) = \nabla \cdot (\rho_f D_f \nabla Y_v) + S_v
\]  

(2.8)

where, \( S_v \) represents the mass transfer source. To obtain the desired form of the energy equation, the enthalpy needs to be cast into a form suitable to characterize the mixture. The specific enthalpy of each species can be described as a sum of sensible and latent components as shown below

\[
h_i = c_{p,i}T_i + h_{fg,i}
\]

(2.9)

where the species number \( i = 1,2,\ldots,N \), and for the present work, \( N \) is equal to 2 (1=air, 2=water vapour). For dry air, only the sensible component exists (i.e. \( h_{fg,1} = 0 \)), but, for water vapour both components have to be considered. If the mathematical operation of summation is applied to the above expression then the total specific enthalpy of a moist air mixture can be expressed as

\[
h = \sum_i Y_i c_{p,i}T_i + Y_i h_{fg,i}
\]

(2.10)

Then, the energy transport equation of the air-water vapour mixture in the pure fluid region can be expressed as [31]

\[
\sum_i c_{p,i} \frac{\partial (\rho_f Y_i T_i)}{\partial t} + \sum_i h_{fg,i} \frac{\partial (\rho_f Y_i)}{\partial t} + \sum_i c_{p,i} \nabla \cdot (\rho_f Y_i \mathbf{v}) + \sum_i h_{fg,i} \nabla \cdot (\rho_f Y_i \mathbf{v}) \]

\[
= k_f \nabla^2 T + \sum_i \nabla \cdot [\rho_f D_f \nabla Y_i (c_{p,i} T_i + h_{fg,i})] + S_e
\]

(2.11)

The first two terms on the left hand side of Eq. 2.11 represent energy transfer due to unsteady effects. The third and fourth terms on the left hand side represent energy transfer due to advection. The first term on the right hand side represents conduction, while the second term on the right hand side accounts for energy transfer due to species diffusion. \( S_e \) represents the source of energy, which in the pure fluid region is zero. The
sensible and the latent energy components of the unsteady, advective, and species diffusion terms have been separated for clarity.

2.2.2 Porous region

In the porous region, volume-averaged forms of the transport equations (Eqs. 2.6-2.8, 2.11) are required such that the porous media is considered as a continuum. In volume-averaging, the transport equations are integrated over a representative elementary volume of a porous media. The basic concept of volume-averaging is that at every point in space, there exists a volume-averaged value of a quantity \((\varphi_f)\) defined by following expression [32]

\[
\langle \varphi_f \rangle = \frac{1}{V} \int_{V_f} \varphi_f \, dV
\] (2.12)

where, \(V\) is the volume over which the averaging is carried out, \(V_f\) is the fluid volume inside \(V\), and \(\langle \varphi_f \rangle\) is called the extrinsic-averaged quantity. In a similar manner, an intrinsic-averaged quantity \(\langle \varphi_f \rangle^f\) can be defined as [32]

\[
\langle \varphi_f \rangle^f = \frac{1}{V_f} \int_{V_f} \varphi_f \, dV
\] (2.13)

The relation between the intrinsic and extrinsic-averaged quantity is defined as [32]

\[
\langle \varphi_f \rangle = \varepsilon \langle \varphi_f \rangle^f
\] (2.14)

where, \(\varepsilon\) is the porosity of porous media, and is defined as the ratio of fluid volume \((V_f)\) to the total volume \((V)\). In general, volume-averaging creates additional terms in the transport equations, which require closure before a solution can be obtained. Here, we present the closed forms of the transport equations. The extrinsic form of the volume-averaged conservation of mass and momentum equations are given as [1]

\[
\varepsilon \frac{\partial \langle \rho_f \rangle^f}{\partial t} + \nabla \cdot \left( \langle \rho_f \rangle^f \langle \mathbf{v} \rangle \right) = 0
\] (2.15)
\[
\frac{\partial \left( \langle \rho_f \rangle^f \langle v \rangle \right)}{\partial t} + \frac{1}{\varepsilon} \nabla \cdot \left( \langle \rho_f \rangle^f \langle v \rangle \langle v \rangle \right) = -\varepsilon \nabla \langle p \rangle^f + \mu_f \nabla^2 \langle v \rangle + \varepsilon \langle \rho_f \rangle^f f - \frac{\varepsilon \mu_f}{K} \langle v \rangle - \frac{\varepsilon \langle \rho_f \rangle^f c_E}{\sqrt{K}} \langle v \rangle \langle v \rangle
\]

where, the last two terms on the right-hand side of Eq. 2.16 are the Darcy and Forchheimer terms, respectively, which represent the viscous and form drag resulting from the interaction between the solid and fluid-constituents in the porous media \[1\]. While the structure of the porous material is not accounted for specifically, the porosity \( \varepsilon \), permeability \( K \), and the inertial coefficient \( c_E \), are used to characterize the resistance of the porous material to fluid flow. Values of these coefficients are introduced in subsequent sections.

To accurately capture the physics of different problems involving mass and heat transfer, non-equilibrium mass and heat transport equations are utilized in the porous media. Such formulation is then capable of accounting for mass transfer, and sensible and latent exchange of energy between the air-water vapor mixture and a moisture-permeable solid-constituent of the porous region. As such, the fluid region (void phase in the porous region) contains air and water vapor, and the solid-constituent of the porous region contains solid and liquid. Moisture permeable solids include, for example, produce, desiccants, and wood or cellulose products. In such cases, moisture can reside inside the solid-constituent in the liquid state. Therefore, the present numerical model considers the presence of liquid water inside the solid-constituent of the porous media, and solves the moisture mass fraction \( Y_w \) transport equation in the solid phase of the porous media.

The extrinsic form of the volume-averaged moisture transport equations for the pure fluid (i.e. air-vapor mixture) and the moisture-permeable solid, respectively, are expressed as

\[
\varepsilon \frac{\partial \left( \langle \rho_f \rangle^f \langle Y_{v,f} \rangle \right)}{\partial t} + \nabla \cdot \left( \langle \rho_f \rangle^f \langle Y_{v,f} \rangle \langle v \rangle \right) = \nabla \cdot \left( \langle \rho_f \rangle^f D_{eff,f} \nabla \langle Y_{v,f} \rangle \right) + \varepsilon S_{v,f} + \langle \dot{m}_{fs} \rangle
\]
\[ (1 - \varepsilon) \frac{\partial (\rho_s s) (Y_{w,s})^s}{\partial t} = \nabla \cdot \left( (\rho_s s) D_{\text{eff},s} \nabla (Y_{w,s})^s \right) + (1 - \varepsilon) S_{w,s} - \langle \dot{m}_{fs} \rangle \quad (2.18) \]

The diffusion coefficient \(D_{\text{eff}}\) represents the effective diffusivity, which results from the closure of different terms present in the volume-averaged moisture transport equations. As a result of closure, \(D_{\text{eff}}\) represents the effect of porous media on the ability of fluid or solid-constituent to diffuse moisture.

The last two terms in Eqs. 2.17-2.18 represent the interfacial mass transfer i.e. moisture transfer from one constituent of porous media to another. In other words, these terms represent the connection between the air-vapor mixture and the solid-constituent of the porous media. These terms remain undefined for now, as their definition is unique to a specific type of problem. In section 2.5, these terms will be expressed in a manner appropriate to simulate evaporative cooling.

Similar to the moisture transport equations, the extrinsic form of the volume-averaged energy transport equation for both the air-water vapor mixture and the solid-constituent, respectively, are expressed as

\[
\sum_i \varepsilon c_{p,i} \frac{\partial (\langle \rho_f \rangle^f (Y_{i,f})^f (T_f)^f)}{\partial t} + \sum_i \varepsilon h_{f,g,i} \frac{\partial (\langle \rho_f \rangle^f (Y_{i,f})^f)}{\partial t} \\
+ \sum_i c_{p,i} \nabla \cdot (\langle \rho_f \rangle^f (Y_{i,f})^f (T_f)^f (\mathbf{v})) \\
+ \sum_i h_{f,g,i} \nabla \cdot (\langle \rho_f \rangle^f (Y_{i,f})^f (\mathbf{v})) \\
= k_{\text{eff},f} \nabla^2 (T_f)^f \\
+ \sum_i \nabla \cdot [\langle \rho_f \rangle^f D_{\text{eff},f} \nabla (Y_{i,f})^f (c_{p,i} (T_f)^f + h_{f,g,i})] + \varepsilon S_{e,f} \\
+ h_{fs} A_{fs} (\langle T_s \rangle^s - \langle T_f \rangle^f) \quad (2.19)
\]
\[
\sum_i (1 - \varepsilon) c_{ps,i} \frac{\partial ((\rho_s)^s (Y_{i,s})^s (T_s)^s)}{\partial t} = k_{eff,s} \nabla^2 (T_s)^s + \sum_i \nabla \cdot \left[ (\rho_s)^s D_{eff,s} \nabla (Y_{i,s})^s (c_{ps,i} (T_s)^s) \right] \\
+ (1 - \varepsilon) S_{e,s} - h_{fs} A_{fs} \left( (T_s)^s - (T_f)^f \right)
\]  

(2.20)

where, Eqs. 2.19-2.20 represent energy transport in fluid and solid-constituents, respectively. Because we only consider the solid-constituent of the porous domain to contain solid and liquid, no latent enthalpy is included in Eq. 2.20. The last two terms of Eqs. 2.19-2.20 represent the interfacial heat transfer between the fluid and solid-constituents of the porous media.

As discussed earlier, the latent energy components of the unsteady, advective, and species diffusion terms have been separated from the sensible energy components. It is interesting to note that the sum of the latent components of the unsteady, advective, and species diffusion terms in the air-vapor mixture energy equation account for the latent energy of water vapour evaporation. Thus, by considering the total mixture enthalpy for each term of the energy transport equation, we inherently account for the latent heat of evaporation of water vapor. The key feature of the present approach is that it takes its roots from the first law of thermodynamics, where the focus is to track the total system energy. Another approach to account for the latent energy of water vapor evaporation has been adopted by other research groups [13, 15-17]. Their approach considers only the sensible energy component in unsteady, advective and species diffusion terms of the energy equation, and then accounts for the latent energy of water vapour evaporation by a source term equivalent to \( h_{fg} \langle \dot{m}_{fs} \rangle \). It is verified that both the approaches produce identical steady-state results. However, the present approach does not require \( h_{fg} \langle \dot{m}_{fs} \rangle \) term to account for the latent energy of evaporation of water vapour.

### 2.2.3 Solid region

In the solid region, it is unnecessary to solve the momentum equations, and transport equations are only required for liquid water transport and energy, given respectively as
\[
\frac{\partial (\rho_s Y_w)}{\partial t} = \nabla \cdot (\rho_s D_s \nabla Y_w) + S_w
\]  (2.21)

\[
\sum_l c_{ps,l} \frac{\partial (\rho_s Y_i T)}{\partial t} = k_s \nabla^2 T + \sum_l \nabla \cdot \left[ \rho_s D_s \nabla Y_i (c_{ps,l} T) \right] + S_e
\]  (2.22)

2.3 Interface conditions

To ensure that momentum, heat and mass transfer is accurately simulated across interfaces, special mathematical conditions are developed for the interfaces between all conjugate regions.

2.3.1 Interface between fluid and porous regions

The extrinsic velocity is continuous at fluid-porous interfaces and is represented by the following condition [1]

\[
v_{fl} = \langle v \rangle_{por}
\]  (2.23)

The continuity of both the normal and shear stresses is also imposed by assuming that the fluid-constituent on the porous side receives \( \epsilon \) amount of the total stresses from the pure fluid side while the remaining stresses are carried by the solid-constituent [1]. The continuity of pressure at the interface is enforced by keeping the fluid region pressure continuous with the porous side intrinsically averaged pressure given as [1]

\[
P_{fl} = \langle P \rangle_{por}
\]  (2.24)

For thermal energy transport, the following condition of continuity exists at fluid-porous interfaces [1]

\[
\left( -k_f \frac{\partial T}{\partial n} \right)_{fl} = \left( -k_{eff,f} \frac{\partial \langle T_f \rangle}{\partial n} - k_{eff,s} \frac{\partial \langle T_s \rangle}{\partial n} \right)_{por}
\]  (2.25)

It can be observed from the above expression that the heat transfer from the pure fluid region splits at the interface; an amount goes to the fluid-constituent and the remaining
goes to the solid-constituent. The use of the thermal non-equilibrium approach in the porous region requires this split of thermal energy at the interface.

Since the present formulation also incorporates non-equilibrium mass transfer in the porous region, it is necessary to develop a condition that facilitates such transport at fluid-porous interfaces. Using an approach similar to that used in [1] for heat transport, the mass transfer condition at a fluid-porous interface can be expressed as

\[
\left( -\rho_f D_f \frac{\partial Y_v}{\partial n} \right)_{fl} = \left( -\langle \rho_f \rangle f D_{eff,f} \frac{\partial \langle Y_{v,f} \rangle f}{\partial n} - \langle \rho_s \rangle s D_{eff,s} \frac{\partial \langle Y_{w,s} \rangle s}{\partial n} \right)_{por}
\]

(2.26)

The physical interpretation of Eq. 2.26, using electrical circuit analogy, is presented in Fig. 2.1, which shows the split of vapour transport \((\dot{m}_v)\) at the fluid/porous interface. The figure also shows a streamwise view of a generic fluid/porous interface from the side of the pure fluid region. This serves to illustrate the fact that the flow of moisture coming from the fluid region sees both fluid and solid-constituents in the porous region. The amount of moisture entering the fluid and solid-constituents \((\dot{m}_{v,f} \text{ and } \dot{m}_{w,s})\) are dependent upon the resistances \((R_v, R_{v,f} \text{ and } R_{w,s})\) and the nodal values of moisture mass fraction \((Y_v, Y_{v,f} \text{ and } Y_{w,s})\) across the interface.

The division of \(\dot{m}_v\) into \(\dot{m}_{v,f}\) and \(\dot{m}_{w,s}\) cannot be controlled by the nodal values of moisture mass fraction as they are part of the required solution. The mass transport split is dictated by the mass fraction potentials, \(\Delta Y\), and the relative resistances \(R_{v,f} \text{ and } R_{w,s}\), which are represented as competing paths in Fig. 2.1. The relevant resistances are characterized as

\[
R_v = \frac{\Delta x_{f-i}}{A \rho_f D_f}, \quad R_{v,f} = \frac{\Delta x_{i-p}}{\varepsilon A \rho_f D_{eff,f}}, \quad R_{w,s} = \frac{\Delta x_{i-p}}{(1 - \varepsilon) A \rho_s D_{eff,s}}
\]

(2.27)

where, \(A\) is the total area of the control volume face adjacent to the interface, \(\rho\) is the mixture density of the pure fluid (air-vapor), \(D\) is the moisture diffusion coefficient, \(\Delta x_{f-i}\) is the distance between the node in the fluid region and the interface, and \(\Delta x_{i-p}\) is the distance between the interface and the porous region node. Eq. 2.27 clearly represents
the effect of each variable on the respective resistance. In general, these resistances are inversely proportional to $A$, $\rho$, and $D$, while directly proportional to the distance between the nodes and the interface ($\Delta x$). Moreover, a high value of $\varepsilon$ decreases $R_{v,f}$ while increasing $R_{w,s}$ and vice versa. While the preceding discussion considered flow from fluid to porous regions, the formulation is equally suitable for flow from porous to fluid regions without modification.

![Figure 2.1: Depiction of vapour mass transfer condition at fluid/porous interface using resistance analog.](image)

2.3.2 Interface with solid region

The hydrodynamic conditions at interfaces between fluid-solid and porous-solid are no-slip, zero-penetration for velocity, while pressure is extrapolated from the interior fluid or porous regions to the solid surface.

At the interface between the pure fluid and solid conjugate regions, heat transfer is governed by the condition [1]

$$
\left( -k_f \frac{\partial T}{\partial n} \right)_{fl} = \left( -k_s \frac{\partial T}{\partial n} \right)_{sol} 
$$

(2.28)
Similarly, moisture mass transfer between pure fluid and solid conjugate regions is governed by

\[ (-\rho_f D_f \frac{\partial Y_v}{\partial n})_{fl} = (-\rho_s D_s \frac{\partial Y_w}{\partial n})_{sol} \]  \hspace{1cm} (2.29)

For thermal energy and moisture transport at the interface between the solid and porous media regions, conditions identical to Eqs. 2.25-2.26 are imposed and are given as [1]

\[ \left( -k_s \frac{\partial T}{\partial n} \right)_{sol} = \left( -k_{eff,f} \frac{\partial \langle T_f \rangle}{\partial n} - k_{eff,s} \frac{\partial \langle T_s \rangle}{\partial n} \right)_{por} \]  \hspace{1cm} (2.30)

\[ \left( -\rho_s D_s \frac{\partial Y_w}{\partial n} \right)_{sol} = \left( -\langle \rho_f \rangle D_{eff,f} \frac{\partial \langle Y_v,f \rangle}{\partial n} - \langle \rho_s \rangle D_{eff,s} \frac{\partial \langle Y_w,s \rangle}{\partial n} \right)_{por} \]  \hspace{1cm} (2.31)

2.4 Discretization and implementation of transport equations and interface conditions

To discretize the transport equations introduced in section 2.2 using the finite-volume approach, the equations are integrated in space over a control volume \( V_P \). This control volume has NS faces and contains a node \( P \) at its center. The equations are further integrated in time using a fully-implicit scheme with time-interval of \( \Delta t \). The conservation of mass equation, multiplied by a suitable reference variable, is then subtracted from each respective transport equation. The resulting discrete transport equations for the pure fluid region are then given as

\[ \frac{V_P (\rho_{f,P} - \rho_{f,P}^o)}{\Delta t} + \sum_{\gamma} \dot{m}_\gamma = 0 \]  \hspace{1cm} (2.32)

\[ \frac{V_P \rho_{f,P}^o (\mathbf{v}_P - \mathbf{v}_P^2)}{\Delta t} + \sum_{\gamma} \dot{m}_\gamma (\mathbf{v}_\gamma - \mathbf{v}_P) = -V_P (V_P)_P + \sum_{\gamma} \mu_f \left( \frac{\partial \mathbf{v}}{\partial n} \right)_\gamma + V_P \rho_f f_P \]  \hspace{1cm} (2.33)
where, all the faces of a control volume are represented by $\gamma = 1, 2, \ldots, NS$. Coupling between velocity and pressure is controlled using the collocated variable method proposed by Rhie and Chow (see ref. 1 for details). In short, this method utilizes the discretized momentum equation to come up with an advecting velocity at every face of a control volume, which is then utilized to compute the mass flow rate ($\dot{m}$) present in the above discretized equations.

The discretization of the transport equations in porous media region is carried out in the similar manner, and the resulting discretized equations can be written as

\begin{equation}
\frac{\varepsilon V_P}{\Delta t} ((\rho_f)_P^{f,o} - \langle \rho_f \rangle_P^{f,o}) + \sum_{\gamma} \dot{m}_y = 0
\end{equation}

\begin{equation}
\frac{V_P (\rho_f)_P^{f,o}}{\Delta t} (\langle \mathbf{v} \rangle_P - \langle \mathbf{v} \rangle_P^o) + \frac{1}{\varepsilon} \sum_{\gamma} \dot{m}_y ((\mathbf{v})_y - \langle \mathbf{v} \rangle_P) = -\varepsilon V_P (\nabla \langle P \rangle_P^f)_P + \sum_{\gamma} \mu_f \left( A \frac{\partial \langle \mathbf{v} \rangle}{\partial n} \right)_y + \varepsilon V_P (\rho_f)_P^{f} f_P
\end{equation}
\[
\frac{\varepsilon V_p (\rho_f)_P^{f,o}}{\Delta t} \left( (Y_{v,f})_P^f - (Y_{v,f})_P^{f,o} \right) + \sum_y \hat{m}_y (Y_{v,f})_y^f - (Y_{v,f})_y^f
\]
\[
= \sum_y D_{\text{eff},f} \left( A (\rho_f)_f^f \frac{\partial (Y_{v,f})_y^f}{\partial n} \right) + \varepsilon V_p S_{v,f} + V_p \langle \hat{m}_{fs} \rangle
\]

\[
\frac{(1 - \varepsilon) V_p}{\Delta t} \left( (\rho_s)_P^s (Y_{w,s})_P^s - (\rho_s)_P^{s,o} (Y_{w,s})_P^{s,o} \right)
\]
\[
= \sum_y D_{\text{eff},s} \left( A (\rho_s)_s^s \frac{\partial (Y_{w,s})_y^s}{\partial n} \right) + (1 - \varepsilon) V_p S_{w,s} - V_p \langle \hat{m}_{fs} \rangle
\]

\[
\frac{\varepsilon V_p (\rho_f)_P^{f,o}}{\Delta t} \sum_i \left[ c_{p,l} \left( (Y_{i,f})_P^f - (Y_{i,f})_P^{f,o} \right) + h_{f,g,i} \left( (Y_{i,f})_P^f - (Y_{i,f})_P^{f,o} \right) \right]
\]
\[
+ \sum_y \left\{ \hat{m}_y \sum_i c_{p,l} \langle Y_{i,f} \rangle_P^f \left( (T_f)_y^f - (T_f)_P^f \right) \right. \\
+ \left. h_{f,g,i} \left( (Y_{i,f})_P^f - (Y_{i,f})_P^{f,o} \right) \right\}
\]
\[
= \sum_y k_{\text{eff},f} \left( A \frac{\partial (T_f)_y^f}{\partial n} \right)_y \\
+ \sum_y \left\{ \sum_i \left[ A (\rho_f)_f^f D_{\text{eff},f} \frac{\partial (Y_{i,f})_y^f}{\partial n} \left( c_{p,l} (T_f)_y^f + h_{f,g,i} \right) \right] \right\}_y \\
+ \varepsilon V_p S_{e,f} + V_p h_{f,s} A_{fs} (T_s)_P^s - (T_f)_P^f
\]

\[
\frac{(1 - \varepsilon) V_p}{\Delta t} \sum_i \left[ c_{p,s} \left( (\rho_s)_P^s (Y_{i,s})_P^s (T_s)_P^s - (\rho_s)_P^{s,o} (Y_{i,s})_P^{s,o} (T_s)_P^{s,o} \right) \right]
\]
\[
= \sum_y k_{\text{eff},s} \left( A \frac{\partial (T_s)_y^s}{\partial n} \right)_y \\
+ \sum_y \left\{ \sum_i \left[ A (\rho_s)_s^s D_{\text{eff},s} \frac{\partial (Y_{i,s})_y^s}{\partial n} \left( c_{p,s} (T_s)_y^s \right) \right] \right\}_y + (1 - \varepsilon) V_p S_{e,s} \\
- V_p h_{f,s} A_{fs} (T_s)_P^s - (T_f)_P^f
\]
As discussed earlier, the discretization involves subtraction of the discrete mass equation, multiplied by a reference value, from the transport equations. This approach ensures that the advective terms of the transport equations do not produce artificial sources when an iterative solver is used to compute the solution. Moreover, it is evident from the discrete moist air mixture transport equations that only the previous time-step mixture density appears in the transient terms, which simplifies implementation of the present numerical model and also inherently makes the formulation suitable for adaptive and moving grids. If the discrete mass equation is not subtracted, the transient terms would include the mixture density from the previous and current time steps.

In the pure solid region, the discretization of the transport equations is straightforward, resulting in

\[
\frac{V_P}{\Delta t} \left( \rho_{s,P} Y_{w,P} - \rho_{s,P} \rho_{o,P} \right) = \sum_{\gamma} D_s \left( A \rho_s \frac{\partial Y_w}{\partial n} \right)_\gamma + V_P s_w \quad (2.42)
\]

\[
\frac{V_P}{\Delta t} \sum_i \left[ c_{ps,i} \left( \rho_{s,P} Y_{i,P} T_P - \rho_{s,P} \rho_{o,P} \right) \right]
= \sum_{\gamma} k_s \left( A \frac{\partial T}{\partial n} \right)_\gamma + \sum_{\gamma} \left\{ \sum_i \left[ A \rho_s D_s \frac{\partial Y_i}{\partial n} \left( c_{ps,i} T \right) \right] \right\}_\gamma + V_P s_e \quad (2.43)
\]

2.4.1 Interface treatment

At fluid-porous interfaces, special treatment is required to compute the advecting velocity, pressure, diffusive and advective terms. Here, we describe the discretization carried out at the interface for these terms without presenting the mathematical formulation. Complete details can be obtained from the work of Betchen et al. [1]. Discretization is carried out in a manner that the interface conditions presented in Eqs. 2.23-2.26 are enforced. The advecting velocity formulation required to compute \( \dot{m} \) at the interface is a blend of advecting velocity formulations utilized in the pure fluid and porous regions. It also utilizes a specially formulated pressure at the interface. To compute the interface pressure, the pressure from the fluid and porous zones adjacent to
the interface are extrapolated to the interface using a second order Taylor series estimation. The fluid side extrapolated pressure is then corrected using a momentum balance. The corrected pressure from the fluid side is then combined with the extrapolated pressure from the porous side to arrive at the average interface pressure.

The diffusive and advective terms appearing in all transport equations also require special attention at the interface. To enforce the interface conditions expressed in Eqs. 2.23-2.26, the harmonic mean formulation is utilized for the diffusive terms. The harmonic mean formulation is also used to calculate $\mathbf{v}_T$ or $\langle \mathbf{v} \rangle_T$ appearing in the advective term of the discretized momentum equation (Eqs. 2.33 and 2.37). For the discretized energy and vapour transport equations, $T_T$ and $Y_{v,T}$ appearing in the advective terms of Eqs. 2.34, 2.35, 2.38, and 2.40 also require evaluation. To this end, the central differencing scheme and the harmonic mean formulation are utilized. However, the results show unexpected spikes in $T_f$ and $Y_f$ across the fluid/porous interface. This can be justified by reasoning that both schemes use a blend of the quantity from both sides of the interface. Moreover, it can be said that mass transfer occurs more inside the porous region than at the fluid/solid interface itself, which means that central differencing and harmonic mean tend to over or under predict the estimated values of $T_T$ and $Y_{v,T}$ resulting in the spikes around the interface region. As a solution, the present formulation proposes use of an upwinding scheme to calculate $T_T$ and $Y_{v,T}$ at the interface, with suitable grid refinement to ensure that solution accuracy is not sacrificed.

The conditions at fluid-solid and porous-solid interfaces within the computational domain are comparatively simple to incorporate in the formulation. The implementation of hydrodynamic interface conditions given in section 2.3.2 is also straightforward. The thermal and moisture transfer conditions given in Eqs. 2.28-2.31 are also enforced using the harmonic mean formulation described previously.

2.5 Model validation

The validation of the developed formulation is carried out to test its capabilities. The current formulation is capable of simulating heat and mass transfer in conjugate
fluid/porous/solid domains. Therefore, problems involving evaporative cooling are simulated for the purpose of validation as they involve both heat and mass transfer. The three problems simulated are: 1) direct evaporative cooling; 2) drying of the wet porous material utilized in the first problem; and 3) indirect evaporative cooling.

Practically, the process of evaporative cooling using porous media involves forced flow of air through a porous material whose surface is kept moist by a continuous supply of water [13]. To mimic this process, the interstitial interface between the solid and fluid in the porous region is assumed to be moist. When air flow having a relative humidity less than 100% is exposed to this interstitial layer, mass transfer occurs resulting in cooling of the air due to the consumption of energy for evaporation. The moisture transfer occurring from the surface of solid-constituent to the fluid-constituent is captured through the \( \langle \dot{m}_{fs} \rangle \) term in Eqs. 2.17-2.18, which can be expressed as [33]

\[
\langle \dot{m}_{fs} \rangle = \langle \rho_f \rangle f h_{fsm} A_{fs} (\langle Y_v \rangle^f_{fs} - \langle Y_v \rangle^f_{fs})
\]  (2.44)

where, \( \langle Y_v \rangle^f_{fs} \) refers to the vapour mass fraction occurring at the surface of the solid-constituent of the porous media, computed using Eqs. 2.1-2.4, and by assuming the surface relative humidity equal to 100%. The amount of moisture transfer can be tracked by considering the change in specific humidity between the inlet and outlet of the domain. The interfacial mass transfer coefficient \( (h_{fsm}) \) appearing in Eq. 2.44 is found from the following expression

\[
Sh_{fs} = C_m Re_l^{0.5} Sc^{0.37} = \frac{h_{fsm} l_d}{D_f}
\]  (2.45)

where, for the present simulations, \( C_m \) is kept equal to 0.52.

For all the simulations, wood wool is considered as the porous material. The solid-constituent of wood wool is capable of holding moisture in the liquid state (water). Moreover, wood wool is utilized in many applications involving evaporative cooling. The characteristic properties of the porous material such as, porosity (\( \epsilon \)), permeability (\( K \)), and interstitial surface area (\( A_{fs} \)) are considered to be that of a generic porous media,
but with the thermophysical properties of wood wool. The thermophysical properties of wood wool along with the characteristic properties of the porous material are summarized in a subsequent section.

In the fluid-phase energy equations, the sensible energy associated with the water before evaporation is accounted by defining the source term in Eqs. 2.11 and 2.19 as [28]

\[ S_e = h_{\text{water}} \langle \dot{m}_{fs} \rangle \]  

(2.46)

where, \( h_{\text{water}} \) is the enthalpy of water at the local temperature.

In terms of sensible heat transfer, the fluid and solid-constituents of the porous media are coupled together by the interfacial heat transfer term appearing in Eqs. 2.19-2.20, as discussed in section 2.2.2. Here it becomes necessary to define an interfacial heat transfer coefficient (\( h_{fs} \)). In the present study, for the cases that do account for sensible heat transfer, \( h_{fs} \) in Eqs. 2.19-2.20 is computed using the expression [34]

\[ Nu_{fs} = C_T Re_{ld}^{0.5} Pr^{0.37} = \frac{h_{fs} l_d}{k_f} \]  

(2.47)

where, for the present simulations, \( C_T \) is kept equal to 0.52 [34].

For the problems of direct and indirect evaporative cooling, the interstitial surface of the porous media is considered to never run out of moisture, thus, making it unnecessary to solve the solid-constituent water mass fraction equation (Eq. 2.18). Consequently, the diffusive term of the solid-constituent water transport equation is set to zero for these simulations.

### 2.5.1 Direct evaporative cooling

The case of direct evaporative cooling is selected to demonstrate: that the present formulation accurately captures the mass and energy exchange in the porous region; that the trends of cooling and heating are correct with appropriate thresholds for moisture addition/removal; and that the activity at the interfaces between all fluid-porous interfaces is reasonable. The domain considered consists of a wet porous material
inserted into a channel, as shown in Fig. 2.2. The domain contains two fluid/porous interfaces, one where air-vapour flows from fluid to porous regions, and one where air-vapour flows from porous to fluid regions. The (three-dimensional) domain is discretized using structured hexahedral control volumes. After grid-convergence testing, the final grid consists of 21 control volumes in the \( y \)-direction. In the \( x \)-direction, each fluid region contains 20 control volumes and the porous region contains 40 control volumes, for a total grid size of 1680 (1 control volume in \( z \)-direction since 3D effects are not considered). The properties of air and water vapour at 27°C, and the porous material used in the simulations are presented in Tab. 2.1. Because of the small ratio of thermal conductivities between the solid and fluid-constituents, thermal dispersion is ignored in the porous region.

![Figure 2.2: Domain geometry for direct evaporative cooling validation case.](image)

A fully developed velocity profile is imposed at the inlet \((x=0)\), using the expression

\[
u = \frac{6Uy}{H} \left[1 - \frac{y}{H}\right], \quad v = 0
\]

where, \( U \) is the average axial velocity in the channel, set to yield a Reynolds number \( Re_H = 1000 \). The flow enters the domain at 25°C, with relative humidity of 30%. The inlet pressure is extrapolated from the interior of the domain. At the outlet, a zero-derivative condition is imposed for both \( u \) and \( v \) velocity components, for temperature \( T \).
and for moisture mass fraction $Y$. The outlet pressure is set to atmospheric pressure, 101.3 [kPa]. No-slip, hydrodynamic conditions are imposed at the walls, combined with extrapolation of pressure from the domain interior. The walls are also considered adiabatic and impermeable to moisture.

Table 2.1: Fluid and porous media properties.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td><strong>Air [28]</strong></td>
<td></td>
</tr>
<tr>
<td>$c_p$ [J/(kg.K)]</td>
<td>1005</td>
</tr>
<tr>
<td>$R$ [J/(kg.K)]</td>
<td>287</td>
</tr>
<tr>
<td><strong>Water vapour [28]</strong></td>
<td></td>
</tr>
<tr>
<td>$c_p$ [J/(kg.K)]</td>
<td>1872</td>
</tr>
<tr>
<td>$h_{fg}$ [J/kg]</td>
<td>$2.5 \times 10^5$</td>
</tr>
<tr>
<td>$R$ [J/(kg.K)]</td>
<td>461.5</td>
</tr>
<tr>
<td><strong>Fluid mixture [34-37]</strong></td>
<td></td>
</tr>
<tr>
<td>$D_f$ [m$^2$/s]</td>
<td>$2.6 \times 10^{-5}$</td>
</tr>
<tr>
<td>$D_{eff,f}$ [m$^2$/s]</td>
<td>$1.52 \times 10^{-5}$</td>
</tr>
<tr>
<td>$k_f$ [W/(m.K)]</td>
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<tr>
<td>$k_{eff,f}$ [W/(m.K)]</td>
<td>0.0237</td>
</tr>
<tr>
<td>$\mu_f$ [N.s/m$^2$]</td>
<td>$1.83 \times 10^{-5}$</td>
</tr>
<tr>
<td><strong>Domain</strong></td>
<td></td>
</tr>
<tr>
<td>$H$ [m]</td>
<td>0.02</td>
</tr>
<tr>
<td><strong>Porous material [1, 34, 35]</strong></td>
<td></td>
</tr>
<tr>
<td>$A_{fs}$ [m$^2$]</td>
<td>917.7</td>
</tr>
<tr>
<td>$c_{ps}$ [J/(kg.K)]</td>
<td>1590</td>
</tr>
<tr>
<td>$c_E$</td>
<td>0.244</td>
</tr>
<tr>
<td>$K$ [m$^3$]</td>
<td>$4.0 \times 10^6$</td>
</tr>
<tr>
<td>$k_{eff,s}$ [W/(m.K)]</td>
<td>0.087</td>
</tr>
<tr>
<td>$l_d$ [m]</td>
<td>$0.55 \times 10^{-3}$</td>
</tr>
<tr>
<td>$\rho_s$ [kg/m$^3$]</td>
<td>350</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>0.7</td>
</tr>
</tbody>
</table>

For advection schemes in fluid and porous regions, Peclet-weighted upwinding and central differencing schemes are utilized. The results show less than 0.1% change when central differencing scheme is selected instead of upwinding scheme due to the unidirectional flow field. The solution procedure advances in time taking a single iteration per time-step towards its steady-state. The solution is said to be converged when the maximum normalized residual of all the transport equations decreases below $10^{-9}$. The residual convergence of the transport equations is presented in Fig. 2.3, which
shows the reduction of the maximum residual values with the number of carried out iterations. The residuals of the fluid energy equation and vapour transport equation are normalized by the average domain values of $T_f$ and $Y_f$, respectively. The criterion of convergence was also checked by increasing and decreasing it one order of magnitude, and the results showed further variation of less than 0.8%, indicating that a criterion of $10^{-9}$ was sufficient. A time-step size of 0.02s was selected for the current simulations, based on the inlet flow velocity and duct size. Variation of the time-step size from 0.2 to 0.002s showed no significant change in terms of computational time nor convergence behavior.

![Graph showing the reduction of the maximum residuals of the transport equations for the direct evaporative cooling case.](image)

**Figure 2.3:** Reduction of the maximum residuals of the transport equations for the direct evaporative cooling case.

Three simulations were carried out for direct evaporative cooling. In case 1, the interfacial heat transfer between the solid and fluid-constituent of porous media is neglected. In cases 2 and 3, the solid-constituent is kept at a temperature of 10°C and 40°C, respectively. The results of specific and relative humidity and the variation temperature for all the three cases are presented in Figs. 2.4, 2.5, and 2.6, respectively.
For case 1, it can be observed from Fig. 2.4 that the specific humidity starts to increase as the flow enters the porous zone, which indicates the addition of moisture to the air. This moisture addition results in an increase in relative humidity and decrease in temperature as observed from Figs. 2.5 and 2.6, respectively. The decrease in fluid temperature due to moisture addition indicates the occurrence of evaporative cooling. Moreover, as soon as the relative humidity reaches 100% no further moisture addition occurs, resulting in constant relative humidity and temperature for the remainder of the region. Case 1 mimics an adiabatic saturation process, which means that the air flow is expected to achieve the wet bulb temperature. The outlet fluid temperature, relative and specific humidities obtained from the simulation are 14.1 °C, 100%, and 10.03 gm\textsubscript{water/kg\textsubscript{air}}, respectively. Compared to a psychrometric chart (for standard barometric pressure), the predicted outlet fluid temperature is approximately 1.5% lower than the charted value of 14.3 °C, while the specific humidity is predicted to be 1.4% higher than the charted value of 9.88 gm\textsubscript{water/kg\textsubscript{air}}. These errors are considered small, and can attributed mainly to the correlation used to compute the saturation pressure of water, which has an error of approximately 0.5%, and to numerical and discretization errors.

![Figure 2.4](image.png)

**Figure 2.4**: Centerline specific humidity along the domain length for the direct evaporative cooling case.
Figure 2.5: Centerline relative humidity along the domain length for the direct evaporative cooling case.

Figure 2.6: Centerline fluid temperature along the domain length for the direct evaporative cooling case.
For case 2, in the porous region close to the upstream interface, moisture addition takes place, but then appears to overshoot the 100% relative humidity threshold. This apparent overshoot is due to sensible cooling of the air, which results in a reduction of moisture capacity. To maintain its 100% relative humidity threshold, the moist air begins to reject moisture as it flows through the remainder of the porous domain, although the threshold is never reached due to the continuous reduction in temperature of the air; see Fig. 2.4. It is clear from the trends shown in Figs. 2.4-2.6 that if the porous region was longer, steady-state values of air temperature and 100% relative humidity would be reached.

Case 3 considers sensible heating of the air, which produces the opposite effect to that shown in Case 2. In this case, moisture addition occurs throughout the porous region due to the sensible heating and continuously increasing moisture capacity of the air. The slight drop in temperature that occurs close to the upstream interface of the porous region can be explained by the fact that initially the relative humidity of the air is very low, which results in very high moisture transfer rates which lowers the air temperature despite the sensible heating. Once the relative humidity of the air increases, less moisture addition occurs, which results in the sensible heating of the air dominating the evaporative cooling effect. Once again, the trends in Figs. 2.4-2.6 indicate that if the porous region were longer, the air would eventually become saturated at the elevated temperature of the solid.

The specific humidity plots illustrate the capability of air to absorb or shed moisture with or without sensible heat transfer, which shows the robustness of the formulation to capture the natural phenomena. Moreover, the relative humidity plots show the excellent coupling of energy and vapour mass fraction, which again shows the efficacy of the developed formulation. The results also illustrate that heat and mass are transferred smoothly across the fluid/porous interfaces without over/under-shoots or wiggles, indicating the robustness of the implemented interface conditions even at a reasonably high Reynolds number ($Re=1000$).
2.5.2 Drying of wet porous material

The previous case has demonstrated that the present formulation accurately simulates heat and mass transfer in conjugate fluid/porous domains. However, the previous case did not require a solution for the mass fraction of water inside the solid-constituent. The case of drying of the initially wet porous material used in the previous problem is now simulated to demonstrate the non-equilibrium mass transfer feature of the present formulation.

To simulate the drying of an initially wet porous material, the solid-constituent of the porous media is considered to hold water. Thus, one can consider the solid-constituent to be made up of the actual solid structure (wood) and liquid water. As the air-vapour mixture passes through the wet porous material, moisture transfer occurs from the solid-constituent to the air-vapour mixture. As the process proceeds in time, it is expected that the moisture residing in the solid-constituent of the porous material gradually “dries up”. In this respect, the solid-constituent density \( \langle \rho_s \rangle^s \) found in Eq. 2.18 is continuously updated to account for the moisture loss by the following expression

\[
\langle \rho_s \rangle^s = \alpha_{st} \rho_{st} + \alpha_w \rho_w
\]  

(2.48)

where, \( \rho_{st} \) and \( \rho_w \) are the density of the solid structure and water, respectively, \( \alpha_{st} \) and \( \alpha_w \) represent the volume fraction of the solid structure and water, respectively. Due to the moisture loss, \( \alpha_w \) is also continuously updated using the latest water mass fraction \( Y_w \).

Special consideration is required to simulate the process of drying. In reality, when the moisture inside the solid-constituent is close to being “dried up”, the interfacial mass transfer coefficient \( h_{fsm} \) declines with the declining moisture content; that is, the process diminishes smoothly as dry-out is approached. Furthermore, the solid-constituent cannot be “over-dried”, meaning that the formulation must ensure that mass transfer is not over-shot. To ensure that this occurs in the numerical model, \( h_{fsm} \) is set to decline when \( Y_w \) falls below \( Y_o \), where \( Y_o \) represents the threshold value of \( Y_w \) indicating that “drying out” of the solid-constituent is imminent. The reduction of \( h_{fsm} \) is first carried
out by simply multiplying it by $Y_w/Y_o$. Then, in each iteration, a check is done to see whether enough water is available in the solid-constituent to carry out the mass transfer ($\langle \dot{m}_{fs} \rangle$) calculated by Eq. 2.44. If the available water content is insufficient then the mass transfer is reduced to the available water content. This computational procedure ensures that the simulated drying process follows trends observed in a real drying processes, however, to obtain accurate absolute results for drying, the value of $h_{fsm}$ would have to be calibrated.

The half portion of the previous case porous material is considered as the domain; i.e. length (L) and height (H) equal to 2cm. Hexahedral control volumes are utilized to create a structured grid that contains 21 control volumes in both the x and y direction. A single control volume in z-direction is used due to the 2D nature of the simulation. The properties of porous media and air are kept as mentioned in Tab. 2.1. Since the present problem requires solution for the mass fraction of water inside the solid-constituent, the mass diffusivity coefficient ($D_{eff_s}$) of water in wood is set to $1.489 \times 10^{-6}$ m$^2$/s [38]. The interfacial heat transfer between the solid and fluid-constituents of porous media is neglected for the present simulation.

The boundary conditions imposed are kept identical to that of the previous case. However, since a solution inside the solid-constituent is sought, the initial condition of the solid-constituent is necessary. It is assumed that initially 20% of the solid-constituent volume of the porous material is occupied by water, while the remaining volume is occupied by wood material, i.e., $\alpha_{s0} = 0.80$ and $\alpha_w = 0.20$ (see Eq. 2.48). Air flow is considered to enter the material at 25°C with 30% relative humidity.

The advective scheme utilized for this case is the same as utilized for the previous case. After conducting the time step convergence test, time step of 0.02s is utilized to advance in time. The simulation advances in time up to the point where no further mass transfer between the air mixture and the solid-constituent occurs, that is, to the point where the solid-constituent contains no more liquid (dry-out). At each time step, a convergence criteria of $5 \times 10^{-6}$ is achieved for all the transport equations before moving forward to the next time step.
The loss of water content from the solid-constituent of porous media along the domain centerline at different times is presented in Fig. 2.7. The reduction in moisture content throughout the porous material with time indicates the occurrence of drying. As expected, drying of the porous material starts at the inlet and then gradually progresses to the outlet. Early in the transient, most of the moisture is transferred near the inlet because of the high transfer potential (high mass-fraction difference). As the inlet region “dries”, this potential disappears and the moisture transfer occurs further into the porous material. The process eventually ends when all of the moisture has been removed. Fig. 2.7 shows that for the mass exchange coefficient utilized in the simulation, complete drying has occurred by 300s. Fig. 2.8 shows the change in the relative humidity of air at the same time intervals indicated in Fig. 2.7. The results from both plots (Figs. 2.7 and 2.8) demonstrate correct coupling of vapour content present in the moist air (water vapour mass fraction equation) with the water residing inside the solid-constituent of the porous material (water mass fraction equation).

**Figure 2.7: Variation of water content in the solid-constituent along the porous material centerline at different time instances.**
In the light of the previous results, one can say that the present model is able to properly simulate the drying process of a wet porous material. However, it is also worth investigating whether the developed model captures the physical trends observed by varying different problem parameters. In this respect, the Reynolds number and the relative humidity of the moist air flow at the inlet will be varied. The effect of the flow Reynolds number on the water mass fraction at the domain center is shown in Fig. 2.9. It can be observed that the Reynolds number is inversely proportional to the porous material drying time; i.e. an increase in the Reynolds number reduces the time required to dry the porous material. Fig. 2.10 presents the influence of the flow inlet relative humidity on the drying time. The plot demonstrates that the drying time increases with increases of the inlet relative humidity, resulting in longer drying times. Moreover, the figure also shows the capability of the present model to correctly simulate the two extreme cases (0% and 100%) of the inlet relative humidity. For the case of 0% relative humidity of the inlet air, the highest moisture removal rates are observed, resulting in the fastest drying time. On the other hand, no moisture transfer occurs when the inlet relative

**Figure 2.8: Variation of moist air relative humidity along the porous material centerline at different time instances.**
humidity is increased to 100%, since the moist air has no capacity to take on more moisture.

Figure 2.9: Variation of water content in the solid-constituent at the porous material center with time. Results are for 3 different Reynolds numbers and a constant inlet relative humidity of 30%.

Figure 2.10: Variation of water content in the solid-constituent at the porous material center with time. Results are for a fixed Reynolds number of 1000 and 4 different inlet relative humidities.
Consequently, it is clear that the present model is capable of simulating the drying process of a wet porous material, which demonstrates the capability of the present formulation to correctly simulate the non-equilibrium moisture transfer. The plots (Figs. 2.7-2.10) results confirm the expected physical trends, which further shows the capability of the developed formulation.

2.5.3 Indirect evaporative cooling

The test case of indirect evaporative cooling is introduced to illustrate three-dimensional heat and mass transfer comprising fluid, porous and solid domains. In indirect evaporative cooling, the temperature of product air is lowered without altering its specific humidity. This is achieved by utilizing a secondary flow of working air, which is isolated from the product stream and cooled by evaporative cooling. The experimental setup of Gómez et al. [39] is selected as a test case due to availability of all the necessary information. Gómez et al. [39] carried out a series of experiments to determine the heat exchange over a range of inlet temperatures and flow rates of the product stream.

Fig. 2.11 shows a schematic of the experimental setup, reduced to a computational domain (a) with all relevant boundaries (b). The domain considered comprises one section of the heat exchanger studied in Gómez et al. [39]. As such, one half of a working channel and one half of a product channel, separated by a polycarbonate wall are modelled, with symmetry conditions at the external x-z faces to indicate that this arrangement is mirrored several times in each direction in the overall unit. The air streams enter the core of the heat exchanger in a cross-flow, and all the heat transfer between the streams takes place through the polycarbonate wall. In the working air channel, evaporative cooling is achieved in the experimental arrangement by spraying water from the top into the hollow working air channels. In the computational model, we replace the hollow working channel with a porous region that has interstitial surfaces that are assumed to be always wet. Since the pressure drop on the working side of the heat exchanger is not of interest, the porosity and the permeability are simply adopted from the previous cases. The thermophysical properties of the porous region are kept same as mentioned in Tab. 2.1. The Nusselt and Sherwood numbers are also assumed to be the same as those used in the previous problems, but the interstitial surface area $A_{fs}$ is
adjusted in a calibration step to achieve moisture exchange in the working channel and heat transfer from product to working air similar to that reported in the experiments (for case 3; see Tab. 2.2).

The computational domain has a height \( H = 0.62 \text{m} \) and width \( W = 0.18 \text{m} \). Each fluid half-channel is 2mm thick, and the separating wall has a thickness of 0.1mm, which yields \( t = 4.1 \text{mm} \). In this manner, the simulation domain consists of fluid and porous regions separated by a thin solid region. The domain is discretized using hexahedral control volumes. After grid convergence testing, the final grid consists of 44 control-volumes in the \( x \)-direction and 20 control-volumes in the \( z \)-direction. In the \( y \)-direction, the grid contains 14 control-volumes for each fluid stream and 5 control-volumes across the solid wall.

The boundaries of the computational domain are indicated in Fig. 2.11b. Boundary conditions are imposed as follows:

**Outlets:** zero normal derivatives for all velocities, temperature and moisture mass fraction are imposed on the outlets of the product and working streams; atmospheric pressure (101.3 kPa) is set as a reference pressure on the outlet faces.

**Walls (edges of the working and product channels only):** velocities are set to zero; pressure is extrapolated from inside the domain; adiabatic conditions on temperature; zero moisture penetration imposed on moisture mass fraction.

**Symmetry planes:** zero normal derivatives are imposed on all variables, with the exception of the \( v \) velocity is set to zero, to enforce a zero mass flux.

**Inlets:** The results selected for validation have a product stream flow rate of 125 m\(^3\)/h at inlet temperatures between 25-40°C and relative humidity between 20-50%. For all the simulations, the working air enters at a temperature of 22°C and flow rate of 260 m\(^3\)/h. The inlet relative humidity of the working air is kept between 53-61% to match the experimental conditions. The exact product and working air inlet conditions for the simulations presented in Tab. 2.2 were obtained by personal communication with the authors of Gómez et al. [39].
The properties of air and water vapour used in the simulations are the same as those used for the previous two problems (see Tab. 2.1). The effects of thermal dispersion are neglected in the porous region. The separating wall is polycarbonate and has density 1200 kg/m$^3$, thermal conductivity 0.2 W/(m.K), and specific heat capacity 1200 J/(kg.K) [40].

The advection models and solution procedure are the same as for the direct evaporative cooling case. A time-step of 10s is used to proceed towards the steady-state solution. The convergence behaviour of the simulation is illustrated in Fig. 2.12 for case 3 (from Tab. 2.2).

The work of Gómez et al. [39] reports the temperature drop of product air as a function of its inlet bulk temperature. The comparison between the experimental and simulation results is presented in Fig. 2.13, which shows that the predicted temperature drop deviates from the experimental results by less than 0.6 °C. In terms of the product air outlet temperature, the numerical results deviate by a maximum of 2%. These results are
satisfactory given that the inlet temperature of working air fluctuated ± 0.5 °C during the experimental runs [41].

**Table 2.2: Product and working air inlet conditions for indirect evaporative cooling simulations Gómez et al. [39]**

<table>
<thead>
<tr>
<th>Case</th>
<th>Product air inlet</th>
<th>Working air inlet</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Flow rate (m³/h)</td>
<td>Temperature (°C)</td>
</tr>
<tr>
<td>Case 1</td>
<td>125</td>
<td>27.24</td>
</tr>
<tr>
<td>Case 2</td>
<td>125</td>
<td>30.50</td>
</tr>
<tr>
<td>Case 3</td>
<td>125</td>
<td>35.00</td>
</tr>
<tr>
<td>Case 4</td>
<td>125</td>
<td>39.68</td>
</tr>
</tbody>
</table>

**Figure 2.12: Reduction in the maximum residual of the transport equations for indirect evaporative cooling case 3.**
Figure 2.13: Comparison of experimental and numerical results for indirect evaporative cooling, showing the bulk temperature drop of the product air stream as a function of product inlet air temperature.

In light of the results for bulk temperature, it can be inferred that the developed formulation accurately simulates the indirect evaporative cooling problem. It is also of interest to investigate the temperature and moisture distributions inside the domain to show how heat and mass transfer occur throughout the domain, and at the interfaces between the porous-solid and solid-fluid domains. The temperature contours presented in Fig. 2.14 show the temperature distribution of both air streams at 5 different y-z planes between the inlet and outlet of the working air channel. Considering the product stream, the temperature decreases on every plane in the streamwise direction and is cooler at the bottom part of the channel, which is adjacent to the inlet of the working channel. In addition, on each plane, the temperature is seen to decrease towards the solid wall where heat is removed.

In the working channel, the air stream warms in the streamwise direction and towards the inlet of the product channel. Temperature is also seen to increase towards the solid dividing wall where heat from the product channel is transferred. Fig. 2.15 shows a
comparison of fluid and solid temperatures in the middle plane of the domain, mainly to show the thermal non-equilibrium in the porous region. While the plot on the left is a reproduction of that shown in Fig. 2.14, the plot on the right shows the temperature of the solid phase of the porous region and the solid wall. The plot shows that the separating wall has a temperature distribution consistent with the adjacent porous region and near the temperatures of the adjacent airstreams. Consequently, the plots show that distributions throughout the different regions of the domain, and through the interfaces between regions are smooth and without discontinuities, which, once again, shows the robustness of the interface formulation.

**Figure 2.14: Temperature (in °C) distribution of product and working air inside the domain of case 4.**

The distribution of vapour mass fraction throughout the domain is presented in Fig. 2.16. As expected, the vapour mass fraction in the working air increases along the channel due to evaporation. Moreover, high vapor mass fractions are observed in regions having high temperatures, which is due to the fact that rise in temperature increases the capacity of air to absorb moisture, as discussed previously. However, no change in vapor mass fraction occurs in the product air channel, as expected since no vapor mass transfer occurs across
the separating wall. To enforce that no vapour transfer occurs across the separating wall, the effective diffusivities, $D_{\text{eff},s}$ and $D_s$, in Eqs. 2.29 and 2.31 are set to zero. This modification also points to the fact that the general moisture transfer conditions at interfaces presented earlier can easily be modified to suit the specific problem requirements.

Figure 2.15: Temperature (in °C) distribution in the middle plane of Fig. 2.14 along with the mesh for case 4
2.6 Summary

In the present study, numerical modeling of heat and mass transfer in conjugate fluid/solid/porous 3D domains was studied. A formulation capable of simulating non-equilibrium heat and mass transfer in conjugate fluid/porous/solid domains was presented, with special consideration towards the manner in which moisture was tracked in the transport equations. Then, to ensure that heat and mass transfer occurred smoothly at all the interfaces, special mathematical conditions were presented in both mathematical and discrete mathematical forms.

Cases of direct and indirect evaporative cooling, and drying were presented to demonstrate the utility of the developed numerical formulation. The case(s) of direct evaporative cooling (adiabatic saturation) showed deviations of less than 1.5% compared to psychrometric chart values. Heat and mass transfer were shown to occur smoothly at fluid/porous interfaces, illustrating the robustness of the interface treatment. The case of indirect evaporative cooling demonstrated the capability of the model to simulate heat
and mass transfer in more complex conjugate fluid/solid/porous 3D domains. Physically realistic solutions were obtained with deviations less than 2% compared to the experimental data, with no discontinuities at fluid-porous and porous-solid interfaces. The non-equilibrium mass transfer capability of the present formulation was demonstrated by simulating the unsteady case of drying of an initially wet porous material. The results show that model predictions follow the expected trends with respect to flow Reynolds number and inlet relative humidity.

As such, the present model formulation is shown to be robust and capable of simulating a large class of problems associated with non-equilibrium heat and mass transfer in conjugate domains.
References


[38] Louis, M., Max, A. O. L., Adeline, C. N., & Florent, M. A. (2013). Determination of the diffusion coefficient and the activation energy of water desorption in IROKO wood


Chapter 3

3 Convective drying of wet porous materials using a conjugate domain approach*

3.1 Introduction

Convective drying of porous materials is of interest due to its applicability in engineering applications such as building materials production, processing and dehydration of foods, paper production, among others [1]. The porous materials to be dried in such applications range from bricks, concrete and wood to fruits, vegetables, and grains. Such materials can be classified based on their hygroscopic nature. For example, potato, carrot, wood, etc. are hygroscopic materials [2,3], while, sand, ceramic, etc. are considered to be non-hygroscopic [3].

In convective drying of porous materials, air with low relative humidity is forced across (and through) a wet porous media. Because of its capacity to hold fluids in their vapour state, the air absorbs moisture as it flows across the porous material, which results in drying or dehydration. The capacity of the airstream to take on moisture increases with increasing temperature (and vice-versa), and has its upper threshold for a given temperature at the dew-point, which is defined by 100% relative humidity. The porous material to be dried consists of a solid structure (or solid matrix), water, and void space [4]. The moist air – comprised of dry air and water vapour – occupies the void space [4], and the liquid water can be considered to be held inside the microstructure of the solid component of the porous material. As such, moisture transport in the form of water vapour and liquid water occurs inside the porous materials [5-8]. Thus, complete modelling of a drying process requires the consideration of (moist) air passing across the material to be dried with dynamic coupling between the constituents to enable exchanges of heat and moisture to evolve based on local conditions (i.e. temperature, water activity, etc.)

Numerical modeling has been widely used to simulate convective drying. Previous numerical models can be broadly classified into categories based on their level of

*A version of this chapter entitled “A conjugate fluid-porous approach to convective heat and mass transfer with application to produce drying” has been published in Journal of Food Engineering 179 (2016) 55-67.
sophistication. In this respect, the most basic are drying curve models (see, for example Akpinar et al. [9], Demir et al. [10], Menges and Ertekin [11], and Seiiedlou et al. [12]), which utilize a single moisture equation to evaluate moisture loss from a porous material as a function of temperature and other parameters. These models provide overall drying rates, however, they are not capable of accounting for the local variations of different quantities inside the porous domain.

The next category of models use differential energy and moisture transport equations to model the drying process inside the porous domain (see, for example Barati and Esfahani [13-15], Golestani et al. [16], Kumar et al. [17], Perussello et al. [18], Srikiatden and Roberts [19], and Younsi et al. [20]). As a result, these models predict the local variations of temperature and moisture content inside the drying material by solving a single equation for each of energy and moisture transport. The transport equations employed, in general, contain only unsteady and diffusion terms, and Fourier and Fick’s Laws are used to model diffusion in the energy and moisture equations, respectively. In such models, convective boundary conditions are imposed at the surface of the material to be dried. In this respect, convective heat and mass transfer coefficients are evaluated using empirical correlations based on $Nu = f(Re, Pr)$ and $Sh = f(Re, Sc)$, which means that the simulation results are dependent upon the empirical correlations used.

The third category of models enables improvement in the evaluation of convective heat and mass transfer inside the porous domain. Such models (see, for example Ateeque et al. [21], Esfahani et al. [22], Kaya et al. [23], Mohan and Talukdar [24], and Tzempelikos et al. [25]) solve single energy and moisture transport equations inside the drying material, but also consider the fluid region surrounding the material, although not in a direct-coupled, conjugate manner. The surrounding airflow is first resolved by solving the mass and momentum transport equations along with the transport equation of energy to calculate the heat transfer coefficient at the surface of the material. The thermal and concentration boundary layer analogy is then used to compute the surface mass transfer coefficient. The evaluated coefficients are then utilized to impose convective boundary conditions at the material’s surface to obtain a solution inside the drying material. The term “non-conjugate approach” is often used to refer to this category of models [1].
While the non-conjugate approach considers one domain at a time, a conjugate approach involves simultaneous modeling of both the drying material and the surrounding airflow region. These models introduce mathematical conditions to enforce continuity of heat and mass transfer at the fluid-porous interface, which eliminates the requirement for imposing convective heat and mass transfer coefficients between regions of the domain. The conjugate models proposed by Lamnatou et al. [26] and Sabarez [27] use single energy and moisture transport equations for each region to model energy and mass transfer. In this respect, it is the effective heat and moisture transport that is solved for, and the temperature and mass fraction characterize the local conditions. This approach is suitable for predicting temperature and moisture distributions in the porous region, but local transport between the phases of the porous media are not provided.

When the material subjected to drying is comprised of a micro-porous solid structure and void space, which is generally the case for biologically derived systems, moisture transport occurs mainly due to capillary forces, pressure gradients, and temperature gradients [7,8]. In such cases, it becomes important to account for both the vapour and liquid transport inside the porous material. In this respect, several studies [5-8,28,29] focused on convective drying of porous materials using a conjugate approach, except that moisture transfer inside the drying material was modeled by combining the vapour and water transport into a single moisture transport equation. The work of De Bonis and Ruocco [30] took a non-equilibrium approach to mass transport by employing separate vapour and water transport equations inside the drying material, but they did not consider advection or thermal non-equilibrium inside the porous material. Defraeye et al. [5], Younsi et al. [8], Erriguible et al. [28], and Perré and Turner [31] have utilized volume-averaged energy and moisture transport equations. In addition, Erriguible et al. [28], and Perré and Turner [31] considered the advection term in the energy and moisture transport equations, and used Darcy’s Law to calculate the flow velocity inside porous material.

The literature survey reveals that a majority of the most advanced prior work models heat and mass transport inside the porous materials or porous solids [5-8] using single energy and moisture transport equations. In other words, the fluid and solid-constituents in a given cell inside the porous media are generally characterized using single temperature
and fluid mass-fraction values. This approach is found to provide reasonable results for temperature and moisture distributions and for overall drying times, provided the effective transport coefficients for heat and mass are carefully calibrated. However, such an approach is not capable of predicting local exchanges of energy and moisture between constituents inside a cell. The main objective of the present work is to demonstrate the capability of the proposed formulation to accurately simulate the convective drying process of porous materials. Moreover, the proposed framework is generic and can be applied to wide range of porous materials. In this respect, the present work utilizes a conjugate domain approach, wherein mass, momentum, energy, and moisture transport equations are solved in the fluid and porous region. The model also accounts for thermal and mass non-equilibrium in the porous region such that both the vapour and water exchanges between the constituents are considered. In this respect, we further demonstrate that a conjugate, non-equilibrium model can provide information necessary to make the next important step towards direct, dynamic coupling of the phases.

Modeling of the porous material at this level of detail requires thermophysical properties of both the fluid and solid constituents, as well as quantification of the key geometric parameters of the porous material. To the best of authors’ knowledge, no study, as yet, has provided such a level of detail of the porous material even though such characterization is essential for modelling the different mechanisms of heat and moisture transport inside the porous region and at the fluid-porous interface. The present study models the interfacial moisture transfer using a circuit analogy, which accounts for all interfacial exchanges, and additional parameters required to achieve the physical moisture thresholds observed in the convective drying process. The performance of the complete model is assessed by application to the drying of apple flesh. In this respect, the results of Velić et al. [32] are used as a reference.

### 3.2 Formulation

As described earlier, the airflow surrounding the porous material plays a crucial role in the convective drying process. From the numerical modeling perspective, moist air can be considered as a mixture of dry air (comprised of all the gaseous components) and water vapour. The vapour content of the moist airflow is evaluated by solving a transport
equation in the form of vapour mass fraction ($Y_v$). The moist air is then treated as a mixture of dry air and water vapour, and its flow is evaluated by solving the conventional mass-momentum transport equations. The moist air density ($\rho_f$) used in the transport equations is continuously updated to account for the moisture gain/loss of the air by the expression

$$\rho_f = \rho_a + \rho_v = \frac{P_a}{R_a T} + \frac{P_v}{R_v T}$$

(3.1)

where, $P_a$ is the partial pressure of dry air, $P_v$ is the vapour partial pressure, $R_a$ and $R_v$ are the air and vapour gas constants, respectively. The moist air temperature ($T$) is obtained by solving the energy transport equation. Complete details on the calculation of $\rho_f$ can be found in Khan et al. [33].

Since the present study models the convective drying using a conjugate approach, we present the transport equations required in both the fluid and porous regions along with the fluid-porous interface conditions.

### 3.2.1 Fluid region

In the fluid region, the mass and momentum conservation equations for the air-water vapour mixture are expressed as

$$\frac{\partial \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{v}) = 0$$

(3.2)

$$\frac{\partial (\rho_f \mathbf{v})}{\partial t} + \nabla \cdot (\rho_f \mathbf{v} \mathbf{v}) = -\nabla P + \mu_f \nabla^2 \mathbf{v} + \rho_f \mathbf{f}$$

(3.3)

The transport equation for the mass fraction of water vapour is expressed as [34]

$$\frac{\partial (\rho_f Y_v)}{\partial t} + \nabla \cdot (\rho_f Y_v \mathbf{v}) = \nabla \cdot (\rho_f D_f \nabla Y_v) + S_v$$

(3.4)

The energy transport equation of the air-water vapour mixture takes a form to account for the latent energy of water vapour evaporation. In this respect, we consider that the
specific enthalpy of each species is the sum of sensible and latent energy components, which can be expressed as

\[ h_i = c_{p,i}T + h_{fg,i} \]  \hspace{1cm} (3.5)

where, \( i \) represents the species number. Since we have two species in the present formulation, \( i = 1 \) (dry air) and 2 (water vapour), and the latent component for dry air is \( h_{fg,1} = 0 \). The total specific enthalpy of the air-water vapour mixture is obtained by summing the specific enthalpy of dry air and water vapour. Using Eq. 3.5, the energy transport of the moist air in the fluid region takes the form

\[
\begin{align*}
\sum_i c_{p,i} \frac{\partial (\rho_f Y_i T)}{\partial t} + \sum_i h_{fg,i} \frac{\partial (\rho_f Y_i)}{\partial t} + \sum_i c_{p,i} \nabla \cdot (\rho_f Y_i T \mathbf{v}) + \sum_i h_{fg,i} \nabla \cdot (\rho_f Y_i \mathbf{v}) \\
= k_f \nabla^2 T + \sum_i \nabla \cdot [\rho_f D_f \nabla Y_i (c_{p,i} T + h_{fg,i})] + S_e
\end{align*}
\]  \hspace{1cm} (3.6)

Energy transfer due to the unsteady effects is represented by the first two terms on the left hand side of Eq. 3.6. The third and fourth terms on the left hand side account for energy transfer caused by advection. On the right hand side, the first term accounts for conduction, while the second term represents energy transfer due to species diffusion.

### 3.2.2 Porous region

In the porous region, volume-averaging of the transport equations is carried out to characterize the porous material as porous continuum. The process of volume-averaging involves integration of the transport equations over a representative elementary volume of porous material. The volume-averaging of a quantity \( \varphi_f \), as described in Whitaker [35], is carried out as

\[
\langle \varphi_f \rangle = \frac{1}{V} \int_{V_f} \varphi_f \, dV
\]  \hspace{1cm} (3.7)
where, $V$ represents the volume over which the averaging is conducted, $V_f$ is the volume of fluid inside $V$, and $\langle \varphi_f \rangle$ is termed as the extrinsic-average of $\varphi_f$. In the similar fashion, an intrinsic-averaged quantity $\langle \varphi_f \rangle^f$ can be expressed as

$$
\langle \varphi_f \rangle^f = \frac{1}{V_f} \int_{V_f} \varphi_f \, dV
$$

(3.8)

The porosity $\varepsilon$ of the porous material is then defined as $\varepsilon = \langle \varphi_f \rangle / \langle \varphi_f \rangle^f$. Complete details of the closed-forms of Eqs. 3.2-3.4 and 3.6 can be found in Khan et al. [33] and is not repeated herein. The volume-averaged mass and momentum conservation equations take the form

$$
\varepsilon \frac{\partial (\rho_f)^f}{\partial t} + \nabla \cdot \left( (\rho_f)^f \langle \mathbf{v} \rangle \right) = 0
$$

(3.9)

$$
\frac{\partial (\langle \rho_f \rangle^f \langle \mathbf{v} \rangle)}{\partial t} + \frac{1}{\varepsilon} \nabla \cdot \left( \langle \rho_f \rangle^f \langle \mathbf{v} \rangle \langle \mathbf{v} \rangle \right)
= -\varepsilon \nabla \langle P \rangle^f + \mu_f \nabla^2 \langle \mathbf{v} \rangle + \varepsilon \langle \rho_f \rangle^f \mathbf{f} - \frac{\varepsilon \mu_f}{K} \langle \mathbf{v} \rangle - \frac{\varepsilon \langle \rho_f \rangle^f c_E}{\sqrt{K}} |\langle \mathbf{v} \rangle| \langle \mathbf{v} \rangle
$$

(3.10)

where the last two terms on the right hand side of Eq. 3.10, are closure terms referred to as Darcy and Forchheimer terms, respectively. These two terms represent viscous (Darcy) and form (Forchheimer) drag experienced by the fluid as it flows through the porous material.

The present model considers a non-equilibrium approach for moisture and energy transport inside the porous material, which means that separate energy and moisture transport equations are employed for each of the fluid and solid-constituents of the porous media. As mentioned previously, the porous materials considered consist of a solid-structure (or solid-matrix), water, and voids. In the present study, the solid-constituent is considered to be holding water within its interconnected micro-pores, while the void space characterized by the volume fraction $\varepsilon$ contains the air-water vapour mixture (fluid-constituent). Water transport inside the solid-constituent is evaluated by
solving a water mass fraction \( Y_w \) transport equation. For the fluid-constituent, the volume-averaged version of Eq. 3.4 is included in the formulation. Thus, the present formulation considers both the water and water vapour transport inside the porous material. The extrinsically volume-averaged moisture transport equations for the fluid and solid-constituents, respectively, are expressed as

\[
\frac{\varepsilon}{\partial t} \frac{\partial (\rho_f Y_{v,f})}{\partial t} + \nabla \cdot (\rho_f Y_{v,f} \mathbf{v}) = \nabla \cdot (D_{eff,f} \nabla Y_{v,f}) + \varepsilon S_{v,f} + \dot{m}_{fs} \tag{3.11}
\]

\[
(1 - \varepsilon) \frac{\partial (\rho_s Y_{w,s})}{\partial t} = \nabla \cdot (D_{eff,s} \nabla Y_{w,s}) + (1 - \varepsilon) S_{w,s} - \dot{m}_{fs} \tag{3.12}
\]

The last two terms on the right hand side of Eqs. 3.11 and 3.12, account for the interfacial moisture transfer between the fluid and solid-constituents inside the porous material. The evaluation of \( \dot{m}_{fs} \) is based on the water content available within the solid-constituent. First, the maximum amount of \( \dot{m}_{fs} \) is evaluated as [36]

\[
\dot{m}_{fs} = \rho_f h_{fs} A_{fs} (Y_{v}^{fs} - Y_{v,f}) \tag{3.13}
\]

where, \( Y_{v}^{fs} \) quantifies the vapour mass fraction at the surface of the solid-constituent, which is evaluated by considering the surface to be saturated with vapor; i.e. relative humidity of 100%. If the available water content is less than the \( \dot{m}_{fs} \) calculated using Eq. 3.13 then \( \dot{m}_{fs} \) is computed based on the available water content (see Khan et al. [33] for details).

Similar to the transport equations for moisture, the extrinsically volume-averaged energy transport equations for the fluid and solid-constituents, respectively, are given as
\[ \sum_l \varepsilon c_{p,l} \frac{\partial \langle (\rho_f)^f (Y_{i,f})^f (T_f)^f \rangle}{\partial t} + \sum_l \varepsilon h_{f,g,l} \frac{\partial \langle (\rho_f)^f (Y_{i,f})^f \rangle}{\partial t} + \sum_l c_{p,l} \nabla. \langle (\rho_f)^f (Y_{i,f})^f (T_f)^f \rangle (\mathbf{v}) + \sum_l h_{f,g,l} \nabla. \langle (\rho_f)^f (Y_{i,f})^f \rangle (\mathbf{v}) = k_{eff,f} \nabla^2 \langle T_f \rangle^f \\
+ \sum_l \nabla. \left[ \langle (\rho_f)^f D_{eff,f} \nabla (Y_{i,f})^f (c_{p,l}(T_f)^f + h_{f,g,l}) \rangle \right] + \varepsilon S_{e,f} + h_{fs} A_{fs} \left( \langle T_s \rangle^s - \langle T_f \rangle^f \right) \] (3.14)

\[ \sum_l (1 - \varepsilon) c_{ps,l} \frac{\partial \langle (\rho_s)^s (Y_{i,s})^s (T_s)^s \rangle}{\partial t} = k_{eff,s} \nabla^2 \langle T_s \rangle^s + \sum_l \nabla. \left[ \langle (\rho_s)^s D_{eff,s} \nabla (Y_{i,s})^s (c_{ps,l}(T_s)^s) \rangle \right] + (1 - \varepsilon) S_{e,s} - h_{fs} A_{fs} \left( \langle T_s \rangle^s - \langle T_f \rangle^f \right) \] (3.15)

Since Eq. 3.15 represents energy transport inside the solid-constituent (solid-structure holding water), it does not include the latent energy terms. The last two terms of Eqs. 3.14 and 3.15 model the interfacial heat transfer between the fluid and solid-constituents. The sensible energy of water before evaporation in the fluid-phase energy equations (Eqs. 3.6 and 3.14) is accounted for by modeling the source term as \( S_e = h_{water}(\dot{m}_{fs}) \). The enthalpy of water \( (h_{water}) \) is defined using the local temperature.

Here, it becomes necessary to calculate the local interfacial heat and mass transfer coefficients \( (h_{fs} \text{ and } h_{fsm}) \) appearing in Eqs. 3.11, 3.12, 3.14, and 3.15. In the present formulation, these coefficients are found using the following expressions [37]

\[ Nu_{fs} = C_T Re_{d_p}^{0.5} Pr^{0.37} = \frac{h_{fs} d_p}{k_f} \] (3.16)

\[ Sh_{fs} = C_m Re_{d_p}^{0.5} Sc^{0.37} = \frac{h_{fsm} d_p}{D_f} \] (3.17)
where, in the present case $C_T$ and $C_m$ are held constant at 100.0 and 0.005, respectively. In the case of no airflow i.e. $Re_{dp} = 0$, $h_{fs}$ and $h_{fsm}$ also become zero using Eqs. 3.16 and 3.17. However, in such case, the diffusive transport still exists between the fluid and solid-constituents. Therefore, the lower limit of the interfacial coefficients is evaluated based on the local diffusion coefficients as $h_{fs} = k_{eff,f}$ and $h_{fsm} = D_{eff,f}$.

### 3.2.3 Interface conditions

The interface conditions between the fluid and porous regions of the conjugate domain connect the fluid and porous regions and ensure that momentum, energy and mass transfer occurs smoothly across the interfaces.

At the fluid-porous interface, the continuity of the airflow velocity and pressure are enforced as [38]

$$v_{fl} = \langle v \rangle_{por} \quad (3.18)$$
$$P_{fl} = \langle P \rangle_{por} \quad (3.19)$$

Comprehensive discussions on the hydrodynamic interface conditions expressed in Eqs. 3.18 and 3.19 can be found in Betchen et al. [38]. The thermal energy transfer at the fluid-porous interface is expressed as [38]

$$\left( -k_f \frac{\partial T}{\partial n} \right)_{fl} = \left( -k_{eff,f} \frac{\partial \langle T \rangle_f}{\partial n} - k_{eff,s} \frac{\partial \langle T \rangle_s}{\partial n} \right)_{por} \quad (3.20)$$

The above expression implies that heat transfer from the fluid region splits at the fluid-porous interface to be transported into the fluid and solid-constituents of porous media. The energy split is quantified based on the different thermal conductivity and temperature gradients appearing in Eq. 3.20.

In the convective drying of porous materials, the treatment of moisture transfer at the fluid-porous interface is critical. The continuity of moisture transfer at the fluid-porous interface is enforced as
\[
( - \rho_f D_f \frac{\partial Y_v}{\partial n} )_{fl} = \left( - (\rho_f)^f D_{f_{\text{eff},f}}^f \frac{\partial (Y_{v,f})^f}{\partial n} - (\rho_s)^s D_{s_{\text{eff},s}}^s \frac{\partial (Y_{w,s})^s}{\partial n} \right)_{\text{por}} \tag{3.21}
\]

For elaboration, Eq. 3.21 is expressed using a circuit analogy at the pore-level scale in Fig. 3.1, which shows that the moisture transport split at the interface is dictated by four resistances driven by moisture mass fractions. Since the nodal values of moisture mass fractions are part of the solution, it is essential to correctly model the four resistances, which requires proper evaluation of the different density and mass diffusivity coefficients given in Eq. 3.21. Thus, while this treatment of the interface is general to heat and mass transfer across conjugate domains, its application requires knowledge of many parameters.

![Figure 3.1: Illustration of fluid-porous moisture transfer interface condition using resistance analog at pore-level scale along with the grid.](image)

The complete conjugate formulation described in this section is suitable for modelling non-equilibrium energy and mass transport in conjugate domains of all scales. The formulation inherently provides the capability to couple the phases inside the volume-averaged porous domain and thereby express the local transport in terms of the local conditions. While this approach is extremely thorough in terms of the level of prediction, it requires the specification of transport coefficients that are not required in equilibrium models. The remainder of this chapter elaborates on application of this model formulation...
to predict the drying of apple flesh, as this provides an opportunity to show how the various coefficients are obtained and demonstrates the capability of the present model.

### 3.3 Convective drying of apple flesh

The convective drying of apple flesh is selected to demonstrate the capabilities of the proposed framework. In this respect, the highly-referenced work of Velić et al. [32] is utilized because it provides all the necessary information required to simulate the drying process. The experimental study of Velić et al. [32] focused on convective drying of 20×20×5 mm rectangular apple slices (with peel removed) to study the effects of airflow velocity on the heat transfer and mass diffusivity coefficients. The computational domain considered in the present modeling effort takes advantage of symmetry in two directions and includes a quarter of an apple slice, plus a portion of the surrounding region where moist air flows (see Fig. 3.2a-b). Consequently, the porous region representing the apple has dimensions of 20×10×2.5 mm in the x, y, and z-directions, respectively. The fluid regions in each direction around the slice are obtained by a *boundary position study* to ensure that their position does not affect predictions in the region of interest. The resulting fluid-porous domain used in the simulations is 40×20×7.5 mm in x, y, and z-directions, respectively.

![Figure 3.2: a) Apple slice geometry and orientation along with the symmetry planes; b) meshed fluid-porous domain used for the convective drying simulations.](image-url)
Structured hexahedral control-volumes (CV) were used to discretize the domain. During the grid convergence testing, the grid was refined from 20×15×15 to 30×20×20 and 40×30×30 CVs in x, y, and z-directions, respectively. The grid containing 30×20×20 CV was selected for the simulations because refinement to 40×30×30 CV produced a maximum change of 0.12 % in the predicted moisture content. To ensure the solution accuracy, the grid is refined in the vicinity of all fluid-porous interfaces. The meshed domain used for the simulations is shown in Fig. 3.2b.

The transport equations were discretized using finite volume approach. In brief, the Rhie-Chow approach was used to maintain pressure-velocity coupling, while UDS and QUICK were implemented to model advection in the fluid and porous domains. The interested reader is directed to Khan et al. [33] for a full description of the discretization details. The solution advances in time to simulate the unsteady convective drying process. The solution proceeds to the next time-step when the maximum normalized residual of all the transport equations falls below 5×10^{-6} at the current time-step. A time-step size of 50 seconds is utilized to advance in time as the reduction in the time-step size from 50 to 5 seconds changes the moisture content by only 0.13 %. Furthermore, for the purpose of solution accuracy and stability, the time-step size is gradually increased from 0.02 to 50 seconds at the beginning of the simulation. Initial conditions are discussed in a subsequent subsection describing properties.

The boundary conditions for the conjugate domain shown in Fig. 3.2b are as follows:

Airflow inlet: The moist airflow enters the domain at 60°C with a relative humidity of 9%; the airflow velocity is varied from 0.64 to 2.75 m/s. These inlet conditions are imposed to simulate the results of Velić et al. [32]. The inlet pressure is extrapolated from the domain interior.

Outlet (east face): zero normal derivative condition is imposed for all velocity components, temperature, and moisture mass fraction. The outlet pressure is fixed at atmospheric pressure (101.3 kPa).
Symmetry plane (south face): zero normal derivative condition is enforced on all the variables, excluding the \( v \) velocity component, which is set to zero to ensure zero mass flux.

Symmetry plane (bottom face): zero normal derivative condition is imposed on all the variables, apart from the \( w \) velocity component, which is equal to zero to ensure zero mass flux.

North and top faces: for all the velocity components, temperature, and moisture mass fraction, zero normal derivative condition is imposed to minimize the boundary condition effects on the solution. The pressure is extrapolated from the interior of the domain.

To assess the drying airflow regime, we evaluated the flow Reynolds number based on the largest dimension of the apple slice (20mm). For the airflow velocity of 2.75 m/s, the Reynolds number was found to be below 3500, which ensures that the drying airflows simulated in the present work fall in the laminar regime.

3.3.1 Modeling of apple flesh as a porous material

Modeling of apple flesh as a porous material involves determination of thermophysical properties of the fluid and solid-constituents along with the geometric parameters of the porous material (apple). These properties are necessary for consideration of apple flesh as a porous material. Note that the procedure described in this study is generic and can be applied to other produce or moist porous materials. In addition, this section also covers the moist airflow properties required to simulate the drying process.

As discussed earlier, apple flesh is composed of solid and fluid-constituents. The solid-constituent is considered herein to be comprised of the solid-structure and liquid water, while the fluid-constituent consists of voids filled with moist air. At this point, we recall Eq. 3.21 and define the solid-constituent density \( \langle \rho_s \rangle_s \) as

\[
\langle \rho_s \rangle_s = \alpha_{st} \rho_{st} + \alpha_w \rho_w
\]  

(3.22)

where, \( \alpha_{st} \) and \( \alpha_w \) are the volume fractions of the solid-structure and water, respectively, and \( \rho_{st} \) and \( \rho_w \) represent the density of the solid-structure and water, respectively.
Information on the volume fractions and densities shown in Eq. 3.22 are required to calculate \( \langle \rho_s \rangle^s \). The density of water \( (\rho_w) \) is well-known, however, \( \rho_{st} \), \( \alpha_{st} \) and \( \alpha_w \) are often difficult to obtain. During the drying process, \( \rho_{st} \) and \( \alpha_{st} \) are assumed constant, while \( \alpha_w \) is updated continuously utilizing the latest water mass fraction \( (Y_w) \). To our advantage, the existing literature contains information on the apple moisture content \( (X) \), which is described as the ratio of mass of water to the mass of dry matter (solid-structure) [39]. The averaged moisture content can be normalized by \( X^0 \), which represents the moisture content prior to the drying process. The local moisture content can be calculated as

\[
X = \frac{\alpha_w \rho_w}{\alpha_{st} \rho_{st}}
\]  

(3.23)

To evaluate \( \rho_{st} \), \( \alpha_{st} \) and \( \alpha_w \), Eqs. 3.22 and 3.23 are solved simultaneously, with the assumption that prior to the drying process the sum of \( \alpha_{st} \) and \( \alpha_w \) is equal to one. In this respect, the values of \( \langle \rho_s \rangle^s \) and \( X \) prior to drying are required. Lozano et al. [39] and Rahman [40] describe different density definitions accounting for various aspects of porous materials. In the present study, we consider \( \langle \rho_s \rangle^s \) as substance density, which represents the density of material without pores or voids. For the evaluation, \( \langle \rho_s \rangle^s \) and \( X^0 \) are set as 1055 kg/m³ [41] and 7.45 kg water/kg dry matter [39], respectively. The evaluated properties of the apple flesh along with the other required properties are presented in Tab. 3.1. The thermal conductivity of the fluid and solid-constituents presented in Tab. 3.1 are obtained as \( K_{eff,f} = \varepsilon \times K_{apple} \) and \( K_{eff,s} = (1 - \varepsilon) \times K_{apple} \), where \( K_{apple} \) is obtained from Donsi et al. [45]. The specific heat of the solid-structure \( (c_{ps}) \) is obtained in a similar manner using the apple specific heat provided by Mykhailyk and Lebovka [47].

The pore diameter \( d_p \) is obtained using the Ergun equation [48]. In the present study, \( \varepsilon \) represents the volume fraction of the fluid-constituent (voids). Moreover, the present formulation neglects the shrinkage, which results in constant \( \varepsilon \) during the simulated drying process. Although, the model does account for the voids created due to the removal of water from the solid-constituent. The specific interfacial surface area of porous material \( (A_{fs}) \) is calculated using \( \varepsilon \) and \( d_p \) of the porous material.
At this point, we define the initial conditions of the convective drying simulation. The initial water mass fraction \( Y_w \) of the apple is evaluated as 0.881 by employing \( X^0 \) provided by Lozano et al. [39]. In addition, the fluid and porous regions initial temperatures are set to 60°C.

### Table 3.1: Fluid and porous regions properties

<p>| | | | |</p>
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<th></th>
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<tbody>
<tr>
<td></td>
<td><strong>Air [42]</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( c_p ) [J/(kg.K)]</td>
<td>1005</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( R ) [J/(kg.K)]</td>
<td>287</td>
<td></td>
</tr>
<tr>
<td><strong>Water vapour [42]</strong></td>
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<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( c_p ) [J/(kg.K)]</td>
<td>1872</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( h_{fg} ) [J/kg]</td>
<td>( 2500 \times 10^3 )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( R ) [J/(kg.K)]</td>
<td>461.5</td>
<td></td>
</tr>
<tr>
<td><strong>Fluid mixture [43,44]</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( D_f ) [m²/s]</td>
<td>( 2.600 \times 10^{-5} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( k_f ) [W/(m.K)]</td>
<td>0.0258</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \mu_f ) [N.s/m²]</td>
<td>( 1.830 \times 10^{-5} )</td>
<td></td>
</tr>
<tr>
<td><strong>Porous material [38,39,43-48]</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>( A_{fs} ) [m⁻¹]</td>
<td>11650</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( K ) [m²]</td>
<td>( 8.89 \times 10^{-13} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( \varepsilon )</td>
<td>0.206</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( d_p ) [µm]</td>
<td>103</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( c_{ps} ) [J/(kg.K)]</td>
<td>252</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( c_{pw} ) [J/(kg.K)]</td>
<td>4180.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td>( k_{eff,f} ) [W/(m.K)]</td>
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<td></td>
<td>( k_{eff,s} ) [W/(m.K)]</td>
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<tr>
<td></td>
<td>( \rho_{st} ) [kg/m³]</td>
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<tr>
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<td>( \rho_w ) [kg/m³]</td>
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<tr>
<td></td>
<td>( \alpha_{st} )</td>
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</tr>
<tr>
<td></td>
<td>( \alpha_w )</td>
<td>0.9311</td>
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</tr>
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</table>

It is important to note that Tab. 3.1 lists all the properties required to model the apple flesh as a porous material, with the exception of effective solid and fluid-constituent mass diffusivity coefficients \( D_{eff,s} \) and \( D_{eff,f} \). In the convective drying process, these coefficients have significant importance, as evident from Eq. 3.21. These coefficients characterize the diffusive transport of vapour and water inside the porous media and transport the moisture to the porous surface to be picked up by the surrounding airflow. In the existing literature, no study, as yet, has evaluated \( D_{eff,s} \) and \( D_{eff,f} \) values for non-
equilibrium moisture transfer inside the porous material. Herein, we utilize available information to evaluate $D_{\text{eff},s}$ and $D_{\text{eff},f}$. Earlier, it was stated that the voids are occupied by moist air, which means that the diffusivity coefficient of air-vapour mixture $D_f$ can be utilized to evaluate $D_{\text{eff},f}$. In this respect, as a reasonable approximation, $D_{\text{eff},f}$ is calculated as $D_{\text{eff},f} = D_f \times \varepsilon$.

The evaluation of $D_{\text{eff},s}$ is done using the moisture resistance circuit shown in Fig. 3.1. At this point, it becomes essential to more clearly describe the four resistances given in the figure. $R_1$ and $R_2$ are responsible for vapour and water diffusive transports from the fluid and solid-constituents of the porous media, respectively, up to the fluid-porous interface. The vapour and water transported at the interface are then exchanged with the fluid region by $R_3$ and $R_4$, respectively. These four resistances can be calculated using the harmonic mean formulation described by Betchen et al. [38], and are expressed as

$$
R_1 = \frac{\Delta x_{i-p}}{A(\rho_f)fD_{\text{eff},f}} , \quad R_2 = \frac{\Delta x_{i-p}}{A(\rho_s)sD_{\text{eff},s}} , \quad R_3 = \frac{\Delta x_{f-i}}{\varepsilon A \rho_f D_f} , \quad R_4 = \frac{\Delta x_{f-i}}{(1 - \varepsilon) A \rho_f D_f} \quad (3.24)
$$

where, $\Delta x_{f-i}$ is the distance between the node in the fluid region and the interface, and $\Delta x_{i-p}$ is the distance between the interface and the porous region node, and $A$ is the total area of the control volume face adjacent to the interface. Note that the effects of porosity in $R_1$ and $R_2$ are absorbed by $D_{\text{eff},f}$ and $D_{\text{eff},s}$, respectively. The total diffusive transport resistance of water between the fluid and porous nodes across the interface is obtained by adding $R_2$ and $R_4$. The resulting resistance ($R_{s,i}$) is expressed as

$$
R_{s,i} = \frac{\Delta x_{i-p}}{A(\rho_s)sD_{\text{eff},s}} + \frac{\Delta x_{f-i}}{A(1 - \varepsilon) \rho_f D_f} \quad (3.25)
$$

For the evaluation of $D_{\text{eff},s}$, a case of convective drying is simulated while keeping $D_f$, $D_{\text{eff},s}$, and $D_{\text{eff},f}$ set to the effective diffusivity coefficient of the drying process ($D_{\text{eff}}$) obtained from Velić et al. [32]. Here, we arbitrarily select the case where the airflow velocity is 0.64 m/s, for which $D_{\text{eff}}$ increases from $1.70 \times 10^{-9}$ to $2.91 \times 10^{-9}$ m$^2$/s during the drying process. The simulation produces moisture removal rates that are in excellent agreement to the corresponding rates reported by Velić et al. [32]. Moreover, the
simulation provides the numerical value of $R_{s,i}$ at the fluid-porous interface, which is then employed to calculate $D_{eff,s}$ by fixing $D_f$. In the present case, $D_f$ (value provided in Tab. 3.1) represents the mass diffusivity coefficient of the air-vapour mixture surrounding the porous material. The purpose of using a single diffusivity coefficient value for $D_f$, $D_{eff,s}$, and $D_{eff,f}$ in the simulation is to obtain the correct numerical value of $R_{s,i}$. In other words, this simulation calibrates $R_{s,i}$ to the correct value, which is then utilized to calculate the correct value of $D_{eff,s}$. While this may appear as over-calibration, it is extremely difficult to measure such values experimentally, so such an approach is warranted.

In addition to $R_{s,i}$, the simulation also provides the diffusive resistance to water transport inside the solid-constituent ($R_s$) and the diffusive resistance to vapour transport inside the fluid-constituent ($R_f$) of the porous material. The simulation reveals that, during the entire drying process, $R_f$ is higher than $R_s$ by more than two orders of magnitude. Such a considerable difference between $R_f$ and $R_s$ means that fluid-constituent transport inside the porous material only weakly participates in the drying process. Moreover, it also suggests that it is more important to have the correct value of $D_{eff,s}$ compared to $D_{eff,f}$.

The comparison in magnitude between $R_{s,i}$ and $R_s$ shows that throughout the drying process $R_{s,i}$ stays greater than $R_s$ by at least one order of magnitude, which means that $R_{s,i}$ acts like a barrier to moisture transfer at the fluid-porous interface. Furthermore, $R_s$ increases in time due to the reduction in moisture content within the porous material. It is also found that, at a given instant in time, the local moisture content decreases as we move towards the fluid-porous interface from the inner porous region. Consequently, it is appropriate to consider that the solid-constituent surface exposed to the surrounding airflow is comparatively dry and hinders the removal of moisture from the porous material. This phenomenon of a dry solid-constituent surface forming an additional moisture resistance is also discussed by Defraeye et al. [5]. This additional hindrance to moisture transfer at the interface is modeled by introducing a resistance coefficient ($C_{sl}$). The modified expression for $R_{s,i}$ is then given as
\[ R_{s,i} = \frac{C_{si}\Delta x_{i-p}}{A(\rho_s)^2D_{eff,s}} + \frac{\Delta x_{f-i}}{A(1 - \epsilon)\rho_f D_f} \]  

(3.26)

An iterative approach is used to converge to a realistic value of \( C_{si} \). We start with \( C_{si} = 1 \) to calculate \( D_{eff,s} \), which is then used to simulate the drying process. \( C_{si} \) is then modified until the simulation produces drying rates that are in reasonable agreement with the results of Velić et al. [32]. The computed \( D_{eff,s} \) as the function of moisture content is presented in Fig. 3.3, which shows that, unlike \( D_f \) and \( D_{eff,f} \), \( D_{eff,s} \) is not constant and changes throughout the process of drying. The increasing pattern of \( D_{eff,s} \) is primarily attributed to the diminishing value of \( \langle \rho_s \rangle^2 \) as evident from Eq. 3.26. Cubic polynomial curve-fitting is utilized to input \( D_{eff,s} \) as the function of local moisture content throughout the porous domain.

Figure 3.3: Evaluated \( D_{eff,s} \) as the function of the moisture content.

One final point in terms of modelling concerns the adherence to thresholds of moisture transport, which are required for the model to work correctly under a full range of airflow conditions. The basic concept is that once the drying airflow becomes completely saturated with vapour – that is, having relative humidity of 100% - then it should not pick
up any further moisture from the porous material. In terms of vapour pressure, such condition exists when the airflow vapour pressure \( P_v \) becomes equal to the water saturation pressure \( P_g \) at a given temperature. For this reason, the modeling is carried out in the fluid region adjacent to the fluid-porous interface. In this respect, the moisture condition at the fluid-porous interface (Eq. 3.21) is again utilized. The total diffusive transport resistance of water across the fluid-porous interface \( R_{s,i} \) is given by Eq. 3.26. In a similar way, \( R_1 \) and \( R_3 \) are added together to formulate the total diffusive transport resistance of vapour between the fluid and porous nodes across the interface \( R_{f,i} \), which is expressed as

\[
R_{f,i} = \frac{\Delta x_{i-p}}{A(\rho_f)^F D_{eff,f}} + \frac{\Delta x_{f-i}}{\varepsilon A(1 - \varepsilon) \rho_f D_f}
\]  

(3.27)

In the present formulation, we create a moisture threshold by introducing an additional resistance coefficient \( C_{fi} \) in \( R_3 \) and \( R_4 \). The resulting \( R_{s,i} \) and \( R_{f,i} \) are expressed as

\[
R_{s,i} = \frac{C_{si} \Delta x_{i-p}}{A(\rho_s)^s D_{eff,s}} + \frac{C_{fi} \Delta x_{f-i}}{A(1 - \varepsilon) \rho_f D_f}
\]  

(3.28)

\[
R_{f,i} = \frac{\Delta x_{i-p}}{A(\rho_f)^F D_{eff,f}} + \frac{C_{fi} \Delta x_{f-i}}{\varepsilon A(1 - \varepsilon) \rho_f D_f}
\]  

(3.29)

We model the resistance coefficient \( C_{fi} \) as the function of airflow vapour and saturation pressures. In this respect, the validated cases presented in Fig. 3.4, which have airflow relative humidity of 9\% at 60\ºC, are considered as a reference having \( C_{fi} = 1 \). Moreover, \( C_{fi} \) should approach the maximum value at 100\% relative humidity of airflow to completely cease the drying process. Based on such requirements, \( C_{fi} \) is evaluated as

\[
C_{fi} = \frac{\Delta P}{\Delta P_{ref}}
\]  

where, \( \Delta P = P_g - P_v \). The evaluation of \( \Delta P \) is carried out at the node in the fluid region adjacent to the fluid-porous interface. The \( P_g \) as the function of temperature is evaluated using Antoine equation for water vapour [49]. The \( \Delta P_{ref} \), which is evaluated using the
validated cases, is found equal to 15.8 kPa. Moreover, the constants $c$ and $b$ are set as 5.85 and 10.0, respectively. It is important to mention that the expression used to calculate $C_{fi}$ in Eq. 3.30 is not calibrated using the experimental results. In the present work, its sole purpose is to ensure that the formulation predicts the correct moisture threshold.

With all the evaluated properties, we now demonstrate the viability of the proposed model formulation and property treatment in a convective drying process and show that the influences of various quantities are properly predicted using the calibrated model. As mentioned earlier, the present results are validated using the results of Velić et al. [32], who reported results over the airflow velocity range of 0.64 to 2.75 m/s. Over this range, Velić et al. [32] reported an increment in $D_{eff}$ with increasing airflow velocity. To account for this variation, a process similar to that described above is used to obtain $C_{si}= 860$, 540, and 330 for velocities of 0.64, 1.5, and 2.75 m/s, respectively. The simulated results for the moisture content of the apple slice are shown in Fig. 3.4. The results show excellent agreement with the work of Velić et al. [32]. While not shown in the figures, several computational cases at varying inlet air temperatures and relative humidity confirmed that the trends in drying time are correctly predicted, and that the imposed thresholds for moisture transport take effect for saturated air.

While it might be argued that the agreement is due to the property evaluation approach and the calibration used for the interface treatment, it is critical to note that those steps only form a small part of the simulation strategy. The purpose of this study is to show that the conjugate domain formulation utilizing a complete flow simulation, combined with thermal and mass non-equilibrium can be used to accurately simulate a drying operation. The formulation is generic and extensive, and has not been simplified to take advantage of the low permeability of the apple flesh or the near-thermal equilibrium of the solid and fluid phases inside the flesh. While simplifications could have been made in the simulations presented, one of the main objectives of the study was to demonstrate the value of using the complete framework, since this is required when using a dynamic phase-coupled approach, which is also possible using the present formulation. The most important result from the present case study is the accurate prediction of both the drying
rates and the rate-of-change of drying rates during the process. The present formulation also permits a detailed look in and around the porous domain, as described below.

Figure 3.4: Comparison of predicted drying rates against the experimental results of Velić et al. [32] (the markers show the experimental inlet airflow velocity: ○ = 0.64 m/s, △ = 1.5 m/s and □ = 2.75 m/s).

Fig. 3.5 shows pressure contours and velocity vectors and streamlines on the symmetry planes of the domain. The plot shows that the incoming air flows almost entirely around the porous material as opposed to flowing through it, an expected result, since the apple slice has a very low permeability and behaves almost like a solid material. Though not seen in Fig. 3.5, weak values of all three velocity components are predicted inside the apple flesh due to the pressure difference in the mean flow direction. Fig. 3.5 also shows the wake behind the slice, which is characterized by a three-dimensional recirculation region of low velocities. The distribution of pressure inside the domain shows the correct physical trends. High pressures are observed around the upstream fluid-porous interface due to the airflow impingement on the porous material, while low pressures are predicted in the wake.
Figure 3.5: Distribution of pressure (normalized by $\rho_f U_\infty^2$) on the domain symmetry planes with a) velocity vectors; b) streamlines. The inlet airflow velocity, temperature and relative humidity are 0.64 m/s, 60°C and 9%, respectively.

The moisture content distribution inside the apple slice at different instants in time is presented in Fig. 3.6, which shows that the moisture content inside the apple gradually reduces as the drying process proceeds in time. The local distribution of moisture content further reveals that, at a given time, the lowest moisture content is correctly observed in the vicinity of the fluid-porous interfaces. Furthermore, the moisture content gradually increases towards the inner region of the porous material as described earlier.

A key feature of the present formulation is its capability to model the evaporation of water during the drying process. To illustrate this influence, Fig. 3.7 shows the domain relative humidity and fluid temperature at an integrated moisture content of 0.6. The relative humidity contours indicate that the relative humidity inside the porous region is higher compared to the surrounding airflow region. Higher relative humidity inside the porous region is attributed to the interfacial moisture transfer occurring inside the porous media. Moreover, the relative humidity of the porous region further increases due to increasing incoming airflow relative humidity. It is interesting to note that the margin of the porous region’s relative humidity increment grows with rising incoming airflow relative humidity. Such behaviour can be explained by the resistance coefficient, $C_{fi}$. As the incoming airflow relative humidity increases, the value of $C_{fi}$ rises, which hinders the
vapour loss from the fluid-constituent resulting in higher vapour pressure and relative humidity inside the porous region.

Figure 3.6: Distribution of moisture content on the domain symmetry planes at different time instances. The inlet airflow velocity, temperature and relative humidity are 0.64 m/s, 60°C and 9%, respectively.
Figure 3.7: Distribution of relative humidity (\%, left column) and fluid temperature (°C, right column) on the domain symmetry planes at various inlet relative humidity values. Average moisture content (\(X/X^0\)) of the porous region is 0.6 (excluding 100% inlet relative humidity case). The inlet airflow velocity and temperature are 0.64 m/s and 60°C, respectively.
The fluid temperature distribution in Fig. 3.7 indicates cooling of the fluid inside the porous region, which is due to evaporative cooling. The level of evaporative cooling is correctly captured with the present model. For example, the case of 100% inlet airflow relative humidity correctly produces no cooling, despite the porous region being completely saturated with vapour. As the relative humidity of the incoming airstream is reduced (for a fixed initial moisture content in the apple), the porous apple is shown to cool more and more.

### 3.4 Summary

In the present study, convective drying of porous materials was modeled using a conjugate domain approach, which involves modeling the porous material and the surrounding airflow (fluid region). The proposed framework is general and can be utilized to simulate the drying process of a wide range of porous materials under different drying conditions. The proposed model includes mass and momentum, energy, and moisture transport equations in both the fluid and porous regions. Inside the porous material, both the liquid water and water vapour transports were considered by utilizing the non-equilibrium heat and moisture transfer approach. Mathematical conditions at the fluid-porous interface were enforced to ensure the smooth transfer of momentum, energy and moisture across the interface. Additional modeling was carried out in the fluid region adjacent to the interface to develop the airflow moisture threshold, and in the porous region adjacent to the interface to ensure the model accuracy. In this respect, detailed discussion of interfacial moisture transfer condition was made using electric circuit analogy.

The proposed model was validated by considering apple flesh as a porous material. In this respect, detailed modeling of the apple was required. The solid-structure holding water was considered as the solid-constituent, while the fluid-constituent was occupied by the moist air voids. The present study evaluated the missing apple properties such as solid-structure density and mass fraction, and moisture diffusivity coefficients required to simulate the unsteady convective drying process. The predicted moisture content was found to deviate against the experimental data by a maximum of 3% in time for the airflow velocity range of 0.64 to 2.75 m/s. Moreover, the results of local distribution of
velocity, pressure, temperature, and moisture content inside the domain were also found to be physically realistic. In this respect, we have demonstrated that a conjugate, non-equilibrium model can provide information necessary to make the next important step towards direct, dynamic coupling of the phases.
References


Non-conjugate and conjugate formulations involving the aerodynamic effects. Renewable Energy, 35(7), 1391-1402.


Chapter 4

4 Closure of macroscopic turbulence and turbulent heat and mass transfer model inside porous media*

4.1 Introduction

Packed beds of spheres are widely encountered in engineering applications related to the chemical processing industry, and the food storage and processing industries. The convective drying of produce stacks using warm airflow is one example of such problems. In many such applications, the sphere size is significant and heat and mass transfer are turbulent. Furthermore, it is often necessary to couple the solid and fluid phases of the process, which requires consideration of non-equilibrium heat and mass exchanges. The complex nature of such problems makes numerical modeling an attractive approach for gaining insight into the underlying physical phenomena. In this respect, turbulence modeling inside beds of packed spheres becomes critical.

Two approaches are commonly used to model the aforementioned problems. In one approach, the bed of spheres is modeled at the microscopic scale, which is characterized by the length scale of spheres. At this scale, the transport equations are used in their usual forms. However, extensive computational resources are required to model the problem. The second approach is to model the packed bed as porous continuum. By this approach, the bed of spheres is up-scaled to the macroscopic level, and the domain is considered to be comprised of solid and fluid phases with parameters like porosity and permeability describing the resistance to flow through the domain. The benefit of the macroscopic approach is that it eliminates the necessity of modeling the problem at the scale of spheres, which significantly reduces the required computational effort. However, to use this approach, the detailed information about the pore-level flow field and the energy and mass exchanges have to be determined and provided via constitutive models characterizing the porous region. The up-scaling of the mathematical formulation is carried out by volume-averaging the transport equations for mass, momentum, energy and turbulence.

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The macroscopic, or volume-averaged, approach for modeling turbulent heat and mass transfer inside packed beds of spheres has been widely used for applications related to food storage and refrigeration. For example, Tapsoba et al. [1] and Moureh et al. [2,3] modeled turbulent airflow inside and around slotted-enclosures filled with spheres to understand the airflow distribution of the problem. In another study, Delele et al. [4] simulated a cold storage room containing boxes loaded with spheres to predict airflow, temperature and humidity distribution. Similarly, the distribution of a gas used to control fruit ripening inside cold storage rooms was numerically predicted by Ambaw et al. [5]. In addition, the cooling process of packed food stacks was simulated by Alvarez and Flick [6]. All of these studies considered porous media at the macroscopic scale and modeled turbulence using eddy viscosity based models or Reynolds stress models (RSM).

To better understand the difference between the modelling approaches and the information required for the volume-averaged approach, we shift our discussion briefly to turbulence modeling using the eddy-diffusivity concept at the macroscopic scale of porous media. At the macroscopic scale, the modeling of turbulence generally involves volume- and time-averaging of the transport equations. In the volume-averaging operation, a transport equation is integrated over a Representative Elemental Volume (REV) of porous material. The volume-averaged value of a quantity \( \varphi \), as described by Whitaker [7], is defined as

\[
\langle \varphi \rangle = \frac{1}{V} \int_{V_f} \varphi \, dV
\]  

(4.1)

where, \( V \) refers to the volume over which the averaging process is carried out, \( V_f \) is the fluid volume inside \( V \), and \( \langle \varphi \rangle \) is defined as the extrinsic-average of \( \varphi \). Using a similar approach, an intrinsic-averaged quantity \( \langle \varphi \rangle^f \) is expressed as

\[
\langle \varphi \rangle^f = \frac{1}{V_f} \int_{V_f} \varphi \, dV
\]  

(4.2)

The ratio \( \langle \varphi \rangle / \langle \varphi \rangle^f \) then defines the porosity \( \phi \) of porous media. Moreover, \( \varphi \) can be split into \( \langle \varphi \rangle^f \) and its spatial deviation \( \hat{\varphi} \) as [7]
\[ \varphi = \langle \varphi \rangle_f + \tilde{\varphi} \quad (4.3) \]

Time-averaging can also be utilized in the porous region to characterize the fluctuations of a quantity in time, similar to that done in pure fluid regions. The time-averaging of a quantity \( \varphi \) is given as [8]

\[ \bar{\varphi} = \frac{1}{\Delta t} \int_t^{t+\Delta t} \varphi \, dt \quad (4.4) \]

Then, similar to that done for spatial deviations in Eq. 4.3, \( \varphi \) can be split into \( \bar{\varphi} \) and its temporal deviation \( \varphi' \) as

\[ \varphi = \bar{\varphi} + \varphi' \quad (4.5) \]

To model a quantity fluctuating in time at the macroscopic scale of porous media, both volume- and time-averaging operations are required. In this respect, Pedras and de Lemos (PDL) [8] introduced the concept of double decomposition, which involves volume-averaging followed by time-averaging or vice versa. The group showed that the order of averaging does not change the solution, i.e. \( \langle \bar{\varphi} \rangle_f = \langle \varphi \rangle_f \).

Existing literature on the macroscopic modeling of turbulence inside porous regions mainly utilizes the \( k-\varepsilon \) model, by which turbulence is characterized by the energy \( (k) \) of an average energy-containing eddy and its dissipation rate \( (\varepsilon) \). The basic derivation of the \( k-\varepsilon \) model is beyond the scope of this chapter, and the interested reader is directed to Wilcox [9] for a full mathematical treatment. In general, existing \( k-\varepsilon \) models can be classified based on the manner they define turbulent kinetic energy \( k \). In this respect, early attempts made by Lee and Howell [10], Wang and Takle [11], and Antohe and Lage [12] defined the macroscopic turbulent kinetic energy \( k_m \) as [13]

\[ k_m = \frac{1}{2} \langle \mathbf{v}' \rangle_f \cdot \langle \mathbf{v}' \rangle_f \quad (4.6) \]

This quantity is derived by first carrying out volume-averaging of the microscopic velocity fluctuation \( \mathbf{v}' \), then applying time-averaging to the square of the volume-
averaged velocity fluctuation. This definition of turbulent kinetic energy was considered incomplete by Nakayama and Kuwahara (NK) [14] and PDL, both of whom defined turbulent kinetic energy $k_{NK}$ by first squaring $v'$ followed by time and volume-averaging operations. By this approach, the Reynolds-averaged Navier-Stokes (RANS) equations, along with the usual form of $k$ and $\varepsilon$ equations, were volume-averaged by NK and PDL to arrive at the macroscopic turbulence model. In another study, Chandesris et al. [15] used a similar approach to propose a $k$-$\varepsilon$ model that characterizes turbulence inside porous media composed of pipe, channel, and rod bundles. Mathematically, $k_{NK}$ is defined as [13]

$$k_{NK} = \frac{1}{2} \left( v' \cdot \bar{v} \right)^f$$  \hspace{1cm} (4.7)$$

Lastly, Teruel and Rizwan-uddin (TR) [16,17] proposed a definition of turbulent kinetic energy that also includes the dispersive kinetic energy. The total macroscopic turbulent kinetic energy $k_{total}$ is then defined as [16]

$$k_{total} = k_{NK} + \frac{1}{2} \left( \bar{v} \cdot \bar{v} \right)^f$$  \hspace{1cm} (4.8)$$

where the second term on the right-hand side accounts for the dispersive kinetic energy, which is considered important by TR for the porous domains having low porosity. In their work, TR applied the concept of double decomposition to the usual Navier-Stokes (N-S) equations to arrive at the velocity fluctuation in time and space, $\bar{v}'$, which was then utilized to derive $k$ and $\varepsilon$ equations that inherently include dispersive effects. The concept of including the dispersive portion of $k$ and $\varepsilon$ was taken forward by Drouin et al. [18] when the group proposed transport equations for dispersive $k$ and $\varepsilon$ along with $k_{NK}$ to model turbulence.

Apart from the $k$-$\varepsilon$ model, other models have also been utilized to simulate the macroscopic turbulence inside porous media. In this respect, Kuwata and Suga [19] employed the RSM to capture turbulence, especially at the fluid-porous interface. To avoid the inherent complexity of the RSM, Kuwata et al. [20] proposed a multiscale turbulence model, which utilized the transport equations of $k$ and $\varepsilon$ at the microscopic
and macroscopic scales of porous media. Conversely, Soulaine and Quintard [21] employed a model similar to the Darcy–Forchheimer model to simulate turbulent flow in structured packings. Furthermore, a Large Eddy Simulation (LES) study was carried out by Kuwahara et al. [22] to quantify the accuracy of the $k$-$\varepsilon$ model. The group found that the $k$-$\varepsilon$ model can be effectively used to predict turbulent flow field inside porous media.

Based on the above discussion, it appears feasible to characterize the macroscopic turbulence inside porous media using the $k$-$\varepsilon$ model. However, there is no universal form of the macroscopic $k$-$\varepsilon$ model due to the presence of the additional terms that arise in the volume-averaging operation. Similarly, additional terms also arise in the volume-averaged momentum, heat and mass transport equations. Simply stated, the terms that arise in all volume-averaged equations account for the interactions between the fluid and the specific porous structure under consideration. For accurate simulation at the macroscopic level, these additional terms require closure to complete a given set of the macroscopic transport equations, and in general, this closure is achieved by simulating the problem at the microscopic scale of porous media.

At the microscopic scale, problems involving turbulent flow and heat transfer inside a bed of spheres have been extensively simulated before for various interests. Many studies [23-26] have modeled the entire bed of spheres by placing each sphere in structured manner, along with the walls containing the bed. Utilizing this approach, Guardo et al. [23] employed the various eddy viscosity based turbulence models to assess their influence on solid-to-fluid heat transfer. In continuation of their work, Coussirat et al. [24] utilized the RSM and found that it produced similar results compared to the eddy viscosity based turbulence models. Similarly, Logtenberg and Dixon [25], and Nijemeisland and Dixon [26] used the $k$-$\varepsilon$ model to comprehensively examine flow and temperature fields inside a bed of spheres. To reduce the computational domain size, Jang and Chiu [27] took the advantage of symmetry to simulate the cooling process of a sintered bed of spheres.

In reality, beds of spheres are usually randomly packed, although in the existing literature very few studies consider random packing. To this end, turbulent flow inside a bed of
randomly packed spheres was simulated by Ambaw et al. [5]. Similarly, Delele et al. [28] conducted the study of turbulent airflow through vented boxes containing randomly packed spheres. The group used the Discrete Element Method (DEM) to model the random arrangement of spheres. However, the aim of these studies was not to close the macroscopic model, but, to examine the flow at the pore-level.

At the microscopic scale, porous media are often modeled using a REV to reduce the computational domain. However, few studies have utilized the concept of the REV to model packed spheres at the microscopic scale. Yang et al. [29] used a REV to simulate packed beds composed of different sphere arrangements to observe their effect on turbulent flow and heat transfer. In their work, several REVs were stacked in line to produce spatially periodic flow and heat transfer in the last few downstream REVs. In another study, Gunjal et al. [30] used REVs composed of different sphere arrangements and applied periodic boundary conditions to examine the problem hydrodynamics and heat transfer. Similarly, Mathey [31] modeled turbulence and heat transfer inside a periodic domain (REV) composed of structurally packed spheres. Mathey [31] also modeled packed beds of short cylinders arranged in a random manner to achieve the more realistic packing. However, the random packing was enclosed in the tubular cylinder to mimic the case of tubular reactor.

In terms of macroscopic transport models for packed bed of spheres, we should state that none of the aforementioned microscopic scale simulation studies were focused on the closure of macroscopic models. At present, the literature shows few attempts to close such macroscopic models, even for simple two- and three-dimensional REVs. With respect to the macroscopic $k$-$\varepsilon$ model, NK, PDL, and TR used two-dimensional REVs composed of structured arrays of circular and square rods. Chandesris et al. [15] and Drouin et al. [18] considered three-dimensional circular rods and flat plate arrays as their REVs. For the case of a packed bed of spheres, Alvarez and Flick [6] closed the macroscopic turbulence model using their own experimental data. Recently, Mathey [31] closed the macroscopic $k$-$\varepsilon$ model for the case of structurally packed spheres. In his work, Mathey [31] also included the dispersive effects of $k$ and $\varepsilon$ using the model provided by TR. However, their results show the closure for only a small range of
Reynolds numbers and with constant sphere packing porosity. The closure of the macroscopic energy and mass transport equations for a two-dimensional array of circular, elliptical, and square rods was carried out by de Lemos [32].

To the authors’ knowledge, no existing study has proposed a closure of the macroscopic \( k-\varepsilon \) model for the case of a randomly packed bed of spheres. Moreover, no study in the existing literature has proposed a closure for the macroscopic non-equilibrium turbulent heat and mass transfer model intended for the bed of spheres. In the present work, we propose a complete closure of the macroscopic turbulence and non-equilibrium turbulent heat and mass transfer model for beds of randomly packed spheres, for applications in the food storage and refrigeration industries. Macroscopic turbulence is modeled using the \( k-\varepsilon \) model, and dispersive effects of \( k \) and \( \varepsilon \) are also considered. The macroscopic model is closed by utilizing the microscopic scale information available inside REVs of randomly packed spheres, where the REVs are produced by a recently published three-dimensional approach. The closure of the macroscopic model is extended by including parametric variations of porosity, Reynolds number and sphere diameter of practical interest. The chapter is organized such that the complete macroscopic volume- and time-averaged model is presented first, followed by a discussion on the closure approach and then the microscopic results and the closure operation itself.

### 4.2 The macroscopic model

As discussed earlier, the present work is focused on the closure of a macroscopic \( k-\varepsilon \) turbulence model. To make the required turbulence closure generic, we focus on the \( k-\varepsilon \) models proposed by NK, PDL, and TR, all of which have a similar form. In general, all these models propose additional source terms in the transport equations to characterize porous region effects in the model. The only difference lies in the closure of these additional source terms. Therefore, we present a generic macroscopic \( k-\varepsilon \) turbulence model valid in the porous region.

Based on the work of NK, PDL, and TR, the volume-time-averaged mass and momentum conservation equations take the form
\[ 
\frac{\partial (\overline{p_f})}{\partial t} + \nabla \cdot (\overline{p_f} \overline{v}) = 0 
\] 

(4.9)

\[
\frac{\partial (\overline{p_f} \overline{v})}{\partial t} + \frac{1}{\phi} \nabla \cdot (\overline{p_f} \overline{v}) \\
= -\phi \nabla \left( \overline{p_f} + \frac{2}{3} \overline{p_f} \overline{k} \right) + \nabla \cdot [ (\mu + \mu_t) 2 \overline{D} ] + \phi \overline{p_f} \overline{f} \\
- \frac{\phi \mu_f}{K} \overline{v} - \frac{\phi \overline{p_f} c_E}{\sqrt{K}} |\overline{v}|(\overline{v}) 
\]

(4.10)

and, \( \mathbf{D} \) represents the deformation tensor defined as

\[ 
\overline{\mathbf{D}} = \frac{1}{2} [ \nabla (\overline{v}) + (\nabla (\overline{v}))^T ] 
\] 

(4.11)

where, an overbar indicates a time-averaged quantity, and \( \langle \quad \rangle \) indicates a volume-averaged quantity. It is interesting to note that the application of volume- and time-averaging in a successive manner produces additional terms from both operations. The momentum equation, Eq. 4.10, uses the Boussinesq approximation to model the Reynolds stresses that arise from time-averaging, resulting in the addition of a turbulent eddy viscosity, \( \mu_t \). The last two terms on the right-hand side of Eq. 4.10 are closure models for terms arising from the volume-averaging operation. These two terms, which are commonly referred to as Darcy and Forchheimer terms, respectively, account for the viscous and form drag on the mean flow through the porous media.

The macroscopic \( k-\varepsilon \) equations are expressed as [8,14,16,17]

\[
\frac{\partial (\overline{p_f})}{\partial t} + \nabla \cdot (\overline{p_f} \overline{v}) \\
= \phi \nabla \left[ (\mu_f + \frac{\mu_k}{\sigma_k}) \overline{v} \right] + P_k - \phi \overline{p_f} \overline{f} + \overline{S_k} 
\]

(4.12)
\[
\phi \frac{\partial \langle \rho_f \rangle^f}{\partial t} + \nabla \cdot \langle \rho_f \rangle^f \langle \varepsilon \rangle^f \langle \mathbf{v} \rangle
\]
\[
= \phi \nabla \cdot \left( \left( \mu_f + \frac{\mu_t}{\sigma_k} \right) \nabla \langle \varepsilon \rangle^f \right) + C_{1e} P_k \langle k \rangle^f - \phi C_{2e} \langle \rho_f \rangle^f \langle \varepsilon \rangle^f \langle k \rangle^f
\]
\[
+ S_\varepsilon
\]

where,

\[
\mu_t = C_\mu \langle \rho_f \rangle^f \langle k \rangle^f \langle \varepsilon \rangle^f
\]

\[
P_k = -\langle \rho_f \rangle^f \langle \mathbf{v} \cdot \mathbf{v} \rangle : \nabla \langle \mathbf{v} \rangle = \left( \mu_t 2 \langle \mathbf{D} \rangle - \frac{2}{3} \langle \rho_f \rangle^f \langle k \rangle^f \mathbf{I} \right) : \nabla \langle \mathbf{v} \rangle
\]

The terms \( S_k \) and \( S_\varepsilon \) in Eqs. 4.12 and 4.13 represent additional sources of \( k \) and \( \varepsilon \), respectively, due to the presence of the porous media. In addition, the \( k-\varepsilon \) model constants \( \sigma_k \), \( \sigma_\varepsilon \), \( C_\mu \), \( C_{1e} \), and \( C_{2e} \) have the usual values of 1.0, 1.3, 0.09, 1.44, and 1.92, respectively [9].

At this point, we shift our focus to the modeling of non-equilibrium turbulent heat and mass transfer inside the porous region. We can consider moist air as a mixture of water vapour and dry air (made of all the gaseous components). The turbulent moist air flow is solved using the aforementioned mass, momentum, and \( k \) and \( \varepsilon \) transport equations. In addition, the moisture content of the moist air is quantified by solving an additional transport equation of water vapour mass fraction \( Y_v \). To account for the moisture gain/loss of air in the numerical model, the relevant transport equations constantly update the moist air density \( \rho_f \) by the following expression

\[
\rho_f = \rho_a + \rho_v = \frac{P_a}{R_a T} + \frac{P_v}{R_v T}
\]

where, \( P_a \) is the dry-air partial pressure, \( P_v \) is the vapour partial pressure, and \( R_a \) and \( R_v \) are the air and vapour gas constants, respectively. The moist air temperature \( T \) is obtained by solving its energy transport equation (see Khan et al. [33] for further details).
Since, the present work is intended for turbulent heat and mass transfer in packed bed of spheres for food storage and refrigeration applications, the present model incorporates non-equilibrium heat and mass transfer inside porous region. The heat and mass transfer of turbulent moist air flow, which forms the fluid-constituent of the porous region, is modeled using its energy transport equation and the vapour mass fraction $Y_v$ equation. The solid-constituent, which is comprised of packed spheres, exchanges heat and mass with the moist air flow by solving separate energy and moisture transport equations. Since we consider that moisture resides in the form of water inside the spheres (food or produce), the moisture transport equation is solved for water mass fraction $Y_w$.

The volume-time-averaged non-equilibrium moisture equations can be expressed as

$$\phi \frac{\partial \langle \rho_f \rangle \langle Y_v \rangle}{\partial t} + \nabla \cdot \left( \langle \rho_f \rangle \langle Y_v \rangle \langle \mathbf{v} \rangle \right) = \nabla \cdot \left( \langle \rho_f \rangle D_{eff,f} \nabla \langle Y_v \rangle \right) + \phi S_{v,f} + \langle \dot{m}_{fs} \rangle$$  \hspace{1cm} (4.17)

$$(1 - \phi) \frac{\partial \langle \rho_s \rangle \langle Y_w \rangle}{\partial t} = \nabla \cdot \left( \langle \rho_s \rangle D_{eff,s} \nabla \langle Y_w \rangle \right) + (1 - \phi) S_{w,s} - \langle \dot{m}_{fs} \rangle$$ \hspace{1cm} (4.18)

The interfacial mass transfer between the fluid and solid-constituents is modeled by $\langle \dot{m}_{fs} \rangle$ term appearing in Eqs. 4.17 and 4.18. The $\langle \dot{m}_{fs} \rangle$ term is quantified based on the quantity of water available inside the solid-constituent. The maximum value of $\langle \dot{m}_{fs} \rangle$ is evaluated as [34]

$$\langle \dot{m}_{fs} \rangle = \langle \rho_f \rangle h_{fs}m A_{fs} \left( \langle Y_v \rangle - \langle Y_v \rangle \right)$$ \hspace{1cm} (4.19)

where, $\langle Y_v \rangle$ refers to the vapour mass fraction at the solid-constituent surface, which is calculated by considering the surface to be saturated with vapor; i.e. having 100% relative humidity. For the case where the available water content is less than the $\langle \dot{m}_{fs} \rangle$ computed using Eq. 4.19, $\langle \dot{m}_{fs} \rangle$ is calculated based on the available water content (see Khan et al. [33] for details).
The present work also considers both the sensible and latent energy components of moist air. In this respect, the specific enthalpy of each species is given as

\[ h_i = c_{p,i}T + h_{fg,i} \]  \hspace{1cm} (4.20)

where, \( i \) is the species number. For the present work \( i = 1 \) (dry air) and 2 (water vapour), and the component of latent energy for dry air is \( h_{fg,1} = 0 \). Moreover, the summation of specific enthalpy of dry air and water vapour provides the total specific enthalpy of the air-vapour mixture. The volume- and time-averaged energy transport equations for the fluid and solid-constituents, respectively, are expressed as [33,35]

\[
\sum_l \phi c_{p,i} \frac{\partial \langle \rho f \rangle}{\partial t} \langle \bar{Y}_{i,f} \rangle f \langle \bar{T}_f \rangle f + \sum_l \phi h_{fg,i} \frac{\partial \langle \rho f \rangle}{\partial t} \langle \bar{Y}_{i,f} \rangle f \langle \bar{T}_f \rangle f \\
+ \sum_l c_{p,i} \nabla \cdot \langle \rho f \rangle f \langle \bar{Y}_{i,f} \rangle f \langle \bar{T}_f \rangle f \langle \bar{\nabla} \rangle f \\
+ \sum_l h_{fg,i} \nabla \cdot \langle \rho f \rangle f \langle \bar{Y}_{i,f} \rangle f \langle \bar{\nabla} \rangle f \\
= \lambda_{eff,f} \nabla^2 \langle \bar{T}_f \rangle f \\
+ \sum_l \nabla \cdot \langle \rho f \rangle f D_{eff,f} \nabla \langle \bar{Y}_{i,f} \rangle f \langle c_{p,i} \bar{\bar{T}}_f \rangle f + h_{fg,i} \\
+ h_{fs}A_{fs}(\langle \bar{T}_s \rangle s - \langle \bar{T}_f \rangle f) \\
\]  \hspace{1cm} (4.21)

\[
\sum_l (1 - \phi) c_{ps,l} \frac{\partial \langle \rho s \rangle s \langle \bar{Y}_{i,s} \rangle s \langle \bar{T}_s \rangle s}{\partial t} \\
= \lambda_{eff,s} \nabla^2 \langle \bar{T}_s \rangle s + \sum_l \nabla \cdot \langle \rho s \rangle s D_{eff,s} \nabla \langle \bar{Y}_{i,s} \rangle s \langle c_{ps,l} \bar{\bar{T}}_s \rangle s \]  \hspace{1cm} (4.22)

We note that the latent energy terms are not included in Eq. 4.22 because the solid-constituent is considered to be composed of solid-structure and water. Similar to the non-equilibrium mass transfer equations, the last two terms on the right-hand side of Eqs. 4.21 and 4.22 account for the interfacial heat transfer between the two constituents of the
porous region. The sensible energy of water before evaporation is included by modeling the source term $S_{e,f} = h_{\text{water}} \langle \dot{m}_{fs} \rangle$ [36], where, $h_{\text{water}}$ refers to the water enthalpy at the local temperature.

4.3 Macroscopic model closure approach

Examination of the macroscopic model (Eqs. 4.9-4.10, 4.12-4.13, 4.17-4.18, 4.21-4.22) presented in the last section shows that terms arising due to volume- and time-averaging of the porous region require closure to complete the model. To this end, mathematical models have been introduced for the terms in question, but coefficients are required to characterize a particular porous material. Herein, we provide a short description of the method of closure for each of the constitutive relations appearing in the momentum, turbulence, moisture and energy equations, and the information required. All information required for closure is obtained from pore-level calculations on a REV that characterizes a randomly packed bed of spheres, which will be discussed in detail in a subsequent section.

Closure of the Darcy and Forchheimer drag terms appearing in Eq. 4.10 is achieved by considering the pore-level hydrodynamics of the REV. The predicted pressure drop across the REV is utilized to evaluate the permeability $K$ and inertial coefficient $c_E$ as [37]

$$\frac{\Delta P}{L} = \frac{\mu_f}{K} \langle \tilde{v} \rangle + \sqrt{\frac{\langle \rho_f \rangle c_E}{K}} |\langle \tilde{v} \rangle| \langle \tilde{v} \rangle$$

(4.23)

where, $\Delta P$ is the pressure drop across the length $L$ of the REV. For each geometric model, creeping flow ($Re_d \approx 0.1$) is considered first to calculate $K$; then $c_E$ is evaluated for higher $Re_d$.

Hydrodynamic closure is completed by closing the macroscopic $k$ and $\varepsilon$ equations. To achieve this, models must be implemented for the $S_k$ and $S_\varepsilon$ terms given in Eqs. 4.12 and 4.13, respectively. The closures for these terms proposed by NK, PDL, and TR are given in Tab. 4.1, which shows that each study has modeled them in a slightly different manner. To better understand these models, consider a REV with one-dimensional fully-
developed flow and zero-mean-shear. Under such conditions, the transport terms in Eqs. 4.12 and 4.13 disappear and the equations reduce to a balance of source and sink terms. For example, the $k$ and $\varepsilon$ equations proposed by NK reduce to

$$0 = -\phi\langle \rho_f \rangle f \langle \varepsilon \rangle f + \phi \langle \rho_f \rangle f \varepsilon_{\infty}$$

(4.24)

$$0 = -\phi C_2 \langle \rho_f \rangle f \langle \varepsilon \rangle f \frac{\langle \varepsilon \rangle f}{\langle k \rangle f} + \phi C_2 \langle \rho_f \rangle f \varepsilon_{\infty} \frac{\varepsilon_{\infty}}{k_{\infty}}$$

(4.25)

which, after simplifications yields

$$\langle k \rangle f = k_{\infty} \text{ and } \langle \varepsilon \rangle f = \varepsilon_{\infty}$$

(4.26)

The model constants $k_{\infty}$ and $\varepsilon_{\infty}$ can then be obtained as the intrinsic-averaged value of $k$ and $\varepsilon$ inside the REV. The closure of $S_k$ and $S_{\varepsilon}$ proposed by PDL and TR can also obtained in the similar manner. In addition, if one includes the dispersive effects of $k$ and $\varepsilon$, then based on Eq. 4.8, the total turbulent kinetic energy $k_{\text{total}}$ and its dissipation rate $\varepsilon_{\text{total}}$ can be written as [16,17]

$$k_{\text{total}} = \langle k \rangle f + k_{\text{disp}}$$

(4.27)

$$\varepsilon_{\text{total}} = \langle \varepsilon \rangle f + \varepsilon_{\text{disp}}$$

(4.28)

where, $k_{\text{disp}}$ and $\varepsilon_{\text{disp}}$ are evaluated, using the expressions proposed by TR, as

$$k_{\text{disp}} = \frac{1}{2} \left( \langle \mathbf{v} - \langle \mathbf{v} \rangle f \rangle^2 \right)^f$$

(4.29)

$$\varepsilon_{\text{disp}} = \nu_f \left( \frac{\partial \mathbf{v}}{\partial x} \frac{\partial \mathbf{v}}{\partial x} + \frac{\partial \mathbf{v}}{\partial y} \frac{\partial \mathbf{v}}{\partial y} + \frac{\partial \mathbf{v}}{\partial z} \frac{\partial \mathbf{v}}{\partial z} \right)^f$$

(4.30)

Thus, the generic closure of the macroscopic $k$-$\varepsilon$ turbulence model including the dispersive effects can be obtained from the solutions of the pore-level, time-averaged turbulent flow field inside the REV.
Table 4.1: Models of $S_k$ and $S_\varepsilon$ proposed by NK [14], PDL [8] and TR [16,17].

<table>
<thead>
<tr>
<th>Turbulent model</th>
<th>$S_k$</th>
<th>$S_\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NK</td>
<td>$\phi\langle p_f \rangle^f \varepsilon_\infty$</td>
<td>$\phi C_k \langle p_f \rangle^f \varepsilon_\infty \frac{\varepsilon_\infty}{k_\infty}$</td>
</tr>
<tr>
<td>PDL</td>
<td>$\frac{\phi C_k \langle p_f \rangle^f \langle k \rangle^f}{\sqrt{K}}</td>
<td>\frac{\phi C_k \langle p_f \rangle^f \langle \varepsilon \rangle^f}{\sqrt{K}}</td>
</tr>
<tr>
<td>TR</td>
<td>$\langle \tilde{\nu} \rangle \left( \frac{\phi \mu_f}{K} \langle \tilde{v} \rangle + \frac{\phi \langle p_f \rangle^f c_E}{\sqrt{K}} \langle \tilde{v} \rangle \right)$</td>
<td>$\frac{\phi f (\phi, K) \langle p_f \rangle^f \langle \varepsilon \rangle^f}{\sqrt{K}}</td>
</tr>
</tbody>
</table>

Closure of the macroscopic, non-equilibrium heat and mass transfer equations requires determination of the interfacial heat and mass transfer coefficients ($h_{fs}$ and $h_{fs,m}$) along with the effective thermal conductivity $\lambda_{eff}$ and mass diffusivity coefficients $D_{eff}$ given in Eqs. 4.17, 4.18, 4.21, and 4.22. Under fully-developed conditions and constant surface temperature, $h_{fs}$ can be evaluated as [38]

$$h_{fs} = -\frac{mc_p}{a_{fs}} \ln \left( \frac{T_s - T_{out}}{T_s - T_{in}} \right) \quad (4.31)$$

where, $a_{fs}$ is the interfacial surface area of the REV, $\dot{m}$ is the mass flow rate though the REV, $T_s$ is the constant surface temperature of the solid-constituent, and $T_{in}$ and $T_{out}$ are the mass-averaged bulk fluid temperatures at the inlet and outlet of the REV, respectively. For evaluation of $h_{fs}$, the value of $T_s$ and $T_{in}$ are set as boundary conditions to determine $T_{out}$. However, under fully-developed conditions, $h_{fs}$ is constant, and hence independent of $T_s$ and $T_{in}$. The effective thermal conductivity of the fluid-constituent, $\lambda_{eff,f}$, arises in Eq. 4.21 due to volume- and time-averaging. This quantity represents the net thermal transport and is utilized in a gradient-diffusion type closure model [35]. Volume-averaging of the energy equation produces tortuosity and thermal dispersion terms, which are modeled as [35]

$$\nabla \cdot \left[ \frac{1}{\Delta V} \int_{a_{fs}} n \lambda_f T_f dA \right] = \lambda_{tor} \nabla \langle T_f \rangle^f \quad (4.32)$$

$$\nabla \cdot \left[ \frac{1}{\Delta V} \int_{a_{fs}} n \lambda_f T_f dA \right] = \lambda_{tor} \nabla \langle T_f \rangle^f \quad (4.32)$$
Thermal dispersion: \(-c_p\langle \rho \rangle f^f (\phi (\bar{V}T_f)^f) = \lambda_{disp} \nabla \langle T_f \rangle^f\) (4.33)\\

Following on, time-averaging of the volume-averaged energy equation results in additional terms characterizing turbulent heat flux and turbulent thermal dispersion, which are closed as [35]

\[
\text{Turbulent heat flux: } -c_p\langle \rho \rangle f^f (\phi (\bar{V}'^f (T_f')^f) = \lambda_t \nabla \langle T_f \rangle^f\\
\text{Turbulent thermal dispersion: } -c_p\langle \rho \rangle f^f (\phi (\bar{V}'^f T_f')^f) = \lambda_{disp,t} \nabla \langle T_f \rangle^f (4.35)
\]

The resulting \(\lambda_{eff,f}\) is then given as [35]

\[
\lambda_{eff,f} = \phi \lambda_f + \lambda_{tor} + \lambda_{disp} + \lambda_t + \lambda_{disp,t} (4.36)
\]

In the above expression, \(\lambda_f\) is the usual thermal conductivity of the fluid-constituent. For the present work, the Tortuosity coefficient \(\lambda_{tor}\) becomes zero due to the approximation of a constant \(T_s\), while, \(\lambda_{disp}\) is evaluated as [32]

\[
\lambda_{disp} = -\frac{c_p\langle \rho \rangle f^f \phi}{\nabla \langle T_f \rangle^f} \left( (\bar{V} - \langle \bar{V} \rangle^f) (\bar{T}_f - \langle \bar{T}_f \rangle^f) \right)^f (4.37)
\]

where,

\[
\nabla \langle T_f \rangle^f \approx \frac{\Delta \langle T_f \rangle^f}{L} = \frac{\langle T_f \rangle_{out}^f - \langle T_f \rangle_{in}^f}{L} (4.38)
\]

where, in the present case, \(\langle T_f \rangle_{in}^f\) and \(\langle T_f \rangle_{out}^f\) represent the area-averaged temperature values at the inlet and outlet surfaces, respectively, which are easily calculated from pore-level results of the REV.

The microscopic simulation results cannot be utilized to evaluate \(\lambda_t\) and \(\lambda_{disp,t}\). To this end, the eddy-diffusivity concept is adopted to model these coefficients as [32]

\[
\lambda_t + \lambda_{disp,t} = c_p\langle \rho \rangle f^f \phi \frac{v_t}{\sigma_r} (4.39)
\]
where, $\nu_t$ is the kinematic turbulent viscosity, and $\sigma_T$ is turbulent Prandtl number for the fluid-constituent energy equation. For the present work, $\sigma_T$ is fixed at 0.9 [35].

Compared to $\lambda_{\text{eff},f}$, the modeling of $\lambda_{\text{eff},s}$, which arises in Eq. 4.22, is much more straightforward, and given as [35]

$$
\lambda_{\text{eff},s} = (1 - \phi)\lambda_s + \lambda_{\text{tor}}
$$

(4.40)

With $\lambda_{\text{tor}}$ equal to zero, for the same reason as discussed earlier, $\lambda_{\text{eff},s}$ only requires solid-constituent thermal conductivity $\lambda_s$ and $\phi$ for evaluation.

For closure of the non-equilibrium mass transport equations, we take the advantage of heat and mass transfer analogy. In this respect, the Chilton-Colburn heat and mass transfer analogy is used to evaluate $h_{fsm}$. This analogy was found to be valid for the case of a packed bed of spheres by Gupta and Thodos [39]. The analogy relates $h_{fs}$ and $h_{fsm}$ as [40]

$$
h_{fsm} = h_{fs} \left(\frac{D_f}{\lambda_f}\right) \left(\frac{Sc}{Pr}\right)^{\frac{1}{3}}
$$

(4.41)

where, $\lambda_f$ and $D_f$ refer to the moist air thermal conductivity and its moisture diffusivity, respectively, and $Pr$ and $Sc$ represent the moist air Prandtl and Schmidt numbers, respectively.

Similar to $\lambda_{\text{eff},f}$, the effective mass diffusivity of the fluid-constituent $D_{\text{eff},f}$ accounts for the usual moisture diffusion, but also includes moisture dispersion, turbulent moisture flux, and turbulent mass dispersion, which are modeled as [32]

$$
D_{\text{eff},f} = \phi D_f + D_{\text{disp}} + D_t + D_{\text{disp},t}
$$

(4.42)

For evaluation of $D_{\text{disp}}$, the heat and mass transfer analogy is again utilized. Comparing the $\lambda_{\text{disp}}$ and $D_{\text{disp}}$ results presented by de Lemos [32] for two-dimensional structured REVs, we can propose the following approximate relation
\[
\frac{\lambda_{\text{eff},f}}{\lambda_f} \approx \frac{D_{\text{eff},f}}{D_f}
\]  

(4.43)

The eddy-diffusivity concept is again employed to model \( D_t \) and \( D_{\text{disp},t} \) as [32]

\[
D_t + D_{\text{disp},t} = \frac{\nu_t}{Sc_t}
\]  

(4.44)

where, \( Sc_t \) is the turbulent Schmidt number, which for the present work is approximately 0.7-0.9 [41]. Finally, \( D_{\text{eff},s} \) is evaluated as \( D_{\text{eff},s} = (1 - \phi)D_s \).

### 4.4 The microscopic model

This section covers the details of the microscopic (pore-level) simulations carried out to evaluate the closure coefficients using the approach described in section 4.3 for the macroscopic model presented in section 4.2. As mentioned earlier, closure is sought herein for a randomly packed bed of spheres. From the computational perspective, geometric modeling of an entire bed of packed spheres is not feasible. Therefore, we utilize REVs having random arrangements of spheres that characterize a small portion of a much larger packed bed. The approach adopted to create the REVs used the formulation developed by Dyck and Straatman [42], except using a modified contact law [43] that was suitable for spherical particles as opposed to spherical voids. Their approach produces three-dimensional domains of randomly packed spheres using YADE [44], with spatial periodicity maintained in the \( x, y \) and \( z \) directions. CAD models of the REVs are created using Solidworks™ [45] and then discretized using the ANSYS® Meshing™ tool [46].

The approach to generating a particular REV is to specify the number of spheres inside the REV along with their diameter (and standard deviation in the case of non-equal sized spheres), and the target porosity of the REV. The model places the spheres (so-called “primitives”) inside of a three-dimensional box and then compresses the box allowing the spheres to collide and reorient until the target porosity is achieved. Though the approach can build REVs where the spheres are rigid solids, slight deformation was allowed to
avoid having point contacts, which can cause issues with mesh generation in the space between the spheres. It was found that at least 50 spheres are required to ensure that the CFD results on the REV are independent of the REV size. Fig. 4.1 shows a sample REV comprised of 50 spheres of equal size randomly oriented to achieve a porosity of 0.47. Fig. 4.1a shows the randomly oriented spheres and the box that represents the REV. The spheres that are outside the box are those that penetrate the boundaries on the opposite periodic face and are simply shown to illustrate how the REV is trimmed out of the random packing. Fig. 4.1b shows the portion of the REV that requires discretization for CFD simulation; i.e. the spheres are subtracted and the fluid space between them remains.

![Image of 50 randomly oriented spheres and REV box]

**Figure 4.1:** a) Geometric model showing 50 randomly oriented spheres of constant $d_s$ and outline of REV box; b) Resulting REV sample with porosity of 0.47.

The fluid space between in the REV was discretized using the ANSYS® Meshing™ tool [46], and pore-level simulations in the REVs were carried out using the commercial CFD software Fluent™ [47]. Since the meshing volume of the REV varies with porosity and sphere diameter, the grid convergence of the domain was based on the ratio of mean sphere diameter $d_s$ to the meshing element size. Tab. 4.2 shows that grid convergence based upon normalized pressure difference, $\Delta \bar{P}/L$, and normalized $\langle k \rangle^f$ and $\langle \varepsilon \rangle^f$ is achieved to within 1% when the ratio is kept to approximately 36.
For consistency, turbulence was modeled in the pore-level (microscopic) simulations using the $k$-$\varepsilon$ model. As the robustness of the macroscopic closure depends on the accuracy of the microscopic simulations, different variations of the $k$-$\varepsilon$ model were tested. The \textit{Realizable} variation compared to the standard model was found to improve the solution convergence as it is better suited to flows having rotation, separation, and recirculation [48]. Moreover, the effects of curvature were incorporated in the model by applying the \textit{curvature correction}, which modifies the turbulence production term in the $k$ and $\varepsilon$ equations [48]. Near-wall effects were accounted for by employing \textit{Enhanced wall treatment}, which resolves the viscous sublayer in the finely meshed regions and employs the law-of-the-wall in the coarsely meshed areas [48]. The use of \textit{Enhanced wall treatment} is necessary in the microscopic model because the meshed REVs have numerous regions of fine mesh, which occur near the contact regions of the spheres. Heat transfer was incorporated by solving the energy transport equation; mass transfer between and among the phases was not included in the pore-level calculations. The advection scheme \textit{QUICK} was utilized for all the transport equations, and pressure-velocity coupling was achieved by employing the \textit{SIMPLEC} algorithm. Air was defined as the working fluid with constant thermophysical properties at standard temperature and pressure. The steady-state problem was simulated until the scaled residuals of all the transport equations dropped below $10^{-3}$.

Periodic boundary conditions were imposed on all pairs of faces of the REV; i.e. $x \rightarrow x + L, y \rightarrow y + L, z \rightarrow z + L$. The mass flow rate along the flow direction was used to impose a flow Reynolds number. Though periodic boundary conditions are imposed on all pairs of faces, we refer to the inlet and outlet faces to be those perpendicular to the flow direction. The mass flow rate is evaluated as

$$\dot{m} = \rho_f L^2 U$$

where, the side length $L$ of the REV is obtained from \textit{YADE} [44] following geometry generation, and the extrinsic flow velocity $U$ is calculated from the Reynolds number, which is defined as
\[ Re_d = \frac{\rho_f U d_s}{\mu_f} \]  

(4.46)

No-slip hydrodynamic conditions were imposed at the surfaces of the spheres. In terms of energy, a mass-weighted bulk inlet temperature \( T_{in} \) was specified, and the surface temperature of the sphere surfaces inside the REV were maintained at \( T_s \). In the present work, \( T_{in} \) and \( T_s \) were set to 5°C and 55°C, respectively, for all the simulations (see Fluent™ Theory Guide [48] for the details of periodic boundary condition implementation).

<table>
<thead>
<tr>
<th>( d_s )/mesh element size</th>
<th>Cell count (million)</th>
<th>Normalized ( \Delta P/L )</th>
<th>Normalized ( \langle k \rangle^f )</th>
<th>Normalized ( \langle \varepsilon \rangle^f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>0.32</td>
<td>63.87</td>
<td>2.13</td>
<td>25.43</td>
</tr>
<tr>
<td>23.5</td>
<td>0.70</td>
<td>65.27</td>
<td>2.91</td>
<td>37.17</td>
</tr>
<tr>
<td>28.6</td>
<td>1.10</td>
<td>65.87</td>
<td>3.07</td>
<td>39.76</td>
</tr>
<tr>
<td>33.3</td>
<td>1.70</td>
<td>66.26</td>
<td>3.18</td>
<td>41.38</td>
</tr>
<tr>
<td>36.4</td>
<td>2.20</td>
<td>67.11</td>
<td>3.25</td>
<td>42.64</td>
</tr>
<tr>
<td>40.0</td>
<td>2.7</td>
<td>67.26</td>
<td>3.27</td>
<td>42.96</td>
</tr>
</tbody>
</table>

The developed microscopic model was validated using the results of Yang et al. [49], which focused on forced convection heat transfer in various structured beds of packed spheres. Their experimental work provides measurements of pressure drop and Nusselt number for packed beds composed of ellipsoidal and spherical particles. Measurements were obtained during the cooling process of initially heated particles. The packed bed was composed of enough particles to ensure that fully-developed flow and heat transfer occurred inside the bed. In addition, the measurements were only taken for the central packed channel to minimize the wall effects of the channel containing the bed.

To mimic this case, simple cubic packing (SC), shown in Fig. 4.2, and body center cubic packing (BCC) REVs based on the information provided by Yang et al. [49] were produced in Solidworks™ [45]. To closely match the experimental conditions, periodic
boundary conditions were imposed on the REV faces normal to the flow, and symmetry boundary conditions were imposed on the remaining REV faces. The flow and temperature boundary conditions were set to match the conditions provided by Yang et al. [49]. The transient problem of cooling was simplified to the steady-state based on the fact that in the fully-developed region, the Nusselt number does not change in time. The domain was discretized using the approach described earlier. The predicted pressure drop and Nusselt number for SC and BBC are shown in Figs. 4.3 and 4.4, respectively. The plots show that the present microscopic model predicts the hydraulic resistance and the heat transfer with reasonable accuracy; trends of both quantities are also correctly predicted as a function of Reynolds number. In this manner, the present model formulation is considered to be suitable and applicable to cases where the packing structure is random. In addition, comparison of Figs. 4.1 and 4.2 clearly demonstrates the inability of structured REVs (Fig. 4.2) to mimic the realistic random packing of spheres.

Figure 4.2: a) Box and spheres for simple cubic packing (SC); b) Resulting SC REV sample with porosity of 0.47.
Figure 4.3: Comparison of predicted pressure drop as a function of Reynolds number for different sphere packings to the experimental results of Yang et al. [49].

Figure 4.4: Comparison of predicted Nusselt number as a function of Reynolds number for different sphere packings to the experimental results of Yang et al. [49].
4.5 Closure results

Results of the pore-level simulations of the REVs are used in this section to close the macroscopic model presented in section 4.2. Results have been obtained for 20 different geometric cases by parametrically varying the mean sphere diameter $d_s$ (along with its statistical variation $d_{\text{var}}$), and porosity $\phi$. The variable $d_{\text{var}}$ defines the local variation of diameter in terms of percentage (or fraction) of $d_s$. For example, with $d_{\text{var}} = 20\%$, spheres inside the REV are uniformly distributed over the range $d_s \pm 0.2 d_s$. As one target application of the present work is food and produce storage industry, the mean sphere diameter was varied over the range $1 \leq d_s \leq 10$ cm, which covers a wide variety of berries and nuts to apples, oranges and potatoes. Specifically, REVs considering $d_s \in \{1 \text{ cm}, 5 \text{ cm}, 10 \text{ cm}\}$ were constructed and discretized, with local variations of sphere diameter of $d_{\text{var}} \in \{0\%, 20\%, 35\%, 50\%\}$.

The porosity of a bed of packed spheres is dependent upon the arrangement of spheres within the packing. The thinnest or loosest packing of spheres has porosity of around 0.476, while the packing of highest density produces a minimum porosity of approximately 0.26 [50]. Based on these limits, the porosity of the randomly packed REVs varied across the range $0.27 \leq \phi \leq 0.47$, specifically for the values: $\phi \in \{0.27, 0.32, 0.37, 0.42, 0.47\}$.

Tab. 4.3 gives a summary of geometric parameterization of the REVs considered herein. The side length $L$ and the interfacial surface area $a_{fs}$ of the generated REVs are required for various calculations, and are included in Tab. 4.3. Note that the specific interfacial surface area $A_{fs}$ can be calculated as $A_{fs} = a_{fs}/L^3$.

As YADE [44] produces random packings of spheres inside the REV, each REV produced is slightly different in terms of its geometry, and within a particular REV the structure in the $x$, $y$ and $z$ directions are all slightly different, even though spatial periodicity is enforced in all principle directions. In this manner, there is no preferred direction for the prescribed flow, so each REV produced was used to simulate three cases of flow and heat transfer; one where the principle flow was prescribed in the $x$-direction, one for the $y$-
direction, and one for the $z$-direction. The results of the three simulations were then averaged to obtain mean values for all quantities.

### Table 4.3: Summary of geometric parameters for the REVs produced using YADE [44]. Side length $L$ and interfacial surface area $a_{fs}$ are also given.

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$d_s$ (cm)</th>
<th>$d_{\text{var}}$ (%)</th>
<th>$L/d_s$</th>
<th>$a_{fs}/d_s^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.27</td>
<td>10</td>
<td>0</td>
<td>3.26</td>
<td>114.65</td>
</tr>
<tr>
<td>0.32</td>
<td>10</td>
<td>0</td>
<td>3.36</td>
<td>129.24</td>
</tr>
<tr>
<td>0.37</td>
<td>10</td>
<td>0</td>
<td>3.45</td>
<td>139.31</td>
</tr>
<tr>
<td>0.42</td>
<td>10</td>
<td>0</td>
<td>3.56</td>
<td>147.81</td>
</tr>
<tr>
<td>0.47</td>
<td>10</td>
<td>0</td>
<td>3.67</td>
<td>150.72</td>
</tr>
<tr>
<td>0.27</td>
<td>5</td>
<td>0</td>
<td>3.26</td>
<td>114.65</td>
</tr>
<tr>
<td>0.37</td>
<td>5</td>
<td>0</td>
<td>3.45</td>
<td>139.31</td>
</tr>
<tr>
<td>0.47</td>
<td>5</td>
<td>0</td>
<td>3.67</td>
<td>150.72</td>
</tr>
<tr>
<td>0.27</td>
<td>1</td>
<td>0</td>
<td>3.26</td>
<td>114.65</td>
</tr>
<tr>
<td>0.37</td>
<td>1</td>
<td>0</td>
<td>3.45</td>
<td>139.31</td>
</tr>
<tr>
<td>0.47</td>
<td>1</td>
<td>0</td>
<td>3.67</td>
<td>150.72</td>
</tr>
<tr>
<td>0.27</td>
<td>10</td>
<td>20</td>
<td>3.32</td>
<td>123.28</td>
</tr>
<tr>
<td>0.37</td>
<td>10</td>
<td>20</td>
<td>3.51</td>
<td>141.90</td>
</tr>
<tr>
<td>0.47</td>
<td>10</td>
<td>20</td>
<td>3.73</td>
<td>156.97</td>
</tr>
<tr>
<td>0.27</td>
<td>10</td>
<td>35</td>
<td>3.41</td>
<td>125.29</td>
</tr>
<tr>
<td>0.37</td>
<td>10</td>
<td>35</td>
<td>3.61</td>
<td>147.76</td>
</tr>
<tr>
<td>0.47</td>
<td>10</td>
<td>35</td>
<td>3.83</td>
<td>160.33</td>
</tr>
<tr>
<td>0.27</td>
<td>10</td>
<td>50</td>
<td>3.54</td>
<td>131.10</td>
</tr>
<tr>
<td>0.37</td>
<td>10</td>
<td>50</td>
<td>3.75</td>
<td>156.55</td>
</tr>
<tr>
<td>0.47</td>
<td>10</td>
<td>50</td>
<td>3.97</td>
<td>168.16</td>
</tr>
</tbody>
</table>

Finally, as fully turbulent flow is found to occur inside a porous media comprised of packed spheres when $Re_d > 300$ [8,34], to provide a wide range of applicability of the closure, the considered range of Reynolds number is $1000 \leq Re_d \leq 100,000$, specifically for the values: $Re_d \in \{1, 5, 10, 25, 100\} \times 10^3$. In addition, cases of $Re_d = 0.1$ were simulated to obtain the permeability of porous media. Accounting for the number of geometric models developed (Tab. 4.3), the fact that each model is run in three directions, and the range of Reynolds number considered, a total of 186 computational runs were made to produce results for the macroscopic model closure.

Before discussing the closure results, in Fig. 4.5, we present the distribution of temperature and velocity inside a typical REV to inform the reader about the complex
nature of flow and other transports occurring inside the bed of packed spheres. The plot shows considerable spatial deviation in fluid temperature due to the presence of highly chaotic turbulent flow.

![Figure 4.5: Distribution of normalized fluid temperature and velocity vectors on planes inside a sample REV. Temperature is normalized as \( (T - T_s)/(T_{in} - T_s) \). Results are for the case of \( Re_d = 10^4, d_s = 10 \text{cm, } d_{\text{var}} = 0\%, \text{ and } \phi = 0.47 \).](image)

To obtain the closure of the volume-time-averaged momentum equation, the permeability \( K \) and inertial coefficient \( c_E \) for the Darcy and Forchheimer models are computed using the procedure described following Eq. 4.23. Plots of these quantities are given in Figs. 4.6 and 4.7, respectively. The permeability is found to be monotonically proportional to porosity. This trend occurs due to the increasing gaps that allow the flow to pass between the spheres more easily. On the other hand, \( c_E \) reduces with increasing porosity, due to a reduction in the intrinsic-velocity and pressure drop of the flow. It can also be observed that \( c_E \) is inversely proportional to \( Re_d \). In addition, \( K \) and \( c_E \) are also found to be only weakly dependent upon \( d_{\text{var}} \). The evaluated permeability was found to match well with the existing correlations for bed of packed spheres [6].
Chapter 4

Figure 4.6: Variation of permeability $K$ with porosity, mean sphere diameter, and its local variation.

Figure 4.7: Variation of inertial coefficient $c_E$ with porosity, Reynolds number, mean sphere diameter, and its local variation.

We obtain closure of the macroscopic $k$-$\epsilon$ model, given in Eqs. 4.12-4.13 by determining the intrinsic-averaged and dispersive components of $k$ and $\epsilon$, as shown in Eqs. 4.27-4.28.
For clarity, the results of $k$ and $\varepsilon$ given in Figs. 4.8 and 4.9, respectively, only consider the parametric variation of porosity and Reynolds number. The plot of $k$ shows that the dispersive component is considerably higher than the intrinsic-averaged component for all the cases. Mathey [31] also found such differences in magnitude between the dispersive and intrinsic-averaged components of $k$ for the case of structurally packed spheres. Similar observations were also made by TR for two-dimensional array of square cylinders. They attribute the dispersive component of $k$ to the presence of recirculation regions, which produce spatial deviations in velocity, and result in a high level of dispersive $k$ as evident from Eq. 4.29. Conversely, the dispersive component of $\varepsilon$ remains low compared to the intrinsic-averaged component. This observation is consistent with that of TR. It can also be observed that both components of $k$ and $\varepsilon$ increase with reducing porosity. This occurs due to the increasing intrinsic-averaged velocity, which ultimately increases velocity fluctuations in space and time. However, $k$ and $\varepsilon$ are found to be reasonably independent of Reynolds number. Moreover, these observed porosity and Reynolds number trends match with the results of NK and TR.

![Figure 4.8](image_url)

**Figure 4.8**: Comparison of the dispersive and intrinsic-averaged components of $k$ as a function of porosity and Reynolds number. The mean sphere diameter and its local variation inside the REVs are equal to 10 cm and 0%, respectively.
Figure 4.9: Comparison of the dispersive and intrinsic-averaged components of $\varepsilon$ as a function of porosity and Reynolds number. The mean sphere diameter and its local variation inside the REVs are equal to 10 cm and 0%, respectively.

The total turbulent kinetic energy and dissipation rate, $k_{total}$ and $\varepsilon_{total}$, are given in Figs. 4.10 and 4.11, respectively. The plots clearly show that mean sphere diameter and its local variation have an insignificant effect on the $k$ and $\varepsilon$ distribution. Thus, $k_{total}$ and $\varepsilon_{total}$ can be considered to be a function of porosity and Reynolds number.

Figure 4.10: Variation of the total turbulent kinetic energy $k_{total}$ with porosity, Reynolds number, mean sphere diameter, and its local variation.
Figure 4.11: Variation of the total dissipation rate of turbulent kinetic energy $\varepsilon_{total}$ with porosity, Reynolds number, mean sphere diameter, and its local variation.

As described in section 4.3, closure of the volume-time-averaged non-equilibrium energy transport equations requires the determination of $h_{fs}$, $\lambda_{disp}$, and $\nu_t$. The kinematic turbulent viscosity $\nu_t$ is obtained from the results of $k_{total}$ and $\varepsilon_{total}$ presented earlier. To make the results generic, $h_{fs}$ is described by an interfacial Nusselt number as $N_u_{fs} = h_{fs}d_s/\lambda_f$. Figs. 4.12 and 4.13 show the results of $N_u_{fs}$ and $\lambda_{disp}$, respectively. As expected, the value of both quantities increases significantly with the flow Reynolds number. However, $N_u_{fs}$ and $\lambda_{disp}$ show comparatively less dependence on porosity. Moreover, $\lambda_{disp}$ is found to be only weakly affected by $d_{var}$. The evaluation of $\lambda_{disp}$ also shows that thermal dispersion is considerably higher for all cases, which is similar to the higher values of $k_{disp}$ and $\varepsilon_{disp}$.

The analysis of velocity, turbulence, and temperature fields inside the REVs reveal high spatial variations. As discussed earlier, the main cause of such high spatial variations is the turbulent flow inside the complex packed spheres domain, which produces complex recirculation, separation, and reattachment regions. Lastly, all the presented results are found to be independent of the mean sphere diameter $d_s$ as shown in Figs. 4.6-4.13.
At this point, we propose a correlation for each closure variable evaluated for the macroscopic model, such that the closure results can be easily implemented in a volume-
averaged porous media framework. The correlations are proposed in the form of a power law for porosity and Reynolds number because the results presented in Figs. 4.6-4.13 show logarithmic trends. Where necessary, a linear component is used to correlate $d_{var}$.

To evaluate the correlations, the MATLAB Curve/Surface Fitting Toolbox™ was used, which utilizes the method of least squares to fit the data. The evaluated correlations are given in Tab. 4.4, where $d_s$ is utilized in meter instead of cm. The table also lists the coefficient of determination ($R^2$) to show how well the correlations fit the data. For all the closure variables, values obtained from the simulations are plotted as a function of the value predicted from the proposed correlation in Fig. 4.14. The plots show that power law-based correlations provide reasonable predictions for all variables. Though in some cases, second degree polynomial-based correlations more accurately predict the values, power law correlations were selected because of their conciseness.

**Table 4.4: Proposed correlations for $k_{total}$, $\epsilon_{total}$, $K$, $c_E$, $Nu_{fs}$, and $\lambda_{disp}$. Valid range of correlations: $0.01 \leq d_s \leq 0.1$ m, $0 \leq d_{var} \leq 50$ %, $0.27 \leq \phi \leq 0.47$ and $10^3 \leq Re_d \leq 10^5$.**

<table>
<thead>
<tr>
<th>Closure variable</th>
<th>Proposed closure correlation</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total turbulent kinetic energy</td>
<td>$\frac{k_{total}}{U^2} = 0.424 \phi^{-3.084} Re_d^{-0.029}$</td>
<td>0.99</td>
</tr>
<tr>
<td>Total dissipation rate of</td>
<td>$\frac{\epsilon_{total} d_s}{U^3} = 0.818 \phi^{-4.59} Re_d^{-0.0916}$</td>
<td>0.99</td>
</tr>
<tr>
<td>turbulent kinetic energy</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Permeability of porous media</td>
<td>$K = 0.0335 \phi^{3.58} + (3.063 \times 10^{-6}) d_{var}$</td>
<td>0.99</td>
</tr>
<tr>
<td>$d_s^2$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inertial coefficient of porous</td>
<td>$c_E = 0.103 \phi^{-2.054} Re_d^{-0.064} - 0.001 d_{var}$</td>
<td>0.97</td>
</tr>
<tr>
<td>media $c_E$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Interfacial Nusselt number</td>
<td>$Nu_{fs} = 0.142 \phi^{-1.07} Re_d^{0.746}$</td>
<td>0.98</td>
</tr>
<tr>
<td>$Nu_{fs}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Thermal dispersion coefficient</td>
<td>$\frac{\lambda_{disp}}{\lambda_f} = 1.59 \phi^{0.8} Re_d^{0.953} + 10.0 d_{var}$</td>
<td>0.99</td>
</tr>
<tr>
<td>$\lambda_{disp}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Heat transfer inside the packed beds has been extensively studied. Since we have proposed a $Nu_{fs}$ correlation, it is worth comparing the correlation and the obtained results against the existing $Nu_{fs}$ literature. In this respect, the correlations and their derived results proposed by Wakao et al. [51], Gillespie et al. [52] and Achenbach [53] were found to be in the similar range as proposed by the present work.
Figure 4.14: Comparison of the correlations given in Tab. 4.4 versus the values of $k_{\text{total}}$, $\varepsilon_{\text{total}}$, $K$, $c_E$, $N_{uf_s}$, and $\lambda_{\text{disp}}$ obtained from the numerical simulations.
4.6 Summary

The present study focused on the closure of the macroscopic turbulence, and non-equilibrium turbulent heat and mass transfer model inside porous media composed of randomly packed spheres. The closures were required to model the additional terms that arise due to volume- and time-averaging of the transport equations. The closure of Darcy and Forchheimer terms appearing in the momentum equation required determination of porous media permeability and its inertial coefficient. For the non-equilibrium heat and mass transport equations, interfacial heat and mass transfer coefficients were needed to close the interfacial heat and mass transfer terms, respectively. Using a gradient-diffusion type model, closures were also obtained for the heat and mass transfer terms for dispersion, turbulent flux, and turbulent dispersion. The macroscopic turbulence inside porous media was modeled using the $k$-$\varepsilon$ model. The dispersive effects of $k$ and $\varepsilon$ were also included to entirely capture the turbulence flow field.

The macroscopic model closure was obtained by simulating the problem at the pore-level or microscopic scale. In this respect, the REVs composed of randomly arranged spheres were subjected to turbulent flow and heat transfer. The conditions of fully-developed unidirectional flow with zero-mean-shear were employed to obtain the closure using the solution fields available at the microscopic scale. The developed microscopic scale model was validated using the experimental data of pressure drop and Nusselt number. The parametric variation of porosity, Reynolds number, mean sphere diameter and its local variation inside the REVs was carried out to increase the applicability of the closure results. In general, all the closure variables were found to be dependent upon the porosity and Reynolds number. However, the mean sphere diameter did not change the results. While, the local variation in spheres’ diameter weakly effected the results. Lastly, the closure results were fitted using the power law-based correlations for ease of implementation into a volume-averaged framework.
References


Chapter 5

5  Thesis summary

In this chapter, we present the overall summary of the thesis. Moreover, we also discuss the novel contributions of the present work. Lastly, recommendations are made to further extend the present work.

5.1  Summary of chapters

In the thesis, a formulation was developed that simulates non-equilibrium heat and mass transfer in conjugate fluid/porous/solid framework. Moreover, the formulation is capable of simulating complex heat and mass transfer problems from laminar to turbulent flow regimes. Complex heat and mass transport problems related to evaporative cooling and convective drying of wet porous materials were simulated to demonstrate and validate the developed formulation. The model was discretized using the finite-volume approach.

In chapter 2, a numerical formulation was developed capable of simulating non-equilibrium heat and mass transfer in three-dimensional conjugate fluid/solid/porous frameworks. The governing transport equations were presented for the fluid, solid, and porous regions. Mathematical conditions were also presented to ensure that heat and mass transfer occurred smoothly across fluid-porous, fluid-solid and porous-solid interfaces. The developed formulation was validated by simulating problems related to evaporative cooling and drying of wet porous media. The simulated cases showed that the results were accurate compared to the available experimental results, and were physically realistic, which demonstrated the robustness of the developed formulation.

In chapter 3, the formulation developed in chapter 2 was employed to simulate the convective drying of wet porous materials. The material to be dried was considered as the porous region, which was coupled through interfaces to the surrounding pure fluid region. The model included non-equilibrium heat and moisture transport in the porous region such that the fluid and solid constituents, and the exchanges between them, were captured. The complexity of the problem required additional modeling for interfacial
moisture transfer between the porous and pure fluid regions. The study considered the
drying of an apple slice to validate the developed drying model against available
experimental data. The results showed accurate prediction of moisture content as a
function of drying time for different airflow velocities, and correctly captured the
influences of relative humidity and temperature on the drying rate.

In chapter 4, the model was extended to include turbulent flow regimes. To this end, the
focus turned to turbulence modeling inside porous media, since, turbulence modeling in
pure fluid region and at fluid-porous interfaces has already been studied. As such, the
chapter was focused on obtaining the closure of the macroscopic turbulent and turbulent
non-equilibrium heat and mass transfer inside porous media comprised of a randomly
packed bed of spheres. In this respect, the closure results were derived from pore-level
information obtained from numerical simulations of turbulent heat transfer and fluid
flow. The $k$-$\varepsilon$ model was utilized to incorporate turbulence at both the levels, and the
dispersive effects of turbulence were also considered. The closure results were found to
be dependent upon the porosity and Reynolds number. However, the mean sphere
diameter and its local variation inside the bed of spheres only weakly affected the results.
The closure results were presented as power law-based correlations, such that they can be
easily implemented in the macroscopic model.

Based on the summary of the thesis, we can conclude that we were able to successfully
develop a formulation for complex heat and mass transfer problems involving porous
media over a wide range of Reynolds numbers. It has been demonstrated that the
formulation is generic and yet capable of being modified to the specific requirements of a
problem. Moreover, the formulation was found capable of being extended in different
directions to further enhance its applicability.

5.2 Summary of novel contributions

- The first and most significant novel contribution of the thesis is the development
  of a formulation presented in chapter 2 that simulates non-equilibrium heat and
  mass transfer in conjugate fluid/porous/solid framework. In the existing
  literature, prior to this work, no such generic formulation existed that combined
the non-equilibrium heat and mass transfer inside porous media with the conjugate fluid/porous/solid framework. Moreover, with all the required capabilities, the developed formulation accurately simulated various types of complex heat and mass transfer problems.

- Also in chapter 2, the air-water vapor mixture energy equation was shown to also account for the latent heat of evaporation of water by constantly tracking the energy of the mixture, which is the second novel contribution of the thesis. This approach, unlike other studies [1-4], does not require a source term in the energy equation to account for the latent heat of evaporation of water.

- With respect to the modeling of convective drying of an apple slice in chapter 3, the detailed modeling of interfacial moisture transport at fluid-porous interfaces is the third novel contribution. Earlier, a few studies [5-9] had employed a conjugate fluid/porous framework to model a convective drying process, but, none of these studies comprehensively discussed moisture transport at fluid-porous interfaces, which is essential to capture the physics of the problem. Conversely, the present study utilized resistance circuit analogy to clearly demonstrate moisture transport at fluid-porous interfaces.

- The fourth novel contribution is the detailed modeling of apple as porous material carried out in chapter 3. With respect to the modeling of porous materials, the existing literature [5,10,11] generally utilized bulk thermophysical properties of porous materials. In the present work, we modeled the apple flesh as porous material with great detail by providing thermophysical properties of both the fluid and solid-constituents. Moreover, volume fraction and density of different components of the apple were also provided. Such detailed modeling of the apple enabled us to capture the intricate details of the drying process. In addition, the modeling procedure is generic, and applicable to other produce or porous materials.

- In chapter 4, the closure of the macroscopic turbulence and turbulent non-equilibrium heat and mass transfer model inside a porous media comprised of a
randomly packed bed of spheres is the fifth novel contribution of the thesis. The closure was derived for the entire macroscopic model that included mass, momentum, turbulence, non-equilibrium heat and mass transport equations. Although, such detailed closure is necessary to complete the macroscopic model, however, no studies in the past were focused on such detailed three-dimensional closures. Moreover, the existing literature also lacked the parametric variations carried out in the present work to derive the closure.

5.3 Future recommendations

To further extend the capabilities of the developed formulation, the following points should be considered

i. In chapter 1, we derived the volume-averaged version of the transport equations for porous region by neglecting the spatial variation of the moist air density (Eq 1.22). Although, this assumption holds valid for the present work and it has provided results that are in good agreement with experimental data, it will be worth to consider the spatial variation of moist air density during the volume-averaging operation. Such consideration may result in new terms that can capture new features of complex heat and mass transfer problems.

ii. As mentioned earlier, in terms of the extension of the model developed in chapter 2, chapter 3 serves as an intermediate step towards implicit dynamic coupling of porous media phases for the applications related to food storage and processing industries. Such extension will allow us to capture many natural processes occurring inside food or produce stacks.

iii. The turbulent heat and mass transport equations for fluid-constituent of porous media presented in chapter 4 were derived by de Lemos [12], who derived these equations for pure fluid rather than air-water vapour mixture considered in the present work. If we time- and volume-average the transport equations by considering air-water vapour mixture then it would result in new terms requiring closure. However, based on our judgement, such terms may not be as significant
as the ones derived by de Lemos [12]. Nevertheless, we can expect some advancement in our knowledge going forward in this direction.

iv. Finally, the incorporation of shrinkage effects in the present model will allow us to more accurately capture the phenomena related to convective drying and produce storage. In this respect, the present model has all the capabilities to be extended in this direction.
References


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