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# FUNDAMENTAL DERIVATION OF CONTINUUM THERMODYNAMIC GOVERNING ENERGY EQUATIONS AND ORDER OF MAGNITUDE ESTIMATES

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### ABSTRACT

This paper is concerned with the volume-averaged mathematical description of heat transfer through packed pebble beds, with special application to pebbled bed modular nuclear reactors. Allthough much work has been done on constructing such mathematical equations, very little is available for systems which are in a state of local-thermal-non-equilibrium. The latter is the case when the solid and fluid are at different temperatures on a volume averaged level, which is prevalent the in the work under consideration. This paper details the fundamental derivation of the implicated governing equations viz. fluid and solid energy conservation. This is followed by order of magnitude estimates for the case of helium flow through a bed of randomly packed graphite spheres in order to identify the dominant heat diffusive type heat transfer modes. Conclusive deductions are made from the study.

### INTRODUCTION

The microscopic (pore-scale) description of the heat transfer phenomenon prevalent in the packed beds found in the pebble bed modular reactor is prohibitively expensive from a numerical modelling point of view. A viable alternative is setting up governing equations in terms of macroscopic (microscopic-volumeaveraged) quantities, and thus reducing the porous system to a continuum. The macroscopic approach results in a set of nonlinear coupled partial differential equations which are written in terms of microscopically-volume-averaged hydrodynamic quantities (density, temperature, velocity etc.). It therefore circumvents the explicit modelling of microscopic phenomenon, which may be accounted for in a microscopic-volume-averaged sense via empirical constitutive relations.

This work is concerned with the continuum (macroscopic)

mathematical modeling of the heat and mass transfer processes prevalent during fluid flow through a stationary randomly packed bed of spheres, where the system is in a state of local thermal non-equilibrium. From recent work performed by the authors, it has become clear that there is currently an absence of a *fundamental* derivation for the energy equations which describe the aforementioned. This document serves to, for the first time, develop such a derivation.

For the purpose of the fundamental derivation, the work of Whitaker [9] is considered due to it offering an alternative perspective to those considered to date, and importantly, being mathematically elaborate and rigorous. The aforementioned employs an approach referred to as *the method of volume averaging*, which may be applied to an arbitrary two-phase system shown schematically in Figure 1.

# VOLUME AVERAGED ENERGY CONSERVATION EQUATIONS

The following sections are devoted to the mathematical derivation of the volume averaged energy conservation equations for both fluid and solid phases of the packed bed.

#### SIMPLIFYING ASSUMPTIONS

The simplifying assumptions which are applicable to the two-phase system under consideration are:

1. Due to the relatively low velocities (significantly below sonic velocities), viscous dissipation effects as well as the kinetic energy contribution to the total energy is assumed negligible (this is similar to other researchers such as Kuipers et al. [5], Becker and Laurien [1] and du Toit et al. [2]).

- 2. Further to the previous assumption, fluid material properties are assumed to be invariant with respect to magnitude of the variation in the pressure field. Note however that fluid properties, with the exclusion of specific heat, are to be fully variant with respect to temperature. This is typically the case for the gases employed in reactors.
- 3. Solid material properties are assumed to be invariant with respect to both temperature and pressure, with the exclusion of thermal conductivity.
- 4. The solid matrix is macroscopically rigid and solid particles impermeable.
- 5. No chemical reactions occur.
- 6. On a macroscopic (volume averaged) scale the solid phase is assumed to be isotropic (invariant with respect to coordinate rotation) and heterogeneous (variant with respect to coordinate translation).
- 7. The effect of nuclear fission may be accounted for on microscopic level (volume averaged molecular scales) by a spatially varying but locally continuous (in the region of a fuel pebble where nuclear fuel is present) volumetric heat source.



Figure 1: Schematic of single phase flow through a porous matrix. The volume averaging length scales are also shown. Note that  $\mathcal{V}(\mathbf{x}_{\mathcal{V}})$  is the averaging volume with center at  $\mathbf{x}_{\mathcal{V}}$  and  $\mathbf{n}_{fs} = -\mathbf{n}_{sf}$ .

$$\mathcal{V}(\mathbf{x}) = \mathcal{V}_f(\mathbf{x}) + \mathcal{V}_s(\mathbf{x}) \tag{1}$$

where the subscripts f and s denote fluid and solid phases respectively. Further, in the figure  $R_{\mathcal{V}}$  is the length scale associated with the size of the volume averaged region  $\mathcal{V}$ , and  $\ell_s$  and  $\ell_f$ indicate length scales associated with the solid and fluid phases respectively.

As a rule, all volume averaged quantities are given with respect to  $\mathbf{x}_{\mathcal{V}}$  unless explicitly stated to be a function of  $\mathbf{x}$ . Accordingly, the void-fraction of fluid is given by

$$\varepsilon = \varepsilon(\mathbf{x}_{\mathcal{V}}) = \frac{1}{\mathcal{V}} \int_{\mathcal{V}_f(\mathbf{x})} d\mathcal{V}$$
(2)

Intrinsic microscopic-volume-averaged quantities for a phase  $\gamma$  are calculated as

$$\begin{aligned} \langle \phi_{\gamma} \rangle^{\gamma} &= \langle \phi_{\gamma} \rangle^{\gamma}(t, \mathbf{x}_{\mathcal{V}}) &= \frac{1}{\mathcal{V}_{\gamma}(\mathbf{x}_{\mathcal{V}})} \int_{\mathcal{V}_{\gamma}(\mathbf{x})} \phi_{\gamma}(t, \mathbf{x}_{\mathcal{V}} + \tilde{\mathbf{x}}) d\mathcal{V} \\ &= \frac{1}{\mathcal{V}_{\gamma}} \int_{\mathcal{V}_{\gamma}(\mathbf{x})} \phi_{\gamma}(t, \mathbf{x}) d\mathcal{V} \end{aligned} \tag{3}$$

where  $\mathbf{x} = \mathbf{x}_{\mathcal{V}} + \tilde{\mathbf{x}}$  (see Figure 1),  $\tilde{\mathbf{x}}$  being the position relative to the averaging volume center  $\mathbf{x}_{\mathcal{V}}$ . Further,  $\phi_{\gamma}(t, \mathbf{x} \in \mathcal{V}_{\gamma})$  describes a property/scalar condition on microscopic level at a time t and spatial position  $\mathbf{x}$ , and  $\mathcal{V}_{\gamma}(\mathbf{x})$  denotes the volume of phase  $\gamma$  over which averaging is applied and such that only spatial locations which contain phase  $\gamma$  are relevant. Importantly, note that in all cases it is assumed that the complete spatial domain over which is being averaged ( $\mathcal{V}(\mathbf{x}_{\mathcal{V}})$ ) is chosen such that both the quantity being averaged  $\phi_{\gamma}$  as well as the solid-matrix is not "disordered" with respect to the averaging volume  $\mathcal{V}$  (Whitaker [9]). Alternatively, the centroid of the domain over which is being volume averaged is to be situated close to the geometric center of  $\mathcal{V}$ .

The superficial volume average of a property  $\phi_{\gamma}$  on  $[t,\mathbf{x}_{\mathcal{V}}]$  is defined as

$$\begin{aligned} \langle \phi_{\gamma} \rangle &= \frac{1}{\mathcal{V}(\mathbf{x}_{\mathcal{V}})} \int_{\mathcal{V}_{\gamma}(\mathbf{x})} \phi_{\gamma}(t, \mathbf{x}_{\mathcal{V}} + \tilde{\mathbf{x}}) d\mathcal{V} \\ &= \frac{1}{\mathcal{V}} \int_{\mathcal{V}_{\gamma}(\mathbf{x})} \phi_{\gamma}(t, \mathbf{x}) d\mathcal{V} \end{aligned}$$

## **MATHEMATICAL PRELIMINARIES**

The spatial volume  $\mathcal{V}$  over which microscopic-volume-averaging is applied (see Figure 1) reads

from where it is clear that the relationship between superficial and intrinsic volume averaged quantities are given by

$$\langle \phi_{\gamma} \rangle = \varepsilon \langle \phi_{\gamma} \rangle^{\gamma} \tag{4}$$

As stated previously,  $\varepsilon$  denotes porosity.

A key mathematical concept in the method of volume averaging is the *spatial averaging theorem* (Slattery [7], Whitaker [8]), which is an extension to multi-dimensions of the Leibniz rule for interchanging differentiation and integration. For a twophase system with phases  $\gamma$  and  $\beta$ , the form which operates on a microscopic scalar quantity  $\phi$  of phase  $\gamma$  follows:

$$\left\langle \frac{\partial \phi_{\gamma}}{\partial x_{j}} \right\rangle = \frac{\partial}{\partial x_{j}} \langle \phi_{\gamma} \rangle + \frac{1}{\mathcal{V}} \int_{\mathcal{A}_{\gamma\beta}} \phi_{\gamma}(t, \mathbf{x}) n_{j_{\gamma\beta}} d\mathcal{A}$$
(5)

where  $n_{j_{\gamma\beta}}$  denotes the component of the outward pointing unit vector to the interface between the phases viz.  $A_{\gamma\beta}$  with normal-unit-vector pointing toward phase  $\beta$ . The version of the equation which operates on a microscopic vector quantity  $\mathbf{a}_{\gamma}$  of phase  $\gamma$  reads:

$$\left\langle \frac{\partial a_{j_{\gamma}}}{\partial x_{j}} \right\rangle = \frac{\partial}{\partial x_{j}} \langle a_{j_{\gamma}} \rangle + \frac{1}{\mathcal{V}} \int_{\mathcal{A}_{\gamma\beta}} a_{j_{\gamma}}(t, \mathbf{x}) n_{j_{\gamma\beta}} d\mathcal{A} \quad (6)$$

where tensor summation is implied.

#### Derivation: Volume Averaged Energy Conservation Equations

This section focuses on the fundamental derivation of the volume averaged energy conservation governing equations for both the fluid and solid phases. In each case the derivation shall commence with the microscopic governing equation as starting point. The final volume-averaged equation will be written in generalised axi-symmetric coordinates, where Cartesian coordinates may be recovered by setting the introduced nondimensional radius term (as described in the next section) to unity.

#### Fluid Phase

Following the simplifying assumptions given in Section, the microscopic energy continuum conservation equation which holds at every point in the fluid, may be written for a Cartesian co-ordinate system as

$$\frac{\partial}{\partial t} \left[ \rho_f C_{p_f} T_f \right] + \frac{\partial}{\partial x_j} \left[ \rho_f C_{p_f} u_j T_f \right] = \frac{\partial}{\partial x_j} \left( k_f \frac{\partial T_f}{\partial x_j} \right) \quad (7)$$

where  $\rho_f$ ,  $C_{p_f}$ ,  $T_f$  and  $k_f$  respectively denote the fluid density, specific heat at constant pressure, temperature and fluid conductivity. Further,  $u_j$  denotes the velocity of the fluid in coordinate direction  $x_j$ . The associated boundary conditions at the fluid-solid interface are

where the velocity no-slip condition has been applied and  $\mathcal{I}$  denotes the relevant temporal domain.

Volume-averaging commences by integrating Equation (7) over the averaging volume  $\mathcal{V}$ :

$$C_{p_f} \frac{1}{\mathcal{V}} \int_{\mathcal{V}_f} \frac{\partial}{\partial t} \left( \rho_f(T_f) T_f \right) d\mathcal{V} + C_{p_f} \left\langle \frac{\partial}{\partial x_j} \left( \rho_f(T_f) u_j T_f \right) \right\rangle = \left\langle \frac{\partial}{\partial x_j} \left( k_f(T_f) \frac{\partial T_f}{\partial x_j} \right) \right\rangle$$
(9)

where density is taken to be a function of temperature only and  $C_{p_f}$  is constant (refer to Section ).

The above equation is indeterminate in the volume averaged (macroscopic) domain in its present form as it is written in terms of intrinsic values viz.  $T_f$  and  $u_f$ . In the following sections it will be endeavored to cast each of the terms viz. temporal, convective and diffusive, into macroscopically determinate form. We commence by considering the temporal term first.

#### **Temporal Derivative Term**

Considering the temporal derivative term in Equation (9) and noting that  $\mathcal{V}$ ,  $\mathcal{V}_f$  and  $\varepsilon$  are invariant with respect to time in the microscopic domain, it follows that

$$C_{p_f} \frac{1}{\mathcal{V}} \int_{\mathcal{V}_f} \frac{\partial}{\partial t} \left( \rho_f(T_f) T_f \right) d\mathcal{V} = \varepsilon C_{p_f} \frac{\partial}{\partial t} \langle \rho_f(T_f) T_f \rangle^f \quad (10)$$

where Equation (4) has been employed to cast the superficial volume average integral into intrinsic form.

Similar to Kaviany [3], we commence in dealing with the microscopic quantities in the temporal term by defining the following relation between the microscopic and macroscopic scalar fields:

$$\phi_{\gamma}(t, \mathbf{x}) = \langle \phi_{\gamma} \rangle^{\gamma}(t, \mathbf{x}_{\mathcal{V}}) + \tilde{\phi}_{\gamma}(t, \mathbf{x})$$
(11)

where, as opposed to the previous equation,  $\langle \phi_{\gamma} \rangle^{\gamma}$  is defined at the volume averaging center and  $\tilde{\phi}_{\gamma}(t, \mathbf{x})$  denotes the deviation of the microscopic quantity  $\phi_{\gamma}$  from the aforementioned.

By applying the relation (11) to all microscopic quantities in the temporal derivative term (right-hand-side of Equation (10)) it follows that:

$$\varepsilon C_{p_f} \frac{\partial}{\partial t} \langle \rho_f T_f \rangle^f = \varepsilon C_{p_f} \frac{\partial}{\partial t} \left\langle \left( \langle \rho_f \rangle^f + \tilde{\rho}_f(t, \mathbf{x}) \right) \times \left( \langle T_f \rangle^f + \tilde{T}_f(t, \mathbf{x}) \right) \right\rangle^f$$
$$= \varepsilon C_{p_f} \frac{\partial}{\partial t} \left[ \langle \rho_f \rangle^f \langle T_f \rangle^f + \langle \rho_f \tilde{T}_f \rangle^f \right] \quad (12)$$

where the relation  $\langle \tilde{\rho}_f \tilde{T}_f \rangle^f = \langle \rho_f \tilde{T}_f \rangle^f$  has been employed (the latter relation may be easily derived). Within a reactor composed of a randomly packed bed of spheres, it is reasonable to believe that the volume averaged *variation* in temperature  $\tilde{T}_f$  is small in comparison with the absolute temperature as the latter is typically of  $O(100) \sim O(1000)$ . This results in the final form of the temporal derivative term follows:

$$C_{p_f} \frac{1}{\mathcal{V}} \int_{\mathcal{V}_f} \frac{\partial}{\partial t} \left( \rho_f(T_f) T_f \right) d\mathcal{V} = \varepsilon C_{p_f} \frac{\partial}{\partial t} \left[ \langle \rho_f \rangle^f \langle T_f \rangle^f \right]$$
(13)

#### **Convective Term**

The convective term in Equation (9) is considered next. We commence by applying the volume averaging Equation (6) which results in:

$$C_{p_f} \left\langle \frac{\partial}{\partial x_j} \left( \rho_f u_{f_j} T_f \right) \right\rangle = C_{p_f} \frac{\partial}{\partial x_j} \left[ \left\langle \rho_f u_{f_j} T_f \right\rangle \right] + C_{p_f} \frac{1}{\mathcal{V}} \int_{\mathcal{A}_{f_s}} \rho_f u_j T_f n_{j_{f_s}} d\mathcal{A} \quad (14)$$

Applying the no-slip boundary condition from Equation (8) (velocity at the fluid-solid interface is zero), renders the surface integral term zero.

By applying Equation (11) in addition to the approriate order of magnitude estimates, expression for the spatial derivative term follows as

$$C_{p_f} \left\langle \frac{\partial}{\partial x_j} \left( \rho_f u_{f_j} T_f \right) \right\rangle = C_{p_f} \frac{\partial}{\partial x_j} \left[ \varepsilon \langle \rho_f \rangle^f \left( \langle u_{f_j} \rangle^f \langle T_f \rangle^f + \langle \tilde{u}_{f_j} \tilde{T}_f \rangle^f \right) \right]$$
(15)

The last term on the right-hand-side accounts for dispersion. By employing a turbulent modeling analogy Kaviany [3], the velocity-temperature-variation term may be expressed as

$$\langle \tilde{u}_{f_j} \tilde{T}_f \rangle^f = \langle \tilde{u}_{f_j} b_i \rangle^f \frac{\partial \langle T_f \rangle^f}{\partial x_i} = -D^d_{ij} \frac{\partial \langle T_f \rangle^f}{\partial x_i}$$
(16)

where  $D_{ij}^d$  is the *thermal dispersion tensor* of rank two which may be expressed as

$$D_{ij}^{d} = \left[\frac{\langle u_{f_{j}}\rangle\langle u_{f_{i}}\rangle}{\sqrt{\langle u_{f_{j}}\rangle\langle u_{f_{j}}\rangle}}D_{\parallel}^{d} + \left(\delta_{ij} - \frac{\langle u_{f_{j}}\rangle\langle u_{f_{i}}\rangle}{\sqrt{\langle u_{f_{j}}\rangle\langle u_{f_{j}}\rangle}}\right)D_{\perp}^{d}\right] (17)$$

where  $\delta_{ij}$  denotes the Kronecker delta and  $D_{\parallel}^d$  and  $D_{\perp}^d$  are respectively the components of the thermal dispersion tensor in the directions normal and perpendicular to the direction of the superficial or intrinsic volume averaged velocity vector. As noted above, correlations for the latter are as per Koch and Brady [4] for the case where  $k_s = 0$ .

The volume averaged convective term in final form now follows

$$C_{p_f} \left\langle \frac{\partial}{\partial x_j} \left( \rho_f u_{f_j} T_f \right) \right\rangle = C_{p_f} \frac{\partial}{\partial x_j} \left[ \varepsilon \langle \rho_f \rangle^f \langle u_{f_j} \rangle^f \langle T_f \rangle^f \right] - C_{p_f} \frac{\partial}{\partial x_j} \left[ \langle \rho_f \rangle^f \varepsilon D_{ij}^d \frac{\partial \langle T_f \rangle^f}{\partial x_i} \right]$$
(18)

where all terms are determinable on a volume-averaged level.

#### **Diffusive term**

Treatment of the diffusive term in Equation (9) commences by applying the volume averaging theorem for a vector (Equation 6). The mathematical depiction follows

$$\left\langle \frac{\partial}{\partial x_j} \left( k_f(T_f) \frac{\partial T_f}{\partial x_j} \right) \right\rangle = \frac{\partial}{\partial x_j} \left[ \varepsilon \left\langle k_f(T_f) \frac{\partial T_f}{\partial x_j} \right\rangle^f \right] + \frac{1}{\mathcal{V}} \int_{\mathcal{A}_{fs}} k_f(T_f) \frac{\partial T_f}{\partial x_j} n_{j_{fs}} d\mathcal{A} \quad (19)$$

By implementing the above in addition to the volume averaging theorem, it may be proven that

$$\left\langle \frac{\partial}{\partial x_j} \left( k_f(T_f) \frac{\partial T_f}{\partial x_j} \right) \right\rangle = \frac{\partial}{\partial x_j} \left[ k_{f_{eff}}^{cond.} (\langle T_f \rangle^f, \varepsilon) \frac{\partial \langle T_f \rangle^f}{\partial x_j} \right] + \frac{1}{\mathcal{V}} \int_{\mathcal{A}_{fs}} k_f(T_f) \frac{\partial T_f}{\partial x_j} n_{j_{fs}} d\mathcal{A}$$
(20)

where  $k_{f_{eff}}^{cond.}$  is the *superficial* volume averaged effective thermal conductivity in the fluid phase due to *conduction* and is a function of both temperature and porosity. Note that the only simplifying assumption is that the variation in volume averaged fluid thermal conductivity within an averaging volume is greater than linear.

The last term on right-hand-side of Equation (20) is considered next. This term constitutes the *inter-facial heat flux* which consists of heat transfer via *conduction* to and from the fluid at the fluid-solid interface. This term is again indeterminate on a macroscopic level, and similar to Quintard and Whitaker [6] for systems in non-local thermal equilibrium systems, the following heat transfer correlation is employed

$$\frac{1}{\mathcal{V}} \int_{\mathcal{A}_{fs}} k_f(T_f) \frac{\partial T_f}{\partial x_j} n_{j_{fs}} d\mathcal{A} = \frac{1}{\mathcal{V}} \int_{\mathcal{A}_{fs}} q_{fs}^f d\mathcal{A} = -\frac{1}{\mathcal{V}} h_{eff}^f \left( \langle T_f \rangle^f - \langle T_s \rangle^s(r_0) \right) \mathcal{A}_{fs}|_{\mathcal{V}} \quad (21)$$

where  $h_{eff}^{f}$  is an effective *intrinsic* volume averaged heat transfer coefficient empirical (to be determined from experimental data) correlation,  $\mathcal{A}_{fs}|_{\mathcal{V}}$  is the fluid-solid surface interface area within the averaging volume and  $\langle T_s \rangle^s(r_0)$  denotes the surface temperature of a pebble with radius  $r_0$ .

For a packed bed of spheres, an expression may be easily obtained for the fluid-solid surface to averaging-volume ratio:

$$\frac{\mathcal{A}_{fs}|_{\mathcal{V}}}{\mathcal{V}} = (1 - \varepsilon) \frac{6}{d_p} \tag{22}$$

and the volume-averaged diffusion term reads

$$\left\langle \frac{\partial}{\partial x_j} \left( k_f(T_f) \frac{\partial T_f}{\partial x_j} \right) \right\rangle = \frac{\partial}{\partial x_j} \left[ k_{f_{eff}}^{cond.} \frac{\partial \langle T_f \rangle^f}{\partial x_j} \right] - (1 - \varepsilon) \frac{6}{d_p} h_{eff}^f \left( \langle T_f \rangle^f - \langle T_s \rangle^s(r_0) \right)$$
(23)

which is determinate on a macroscopic level.

# Volume-Averaged Energy Conservation Equation: Fluid Phase

The final form of the volume averaged energy governing conservation equation for the fluid phase follows by combining the result of the above volume averaging process, which is reflected in Equations (10), (18) and (23). It will be written in generalised cylindrical coordinates, where the latter concept is introduced (this departs from conventional text) as the resulting governing equations are written in a manner that they hold for both cylindrical and Cartesian coordinate systems:

$$r^{*} \varepsilon C_{p_{f}} \frac{\partial}{\partial t} \left[ \langle \rho_{f} \rangle^{f} \langle T_{f} \rangle^{f} \right] + C_{p_{f}} \frac{\partial}{\partial x_{j}} \left[ r^{*} \varepsilon \langle \rho_{f} \rangle^{f} \langle u_{f_{j}} \rangle^{f} \langle T_{f} \rangle^{f} \right] = \frac{\partial}{\partial x_{j}} \left[ r^{*} \left( k_{f_{eff}}^{cond.} I_{ij} + \varepsilon \langle \rho_{f} \rangle^{f} C_{p_{f}} D_{ij}^{d} \right) \frac{\partial \langle T_{f} \rangle^{f}}{\partial x_{i}} \right] - r^{*} (1 - \varepsilon) \frac{6}{d_{p}} h_{eff}^{f} \left( \langle T_{f} \rangle^{f} - \langle T_{s} \rangle^{s} (r_{0}) \right) \quad (24)$$

where  $I_{ij}$  is the identity matrix and  $r^*$  is the non-dimensional radius (non-dimensionalization may be done with respect to the domain average radius) and is a constant in the case of a Cartesian coordinate system. Note that  $r^*$  is variant in the mathematical macroscopic (volume-averaged) level only i.e. it is invariant in the microscopic domain.

#### Solid Phase

Similar to the fluid phase, we commence the derivation of the solid phase volume averaged equation by considering the microscopic continuum energy conservation equation written in *Cartesian coordinates*. Following the simplifying assumptions given in Section , the resulting microscopic energy continuum conservation equation which holds at every point in the solid reads:

$$\frac{\partial}{\partial t} \left[ \rho_s C_{p_s} T_s \right] = \frac{\partial}{\partial x_j} \left( k_s \frac{\partial T_s}{\partial x_j} \right) + \dot{q}_n^{\prime\prime\prime} \tag{25}$$

where  $\rho_s$ ,  $C_{p_s}$  and  $T_s$  respectively denote the fluid density, specific heat at constant pressure, and temperature. Further,  $\dot{q}_n'''$  is the volumetric nuclear heat production.

The associated boundary condition at the fluid-solid interface is

$$T_f(t, \mathbf{x}) = T_s(\mathbf{x}, t) \quad \forall \ \mathbf{x} \in \mathcal{A}_{\beta s}, \quad t \in \mathcal{I}$$
(26)

where as before, I is the temporal domain.

As previously, volume-averaging commences by integrating Equation (25) over the averaging volume  $\mathcal{V}$ :

$$C_{p_s}\rho_s \frac{1}{\mathcal{V}} \int_{\mathcal{V}_s} \frac{\partial}{\partial t} \left(T_s\right) d\mathcal{V} = \left\langle \frac{\partial}{\partial x_j} \left(k_s(T_s) \frac{\partial T_s}{\partial x_j}\right) \right\rangle + \left\langle \dot{q}_n^{\prime\prime\prime} \right\rangle (27)$$

where specific heat and density are assumed constant (refer to Section ). By applying a similar methodology to previously, the temporal derivative term follows trivially as

$$C_{p_s}\rho_s(1-\varepsilon)\frac{\partial}{\partial t}\langle T_s\rangle^s = \left\langle \frac{\partial}{\partial x_j} \left( k_s(T_s)\frac{\partial T_s}{\partial x_j} \right) \right\rangle + (1-\varepsilon)\langle \dot{q}_n^{\prime\prime\prime}\rangle^s$$
(28)

where the volume averaged nuclear heat source is expressed in terms of the intrinsic value  $\langle \dot{q}_n^{\prime\prime\prime} \rangle^s$ .

In the following section the diffusive term is cast into volume averaged form.

#### **Diffusive term**

Treatment of the diffusive term in Equation (28) commences by applying the volume averaging theorem for a vector (Equation 6) as

$$\left\langle \frac{\partial}{\partial x_j} \left( k_s(T_s) \frac{\partial T_s}{\partial x_j} \right) \right\rangle = \frac{\partial}{\partial x_j} \left[ (1 - \varepsilon) \left\langle k_s(T_s) \frac{\partial T_s}{\partial x_j} \right\rangle^s \right] + \frac{1}{\mathcal{V}} \int_{\mathcal{A}_{fs}} k_s(T_s) \frac{\partial T_s}{\partial x_j} n_{j_{sf}} d\mathcal{A}$$
(29)

By again employing the volume-averaged theorems followed by order-of-magnitude estimates, it may be proven that

$$\left\langle \frac{\partial}{\partial x_j} \left( k_s(T_s) \frac{\partial T_s}{\partial x_j} \right) \right\rangle = \frac{\partial}{\partial x_j} \left[ \left( k_{s_{eff}}^{cond.} \left( \langle T_s \rangle^s, \varepsilon \right) + k_{s_{eff}}^{cont.} \left( \langle T_s \rangle^s, \varepsilon \right) + k_{s_{eff}}^{rad.} \left( \langle T_s \rangle^s, \varepsilon \right) \right) \frac{\partial \langle T_s \rangle^s(r_0)}{\partial x_j} \right] + \left( 1 - \varepsilon \right) \frac{6}{d_p} h_{eff}^f \left( \langle T_f \rangle^f - \langle T_s \rangle^s(r_0) \right) \right)$$
(30)

where the approximation is made that heat flux due to the effective thermal conductivity is due to the gradient in volume averaged solid surface temperatures. In the above expression,  $k_{s_{eff}}^{cont.}$  and  $k_{s_{eff}}^{rad.}$  respectively denote superficial volume averaged heat transfer in the solid phase through solid contact and radiation and the associated associated temperature gradient is that of the volume averaged pebble *surface* temperatures.

The volume averaged solid energy conservation equation in macroscopically determinate form is compiled in the next section.

# Volume-Averaged Energy Conservation Equation: Solid Phase

The final form of the volume averaged solid energy governing conservation equation follows by combining Equations (28) and (30). As previously the result is written in generalised cylindrical coordinates:

$$r^{*}C_{p_{s}}\rho_{s}(1-\varepsilon)\frac{\partial}{\partial t}\langle T_{s}\rangle^{s} = \frac{\partial}{\partial x_{j}}\left[r^{*}\left(k_{s_{eff}}^{cond.} + k_{s_{eff}}^{cont.} + k_{s_{eff}}^{rad.}\right)\frac{\partial\langle T_{s}\rangle^{s}(r_{0})}{\partial x_{j}}\right] + r^{*}(1-\varepsilon)\frac{6}{d_{p}}h_{eff}^{f}\left(\langle T_{f}\rangle^{f} - \langle T_{s}\rangle^{s}(r_{0})\right) + r^{*}(1-\varepsilon)\langle \dot{q}_{n}^{\prime\prime\prime}\rangle^{s}$$

$$(31)$$

It is important to note that  $k_{s_{eff}}$  is a function of porosity as well as solid temperature, but *not* of fluid related material properties or fluid thermodynamic conditions.

# Volume-Averaged Energy Conservation Equation: Local Thermal Equilibrium

The above derivation detailed the governing equations for the case of local thermal disequilibrium which is a more general case of local thermal equilibrium. Therefore, in the latter case, the derived equations should reduce to the classical single energy equation. This is proven by replacing the intrinsic phase temperatures  $\langle T_f \rangle^f$  and  $\langle T_s \rangle^s$  in the final volume averaged equations (24) and (31) by the single fluid-solid temperature  $\langle T_{fs} \rangle^{fs}$  and adding the resulting equations together. The result follows

$$r^{*} \left[ \varepsilon C_{p_{f}} \rho_{f} + (1 - \varepsilon) C_{p_{s}} \rho_{s} \right] \frac{\partial}{\partial t} \langle T_{fs} \rangle^{fs} = \frac{\partial}{\partial x_{j}} \left[ r^{*} \left( k_{eff}^{all} I_{ij} + \varepsilon \langle \rho_{f} \rangle^{f} C_{p_{f}} D_{ij}^{d} \right) \frac{\partial \langle T_{fs} \rangle^{fs}}{\partial x_{i}} \right] + r^{*} (1 - \varepsilon) \langle \dot{q}_{n}^{\prime\prime\prime} \rangle^{s} \quad (32)$$

where  $k_{eff}^{all}$  is the total effective thermal conductivity as given by the Zehner and Schlünder [10] correlation. The above equation is indeed as hoped for.

ORDER OF MAGNITUDE ESTIMATES ON THE

## RELATIVE CONTRIBUTION OF VARIOUS HEAT TRANSFER MECHANISMS

In the preceding paragraphs, the effective thermal conductivity and thermal dispersion terms were introduced (these are as contained in Equations (17), (24) and (31)). These are correlations which are based on experimental data, and therefore mathematically not as rigorous as the remainder of the governing equation, as well as there being concerns around their accuracy and applicability to certain regions of a packed bed. For this reason, it is of importance to assess the relative contribution of each to heat transfer to identify the most important mechanisms.

For the above purpose, the mentioned correlations were compared to each other in magnitude as a function of porosity, temperature as well as volume averaged fluid flow velocity for a randomly packed bed of graphite pebbled with helium as working fluid. The latter was done to ensure relevance to the PBMR reactor. Note that in all cases temperature dependence of the helium and graphite material properties are fully accounted for while porosity was kept to below 0.9 as this is the upper limit for which the employed correlations are stated to be accurate. The most important findings of the exercise now follows:

- With regards the components of  $k_{eff}$ 
  - Conduction in the fluid itself is insignificant in all cases.
  - $\langle T \rangle > 800$ K: radiation is completely dominant i.e. heat transfer via conduction and contact is insignificant for all porosity values.
- $\varepsilon \langle \rho_f \rangle^f C_{p_f} D^d_{\perp}$  vs.  $k_{eff}$  in the case of natural convection where  $(\langle u_f \rangle = 0.15m/s)$ :
  - $\langle T \rangle > 800$  Thermal dispersion is one order of magnitude less than  $k_{eff}$  i.e. the latter is dominant.
- $\varepsilon \langle \rho_f \rangle^f C_{p_f} D^d_{\perp}$  vs.  $k_{eff}$  in the case of natural convection where  $(\langle u_f \rangle = 5.0m/s)$ :
  - $D^d_{\parallel}$  is one order of magnitude larger than the  $k_{eff}$ and  $D^d_{\perp}$  terms in all cases except for  $\langle T \rangle > 1100K$ when  $\varepsilon > 0.9$ .
  - $\langle T \rangle > 500$ : The  $k_{eff}$  term is orders larger than  $D^d_\perp.$

Note from the above that, contrary to popular believe, heat transfer via thermal dispersion from a solid wall is not dominated by thermal dispersion. This is as  $D_{\perp}^d$  is the dispersion related term which effect heat transfer here (and not the  $D_{\parallel}^d$ ), with the former being orders of magnitude less than  $k_{eff}$  for temperatures exceeding 800K. This clearly points to a major shortcoming in available experimental data as  $k_{eff}$  is not well known near to a solid boundary wall.

### CONCLUSION

This paper was concerned with the volume-averaged mathematical description of heat transfer through packed pebble beds, with special application to pebbled bed modular nuclear reactors. Allthough much work has been done on constructing such mathematical equations, very little is available for systems which are in a state of local-thermal-non-equilibrium. The latter is the case when the solid and fluid are at different temperatures on a volume averaged level, which is prevalent the in the work under consideration. This paper details the fundamental derivation of the implicated governing equations viz. fluid and solid energy conservation. This was followed by order of magnitude estimates for the case of helium flow through a bed of randomly packed graphite spheres in order to identify the dominant heat diffusive type heat transfer modes. Conclusive deductions were made from the study.

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