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EULERIAN-LAGRANGIAN APPROACH TO MODELING HEAT TRANSFER IN GAS-PARTICLE MIXTURES: VOLUME-AVERAGED EQUATIONS, MULTI-SCALE MODELING AND COMPARISON WITH NUMERICAL EXPERIMENTS

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ABSTRACT

In this paper, a macro-scale model is proposed to describe heat transfer in a dilute gas-particle mixture. The continuous phase is described by a filtered Eulerian approach while the dispersed one is represented as Lagrangian particles. The filtered model, which is obtained using an up-scaling methodology, consists of a macroscopic heat transfer model for the continuous phase with a matrix of heat exchange coefficients that captures both particle-particle and particle-fluid interactions. The up-scaling methodology further provides closure problems that link these coefficients to the particle scale and can be used to calculate the matrix explicitly. The validity of lumped and diagonal approximations of the matrix is studied, therefore providing a direct link between our approach and classical models of dilute gas-particle mixtures considering that the temperature field in the vicinity of each particle is not influenced by the presence of other particles. We also discuss the influence of the number of particles in the REV (Representative Elementary Volume) on the solution of the closure problems and compare numerical solutions of the exchange coefficients with analytical results obtained in the case of an isolated particle. Finally, we study a model system with immobile particles in a purely diffusive case and compare results of the macro-scale representation to those obtained from numerical experiments for different volume fractions. We show good agreement of our model with the numerical experiments and discuss the accuracy of lumped and diagonal approximations.

KEY WORDS: Two-phase/Multiphase flow; Conduction; Heat exchange; Euler-Lagrange; Volume averaging method; Closure problem; Numerical experiments.

1. INTRODUCTION

Dust explosion hazard appears in many industrial installations such as in coal mines or in the cereal industry. In nuclear safety analysis, one of the scenarios is the risk of graphite dust explosion that may occur during decommissioning operation of UNGG (Uranium Natural Graphite Gas) reactors [12] or during a loss of vacuum accident in the vessel of fusion reactors [5]. In such a case, the gas-particle mixture yields a dilute and dispersed two-phase flow with particle sizes typically ranging from 1 to 100 μm and a volume fraction of particles in the order of 10^{-3} [3]. The macro-scale modeling of such reactive dispersed two-phase flows is usually done through Euler-Lagrange approaches for which the continuous phase is described by a filtered Eulerian description while

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the dispersed one is represented as Lagrangian particles. The macro-scale exchange between the two phases is usually modeled from the boundary layer description in the vicinity of an isolated particle [8]. In this paper, we propose an alternate route to derive the Euler-Lagrange formulation, using an up-scaling methodology based on spatial averaging. We focus here on macro-scale heat exchange, the oxidation of particles will thus simply be modeled by a constant homogeneous heat source. The proposed methodology allows us to determine the heat exchange coefficients between the continuous phase and the particles, taking into account particle-particle and particle-fluid interactions, from the resolution of closure problems. A discussion is provided regarding the link of the proposed model with classical macro-scale models.

2. MICRO-SCALE HEAT TRANSFER PROBLEM

As stated in the introduction, the problem under consideration corresponds to heat transfer in a dispersed two-phase system. The continuous phase is identified as the β -phase while the dispersed one that consists in solid particles is identified as the σ -phase. In this study we consider rigid spherical particles of diameter d and the physical properties of both phases are considered to be constants. The micro-scale problem that describes the considered heat transfer process reads

$$\partial_t ((\rho c_p)_\beta T_\beta) + \nabla \cdot ((\rho c_p)_\beta T_\beta \mathbf{u}_\beta) = \nabla \cdot (\lambda_\beta \nabla T_\beta) , \text{ in the } \beta\text{-phase} \quad (1)$$

$$\mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla T_\beta = \mathbf{n}_{\beta\sigma} \cdot \lambda_\sigma \nabla T_\sigma , \text{ at } A_{\beta\sigma} \text{ (BC1)} \quad (2)$$

$$T_\beta = T_\sigma , \text{ at } A_{\beta\sigma} \text{ (BC2)} \quad (3)$$

$$\partial_t ((\rho c_p)_\sigma T_\sigma) + \nabla \cdot ((\rho c_p)_\sigma T_\sigma \mathbf{u}_\sigma) = \nabla \cdot (\lambda_\sigma \nabla T_\sigma) + \omega_\sigma , \text{ in the } \sigma\text{-phase} \quad (4)$$

where λ_γ , $(\rho c_p)_\gamma$ and \mathbf{u}_γ are respectively the thermal conductivity, the volumetric heat and the velocity of the γ -phase ($\gamma = \beta, \sigma$). In the boundary conditions Eqs. (2)-(3), $A_{\beta\sigma}$ refers to the β - σ interface and $\mathbf{n}_{\beta\sigma}$ represents the unit normal from the β -phase towards the σ -phase. The source term that appears in the right hand side of Eq. (4) corresponds to a constant homogeneous heat source in the σ -phase (i.e., that does not depend on temperature). The boundary conditions at the entrance and exit of the two-phase system together with the initial conditions have to be specified, but it is not necessary to prescribe them at this stage. The reader can refer to [13] for a more detailed description of their treatment in a macro-scale description. In our study, the σ -phase thermal conductivity is much larger than the β -phase thermal conductivity, typically $\lambda_\sigma/\lambda_\beta \sim 10^3$. In all subsequent developments, we therefore assume that $\lambda_\sigma/\lambda_\beta \gg 1$. This implies that the Biot number for the particle is much smaller than unity ($Bi \ll 1$). Accordingly, the temperature of the σ -phase will be considered homogeneous within each particle (This assumption is also sustained by the small size of the particles compared to other characteristic lengths). We further assume in this work that the problem of the two-phase flow can be decoupled from the heat transfer and can be solved independently. The two phase flow macroscopic description has been largely studied using the up-scaling methodology and the interested reader is encouraged to read [6].

3. MACRO-SCALE EULERIAN-LAGRANGIAN DESCRIPTION

In the Eulerian-Lagrangian description, the continuous phase is described in an Eulerian frame while the dispersed phase is described in a Lagrangian frame by tracking each individual particle into the carrying continuous phase. As the characteristic size d of particles is much smaller than the characteristic scale L of the large-scale temperature gradients, heat transfer in the vicinity of each particle is difficult or even impossible to resolve owing to the amount of needed computer resources. Accordingly, the micro-scale heat transfer problem for the continuous phase is filtered at a scale r_0 such that $d \ll r_0 \ll L$. The up-scaling methodology is based here on volume averaging that consists in applying a local volume filtering operator to the micro-scale continuous phase heat transfer governing equations. For any variable ψ_β defined in the β -phase, the spatial

average $\langle \psi_\beta \rangle$ and the intrinsic phase average $\langle \psi_\beta \rangle^\beta$ are defined by:

$$\langle \psi_\beta \rangle = \varepsilon_\beta \langle \psi_\beta \rangle^\beta = \frac{1}{\mathcal{V}} \int_{\mathcal{V}_\beta} \psi_\beta \, dV \quad (5)$$

where \mathcal{V}_β denotes the volume of the β -phase contained in the averaging volume \mathcal{V} and $\varepsilon_\beta = \mathcal{V}_\beta/\mathcal{V}$ is the β -phase volume fraction. By applying averaging theorems (e.g. [2, 10]), the averaging of Eq. (1) leads to the following macro-scale heat transfer equation for the filtered temperature $\langle T_\beta \rangle^\beta$

$$\partial_t \left(\varepsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta \right) + \nabla \cdot \left(\varepsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta \langle \mathbf{u}_\beta \rangle^\beta \right) = \nabla \cdot \left(\varepsilon_\beta \lambda_\beta^* \nabla \langle T_\beta \rangle^\beta \right) - \frac{1}{\mathcal{V}} \sum_{k=1}^{N_\mathcal{V}} Q_{\beta k} \quad (6)$$

where λ_β^* refers to some effective thermal conductivity that remains to be specified, $N_\mathcal{V}$ is the number of particles contained in the averaging volume \mathcal{V} and $Q_{\beta k}$ correspond to the macro-scale heat transfer between the continuous phase and the particle k defined by:

$$Q_{\beta k} = - \int_{A_k} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla T_\beta \, dS \quad (7)$$

On the other hand, the Lagrangian description for the dispersed phase is usually obtained by integrating the micro-scale heat transfer equation Eq. (4) over the volume of each particle [3]. Making use of the boundary condition Eq. (2) leads to the following equation for the averaged particle temperature T_k :

$$(m c_p)_k \frac{dT_k}{dt} = Q_{\beta k} \quad (8)$$

In addition, as expected, the Lagrangian description requires an equation for the location $\mathbf{x}_k(t)$ of each particle. As mentioned in the introduction, we focus in this paper on macro-scale heat exchange. As a result, it will be assumed that the particles move with the same velocity than the continuous phase in order to facilitate the numerical experiments. We also consider that the velocity of the continuous phase is uniform. As a result, without slip between the two phases, the particle location can be viewed as fixed in the moving coordinate system attached to the continuous phase. In addition, using this simplifying assumption, the macro-scale convective term in Eq. (6) can be removed in this moving coordinate system. The modeling of heat transfer between the filtered continuous phase and particles is usually based on the description of heat transfer from an isolated particle [3, 8]. This description uses a decomposition of the surrounding phase temperature into an undisturbed thermal field and a disturbance due to the presence of the particle to solve the heat transfer problem. The undisturbed field is usually viewed as the macro-scale temperature $\langle T_\beta \rangle^\beta$ and the resulting heat exchange reads [7, 8]:

$$Q_{\beta k} = - \int_{A_k} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla \langle T_\beta \rangle^\beta \, dS + \lambda_\beta \pi d_k \text{Nu}_k \left(\langle T_\beta \rangle^\beta - T_k \right) + \lambda_\beta \pi d_k^2 \text{Nu}_k \int_0^t \frac{d(\langle T_\beta \rangle^\beta - T_k)}{d\tau} \frac{d\tau}{2 \left(\pi \frac{\lambda_\beta}{(\rho c_p)_\beta} (t - \tau) \right)^{1/2}} \, d\tau \quad (9)$$

where Nu_k refers to the particle Nusselt number, defined as $\text{Nu}_k = h_k^* d_k / \lambda_\beta$, with h_k^* is the heat exchange coefficient between the continuous phase and the particle k . Of the terms which appear in equation Eq. (9) the first term corresponds to the undisturbed heat flux seen by the particle, which represents the rate of heat that would have entered the control volume occupied by the continuous phase in the absence of the particle, the second term corresponds to the quasi-steady thermal transfer from the particle to the surrounding continuous phase and the last contribution that takes the form of a history integral accounts for unsteady thermal diffusion.

In practice, the first and the last contributions are often neglected following scaling arguments for gas-particle mixtures and we refer to [8] for a detailed discussion. In this study, the modeling of heat transfer between the filtered continuous phase and particles follows the up-scaling methodology. The up-scaling methodology based on the volume averaging method has been extensively discussed elsewhere (*e.g.* [2, 4, 10]) and only the major steps that lead to a closed form of the macro-scale exchange $Q_{\beta k}$ will be outlined below. The first step consists in introducing the deviation \tilde{T}_β from the averaged temperature classically defined as $T_\beta = \langle T_\beta \rangle^\beta + \tilde{T}_\beta$ in the macro-scale heat transfer problem. For instance, introducing the deviation in the macro-scale heat exchange defined by Eq. (7) leads to

$$Q_{\beta k} = - \int_{A_k} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla \langle T_\beta \rangle^\beta dS - \int_{A_k} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla \tilde{T}_\beta dS \quad (10)$$

While the first term corresponds formally to the undisturbed heat flux contribution, the last term represents the contribution due to the deviation, which is due to the influence of the presence of particles in the averaging volume and this term remains to be closed. By introducing the deviation in the micro-scale heat transfer problem and by using the macro-scale transport equations, one obtains a boundary value problem for the deviations that suggests the following quasi-steady representation:

$$\tilde{T}_\beta = - \sum_{j=1}^{N_\nu} s_j \left(\langle T_\beta \rangle^\beta - T_j \right) \quad (11)$$

where s_j refers to the mapping variables that realize an approximate solution of the coupled macro micro-scale heat transfer problem. It is beyond the scope of this paper to present the developments leading to Eq. (11) and we refer the reader to [4] for a detailed presentation. Here we just note that the proposed mapping corresponds to a quasi-steady closure in which the mapping variables are solutions of steady micro-scale boundary value problems provided that the time-scale constraint $\lambda_\beta t / ((\rho c_p)_\beta l_\beta^2) \gg 1$ is satisfied, where l_β is the micro-scale characteristic length. This constraint has been discussed in details elsewhere (*e.g.* [10]) and here it will be assumed to be valid for the system under consideration. By substituting Eq. (11) into Eq. (10), the closed form of the macro-scale heat exchange reads

$$Q_{\beta k} = - \int_{A_k} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla \langle T_\beta \rangle^\beta dS + \sum_{j=1}^{N_\nu} h_{kj} \left(\langle T_\beta \rangle^\beta - T_j \right) \quad (12)$$

where h_{kj} denotes the effective heat exchange coefficients that are calculated from the closure variables s_j as

$$h_{kj} = \int_{A_k} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla s_j dS \quad (13)$$

When comparing to Eq. (9), the proposed macro-scale heat exchange involves additional contributions coming from particles contained within the averaging volume that look like particle-particle heat exchanges. To be clear about particle-particle heat exchanges, neglecting the first contribution in the right hand side of Eq. (12), the macro-scale heat exchange can be rewritten as:

$$Q_{\beta k} = h_k \left(\langle T_\beta \rangle^\beta - T_k \right) - \sum_{j=1}^{N_\nu} h_{kj} (T_j - T_k), \quad h_k = \sum_{j=1}^{N_\nu} h_{kj} \quad (14)$$

In addition, history effects are absent from the proposed heat exchange but this is a direct consequence of the quasi-steady closure. It is beyond the scope of this paper to deal with an unsteady-state closure but we just mention here that following [9], by writing the representation Eq. (11) as a convolution product in time leads formally to the same macro-scale heat exchange that includes history contributions.

4. CALCULATION OF HEAT EXCHANGE COEFFICIENTS

The effective heat exchange coefficients can be calculated from the micro-scale properties by solving the closure problem given in appendix. This problem has to be solved on the averaging volume \mathcal{V} whose characteristic size r_0 has to satisfy the constraint $d \ll r_0 \ll L$ mentioned previously. This can be recast here as the number of particles $N_{\mathcal{V}}$ contained within the averaging volume. We consider a two-dimensional geometry illustrated in Fig. (1) that consists in an array of particles with the same diameter d and where l_{β} is the distance between two successive particles. In practice, the averaging volume is assumed to be spatially periodic [4, 10] and this means here that taking into account symmetry with respect to the center of the particle 1, the matrix of heat exchange coefficients is symmetric $h_{kj} = h_{jk}$. Moreover the considered geometry allows to determine all the coefficients from $h_{11}, h_{12}, \dots, h_{1n}$.

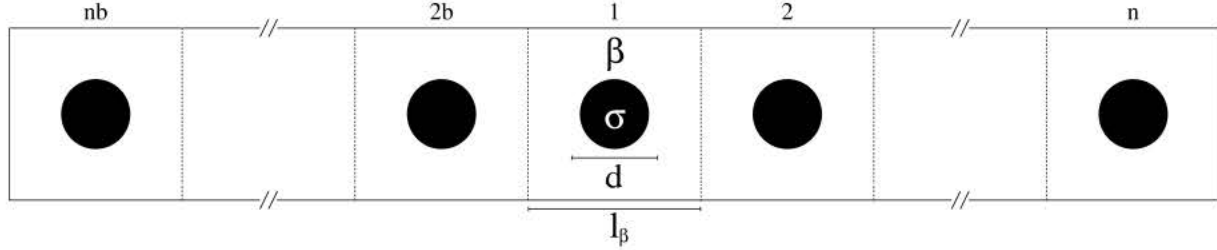


Fig. 1 Two-dimensional geometry with $N_{\mathcal{V}} = 2n + 1$ particles

As we are interested in dilute gas-particle mixtures, the solid volume fraction $\varepsilon_{\sigma} = 1 - \varepsilon_{\beta}$ is expected not to exceed at least 10^{-3} . Using this upper bound, the values of the heat exchange coefficients are reported in Tab. (1) for $N_{\mathcal{V}}$ ranging from 1 to 13. The results show first that the value of the lumped coefficient h_k defined in Eq. (14) does not depend on $N_{\mathcal{V}}$. Moreover, the value of h_k is much larger than the value of h_{kj} except for the diagonal coefficient h_{kk} which is of the same order of magnitude.

$N_{\mathcal{V}}$	$\frac{h_{11}}{\lambda_{\beta}d}$	$\frac{h_{12}}{\lambda_{\beta}d}$	$\frac{h_{13}}{\lambda_{\beta}d}$	$\frac{h_{14}}{\lambda_{\beta}d}$	$\frac{h_{15}}{\lambda_{\beta}d}$	$\frac{h_{16}}{\lambda_{\beta}d}$	$\frac{h_{17}}{\lambda_{\beta}d}$
1	1.163						
3	0.881	0.141					
5	0.746	0.029	0.180				
7	0.681	-0.035	0.123	0.155			
9	0.644	-0.072	0.086	0.120	0.127		
11	0.620	-0.095	0.062	0.096	0.104	0.105	
13	0.604	-0.112	0.046	0.080	0.088	0.089	0.090

Table 1 Dimensionless heat exchange coefficients for different values of $N_{\mathcal{V}}$ and $\varepsilon_{\sigma} = 10^{-3}$

The results obtained for the lumped coefficient are in fact a general property when looking at the structure of the closure problems given in appendix. The lumped coefficient can be obtained from a closure problems for the lumped mapping variable that can be solved here for the spatially periodic cell show in Fig. (2). In this case, the closure problems can be solved analytically for the Chang's unit cell also shown in Fig. (2), where the condition of periodicity has been replaced by a symmetry condition [11]. The correspondence between the two cells requires their volume fraction to be equal [11]. This leads to $\pi R^2 = l_{\beta}^2$, where R is the radius of Chang's unit cell. The resulting heat exchange coefficient reads

$$\frac{h}{\lambda_{\beta}d} = -\frac{8\pi(1 - \varepsilon_{\sigma})^2}{2 \log \varepsilon_{\sigma} + \varepsilon_{\beta}(1 + \varepsilon_{\sigma})} \quad (15)$$

Following [11], we compare for various particle volume fraction ε_σ the analytical solution obtained for Chang's unit cell with the numerical solution of the closure problems obtained for the spatially periodic unit cell. The results illustrated in Fig. (2) show a good agreement between the analytical solution and the numerical one. While this work is restricted to two-dimensional geometry, we just note here that solving Chang's unit cell in spherical coordinates and taking the limit $\varepsilon_\sigma = 0$ leads to the quasi-steady heat exchange coefficient obtained in [8].

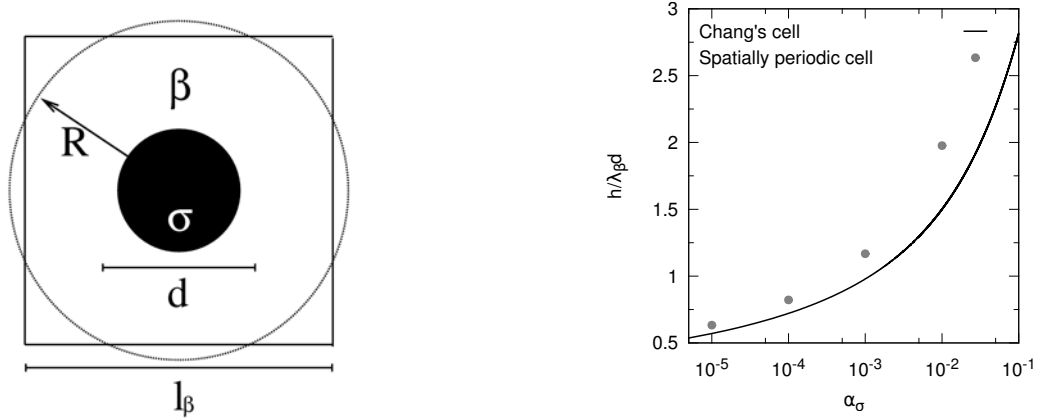


Fig. 2 Comparison of Chang's unit cell with a spatially periodic cell

5. NUMERICAL EXPERIMENTS

The main purpose of this section is to assess the validity of the proposed macro-scale description together with two simplified models that correspond to the lumped and the diagonal approximation of the heat exchange coefficients h_{kj} . When looking at the macro-scale heat exchange Eq. (14), these two simplified models consist roughly in neglecting particle-particle heat exchange and read formally as the classical model. In this regard, the results of the macro-scale models are compared with those obtained by averaging the numerical solution of the 2D micro-scale problem obtained from an unstructured finite volume solver [1]. In order to focus on the macro-scale heat exchange, we assume here that the system illustrated in Fig. (1) is infinite in all direction so that there is no averaged temperature gradient. The homogeneous source term is assumed to be zero in all particles except for the particle 1. Calculations have been carried out for typical parameters of dust explosion scenarios in nuclear safety analysis. These parameters are given in Tab. (2) where T_0 is the initial temperature for both phases and Da is the Damköhler number defined as $Da = \omega_1 d^2 / (T_0 \lambda_\sigma)$, where ω_1 is the heat energy generated in the particle 1.

Parameter	$\frac{\lambda_\sigma}{\lambda_\beta}$	$\frac{(\rho c_p)_\sigma}{(\rho c_p)_\beta}$	ε_σ	N_V	T_0	Da
Value	10^3	10^3	10^{-3}	7	300	0.1

Table 2 Model parameters

The average temperature $\langle T_\beta \rangle^\beta$ and the temperatures of particles 1, 2, 3, and 4 obtained from direct micro-scale simulations are compared with those obtained from the macro-scale Eulerian-Lagrangian description using the heat exchange coefficients given in the previous section (Tab. (1) with $N_V = 7$). The results are reported in Fig. (3) where T^* and t^* refer respectively to the dimensionless temperature T/T_0 and the dimensionless time $t \lambda_\beta / ((\rho c_p)_\beta l_\beta^2)$. These results show that the values obtained by the model are found to be in good agreement with the numerical experiments values for a time greater than 5. One must remember that the closure problems are taken to be quasi-steady by imposing the time scale constraints $t^* \gg 1$.

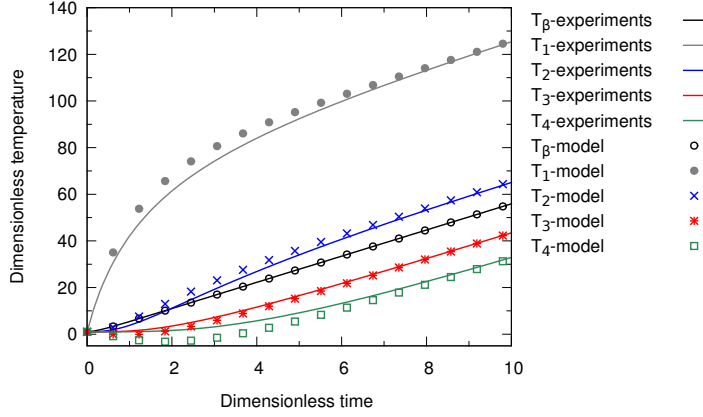


Fig. 3 Comparison of numerical experiments with the macro-scale model for $\varepsilon_\sigma = 10^{-3}$

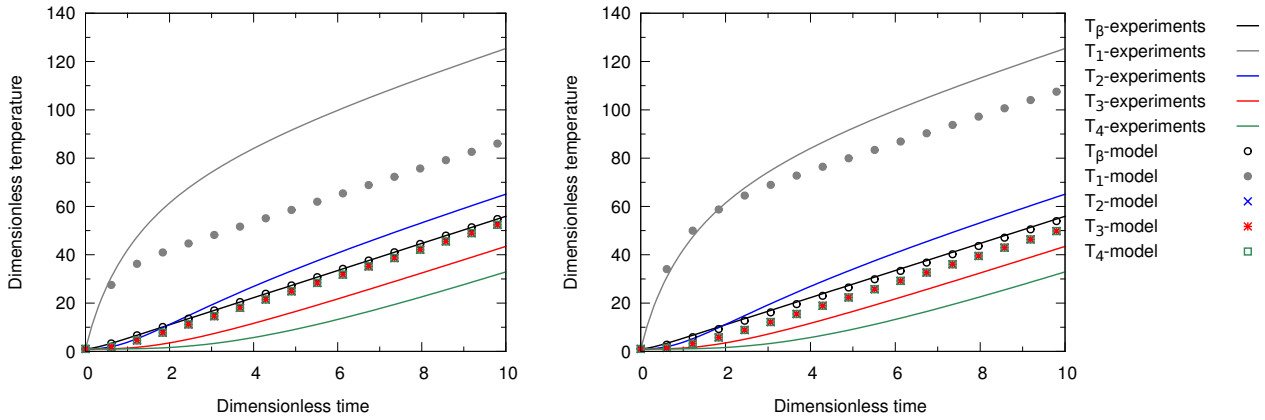


Fig. 4 Comparison of numerical experiments with the lumped (left) and diagonal (right) approximation

Regarding the lumped and the diagonal approximations, the results are reported in Fig. (4). Here again, a good agreement between numerical experiments and the macro-scale is observed for the averaged β -phase temperature $\langle T_\beta \rangle^\beta$ for both the lumped and the diagonal approximations. However, both approximations predict the same temperature for particles 2, 3 and 4 close to the average temperature $\langle T_\beta \rangle^\beta$ and this is in clear contradiction with numerical experiments results. Moving to the particle 1 for which the homogeneous source term is non zero, the diagonal approximation seems to be more attractive than the lumped one.

6. CONCLUSION

In this study, an Eulerian-Lagrangian macro-scale model has been proposed following an up-scaling methodology to describe heat transfer in a dilute gas-particle mixture. The major difference between the proposed model and the classical one is the presence of additional terms that involves particle-particle heat exchanges. The up-scaling methodology provides closure problems to determine the macro-scale heat exchange coefficients. These coefficients have been computed for a two-dimensional micro-scale geometry and different numbers of particles contained within the averaging volume and different particle volume fraction. In addition, two approximations have been proposed to establish a link with the classical model. In order to assess the validity of the proposed model and its approximate versions, the macro-scale predictions have been compared with a numerical experiments of the micro-scale problem. The predictions of the macro-scale model with the averaged solution of the micro-scale problem are in very good agreement. The proposed lumped and diagonal approximations are still capable of predicting correctly the continuous phase averaged temperature whereas it fails to estimate accurately the particles temperature.

Appendix A. CLOSURE PROBLEMS

The closure problems for the mapping variable s_j reads

$$\begin{aligned}\lambda_\beta \nabla^2 s_j - \varepsilon_\beta^{-1} \frac{1}{V} \sum_{k=1}^N h_{kj} &= 0, \text{ in the } \beta\text{-phase} \\ s_j &= 1, \text{ at } A_j \\ s_j &= 0, \text{ at } A_p, \text{ with } p \neq j \\ \langle s_j \rangle^\beta &= 0\end{aligned}$$

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