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Up-scaling heat transfer in gas-particle mixtures: Eulerian-Lagrangian macro-scale description through volume averaging

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1. Introduction

The risk of dust explosion appears in many industrial situations. In nuclear safety analysis, one of the scenarios is the risk of graphite dust explosion that may occur during decommissioning operations of UNGG reactors [6]. In such a case, the problem is considered as a dispersed two-phase flow with particle size typically ranging from 1 to 100 μ m and a particle volume fraction up to 10⁻³. The modeling of such reactive dispersed two-phase flows is usually done through a macro-scale Euler-Lagrange approach for which the continuous phase β is described in macro-scale Eulerian frame while the dispersed phase σ is described in a Lagrangian frame by tracking each individual particle into the carrying filtered continuous phase. The modeling of the macro-scale heat exchanges between the filtered continuous phase and particles is usually based on the description of heat transfer from an isolated particle [3, 5]. In this paper, we propose an alternate route to derive the macro-scale Eulerian-Lagrangian description, using the upscaling methodology based on spatial averaging. The proposed methodology allows us to determine the macro-scale exchange between the continuous phase and the particles directly from the resolution of closure problems on a representative element volume.

2. Methods and models

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 equation [1, 4] which leads to the following macro-scale heat transfer equation for the filtered temperature $\langle T_\beta \rangle^{\beta}$

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

where ε_{β} , $(\rho c_p)_{\beta}$ and \mathbf{u}_{β} are respectively the volume fraction, the volumetric heat and velocity of the β-phase. λ^*_{β} refers to some effective thermal conductivity that remains to be specified, $N_{\mathcal{V}}$ is the number of particles contained within the averaging volume V. $Q_{\beta k}$ correspond to the macro-scale heat transfer between the continuous phase and the k -particle defined by:

$$
Q_{\beta k} = -\int_{A_k} \mathbf{n}_{\beta \sigma} \cdot \lambda_{\beta} \nabla T_{\beta} dS \tag{2}
$$

where A_k refers to the β - σ interface, λ_{β} is the thermal conductivity of the β -phase and $\mathbf{n}_{\beta\sigma}$ represents the unit normal from the β -phase towards the σ -phase. On the other hand, the Lagrangian description for the dispersed phase is usually obtained by integrating the micro-scale heat transfer equation for the dispersed phase over the volume of each particle, this leads to the following equation for the averaged particle temperature T_k :

$$
(mc_p)_k \frac{dT_k}{dt} = Q_{\beta k} \tag{3}
$$

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By introducing the deviation T_β from the averaged temperature defined as $T_\beta = \langle T_\beta \rangle^\beta + T_\beta$ in the microscale heat transfer problem and by using the macro-scale transport equations, one obtains a boundary value problem for the deviations that suggests the following unsteady representation $[4, 2]$:

$$
\widetilde{T}_{\beta}|_{(\mathbf{x},t)} = -\sum_{j=1}^{N_{\mathcal{V}}} s_j|_{(\mathbf{x},t)} * \partial_t \left(\langle T_{\beta} \rangle^{\beta} |_{(\mathbf{x}_j,t)} - T_j |_{(\mathbf{x}_j,t)} \right) \tag{4}
$$

where $*$ refers to time convolution, x_j is the location of the k-particle and s_j is the mapping variables that realize an approximate solution of the coupled macro micro-scale heat transfer problem. By substituting Eq. (4) into Eq. (2), the closed form of the macro-scale heat exchange reads

$$
Q_{\beta k} = -\int_{A_k} \mathbf{n}_{\beta \sigma} \cdot \lambda_{\beta} \nabla \langle T_{\beta} \rangle^{\beta} \, \mathrm{d}S + \sum_{j=1}^{N_{\mathcal{V}}} h_{kj} * \partial_t \left(\langle T_{\beta} \rangle^{\beta} |_{(\mathbf{x}_j, t)} - T_j |_{(\mathbf{x}_j, t)} \right) \,, \quad h_{kj} = \int_{A_k} \mathbf{n}_{\beta \sigma} \cdot \lambda_{\beta} \nabla s_j \, \mathrm{d}S \tag{5}
$$

The unsteady solution of the closure problems must converge towards quasi-stationary solution when the macroscopic times are significantly greater than the characteristic times associated with the relaxation of s_j towards s_j^{∞} . This asymptotic behavior corresponds to the transition from s_j to the limit $u(t)s_j^{\infty}$ in the convolution product defined by Eq. (4) , where $u(t)$ is the Heaviside function. This decomposition can be written as: $s_j|_{(\mathbf{x},t)} - u(t)s_j^{\infty}|_{(\mathbf{x})} = s_j^*|_{(\mathbf{x},t)}$, where s_j^* represents the contribution of some history effects in the unsteady closure problem and verifies $\lim_{t\to+\infty} s_j^*|_{(\mathbf{x},t)} = 0$. By substituting the decomposition of s_j in a quasi-steady and memory contribution, the macro-scale heat exchange can be rewritten as :

$$
Q_{\beta k} = -\int_{A_k} \mathbf{n}_{\beta \sigma} \cdot \lambda_{\beta} \nabla \langle T_{\beta} \rangle^{\beta} \, \mathrm{d}S + \sum_{j=1}^{N_{\mathcal{V}}} h_{kj}^{\infty} \left(\langle T_{\beta} \rangle^{\beta} |_{(\mathbf{x}_j, t)} - T_j |_{(\mathbf{x}_j, t)} \right) + \sum_{j=1}^{N_{\mathcal{V}}} h_{kj}^{*} \cdot \partial_t \left(\langle T_{\beta} \rangle^{\beta} |_{(\mathbf{x}_j, t)} - T_j |_{(\mathbf{x}_j, t)} \right) \tag{6}
$$

where h_{kj}^{∞} and h_{kj}^{*} represent respectively the quasi-steady and the "memory" effective heat exchange coefficients that are calculated from the closure variables s_j^{∞} and s_j^* . The first term in Eq. (6) corresponds to the rate of heat that would have entered the volume occupied by the particle. The second term corresponds to the quasi-steady thermal transfer to the particle and the last contribution that takes the form of a history integral accounts for unsteady thermal diffusion.

3. Results

- Solving the closure problems for an isolated particle and taking the limit $\varepsilon_\beta = 1$ leads to the classical macro-scale exchange described in [3].
- The unsteady closure problems and the macro-scale Eulerian-lagrangian equations in a purely diffusive case have been solved analytically in a 1-D case and results have been validated by comparing with direct solution of the micro-scale heat transfer problem.
- Two diagonal approximations of the matrix describing heat exchanges have been proposed to establish a link with the classical model. These approximations are still capable of predicting correctly the continuous phase averaged temperature but they fail to estimate accurately some particle temperature.

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