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3D numerical modelling of the propagation of radiative intensity through a X-ray tomographied ligament

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ABSTRACT

In order to explain the macroscopic radiative behaviour of an open-cell ceramic foam, knowledge of its solid phase distribution in space and the radiative contributions by this solid phase is required. The solid phase in an open-cell ceramic foam is arranged as a porous skeleton, which is itself composed of an interconnected network of ligament. Typically, ligaments being based on the assembly of grains more or less compacted, exhibit an anisotropic geometry with a concave cross section having a lateral size of one hundred microns. Therefore, ligaments are likely to emit, absorb and scatter thermal radiation. This framework explains why experimental investigations at this scale must be developed to extract accurate homogenized radiative properties regardless the shape and size of ligaments. To support this development, a 3D numerical investigation of the radiative intensity propagation through a real world ligament, beforehand scanned by X-Ray micro-tomography, is presented in this paper. The Radiative Transfer Equation (RTE), applied to the resulting meshed volume, is solved by combining Discrete Ordinate Method (DOM) and Streamline upwind Petrov-Garlekin (SUPG) numerical scheme. A particular attention is paid to propose an improved discretization procedure (spatial and angular) based on ordinate parallelization with the aim to reach fast convergence. Towards the end of this article, we present the effects played by the local radiative properties of three ceramic materials (silicon carbide, alumina and zirconia), which are often used for designing open-cell refractory ceramic foams.

1. Introduction

Refractory ceramic open-cell foams offer versatile possibilities for developing high temperature systems ($T \approx 1000\,^{\circ}\mathrm{C}$) in which fluid flow and heat transfers may occur simultaneously. Typical applications are porous gas burners [1], volumetric solar receivers [2] or heat exchangers for recovering sensible heat [3]. A key challenge to increase the thermal efficiency of these energy conversion systems is to integrate properly the contribution of the thermal radiation for establishing an appropriate thermal balance. Dealing accurately with the radiative exchanges involves, firstly robust solving of the radiative transfer equation for these refractory open-cell foams which by nature are generally considered as semi-transparent materials [4] in reason of their high porosity, p, with $p \in [0.7 - 0.95]$. Secondly, the spectral radiative properties such as the absorption coefficient κ_ν, the scattering coefficient σ_{s_ν}, the scattering phase function Φ_ν and the complex refractive index $\tilde{n}(\nu, T)$ must be exactly known for the spectral range $[\nu_{min}, \nu_{max}]$, that corresponds here to wave numbers,ν where the Planck's law takes significant values at the considered temperature. Here T stands for the temperature. This set of parameters is governed by the materials used to manufacture the ceramic open-cell foams. Popular manufacturing materials involved are, silicon carbide [2,5] a typically opaque material for sample thickness higher than few microns and alumina, [6] mullite [7] or zirconia [8] which are rather semi-transparent materials by nature. Being able to work with compact expressions that govern the radiative properties from simple chemical and textural [9] parameters relevant to the foams are useful when global heat and fluid transfers are treated simultaneously for energy optimization [2,5].

However, ceramic open-cell foams are complex materials, from a topological viewpoint, since they are composed from a solid network of ligaments [10] which posses confined macropores most often filled with air. Further, adding to the complications is the multi-scale length organization of open-cell foams, where each element of matter contributes to the global radiative

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behaviours [11]. To detail these lengths, there exist: (i) the crystalline structure of the solid grains at nanometric scale, which is itself imposed by the chemical composition of the foams, (ii) the grains and the micropores constituting the ligaments at micronic scale, (iii) the ligaments and the macropores at millimetric scale that define the architecture of the foams and (iv) the final shape and volume of the foams at centimetric scale when they are used in industrial systems. Adding more to the complexities is the elaboration process used to elaborate the foams [12]. Indeed, the process tends to form solid ligaments that are more or less dense or really hollow [1] and often exhibit, based on the replication methods, a concave shape where the cross sectional area remains nearly constant over the central half of the ligament but increases on its extremities [13]. It has been recently underlined that the ligament geometries influence the determination of the extinction coefficient of metallic foams since computed values can evolve around 10% [14,15]. Let us notify that in the latter case, ligaments are considered as optically thick media. On the other hand, in the case of mullite foam possessing semi-transparent ligaments, authors have successfully extracted the solid phase radiative properties on an available dense ceramic of mullite to compute afterwards the bi-directional reflectance of the foam through a Monte Carlo code [16]. This two-step process proves to be delicate since it requires to find a centimetric sample with a similar textural feature than the one present in the ligaments. However, from an elaboration viewpoint, it is well known that the texture of a ligament can not be strictly the same than in a dense sintered ceramic composed of the same material [1].

This description indicates that the direct investigation of the radiative properties of ligaments at the local scale either for semi-transparent compounds or for opaque compounds constitutes a new domain of development for researchers involved in the design of foam with controlled macroscopic radiative properties. Recently, Guevelou et al. performed infrared microscopy reflectivity measurement on the ligaments of a silicon carbide open-cell foam with the aim to determine their effective complex index of refraction [5]. The authors developed an analytical methodology based on an effective medium law in order to avoid treating directly the effect played by the rough surface of the ligaments. Rochais et al., measured, until 900 °C, through a microscopic photothermal set-up, the thermal diffusivity of mullite foams and developed a meticulous sample preparation for dealing with the semitransparency of the observed lumps [17]. The sample preparation consisted to optically polished a mullite foam, which has been impregnated with a glue ceramic (stable until 900 °C) and to deposit an opaque coating on the surfaces of the lumps. These two experimental works are restricted on microscopic pieces of matter being opaque and the theoretical modeling of the reflected spectra requires to bear on some assumptions. This is why the knowledge of the transport of thermal radiation within the ligament, either opaque or semitransparent, can provide critical information for developing high-quality experimental developments.

This framework shows that investigating the radiative behaviour of the ligaments regardless of their shapes and optical thicknesses, $\tau_\nu = \beta_\nu d$, are today of crucial importance. Let us recall here d is the typical length of the ligament cross-section and β_ν is the extinction coefficient. To go one step further, one proposes to model the 3D radiative transport within a ligament, beforehand 3D imaged by X-ray micro-tomography, and endowed with a set of gradual radiative properties (κ_ν, σ_{s_ν}, Φ_ν, $\tilde{n}_\nu$) that confers to its opacity or semi transparency. The 3D image is entirely meshed within its all volume. To follow the volumetric propagation of the radiative intensity within the ligament which is exposed to a collimated beam of radiation, the radiative transfer equation (RTE) is solved by combining the discrete ordinate method (DOM) and the Streamline upwind Petrov-Galerkin methods (SUPG). The treatment of reflection of radiative intensive on borders is also performed very accurately, following [18]. Such a numerical methodology allows to deal with the specular reflective behaviour of the ligaments. The paper is organized as follows. Part 2 exposes the mathematical models used in this work. Part 3 details the numerical methodologies used to solve the RTE. Then, Part 4 gives the results which are further discussed.

2. Physical model

The steady-state radiative transfer equation (RTE) governs the radiative intensity $I_\nu(\boldsymbol{x}, \boldsymbol{s})$ through a 5 dimensional integro-differential equation that reads [19,20]:

$$\boldsymbol{s}\cdot\nabla I_\nu(\boldsymbol{x}, \boldsymbol{s}) + \beta_\nu I_\nu(\boldsymbol{x}, \boldsymbol{s}) = \sigma_{s_\nu}\oint_{\mathcal{S}^2}\Phi(\boldsymbol{s}' \to \boldsymbol{s})I_\nu(\boldsymbol{x}, \boldsymbol{s}')\mathrm{d}\boldsymbol{s}' + \kappa_\nu I_b(T, \nu) \tag{1}$$

in which $\boldsymbol{x} \in \mathcal{D} \subset \mathbb{R}^3$ represents the space coordinate, $\boldsymbol{s}$ is the unit direction within the sphere (2D) and I_b is the Plancks function dependent on the wavelength as well as on temperature. To model carefully the evolution of the radiative intensity, appropriate intensity attenuations due to reflection effect on the boundaries is to be taken into account. The boundary condition on the borders can be expressed as follows, for $\boldsymbol{x} \in \partial\mathcal{D}^- = \partial\mathcal{D}|\boldsymbol{s}\cdot\boldsymbol{n} < 0$:

$$I_w(\boldsymbol{x}, \boldsymbol{s}) = (1-\alpha)I_\nu^{\Psi}(\boldsymbol{x}, \boldsymbol{s}) + \alpha I_\nu^{\curlyvee}(\boldsymbol{x}, \boldsymbol{s}) \tag{2}$$

The first term in the right-hand-side of (2) is the diffusion contribution of reflection, and the second term represents the specular contribution. The partition ratio coefficient $\alpha \in [0, 1]$, also called “parameter of specularity” [21] yields a linear interpolation between diffuse and specular contributions while dealing with mixed boundary conditions. To add more, the entering beam $\tilde{I}_\nu(\boldsymbol{x}, \boldsymbol{s}_0)$ towards the direction $\boldsymbol{s}_0$ also yields both diffuse and specular refractions. Reflections and refractions brought together for diffuse and specular parts are finally given by, $\forall\, \boldsymbol{x} \in \partial\mathcal{D}^-$:

$$I^{\Psi}(\boldsymbol{x}, \boldsymbol{s}) = -\boldsymbol{s}_0\cdot\boldsymbol{n}\left(1-\rho_d\right)\frac{\tilde{\omega}}{\pi}\tilde{I}(\boldsymbol{x}, \boldsymbol{s}_0) + \frac{\rho_d}{\pi}\int_{\partial\mathcal{D}^+} I(\boldsymbol{x}, \boldsymbol{s}')\boldsymbol{s}'\cdot\boldsymbol{n}\mathrm{d}\boldsymbol{s}' \tag{3}$$

$$I^{\curlyvee}(\boldsymbol{x}, \boldsymbol{s}) = (1-\rho_s(\boldsymbol{s}_0\cdot\boldsymbol{n}))\tilde{I}(\boldsymbol{x}, \boldsymbol{s}_0) + \rho_s(\boldsymbol{s}\cdot\boldsymbol{n})I(\boldsymbol{x}, \xi(\boldsymbol{s})) \tag{4}$$

where $\rho_s(\cdot)$ and ρ_d are respectively the specular and diffuse reflectivity. $\xi(\boldsymbol{s}) = \boldsymbol{s} - 2(\boldsymbol{s}\cdot\boldsymbol{n})\boldsymbol{n}$ is the incident radiation of the reflected direction $\boldsymbol{s}$. The first terms in right hand sides of (3) and (4) actually come from the Dirichlet conditions, while the second terms represent internal reflections. To add more, in (3), $\tilde{\omega}$ denotes the solid angle characterizing the direction $\boldsymbol{s}_0$ of the entering beam. Note that the subscript ν has been dropped here and so forth for readability considerations. Also, the reflectivity ρ_s is a function of the cosine angle between the direction $\boldsymbol{s}$ and the outward normal $\boldsymbol{n}$.

3. Numerical development

To solve the radiative transfer problem involving (1) and (2), numerical methods have to be used. Two major kinds of numerical methods are available to solve such problem: the statistical methods and the deterministic methods. For the statistical approach, the Monte-Carlo [22–25] and Ray-Tracing methods [26,27] are the most popular. These methods are fast, efficient and use little memory to get an exchange between two surfaces, at least for simple geometries and homogeneous media. However, on the other hand, we have the deterministic approach based on discretizations, as it is presented in this paper. For Deterministic