Numerical prediction of the radiative behavior of metallic foams from the microscopic to macroscopic scale

B Rousseau¹, JY Rolland¹, P. Echegut², E. Brun³ and J Vicente⁴

¹LTN, UMR CNRS 6607, Rue Christian Pauc, BP 50609, 44306 Nantes cedex 3, France
²CEMHTI, UPR CNRS 3079, 45071, Orléans cedex 2, France
³ESRF, F38043, Grenoble, France
⁴IUSTI, UMR CNRS 6595, F13453, Marseille France
E-mail of the corresponding author: benoit.rousseau@univ-nantes.fr

Abstract. A parallel C++ numerical code was implemented to quickly and accurately calculate the radiative properties (reflectance and transmittance) of metallic foams that had scattering domains (pores, struts) with mean sizes larger than the wavelengths associated with thermal radiation. For application, the code required experimental knowledge of the material characteristics on several length scales ranging from the microscopic (approximately one micrometer) to macroscopic (approximately one centimeter). In particular, the 3D voxelized image of the investigated material was used, which was previously acquired using x-ray µ-tomography. The radiative properties were obtained by tracking a large number of rays within the numerical medium. On the local scale, rays interacted directly with the fluid/solid interface, which was obtained prior to the calculation by the application of a robust marching cubes algorithm to the entire set of voxels. The code was applied to aluminum foam samples, for which the experimental radiative properties were previously measured at room temperature with a customized instrument based on an infrared spectrometer. The code performance is discussed and the results enabled determination of the effects caused by the fluid/solid interface on the interfacial reflection.

1. Introduction

Understanding the thermal radiative properties of porous materials is of crucial interest when calculating heat transfers within industrial systems that operate at high temperatures. Porous materials are often used as part of the design for high-temperature systems (e.g., heat exchangers, solar thermal receivers [1] and glass melting furnaces [2-3]). However, porous materials have a complex texture that makes study of the radiative properties difficult [4]. The term “texture” describes the spatial arrangement and size distribution of the scattering objects (i.e., pores, cracks, struts and fibers) in the host solid matrix. Currently, an important challenge is to predict the thermal radiative properties of both the pertinent textural parameters (e.g., porosity, specific surface area and pore size distributions) and chemical composition. The achievement of this task will enable engineers to reliably design porous materials with the intended radiative properties.

Since the pioneering work of Gliksman and Torpey [5], several approaches have been developed to firmly connect textural parameters to the radiative properties. Recently, Loretz et al. reported
analytical and experimental methods used to determine radiative properties such as the extinction coefficient, scattering albedo and scattering phase function of metallic foams [6]. The authors suggested that the extinction coefficient can be simply calculated from the strut dimensions. However, for metallic foams, Zhao et al. used relations where the extinction coefficient was dependent on the ratio between the foam’s porosity and the mean strut diameter [7]. The relations defined by Loretz et al. and by Zhao et al. can be used for struts that have nearly optically polished surfaces. However, results from the application of these formulas are less reliable as the struts become optically thin (i.e., the solid phase is semitransparent).

During the last five years, numerical approaches based on the use of 3D images obtained by x-ray µ-tomography provided new insights into the investigation of this topic [8-13]. In particular, in the most favorable cases, x-ray µ-tomography [14] provides easy access to the geometrical position of the fluid/solid interface at the limit of the spatial resolution of the tomographic experiment, as well as a numerical method to draw the interface. Most of the numerical methods that attempt to calculate the radiative properties of metallic foams are based on the stochastic propagation of a huge number of rays within the porous medium. It is noteworthy that if rays propagate within a volumetric domain higher than the representative elementary volume [9, 15-16], the calculated discrete-scale radiative data can be used to solve continuum-scale simulations of heat transfer within the medium [17-18]. As the texture of the porous material becomes more complex (i.e., the material has several populations of scattering objects with different length scales and chemical compositions), the numerical methods, which are only based on the geometrical optics approximations, begin to fail. Rousseau et al. [13] combined the geometrical optics approximation and effective medium approximation to model the radiative properties at T = 1000 K of an optically thick rough coating that contained micropores. For metallic foams, Loretz et al. [6] introduced a parameter of specularity to account for the scattering of light by the rough surfaces of struts. Coquard et al. [19] combined stereoscopic and tomographic imaging approaches to account for surface roughness.

These methods show that accurate modeling of the radiative properties is primarily dependent on an accurate description of the topology of each interface (e.g., fluid/solid) encountered. Furthermore, some studies indicate that trilinear interpolation methods [20] can be used to reconstruct a small piece of curvilinear surface during the propagation of a given ray within the foam at each interaction point [9, 12, 21]. Other investigations used the marching cube approach [22] to create a small flat interface section. For foams with a single solid phase, commercial codes [6, 11] were applied to obtain an entire interface composed of numerous triangles. Once the triangular grid was known, stochastic rays were launched into a given volume.

In this work, a homemade code, titled iMorph [23-24] (IUSTI, Marseille, France), was used to determine the entire fluid/solid interface of an aluminum foam (ERG® Al 20), which was scanned by x-ray µ-tomography prior to the calculations. The fluid/solid interface was determined by applying a robust marching cube algorithm. Then, according to a thorough textural and chemical analysis, an improved Monte Carlo Ray Tracing (MCRT) [25] scheme was applied to the resulting digital image to compute both the normal hemispherical spectral reflectance and transmittance of the foam. Finally, a comparison between the computed data and experimental data acquired by infrared spectroscopy allowed the light-scattering mechanisms that occurred at the fluid/solid interface to be discussed.

2. Experimental procedure and textural study
A highly porous aluminum foam with 20 pores per linear inch (ppi), which was supplied by the Erg company (Oakland, California, US), was investigated. Two small samples (S1 and S2) were machined from the first specimen. S1, which had dimensions of 57×57×55 mm, was used for the textural and chemical investigation. S2 was used to measure the radiative properties. S2 had a paved shape and had dimensions of 57×57×13 mm.

The 2D investigation of the foam morphology was performed with an Environmental Scanning Electron Microscope (ESEM-Philip XL 40 at CEMHTI, Orléans, France) with the detection mode set to be sensitive to Secondary Electrons (SE). This mode was adapted for determining the topographic
contrast. Furthermore, the ESEM apparatus was equipped with an energy dispersive x-ray detector. This device was useful for performing the chemical analysis of the struts that constituted the foam. The results from the investigation were used to determine the complex refractive index of the solid phase. To obtain more quantitative information regarding the foam texture, x-ray μ-computed tomography experiments were performed at the European Synchrotron Radiation Facility on the ID19 beamline (ESRF, Grenoble, France). The absorption images were collected using a fast read out 2048 × 2048 CCD camera, FRELON (Fast Readout LOw Noise), developed at ESRF and described in detail in by Thi et al. [26] and by Coan et al. [27]. A customized gold-coated integrating sphere with a diameter of 150 mm was used to measure the normal hemispherical spectral reflectance at room temperature (CEMHTI, Orléans, France). The sphere was adapted onto a Fourier Transform InfraRed (FTIR) spectrometer (Bruker IFS 113v Ettlingen, Germany) using a customized holder.

In Figure 1, 2D views of the foam are shown, in which the spatial resolution is serially increased: 20 mm (a), 2 mm (b) and 20 µm (c). Inspection of the image indicates that the cell was composed of curved triangular struts of inconstant sizes. Moreover, careful observation of the cross-sections of the struts indicates that they were filled. Investigations at higher magnification show that the surface of the struts was rough (Figure 1c).

Figure 1: (a) A 2D view of the foam acquired with a digital camera at a resolution of 20 mm. (b) The same image with a higher magnification, which was obtained using an ESEM apparatus at a resolution of 2 mm. (c) The same image with a resolution of 20 µm.

Overlapping spherical pits with a mean diameter of 10 µm can be observed in Figure 1c. In the case of opaque media, this type of surface is well known to decrease the directional hemispherical reflectivity [28]. X-ray μ-tomography experiments were performed to acquire quantitative textural parameters (i.e., porosity, pore size distribution and volumetric surface) [6, 29-30]. After binning and filtering the raw data, the final numerical samples were shown as grey-scale images with a maximal size of 760×760×737 voxels and a digital resolution of 74.6 µm. A simple threshold procedure was performed with the iMorph software [24] to separate the solid phase from the fluid phase. The total porosity of the 3D image was determined by computing the ratio between the voxels belonging to the fluid phase to the total number of voxels. A calculated porosity of 92.0 % was determined by applying the iMorph software. It is worthy to note that this calculated porosity was similar to the value determined by the classical weighing method (91.5 %) [31]. The similar values indicate that the segmentation method was exact. To obtain the fluid/solid interface, a marching cubes algorithm was used [22, 32]. The numerical interface was constructed from a regular mesh composed of ordered triangles. A full 3D view of a reconstructed foam is shown in Figure 2.
The implementation of the marching cubes algorithm in iMorph guaranteed that the mesh was continuous: neither holes between each triangle nor degenerated triangles were observed. Both of these artifacts can be very problematic as a ray tracing algorithm is used. The iMorph software also allowed each individualized pore to be segmented to retrieve the shape and size. An unbiased watershed transform was used to extract each cell, which resulted in the composition of the full 3D grey-scale image. The automated extraction of markers for the watershed was based on the maximal, included ball method [33]. The shape of the cell is generally assumed to be ellipsoidal, which was an assumption inspired by previous work on the same type of metallic foam [24, 31]. Upon completion of the segmentation, classical orientation and morphometric analyses (i.e., volume and mass moment of inertia) were used to obtain the shape and size distribution of a set of 1330 cells. The results indicated that the pores could be ellipsoids [31]. The 3 principal axes of the ellipsoids were denoted as $a < b < c$, and the mean values were $a = 2150 \mu m$, $b = 1430 \mu m$, $c = 1120 \mu m$. Moreover, a solid phase granulometry procedure (i.e., growth of the ball) was applied to the complete set of struts that composed the foam, which indicates that the struts had a typical lateral size of approximately 300 $\mu m$.

After the textural features were determined, a study of the chemical composition of the struts was performed. Energy-Dispersive X-ray (EDX) spectra indicated that the struts were mainly composed of aluminum. No other species (e.g., rare earth or transition metal ions) were observed. A small peak was observed at lower energy, which could correspond to oxygen; however, EDX is not a reliable technique for the characterization of species with low atomic numbers. In conclusion, only aluminum was considered in the following calculations for determining the local optical properties of the foam samples. Therefore, the complex refractive index of pure aluminum [34] was used.

### 3. Development of the numerical simulation

In this work, an Monte Carlo Ray Tracing (MCRT) program was implemented for computing the spectral dependence of the radiative properties of opened foams (reflectance and transmittance). The program was directly developed within the iMorph software previously used for the textural analysis and for the construction of the 3D image of the foam. The construction of the code was strictly based on the textural and chemical analysis of the studied sample. The principles of the MCRT code were extensively detailed in previous papers [4, 10, 25]. Briefly, the code launches a large number of parallel and unpolarized rays towards the center face of the numerical sample and tracks the rays until they exit the sample. Thus, the code was able to numerically reproduce experimental conditions required for measuring normal hemispherical reflectance, $\hat{R}(\sigma, T)$, and normal hemispherical transmittance, $T_r(\sigma, T)$, with an integrating gold sphere. Normal normal transmittance can also be computed. For these variables, $\sigma$ represents wave number and $T$ represents temperature.

During the propagation of a ray on the local scale, only reflection occurred. If the ray had a certain energy ($I_i$) before reaching an interface, then the ray transports the reflected energy, $I_{i+1} = rI_i$, after the
reflection event and releases \((1 - r)I_i\) to the solid phase (i.e., a strut), where \(r\) corresponds to the local directional reflectivity given by the Fresnel law for a given incident angle, \(\sigma\) and \(T\) [35]. This scheme is possible because the struts are optically thick. A brief inspection of the value of the index of absorption of pure aluminum [34], \(k\), indicates that for the entire spectral range of this study (i.e., 2-25 \(\mu\)m), the incident light would be completely absorbed for a mean thickness of 190 nm. Consequently, rays are not transmitted as they cross a strut. Reflection events can occur within the foam until the energy of a ray is higher than a cut off criterion, which a value equal to 0.01 was used in this paper. A discussion of the effects produced by the cut-off value was provided in a previous paper [36].

Finally, if rays can exit the sample through the back face, the energies of the rays contribute to the macroscopic normal hemispherical reflectance, \(\tilde{R}(\sigma, T)\). For the 5 other faces, energies supplied by the rays contribute to the normal hemispherical transmittance, \(\tilde{T}_r(\sigma, T)\).

Improvements to the MCRT code were performed. Recall that the order of the triangles in the mesh was determined using the iMorph software. At the voxel scale, special care focused on the optimization of the propagation time of a given ray. The voxels connected to the regular mesh are used to follow the propagation of rays through the sample. A step-by-step procedure is used to propagate rays into the media. This method assures that the algorithm uses a maximum of three triangles per voxel to determine if intersection occurs. If no intersection occurs in a voxel, then the next voxel is evaluated. The technique used in this article was faster and more efficient than the implementation of a more straightforward technique based on the direct calculation of the intersection with each voxel considered [8-9, 12, 21, 37]. Moreover, the step-by-step technique is much more efficient than a computation that uses every triangle for each intersection [6, 11]. For reference, the intersection calculation time for our method was on the order of \(O(1)\), whereas direct computation with \(n\) triangles had a dependence of \(n \log(n)\). Furthermore, in the algorithm used, the initial rays were placed into a “deque” memory structure. To be launched, each ray emerges from the end of the “deque”. A ray is deleted from the “deque” upon intersection with the interface and a new ray, which results from the local interaction, is placed at the end of the deck. The process ends when the deck is empty. Therefore, the algorithm is very easy to parallelize. The initial 10\(^6\) rays were distributed into different “deques” that were managed by separate threads.

Furthermore, a local optical scattering law that was based on the geometrical optics approximation was pragmatically introduced to account for the diffuse reflections induced by the rough surface of the struts (see Figure 1c). In this study, a simulation strategy that was previously employed for studies in the literature was used [6, 19, 38]. The strategy provided results largely comparable with those obtained from the approximated, as well as rigorous, resolution of Maxwell’s equations at the interfaces [39]. If a ray intercepts a triangle while traveling, then the reflected energy is modified by a factor loss of \(r^{n_{\text{impact}}}\), where \(n_{\text{impact}}\) is the mean number of local reflections generated by the surface roughness. The outgoing direction of the rays is randomly decided in the upward-hemisphere, in which the basal plane is defined by the intercepted triangle. An isotropic scattering behavior was assumed. In this work, \(n_{\text{impact}}\) values were obtained by studying the optical behavior of the virtual roughness of aluminum samples with an increasing slope \((\sigma_{\text{rms}}/\tau)\), where \(\sigma_{\text{rms}}\) is the root mean square of the height, and \(\tau\) is the correlation length of the height. A previously known MCRT code that was developed to investigate the optical behavior of an opaque rough surface was applied [13], which allowed for the evolution of \(n_{\text{impact}}\) as a function of \(\sigma_{\text{rms}}/\tau\) to be determined, as shown in Figure 3. The evolution was consistent with the earlier works of Bergstrom et al. [38, 40], where two scattering regimes could be distinguished. For \(\sigma_{\text{rms}}/\tau < 0.25\), simple scattering occurs. However, for \(\sigma_{\text{rms}}/\tau > 0.25\), multiple scattering regimes can occur with a local mean number of reflections, which can reach 5 local reflections if the slope is 2. This method enabled the spatial structure to be integrated in the calculations, which was not “viewed” by the tomographic experiment, at a resolution of 74.62 \(\mu\)m.
4. Results and discussion

The results of the calculations of both the room-temperature normal hemispherical reflectance and transmittance of the numerical foam samples were determined for wave numbers in a spectral range of 400 cm\(^{-1}\) to 5000 cm\(^{-1}\) (i.e., 2-25 µm). As determined in section 2, the mean characteristic sizes of the pores and struts identified in the foam enabled the geometrical optics approximation to be largely suitable for calculating the light-matter interactions. The Mie parameter sizes (\(X_{\text{Mie pore}}\) and \(X_{\text{Mie struts}}\)) were larger than 1 over the entire spectral range investigated. Furthermore, each strut was optically thick at T = 300 K. Consequently, the MCRT code (in C++) implemented in the iMorph software was applied to compute \(\hat{R}(\sigma, T)\) and \(\hat{T}(\sigma, T)\). For each experiment, \(10^6\) rays were launched at the bottom face of a given sample, which was a sensible compromise between statistical stability and computational cost. The statistical fluctuation of \(10^6\) rays was less than 0.5 % over several simulations. An incident beam diameter of 10 mm was used to reproduce the experimental conditions required for the use of the gold integrating sphere installed on the infrared spectrometer. More precisely, the aperture of the collection port for reflectance was virtually modified. Numerical calculations were performed with a commercial HP Z800 workstation equipped with an Intel(R)Xeon(R) Quad-Core processor (2.4 GHz, 12 MB cache, 1066 MHz memory). Using the QT framework that allows the iMorph software to run, parallel computations can be programmed. For a given wave number, 60 seconds was necessary to calculate the entire set of results.

Figure 4 shows the normal hemispherical spectral reflectance and transmittance as a function of the reconstructed foam thickness. When rays interact with the surface of the struts, only specular reflection events are considered, which indicates that the roughness of the struts does not cause peculiar scattering effects. For the normal spectral reflectance, the diameter of the aperture of the collector was set to 50 mm. As expected, the normal normal transmittance decreased exponentially, whereas the normal hemispherical reflectance increased and reached an asymptote at a thickness of 25 mm. The normal normal transmittance reached a value close to 0 for a foam thickness of 40 mm. The normal normal spectral transmittance decreased more rapidly than the normal hemispherical spectral transmittance. According to the procedure used for the calculations, normal normal transmittance was obtained by the ratio between the accumulated transmitted energies that arrived on the top face of the sample (i.e., the face opposite to the face that was impacted by the incident beam) to the initial energies deposited on the bottom face, whereas normal hemispherical transmittance included also the accumulated transmitted energies that reached the 4 side faces (i.e., the 4 faces other than the top face). As the sample thickness increased, the probability for rays to be transmitted to the lateral faces
increased. The energies received on the 4 side faces were identical in value, which indicates that the distribution of energy was symmetric for the samples.

Figure 4: (a) Evolution of the normal hemispherical spectral transmittance for increasing thicknesses of the foam at \( T = 300 \text{ K} \): (1) 5 mm, (2) 10 mm, (3) 15 mm, (4) 20 mm, (5) 25 mm and (6) 30 mm. (b) A room temperature comparison of (1) the normal hemispherical transmittance of the foam at \( \sigma = 2900 \text{ cm}^{-1} \) and (2) the normal normal transmittance at \( \sigma = 2900 \text{ cm}^{-1} \).

Figures 5 and 6 show the evolution of the spatial repartition of the back scattered energies for two aluminum foams with a thickness of 5 mm and 30 mm. The images indicate that as the thickness of foam increases, the back scattering spot becomes more extensive. For the sample with a thickness of 5 mm, 95% of the reflected energy was localized in a circular area of 20 mm, whereas this value decreased to 81% for the 30 mm-thick sample. A collector with an aperture diameter of 30 mm concentrated 99% of the reflected energy from the 5 mm-thick foam, whereas the value increased to 93% for the 30-mm thick foam. This result indicates that the thickness of the sample must be considered to correctly measure the normal hemispherical reflectance with an integrating sphere. For example, in studies with foams that have varied thicknesses and similar textural properties, use of an integrating sphere with the same aperture for the collection port of the reflected light can lead to incorrect experimental results.

To obtain a more quantitative appraisal of the effects on normal spherical reflectance caused by the surface roughness of the struts, numerical simulations were performed on struts with growing roughness slopes, \( \sigma_{rms}/\tau \). As explained in the section 3, calculations were used to integrate the
surface optical scattering due to the solid struts. Increasing values of $n_{\text{impact}}$ were used for different collector diameters, which the results are shown in Figure 7.

![Figure 7: Effect of the surface roughness of the struts on the normal hemispherical reflectance of a reconstructed aluminum foam with dimensions of $57 \times 57 \times 13$ mm ($T = 300$ K, $\sigma = 2900$ cm$^{-1}$): (1) the specular case and diffuse cases for (2) $n_{\text{impact}} = 1$, (3) $n_{\text{impact}} = 1.2$, (4) $n_{\text{impact}} = 1.4$ (5) $n_{\text{impact}} = 1.6$, (6) $n_{\text{impact}} = 1.8$ and (7) $n_{\text{impact}} = 2$.](image)

According to the model, the surface roughness has a noticeable effect on the level of normal hemispherical reflectance. For collector diameters greater than 40 mm, the reflectance values seem to be approaching an upper limit.

![Figure 8: Comparison between the calculated normal hemispherical spectral reflectance for different collector sizes and surface scattering behaviors at a variety of wave numbers: (1) $\Phi_{\text{collector}} = 15$ mm, specular case (2) $\Phi_{\text{collector}} = 20$ mm, specular case (3) $\Phi_{\text{collector}} = 25$ mm, specular case (4) $\Phi_{\text{collector}} = 15$ mm, $n_{\text{impact}} = 1.2$, (5) $\Phi_{\text{collector}} = 20$ mm, $n_{\text{impact}} = 1.2$, (6) $\Phi_{\text{collector}} = 25$ mm, $n_{\text{impact}} = 1.2$, (7) $\Phi_{\text{collector}} = 15$ mm, $n_{\text{impact}} = 1.4$ (8) $\Phi_{\text{collector}} = 20$ mm, $n_{\text{impact}} = 1.4$ (9) $\Phi_{\text{collector}} = 25$ mm, $n_{\text{impact}} = 1.4$ and (10) experimental data ($\Phi_{\text{incident beam}} = 10$ mm).](image)
The main augmentation occurs for \( n_{\text{impact}} = 1 \) (i.e., the scattering regime for which \( \sigma_{\text{rms}}/\tau < 0.25 \)).

For \( n_{\text{impact}} = 1 \), 90% of the reflected rays were concentrated in a spherical area with a diameter of 20 mm, whereas the value decreased to 85% for the specular case. If a backward distribution of the diffuse reflected light at the impact point between a ray and a strut is assumed, then a global enhancement can be observed in the backscattering behavior of the foam. As \( n_{\text{impact}} \) increases, \( \bar{R}(\sigma, T) \) starts to slowly decrease because the amount of energy that is locally absorbed by the matter is equal to 1 − \( r^{n_{\text{impact}}} \).

For a fixed value of the collector size, the value of the roughness of the slope of the real Erg foam can be indirectly estimated by adjusting the experimental measurement and numerical calculation. Figure 8 depicts the comparison of experimental and calculated reflectances with the MCRT code at \( T = 300 \) K.

The best agreements were obtained for \( \phi_{\text{collector}} = 20 \) mm and \( n_{\text{impact}} = 1.2 \) and for \( \phi_{\text{collector}} = 25 \) mm and \( n_{\text{impact}} = 1.4 \), where \( n_{\text{impact}} = 1.2 \) and 1.4 correspond to a slope of 0.35 and 0.45, respectively. The experimental collector had a diameter of 20 mm, which indicates that the mean slope roughness could be close to 1.2. This result indicates that the development of a contactless method to quantitatively probe the mean roughness parameters of the struts that constitute foams should be possible, which is easier than only using SEM images (Figure 1c). In cases where only simulated data can be provided, we would use the results obtained under the experimental acquisition conditions defined by the gold integrating sphere as a starting point.

5. Conclusion
The characterization of an aluminum foam was performed to provide experimental data for numerical software, which was intended to quickly compute the radiative properties. The numerical tool was integrated into a pre-existing software application, iMorph. The software was able to compute normal hemispherical reflectance and transmittance of materials for the following reasons: (i) at the microscopic scale, the interaction between light and fluid/solid interfaces can be treated pragmatically according to the geometrical optics approximation, and (ii) at the macroscopic scale, the dimensions of the reconstructed 3D images correspond to the dimensions of the sample used for the experimental characterization of the radiative behavior.

For a fixed probed volume, the code demonstrated that the effects caused by the experimentally observed micro-roughness on the surface of the struts using SEM (not observed in x-ray \( \mu \)-tomography) can be important. According to the accuracy of the set-up used for measuring the diffuse reflectance and transmittance and to the dimensions of the probed sample, a contactless method may be possible to probe the roughness of struts.

6. References
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