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► **To cite this version:**

Morgan Sans-Laurent, Olivier Farges, Vincent Schick, Christian Moyne, Gilles Parent. Modeling the Flash Method by using a Conducto-Radiative Monte-Carlo Method: Application to Porous Media. 9th International Symposium on Radiative Transfer (RAD-19), Jun 2019, Athènes, Greece. pp.319-326, 10.1615/RAD-19.390 . hal-02410633

HAL Id: hal-02410633

<https://hal.science/hal-02410633>

Submitted on 19 Dec 2019

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MODELING THE FLASH METHOD BY USING A CONDUCTO-RADIATIVE MONTE CARLO ALGORITHM : APPLICATION TO POROUS MEDIA

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ABSTRACT. In the following paper, both conduction and radiation heat transfer were explored **with** a Monte-Carlo method applied to a complex geometry. The algorithm accounted for the coupling of conduction in the solid phase and radiation through the void phase and is used for direct simulation of a flash method. This allowed us to evaluate the effective total conductivity of the equivalent homogenized medium **in function of a wide range of thermal, optical and geometric properties**. The influence of the hemispherical emissivity of **the struts material**, the porosity and the diameter of the cells are investigated. Moreover, this procedure appears to be a useful tool to confirm whether or not the assumption of the **diffuse radiation** (Rosseland) is valid.

1. INTRODUCTION

Because of their interesting thermal, mechanical and optical properties, ceramic and metallic foams are commonly used in many engineering applications [1]. Improvements of the manufacturing processes **allows the fabrication of foams with a very wide range of textural parameters such as porosity, cell size distribution, geometries or materials used**. Foams can be designed and applied to several processes such as catalysis, volumetric solar absorbers, insulators, heat exchangers or gas-phase heat recovery. The complexity of the geometry and the different **physical phenomena** involved (conduction, convection, transport, radiation or chemical reaction) play an important role on the efficiency of the studied system. In order to optimize systems including heterogeneous media, a good understanding of the link between the textural parameters and the heat transfer is needed.

Solving combined heat transfers directly on the complex geometry requires long computation times. Therefore, it is common to simplify the physical problem by working with an effective thermal property. The foam is thus represented by an equivalent homogeneous medium, where the coupled thermal behavior is described only with equivalent properties specific to each mode of heat transfer.

One of the main problems comes from the different nature of the two modes of heat transfer. Purely conductive transfer modeling in this kind of medium was widely studied, see [2,3] for example. It is no more the case for the coupled conductive-radiative transfer. On the one hand, the conduction transfer, which obeys the Energy Balance Equation (EBE), can be solved by using a numerical solver based on classical discretization methods such as finite element method (FEM) or finite volume method (VFM). On the other hand, the radiative transfer is described by the famous radiative transfer equation (RTE), which can be solved by a wide choice of methods (Discrete Ordinate Method, Monte Carlo Method, Moments Methods, etc...). Classically, if the solid is assumed opaque, the radiative transfer is simply an exchange

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between all the surfaces of the solid matrix. Hence, the Radiosity Method, based on the computation of the form factors appears as the most appropriate method. However, during the past decade, Monte Carlo Method (MCM) based on ray tracing became the most popular method [4,5]. It allows the identification of the equivalent radiative property of a wide range of very complex 3D geometries. Nevertheless, an appropriate method, which describes the conductive transfer through the foam is still needed in order to model the coupled transfer.

Recently, Fournier et al. [6] suggested the idea of a complete resolution of conduction, convection, and radiation in a single Monte-Carlo algorithm. Based on an integral formulation, a recursive (backward in time) algorithm computes the temperature at any location of a complex 3D geometry and takes into account a multiphysical problem. The main assumption is that all the set of equations solved in each phase can be written as a Fredholm equation of the second kind. For this, the thermal and optical properties are assumed independent of the temperature and the radiative transfer is linearized. In a stationary case, Caliot et al.[7] applied this algorithm on a structured foam (Kelvin cell). Considering conductive and radiative transfers, the method was developed to describe a numerical hot guarded plate. This approach was validated by comparison with a deterministic method.

The present article continues the work initiated by Caliot et al. [7] in an unsteady case. In a previous study, the thermal characterization of SiC and SiSiC foams was investigated thanks to an experimental Flash method [8]. So, this **work is aimed** at bringing a complementary study of the estimated equivalent thermal parameters **in function of the physical parameters (e.g. porosity, emissivity, investigated temperature, conductivity of the solid)**. A numerical Flash method was applied to a 3D structure. Hence, the temporal evolution of the temperature on the rear face of the sample due to a thermal excitation on its front face was computed with a recursive Monte-Carlo method. Then, the thermal response on the rear face, characteristic of the thermal behaviour of the foam was treated like a classical thermogram which could be measured experimentally [9]. In the following, we first describe the construction of the geometry, then present the principle and the implementation of the Monte-Carlo method. Finally, we investigate the influence of the emissivity of the solid, the porosity and the diameter of the cells. The results obtained on different Kelvin's cell foams are discussed.

2. METHODS

2.1 Geometry construction

All computations were carried out using 3D images defined by structured grids of $N_x \times N_y \times N_z$ voxels, which can be built numerically or obtained from X-ray tomographies. In this article, we only treat the case of purely structured numerical foams based on a repetition of a unitary tetrakaidecahedron (Kelvin's cell), but the procedure can be easily extended to a wide range of geometries such as stochastic numerical foams, fibers, packed spheres or foams from X-ray tomography. The initial raw data was obtained thanks to a numerical foam generator called GenMat, which was developed at Laboratoire de Thermique et d'Energie de Nantes (LTEN). Based on a watershed marker-based method, this open-source software was validated by comparing with a reference SiC foam for the case of the stochastic foams [10].

Experimentally, it is common to put the foams between two soleplates or to cover each face with a black coating [9]. The first soleplate absorbs the deposited energy while the second is used for the measurement of the spatial average of the temperature. Hence, in order to simulate this three-layer system, two stacks of images, which represent the two soleplates were added to the Kelvin's cells structure itself (see Figure 2 a). Then, the surface mesh was generated with a robust marching-cube method. However, the triangular mesh obtained is very dense and, due to a limited orientation of the possible faces, can display a surface with an unrealistic appearance. So, we applied a decimation method and a smoothing (surface preserved) algorithm to reduce the number of elements and improve the quality of the mesh.

2.2 Monte-Carlo Method

The main idea of the Monte Carlo method, in order to compute the temperature at location \vec{r} and at time t , is to follow **a large number** of paths crossing the complex geometry. The temperature is the expectation of a random variable $T(\vec{r}, t)$. This random variable is determined from a path inside the calculation domain. Each path can follow a conductive path in the solid (considered here opaque) or a radiative path in the void phase (considered here perfectly transparent). **A path starts at the location and at the time where the temperature needs be computed.**

In the classical Flash method, the sample, in thermal equilibrium at the desired temperature, is excited in the front face with a heat flux. The temporal evolution of the spatial average of the temperature on the rear face is measured with an infrared camera. In order to reproduce numerically the latter procedure, all the realizations of Monte Carlo start thus from the rear face. Initially, we set $\vec{r} = (x, y, z = e_{foam} + 2e_{sole})$, where e_{foam} and e_{sole} are the thicknesses of the foam and of the soleplates, respectively.

The time is discretised by defining a uniform time step Δt . For each time interval t_i , N_p paths are followed. The j^{th} path in the i^{th} time interval begins at $t_{ij}^{k=0} = t_i + (R - 0.5) \times \Delta t$ (with R a random number). The recursivity arises naturally from the fact that the temperature at the given time t_{ij}^k depends on the temperature at the previous time t_{ij}^{k+1} (which also depends on the previous time t_{ij}^{k+2} etc..) until a **known temperature is achieved (e-g. a boundary or an initial condition)**. A chain of random events is thus constructed. The computed temperature in the i^{th} interval $T(\vec{r}, t_i)$ corresponds to the average of the N_p paths followed in this time interval.

In the solid, the energy equation is solved with a fixed random walk as proposed by Caliot et al. [7]. As represented in Figure 1 a), a sphere with a radius δ_d and centered at the computed temperature is drawn. The new position is sampled uniformly on the sphere (sampling of a direction \vec{u}). If the temperature is still not established or an interface solid/void is not reached, a new sphere is drawn and the algorithm continues the walk through the solid. If the distance between the computed location and solid/void phase interface is shorter than the radius of the sphere, the algorithm jumps directly at the interface with a shorter displacement $\delta_w < \delta_d$.

Moreover, each spatial jump implies a temporal jump. For a given displacement $\delta_c = \min(\delta_w; \delta_d)$, inside a homogeneous and isotropic solid with a_s its diffusivity, the backward temporal jump δ_t is computed by sampling an exponentially distributed random variable with expectation $\delta_c^2/6a_s$ [11].

At the interface \vec{r}_w , under vacuum condition, the balance of the radiative and conductive fluxes is written :

$$-\vec{n} \cdot \lambda_s \vec{\nabla} T = h_r (T(\vec{r}_w) - T_{\text{rad}}(\vec{r}_w)) \quad (1)$$

where $h_r = 4\epsilon\sigma T_{\text{ref}}^3$ is a radiative exchange coefficient, \vec{n} is the outward unit normal vector of the intersected surface, λ_s the conductivity of the solid, ϵ the hemispherical emissivity and σ the Stefan-Boltzmann constant. On the one hand, a reference temperature T_{ref} is defined and corresponds to the linearized radiative term. On the other hand, T_{rad} **represents an average radiative temperature seen at the interface and due to the radiative exchanges through the void phase as demonstrated in [7]**. The temperature gradient in the solid, by defining an infinitesimal length δ_b , **is computed as:**

$$-\vec{n} \cdot \lambda_s \vec{\nabla} T \approx -\frac{\lambda_s}{\delta_b} (T(\vec{r}_w) - T(\vec{r}_w - \delta_b \vec{n})) \quad (2)$$

Injecting this relation into Equation 1, the temperature at the interface is expressed as:

$$T(\vec{r}_w) = \frac{\lambda_s/\delta_b}{\lambda_s/\delta_b + h_r} T(\vec{r}_w - \delta_b \vec{n}) + \frac{h_r}{\lambda_s/\delta_b + h_r} T_{\text{rad}}(\vec{r}_w) = P_{c \rightarrow c} T(\vec{r}_w - \delta_b \vec{n}) + P_{c \rightarrow r} T_{\text{rad}}(\vec{r}_w) \quad (3)$$

According to Equation 3, the temperature at the wall appears as an average of a **conductive and radiative temperature weighted by intrinsic properties (i.e. ϵ and λ_s) and by the investigated reference**

temperature T_{ref} . The weight functions, $P_{c \rightarrow c}$ and $P_{c \rightarrow r}$, corresponds to the probability to follow a conductive or a radiative path, respectively. Hence, a uniform sampling of a random number R_{rad} is compared to $P_{c \rightarrow r}$.

Moreover, let us note that an increase of the hemispherical emissivity and of the reference temperature increase the probability to follow a radiative path while an increase of the conductivity increases the probability of a conductive path. Hence, the impact of the intrinsic properties on the global heat transfer can be studied and allow a better quantification of the major heat transfer mechanism.

If $R_{\text{rad}} \leq P_{c \rightarrow r}$, an emission direction \vec{w} , obeying a lambertian law, is computed. Then, the new position, which corresponds to the intersection between the emitted ray and the geometry through the void phase is set. The distance is traveled along a straight line and no backward temporal jump is performed. In other words, the travel is instantaneous due to the very large light velocity. Then, we estimate if the incident ‘‘ray’’ is absorbed or reflected with a probability equal to the hemispherical reflectivity $1 - \epsilon$. The reflection is assumed purely diffuse. Hence, multiple reflections are computed until an absorption event appears. Finally, after absorption, the position being still set on an interface, we verify if the path will continue in the void phase by reemission or will follow a walk in the solid. On the contrary, if $R_{\text{rad}} > P_{c \rightarrow r}$, the path is positioned with a distance δ_b in the solid according to the direction $-\vec{n}$. All the implemented recursive algorithm is described in **Figure 1 b)**. The extension of the method with any specular reflection and spectral dependency is straightforward. At the lateral boundaries of the domain, a

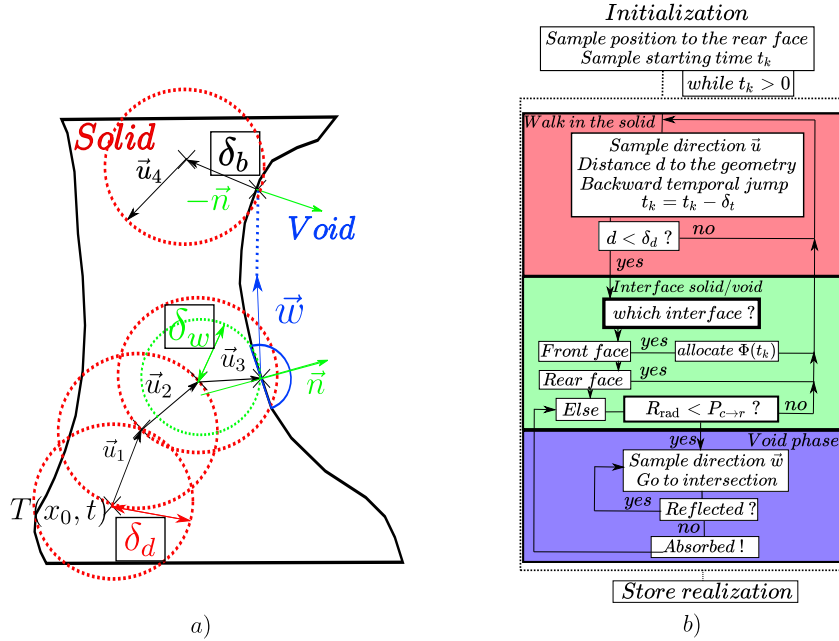


Figure 1. a) Scheme of a coupled conductive and radiative path b) Algorithm to evaluate the temporal evolution of the rear face temperature

periodic boundary condition is used, such that the medium is infinite along \vec{x} and \vec{y} . For both conductive and radiative path, all incident directions are purely reflected. For the upper (rear face) and the lower (front face) bounds, an adiabatic condition is fixed (the conductive flux is null). **Hence, the path is only replaced in the solid with a distance δ_b according to the direction $-\vec{n}$.**

In an experimental Flash method, the temporal distribution of the heat excitation can be assimilated to a Dirac function or at least a very short pulse. However, the probability for a path to be located in the front face at the exact time of the pulse is null. So, we impose a constant heat excitation $\Phi(t)$ during a fixed time t_d , which can be written as :

$$\Phi(t) = Q (H(t) - H(t - t_d)) \quad (4)$$

where H is the Heaviside-step function and Q (W m^{-2}) the deposited flux density. Each time the path

reaches the front face between $[0; t_d]$ a part of the deposited flux density is allocated to the given path (see Equation 5).

Finally, each path is stopped when $t < 0$. Indeed, at this time the temperature is known ($T(\vec{r}, 0) = T_0$). Hence, the computed temperature for the j^{th} path with a starting time included in the i^{th} time interval is:

$$T_{ij} = T_0 + \sum \frac{\delta_b Q}{\lambda_s} \quad (5)$$

In other words, the temperature of the rear face at a time t is simply the temperature at the initial condition ($t = 0$) plus its history, the increase being provided by the deposited energy. The final temperature of the i^{th} time interval is the average of the temperature of all the followed paths.

The temporal evolution of the temperature on the rear face is treated as an experimental thermogram. The standard deviation associated to each value can be seen as an experimental noise, which is proportional to the inverse of the square root of the number of Monte Carlo realizations. The results are thus comparable to the **temperature evolution obtained by a measuring instrument such as a thermocouple or an IR camera. The inversion of the thermogram requires a direct model. The latter assumes a purely one way conductive heat transfer and is built from a quadrupole method [12]. Hence, the foam is treated as a homogeneous medium. A Levenberg-Marquardt algorithm [13] estimates the total equivalent diffusivity, which allows the best match between the curve computed with the MCM and the curve obtained with the quadrupole method.**

3. RESULTS AND DISCUSSION

The proposed algorithm was applied to a porous medium composed by a stack of five Kelvin's cell between two soleplates as depicted on the Figure 2 a). First, the influence of the hemispherical emissivity was studied. Then, we explored the impact of the porosity on the total heat transfer. For each case, the diffusion length was fixed to $\delta_d = D_{cell}/250$ with D_{cell} the diameter of the cells. The arbitrary length defined at the interface was set to $\delta_b = 3 \times \delta_d$. Obviously, the error on the estimated value would decrease with $\delta_d \rightarrow 0$ and $\delta_b \rightarrow 0$. **Unfortunately, a too small diffusion length provides digital error and, on the contrary, a large diffusion length compared to the characteristic length of the system (struts of the foam) provides bias on the final value. For the sake of brevity, validations cases are not presented here and will be detailed in an extended version of the present article.**

3.1 Influence of the emissivity

The objective of the simulation was to understand, through the estimation of the equivalent thermal diffusivity, the thermal behavior of a heterogeneous medium with respect to the temperature and to the emissivity of the foam struts. The conductivity of the solid was fixed to $50 \text{ W m}^{-1} \text{ K}^{-1}$ (SiC at 1000 K), the diameter of the cell was $D_{cell} = 10 \text{ mm}$, the porosity of the foam was $\Phi = 80\%$, the range of the reference temperature investigated was $[300 \text{ K}; 2500 \text{ K}]$ and the emissivity was between 0.25 and 1. The probability to follow a radiative path $P_{c \rightarrow r}$ was lower than 1% due to a high conductive coefficient ($\lambda_s/\delta_b \approx 4.2 \cdot 10^5 \text{ W m}^{-2} \text{ K}^{-1}$) compared to the one for radiation ($\max(h_r) \approx 3.5 \cdot 10^3 \text{ W m}^{-2} \text{ K}^{-1}$). Figure 2 b) and c) shows the path with only conduction and conduction + radiation, respectively. More the probability increases more often a path crosses the void phase instantaneously. So, the mean celerity of the walk is increased. This is also evidenced in the Figure 2 d). The elevation of the temperature is accelerated by the radiative transfer. The estimated total equivalent conductivity quantifies this acceleration. Let us note that the achieved temperatures at the steady state are exactly the same for all the reference temperature because the deposited energy is the same. Each thermogram was computed **using**

2000 Monte-Carlo realizations per 50 time intervals (thus 10^5 total paths). Computation time is strongly dependent on the diffusion length and the maximum time t_f . With a single CPU Intel Xeon X5650, 73h was needed for the pure conduction case while only 1h30 was sufficient for $T_{\text{ref}} = 2500$ K. Thus, the algorithm shows a better interest in case of a high radiative transfer.

Concerning the inversion procedure, the obtained residual indicates that the thermal behavior for a coupled heat transfer in the structure is well described by a purely conductive model inside an equivalent homogeneous medium. Hence, these results confirm the possibility to describe heat transfer with a radiative equivalent conductivity λ_r . In other words, the radiative transfer can be comparable to a conductive one. The diffusion approximation for radiation (Rosseland) is thus valid for this geometry. The similar procedure, not presented here for the sake of brevity, applied to a geometry composed by only two Kelvin's cell between two soleplates, **showed that a purely conductive model cannot describe the thermogram obtained with the MCM. In this configuration, the assumption of the diffuse radiation is no more valid and a model describing both conductive and radiative heat transfer is required.** These results highlight the usefulness of the described tool to investigate the validity field of **this assumption**. Flash experiments also showed that a conducto-radiative model is better than a conductive model for foams having an optical thickness lower than 6 [8].

Figure 3 represents the ratio of the total conductivity $\lambda_{\text{tot}} = \lambda_r + \lambda_c$ to the bulk conductivity λ_s according to the reference temperature. The impact of the radiative transfer is thus quantified. The total conductivity increase appears to be logically proportional to T_{ref}^3 . However, for the intended field of application, the conduction is still the main heat transfer (60%), which is in agreement with [14].

The radiative transfer becomes **predominant** from 1200 K. Above a value of 0.9, the radiative transfer is independent of the emissivity (blue and red curves in Figure 3 are almost superimposed). **These results show that an effective optical thickness β_{eff} , characteristic of the radiative transfer of the medium, is not a pure constant.** It is function of the emissivity, as it was also very recently evidenced by Vignoles et Ortona [15].

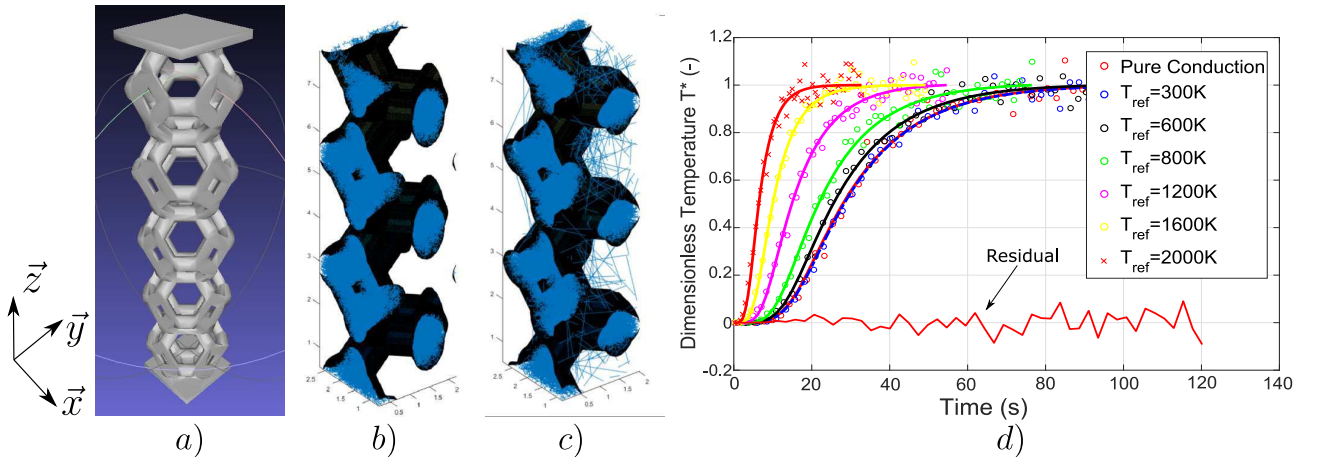


Figure 2. a) Investigated geometry; b) Only conductive transfer (path represented in blue); c) Conductive and Radiative transfer : $T_{\text{ref}} = 2500$ K(path represented in blue); d) Comparison between obtained thermograms and corresponding direct simulation. The drawn residual is for the case : $T_{\text{ref}} = 300$ K.

3.2 Influence of the porosity and the size of the cells

We performed the same procedure in order to investigate the influence of the textural parameters such as porosity or diameter of the cell for fixed thermal properties. The textural parameters were, for the first cases : $D_{\text{cell}} = 5$ mm and $\phi \in [30\%; 90\%]$ and for the second cases : $\phi = 80\%$ and $D_{\text{cell}} \in [1$ mm;10 mm]. The probability to follow a radiative path $P_{c \rightarrow r}$ was increased by decreasing the conductivity of the solid such as $\lambda = 1$ W m⁻¹ K⁻¹. All other parameters were identical to the previous study.

For a low temperature, for which conduction is predominant, the total conductivity decreases according

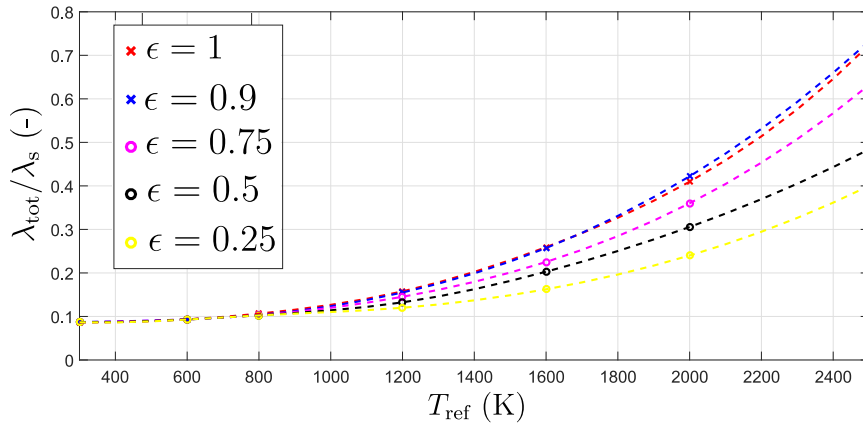


Figure 3. Influence of the emissivity

to the porosity (Figure 4 a)). Then, we observe the exact opposite behavior at higher temperature. The role of the radiation is increased by the vacuum let by the structures with the highest porosity and becomes not negligible, even at ambient temperature. Moreover, the investigated ratios λ_{tot}/λ_s are much higher than the previous case due to a higher probability to follow a radiative path.

Figure 4 b) illustrates the effect of the size of the cell. If we consider only conduction, all the foams present the same equivalent conductivity. This result is in good agreement with the findings of previous studies [14]. Then, it is clear that the radiative contribution is function of the diameter of the cells. This is explained by the fact that the radiative free mean path is higher for the bigger cells, which thus favors the radiative transfer.

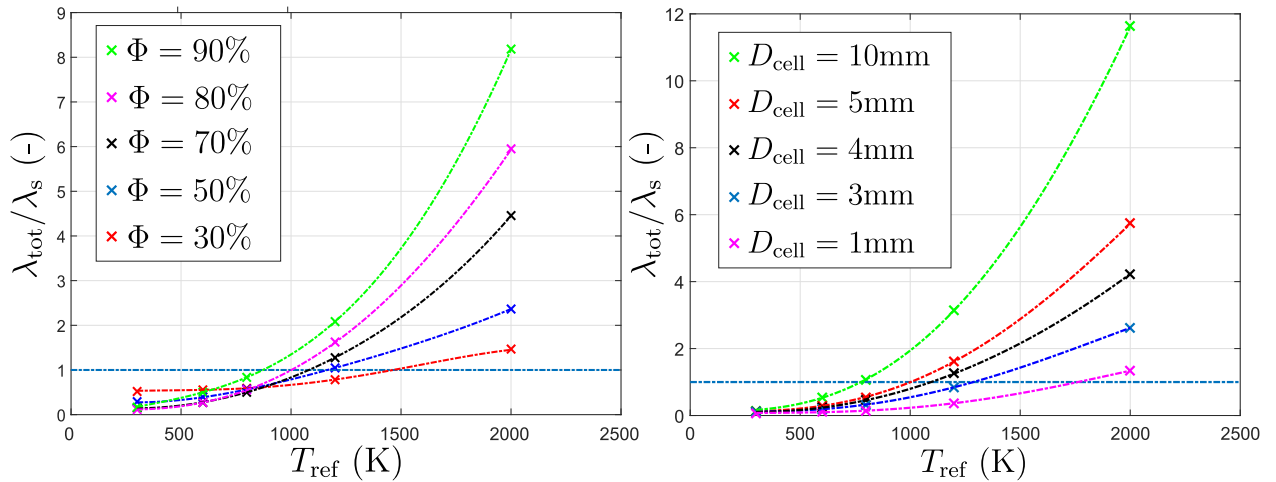


Figure 4. Influence of the textural properties : a) Porosity b) Diameter of the cells

4. CONCLUSION

Following a stochastic method, a **Recursive** Monte Carlo algorithm was designed to solve the combined conductive and radiative heat transfer in 3D heterogeneous media. This work extends previous studies by considering a transient transfer. In order to characterize the total equivalent conductivity, a numerical flash method was implemented and allowed the computation of the thermal response due to a thermal excitation of porous media (Kelvin's cells). The algorithm was detailed and the influence of thermal (emissivity of the solid) and textural (porosity and size of the cell) properties was investigated. The results show good agreement with literature. This new tool allows a better quantification of the link between intrinsic properties and homogenized ones and of the major heat transfer mechanism. Moreover, it is clear

that the procedure is useful to determine whether or not the assumption of the diffusion for the radiation is valid. An extension of this study will concern numerical stochastic foams generated with GenMat or foams issued from X-ray tomography. Upcoming work will also include the characterization of an effective extinction coefficient thanks to a direct model describing the heat transfer in a homogeneous semitransparent medium.

ACKNOWLEDGMENTS

The authors gratefully acknowledge Benoit Rousseau (LTEN) for providing and support regarding the use of GenMat. We also wish to acknowledge Cyril Caliot (Promes), Mouna El Hafi (Rapsodee), Richard Fournier and Stephane Blanco (Laplace) for their motivating advice and the fruitful discussions.

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