Numerical validation of an effective radiation heat-transfer model for fiber preforms

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Direct numerical simulation (DNS) of radiation heat-transfer has enabled the validation of an effective radiative conductivity (semi-analytical) model, for thin layers of two-dimensional carbon-fiber preforms. The effective conductivity is shown to be a function of three parameters: the local temperature, the extinction coefficient, and the sample thickness. The integration of the proposed model, in macroscopic material-response simulation tools, is relatively simple. Only the effective conductivity in Fourier's law needs to be modified, to accurately account for radiation effects. DNS and macroscopic simulations show an excellent agreement even in the transient regime when very strong temperature gradients develop across the thickness.

Nomenclature

A_i	=	surface, m^2
c	=	capacity, J/(kg.K)
d	=	distance, m

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F_{ij}	=	view-factor, -
H_i	=	incident flux, W/(m^2)
k	=	correlation coefficient, -
$\overline{k}$	=	average correlation coefficient, -
q	=	heat flux, W/(m^2)
R_i	=	radiosity, W/(m^2)
T	=	temperature, K
Δx	=	length of the model, m
Δy	=	height of the model, m
Δz	=	depth of the model, m
ϵ_σ	=	emissivity, -
ρ	=	density, kg/(m^3)
λ	=	conductivity, W/(m.K)
σ	=	Stefan-Boltzmann constant, $5.67 \cdot 10^{-8}$ W/(m^2 .K^4)
σ_{ext}	=	specific extinction coefficient, m^2/kg

Sub/Super-script

$_0$	=	apparent value
$_{1,2}$	=	walls
$_i$	=	fiber faces
$_r$	=	radiative
$_\lambda$	=	conductive

I. Introduction

RADIATIVE heat-transfer in fibrous materials has been the subject of numerous investigations.[1–5] Models with different degree of complexity and accuracy have been proposed. They range from semi-analytical models anchored by experimental data,[6] to an accurate analytical modeling of the radiative energy transport through an absorbing and scattering medium.[3] The later method gives excellent results but counts two major drawbacks:

- it is limited to materials with an homogeneous distribution of well defined geometrical features (e.g. spheres, cylinders);
- it is not practical to implement in macroscopic material-response simulation tools.

This study has two complementary short term objectives [with long term goals noted between brackets]:

- extend the applicability of ab-initio methods, with the development of a direct numerical simulation (DNS) tool allowing the treatment of any geometry. [The long term goal is to compute material properties from three-dimensional material-architecture reconstruction obtained by computed X-ray micro-tomography.]
- develop an effective radiative transfer model for thin layers of two-dimensional low-density carbon-fiber preforms, that may be integrated in macroscopic material-response tools. Perform a DNS analysis and validate the effective radiative transfer model. [The long term goal is to generalize the validation or extend the model to any architecture].

The article is organized as follows. In the second section, the material properties are discussed, an effective conductivity model is derived, and the DNS approach is presented. In the third section, the parameters of the effective model are obtained from steady-state DNS. In the fourth section, the accuracy of the effective model in the transient regime is confronted to time-accurate DNS.

II. Model and simulation tool

A. Material model and problem studied

In this first study, we shall consider that the carbon-fiber preform is two-dimensional with fibers parallel to each other. The following carbon-fiber properties, representative of literature data, will be used: conductivity, $\lambda = 10$ W/(m.K); specific heat capacity, c =1000 J/(kg.K); density, $\rho = 1800$ kg/m^3; and emissivity, $\epsilon_\sigma = 0.85$ (gray body). The fibers are treated as perfect cylinders with a diameter of 10 μm. The fiber volume fraction of carbon-fiber preform is typically about 0.1. The model material for the DNS is generated using a Monte-

Carlo procedure: non-overlapping fibers are randomly placed in a 2D box until the required volume fraction is obtained (Fig. 1). Therefore, the model is heterogeneous and two-dimensional at the microscopic scale, and homogeneous isotropic at the macroscopic scale.

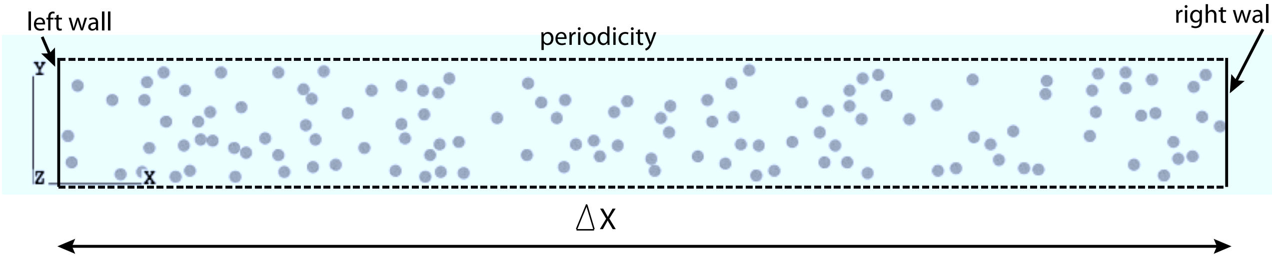

Figure 1. Random distribution of fibers between two walls ($\Delta x = 1$ mm).

We shall study the problem of Deissler;[7] that is, we shall assume that there are imaginary walls on the right hand side and on the left hand side of the box containing the fibers (Fig. 1), with equal emissivities ϵ_σ for both walls and for the fibers. The model is taken periodic in the y-direction. The macroscopic problem is then one-dimensional.

B. Effective radiative transfer model

The diffuse gray radiation model between two infinite parallel planes may be linearized (Fourier's form) and the effective radiation conductivity λ_r can be written as:

$$\lambda_r = \frac{k\epsilon_\sigma}{2-\epsilon_\sigma}\sigma T^3 \Delta x \tag{1}$$

where $k = 4$, is a geometric factor. In the presence of fibers, the value of k is modified.

Under the hypothesis of Rosseland (optically thick medium), the effective conductivity may be expressed as a function of the emissivity (ϵ_σ) and the thickness of the model (Δx):[6]

$$\lambda_r = \frac{4\epsilon_\sigma \sigma T^3 \Delta x}{(2-\epsilon_\sigma) + \sigma_{ext}\epsilon_\sigma \rho_0 \Delta x} \tag{2}$$

where ρ_0 is the effective density of the material and σ_{ext} is the specific effective extinction coefficient that must be obtained for a given fiber configuration. Combining Eq. (1) and (2), the geometric factor k for the fibrous medium may be expressed a function of Δx as

$$k = \frac{4(2-\epsilon_\sigma)}{(2-\epsilon_\sigma) + \sigma_{ext}\epsilon_\sigma \rho_0 \Delta x} \tag{3}$$

The radiation heat flux q_r may be written as

$$q_r = -\frac{k\epsilon_\sigma}{2-\epsilon_\sigma}\sigma T^3 \Delta x \frac{\Delta T}{\Delta x} = -\frac{k\epsilon_\sigma}{2-\epsilon_\sigma}\sigma T^3 \Delta T \quad (4)$$

C. Ab-initio physical model and associated DNS tool

An electromagnetic wave or photon passing through the immediate vicinity of a fiber is either absorbed or scattered. The scattering is due to three separate phenomena, namely, (i) diffraction (waves never come into contact with the fiber, but their direction of propagation is altered by the presence of the fiber), (ii) reflection (waves reflected from the surface of the fiber), and (iii) refraction (waves that penetrate in the fiber and, after partial absorption, reemerge traveling in a different direction).[8] Carbon fibers are opaque, therefore, there is no refraction. The carbon-fiber surface is rough generating a diffuse reflection. Diffraction is critical when the wavelength is not small compared to the fiber diameter. In the case of fibrous media, the size parameter x is defined as:

$$x = \frac{d \cdot \pi}{\lambda} \quad (5)$$

where the fiber diameter d equals 10 μm and where λ is the wavelength of interest. In general, diffraction is negligible for $x \geq 10$.[8] However, the work of Lee[1] has shown that diffraction, for randomly oriented fibers, has a negligible effect on effective heat transfer for values of x larger than unity. Hence, diffraction may be neglected for wavelengths smaller than $\lambda_{lim} = 31.4\,\mu$m. According to Plank's law, 99% of the energy of a black (or gray) body is emitted at wavelengths smaller than $\lambda_{lim} = 31.4\,\mu$m for temperatures higher than about 700 K. Radiative heat transfer is small compared to conduction for temperatures below 800 K in carbon preforms. Therefore, diffraction will be neglected in the following and a gray-body diffuse radiation model will be used.

Numerically, the perimeter of each fiber is discretized into facets (or faces). View-factors, which model the energy exchange between the faces, need to be calculated between the fiber faces:

$$F_{ij} = \frac{\text{Energy absorbed by face } A_j, \text{by direct travel}}{\text{Diffuse energy emitted by face } A_i} = \frac{1}{A_i}\int_{A_j}\int_{A_i} \frac{\cos(\theta_i)\cos(\theta_j)}{d^2}\, dA_i\, dA_j \quad (6)$$

which can be expressed both as an energy balance, or as a geometric quantity (isothermal facets). The view-factors are obtained using a collision-based Monte-Carlo method, to which reciprocity and least-squares closure is applied as described by Zeeb.[9]

In the case of diffuse gray-body radiation, the radiosity of a face R_i, which is defined as the emitted energy of the face plus the portion of the incoming radiation H_i that is reflected by the face, may be written as

$$R_i = \epsilon_\sigma \sigma T_i^4 + (1 - \epsilon_\sigma) H_i \tag{7}$$

By writing the energy balance equation for face i, as either the difference of the incident flux (H_i) and the total radiated flux (R_i), or the absorbed flux and the emitted flux, we obtain the following:

$$q_i = H_i - R_i = \epsilon_\sigma H_i - \epsilon_\sigma \sigma T_i^4 \tag{8}$$

The incident flux on face i can be expressed by the sum of all the radiosities (R_j), times the view-factors between facet i and the rest of the closed cavity.

$$H_i = \sum_{j=1}^{N} R_j F_{ji} \tag{9}$$

Using reciprocity ($A_i F_{ij} = A_j F_{ji}$) and closure ($\sum_{j=1}^{N} F_{ij} = 1$) the final balance equation for facet i equals:

$$\sum_{j=1}^{N} F_{ij} \left(R_j - R_i\right) + \frac{\epsilon_\sigma}{1 - \epsilon_\sigma} \left(\sigma T_i^4 - R_i\right) = 0 \tag{10}$$

This formulation is known as the electrical analogy formulation for radiation heat exchange. It is described in detail by Modest.[8] The heat radiation equations are combined with the standard transient heat transfer equations for solids. This allows the modeling of the conduction and radiation problem in both transient and steady state. All the equations are implemented in the finite-element code SAMCEF, which is used for industrial applications in the aerospace industry.[10]

III. Steady state analysis

The goal of this analysis is to determine the effective radiative conductivity. For the steady state analysis, the temperature on both sides of the model is imposed. This results in a known temperature difference ΔT over the model for a given temperature T (=$(T_1 + T_2)/2$). This analysis is repeated for different temperatures T between 0 K and 4000 K.

A. Test-matrix

The steady state analysis is performed for 5 different configurations. All configurations have the same basic geometric layout (see Fig. 1), with a height Δy and a depth Δz of 100 μm, but with different lengths. The model in Fig. 1 is a finite element model where every fiber is modeled using approximately 55 elements.

- Configuration 1: 63 fibers with a length of $\Delta x = 0.5$ mm.
- Configuration 2: 126 fibers with a length of $\Delta x = 1$ mm.
- Configuration 3: 252 fibers with a length of $\Delta x = 2$ mm.
- Configuration 4: 504 fibers with a length of $\Delta x = 4$ mm.
- Configuration 5: 1008 fibers with a length of $\Delta x = 8$ mm.

All five configurations are generated in such a way that they have the same fiber volume fraction ($\approx 9.76\%$), resulting in an effective density ρ_0 of 175.68 kg/m^3. For all configurations a total of 5 random geometries (seeds) are generated in order to assess the influence of the random fiber placement on the convergence of the solution.

Table 1. Values of k for five random seeds.

Configuration:	1	2	3	4	5
Seed			$k[-]$		
1	0.798	0.432	0.233	0.121	0.062
2	0.785	0.445	0.233	0.121	0.062
3	0.761	0.447	0.238	0.122	0.061
4	0.796	0.447	0.232	0.122	0.062
5	0.758	0.435	0.236	0.121	0.062
$\overline{k} =$	0.779	0.441	0.234	0.121	0.062

B. Effective radiative conductivity

The average effective conductivity curves for the five configurations are plotted in Fig. 2. As expected from the form of Eq. 2, the effective conductivity features an asymptotic behavior as a function of Δx. For all five configurations the values of k are presented in Table 1. The random nature of the geometry has very little effect of the value of k. In Fig. 3, the average $\overline{k}$ values are plotted as a function of the model length Δx. The data are perfectly fitted using Eq. (3) with an extinction coefficient σ_{ext} of 63.11 m^2/kg.

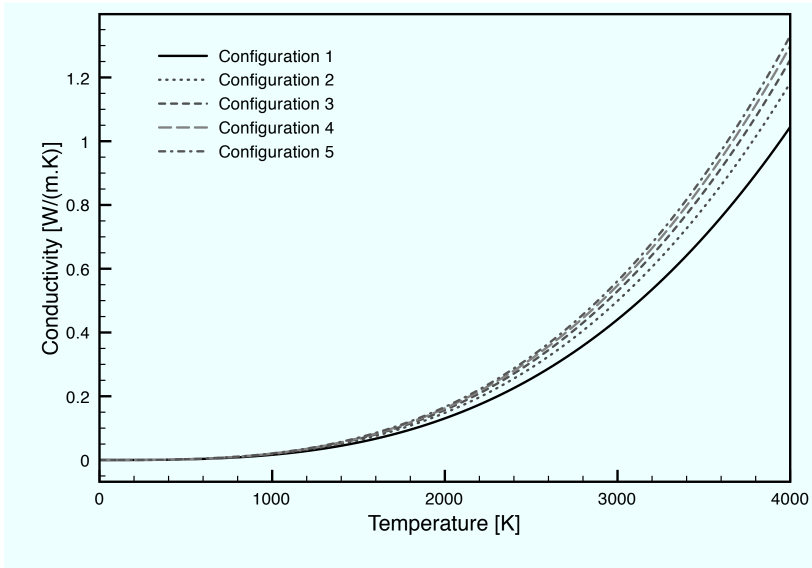

Figure 2. Average effective conductivity λ_r as a function of temperature.

IV. Transient analysis

The objective of the transient analysis is to study the validity of the effective conductivity model in the transient regime. Two models are now compared in a transient regime. The first one is the microscopic radiation model (direct numerical simulations at fiber scale). The second model is the classical macroscopic conduction model (conservation of the enthalpy and Fourier's law for conduction). The goal is to test the validity in the transient regime using the approach developed in the previous section. As indicated in the paper of Marschall et. al.,[5] temperature-dependent effective conductivities are not expected to correctly model the thermal transient response of a porous material, especially in high heating rate environments.

For the transient analysis we will reproduce the arc-jet heating environment test from Marschall et. al.[5] The model is initially at 300 K. The boundary condition is a time-dependent fixed temperature (Dirichlet) on one side of the sample and an adiabatic condition (Neumann) on the other side (see Fig. 4).

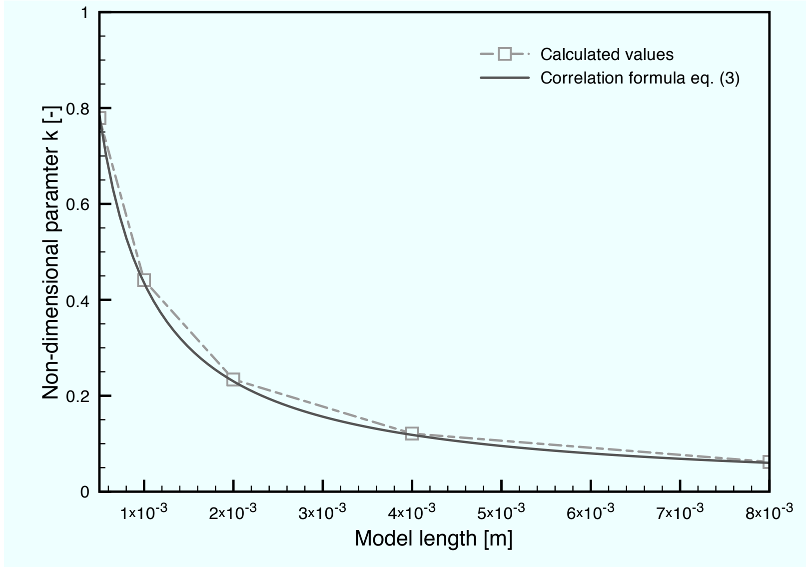

Figure 3. $\overline{k}$-factor as a function of model length Δx.

A. Test-matrix

Calculations are performed for two different values of Δx. For the effective conductive model, the material properties given in Table 2 are used. For the transient radiative model again five runs are performed in order to obtain averaged transient curves. For both the radiation and the equivalent model the temperature

Table 2. Effective conductivity properties

calculation	Δx [m]	ϵ_σ [$-$]	k [$-$]	λ_r [W/(m.K)]
1	$4 \cdot 10^{-3}$	0.85	$1.184 \cdot 10^{-1}$	$1.985 \cdot 10^{-11} \times T^3$
2	$8 \cdot 10^{-3}$	0.85	$6.000 \cdot 10^{-2}$	$2.012 \cdot 10^{-11} \times T^3$

curves of five imaginary thermocouples were generated. The five imaginary thermocouples were positioned at the following places:

- Thermocouple 1: positioned on the left hand surface, where the temperature is imposed.
- Thermocouple 2: is positioned at a depth of $\frac{1}{8}\Delta x$.

- Thermocouple 3: is positioned at a depth of $\frac{1}{4}\Delta x$.
- Thermocouple 4: is positioned at a depth of $\frac{1}{2}\Delta x$.
- Thermocouple 5: is positioned at the right hand surface.

For the microscopic radiation model, the thermocouples measure the average temperature of a group of elements (fibers). We use this approach because at a given position, there might not be any fiber present.

B. Microscopic radiation model

For the transient radiation model, the temperature-dependent evolution of the enthalpy of the fibers is accounted for and the energy equation is solved for each fiber. The results shown in Fig. 4 are the averaged (five random geometries) results of the microscopic radiation model and the results of the equivalent macroscopic model. It is interesting to notice that the thermocouple curves 2,3 and 4 show a distinctive *bend* in the high temperature range (at $t \approx 120$ seconds). The reason for this bend is not directly obvious from looking at the full radiation equations, but the effective conductivity Eq. 4 is more explicit. As it can be seen from this equation, the heat flux q_r depends on both ΔT and T^3. As a consequence at the beginning of the analysis ΔT is high and the structure heats up quickly. This effect will eventually level off, but is taken over in the high temperature range by the T^3 term.

C. Effective macroscopic conductivity model

The macroscopic model consists of a uniform mesh with a total length of Δx, with a material effective density of 175.68 kg/m^3. We use the effective conductivities reported in Table 2. The results of the macroscopic calculation and the radiation calculation are shown in Fig. 4. The macroscopic calculation reproduces the DNS results accurately, even during the high heating-rate transient phase.

V. Conclusion

Direct numerical simulations (DNS) of the radiation heat-transfer in two-dimensional fibrous media, have enabled the validation of a semi-analytical (phenomenological) model for the effective radiative conductivity. The effective conductivity is shown to be a function of three parameters: the local temperature

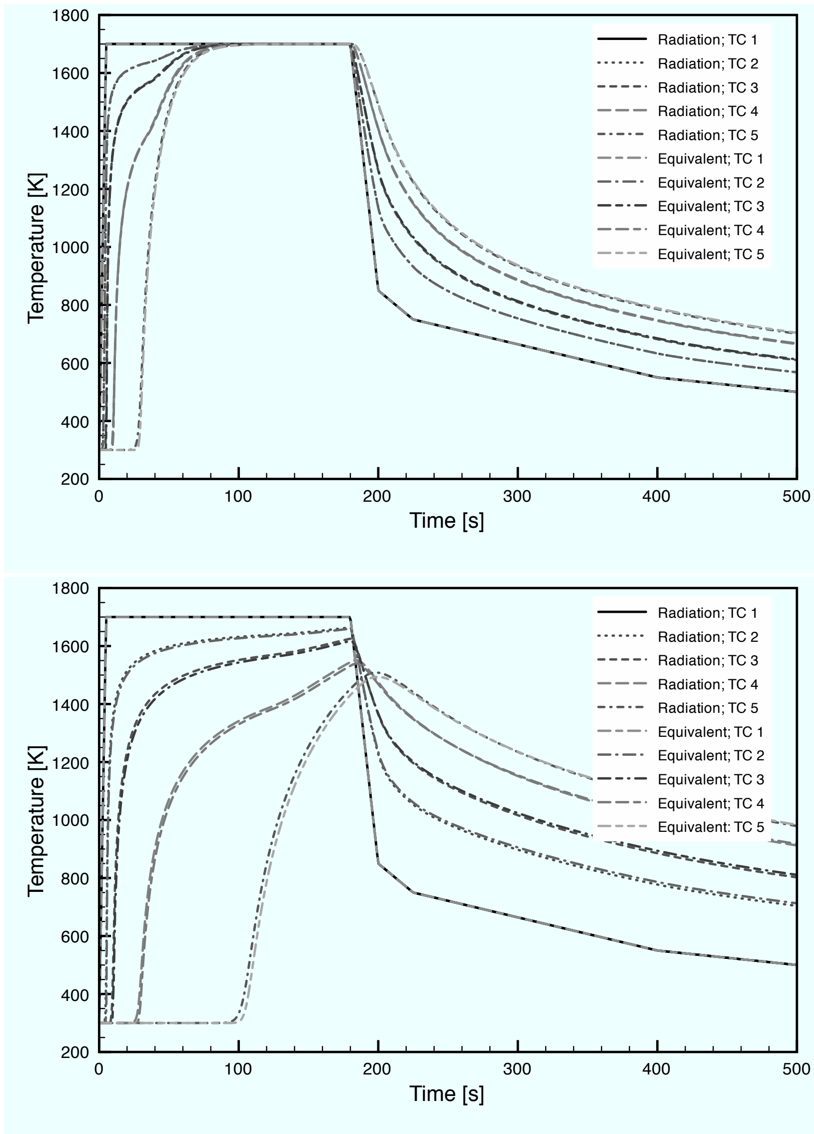

Figure 4. Comparison of the Temperature evolution for the equivalent and the radiation model, [a] Calculation 1, [b] Calculation 2.

(T^3), the extinction coefficient, and the sample thickness. The extinction coefficient of a two-dimensional fiber preform, made of randomly positioned but parallel fibers, has been determined by inverse analysis in steady state. Transient regime simulations have been carried out using both DNS and a macroscopic model for heat transfer (Fourier's law). When the effective radiation conductivity computed in steady state (using DNS) is used as an input to the macroscopic model, the macroscopic model reproduces the transient DNS simulations with an acceptable level of uncertainty. Hence, the results from our study indicate that the proposed correlation can be used for both steady state and transient analysis. The results show that Rosseland hypothesis used to linearize the radiative heat transfer is valid in the two-dimensional case studied.

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