Radiative transfer modelling inside thermal protection system using hybrid homogenization method for a backward Monte Carlo method coupled with Mie theory

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Abstract. A backward Monte Carlo method for modelling the spectral directional emittance of fibrous media has been developed. It uses Mie theory to calculate the radiative properties of single fibres, modelled as infinite cylinders, and the complex refractive index is computed by a Drude-Lorenz model for the dielectric function. The absorption and scattering coefficient are homogenised over several fibres, but the scattering phase function of a single one is used to determine the scattering direction of energy inside the medium. Sensitivity analysis based on several Monte Carlo results has been performed to estimate coefficients for a Multi-Linear Model (MLM) specifically developed for inverse analysis of experimental data. This model concurs with the Monte Carlo method and is highly computationally efficient. In contrast, the surface emissivity model, which assumes an opaque medium, shows poor agreement with the reference Monte Carlo calculations.

1. Introduction

Space vehicles encounter extreme thermal conditions during atmosphere re-entry, as described in Pulci et al. [1], and must be efficiently shielded to protect their contents. One traditional approach to achieve this involves ablative Thermal Protection System (TPS). Furthermore, since weight is a major constraint for space mission, the use of low density fibrous materials is often chosen. These materials are highly porous media and the impact of radiative transfer within them remains an active research area.

Different methods can be used to model radiative transfer inside fibrous media. Farmer and Howell [2] as well as Modest [3] described several Monte Carlo and Backward Monte Carlo methods for the modelling of the transmittance of absorbing and isotropically scattering media that were the starting point of the method presented in this paper. Dombrovsky et al. [4] developed an approximate analytical solution based on the transport approximation and the two-step solution method to compute the normal emittance of an absorbing, scattering, and refracting medium. Results obtained by [4] were reproduced during the early development of our method to ensure its accuracy for gray medium configurations. Milandri et al. [5] used Mie theory (as described for instance by Bohren and Huffman [6]) with the homogenisation method described by Lee [7] to model the directional emittance without axial symmetry for medium made of silica fibres. They computed the spectral bidirectional scattering

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coefficient to take into account anisotropic scattering cases. Mie theory and the homogenization method were used in the present work to test our codes against results provided by [5]. Axial symmetry situations were avoided with the use of the phase function of a single fibre and its orientation in space.

The aim of this paper is to study the possibility to derive a simple model for radiative emission to be used in future work to identify complex refractive index required to model the radiative transfer inside fibrous media. The identification process will be based on the analysis of the radiative emission of samples of carbon felt measured by FTIR spectroscopy. Studied sample is a 3 mm thick low density carbon felt (0.18 g cm\(^{-3}\), 89% porosity) with the fibres’ mean radius of 5 µm. Fibres are randomly oriented in space with a favoured direction in the felt plane. As a first attempt to determine which model should be used for this purpose, several ones were developed to assess their accuracy. This paper presents a Monte Carlo method for the estimation of spectral directional emittance based on Mie theory and using Lee’s method to homogenize the scattering and absorption coefficient of fibres modelled as infinite cylinders. The scattering phase function of a single fibre is used to determine the anisotropic scattering direction. Complex refractive indexes used in Mie theory are obtained with a Drude-Lorenz model for the dielectric function of soot and are assumed in this work to match those of carbon. A surface emissivity model based on the assumption that the fibrous medium emits radiation as an opaque body is also presented. Numerical analyses were also performed on the Monte Carlo model to compute sensitivity coefficients used as building blocks for a multi-linear approximation of the emission factor function.

2. Models for radiative emission

In this section, three different models are presented. The first one is based on the simplifying assumption that the sample emits radiation as an opaque body and only surface emissivity is modelled. This first approximation is motivated by the fact that the medium may be considered as optically thick even for very thin samples. Indeed, this radiative behaviour was observed with preliminary spectroscopic tests performed at room temperature in the 0.2-2.5 µm spectral range. Figure 1 shows an example of the normal hemispherical transmittance and reflectance spectra measured on a 3 mm thick sample with a Perkin Elmer Lambda 900 spectrometer. The second model takes into account the semi-transparent nature of the medium and the apparent directional emission factor is estimated by a Backward Monte Carlo method. The last one is a multi-linear development of the emission factor function based on results from the Monte Carlo model.

![Figure 1. Measured normal hemispherical transmittance and reflectance spectra for a 3 mm thick sample.](image-url)
2.1. Model for surface emissivity of opaque bodies

The assumption of an opaque body is often chosen in multi-physics code used in the space industry to simplify the already complex and time consuming computation. This model will be used here to show the extent of the inaccuracy brought by such an assumption as it does not suit such materials.

The flux balance for radiation incident in the direction \( u \) on an opaque body can be written in spectral form as:

\[
\alpha_v(u) + \rho_v^{\text{dir}}(u) = 1
\]

In Eq. (1) \( \rho_v^{\text{dir}}(u) \) is the spectral directional hemispherical reflectivity. Using Kirchhoff’s law, the spectral directional absorptivity \( \alpha_v(u) \) is equal to the spectral directional emissivity \( F_v(u) \) in the same direction. Hence, the spectral directional emissivity is obtained as:

\[
F_v(u) = 1 - \rho_v^{\text{dir}}(u)
\]

The spectral directional emissivity under unpolarized normal incident radiation for a medium in vacuum can be computed as [8]:

\[
F_v = 1 - \frac{(n-1)^2+k^2}{(n+1)^2+k^2}
\]

Where \( n \) and \( k \) are the real and imaginary part of the complex refractive index respectively \( (m = n + ik, i^2 = -1) \). Results provided by Eq. (3) will be compared to the Monte Carlo data to assess the relevance of such a model in our problem.

2.2. Backward Monte Carlo model for the radiative emission of fibrous media

A backward Monte Carlo method based on the reciprocity of radiation distribution factor [9] is used to model the spectral directional emittance of the fibrous medium. Using this approach, only rays that reach a target (the detector) are taken into account which reduces computational time considerably compared to forward Monte Carlo for equivalent accuracy [10]. The path of the ray is followed back from the target to the medium layer that emitted it with the scattering or absorption events locations obtained with the extinction length

\[
L_{\text{ext}} = -\frac{\log(\text{Rand})}{\sigma^{\text{ext}}}
\]

In Eq. (4) \( \text{Rand} \) is a number randomly generated between 0 and 1 and \( \sigma^{\text{ext}} \) is the extinction coefficients of single fibres. At these locations the ray is absorbed if \( \text{Rand} > \sigma^{\text{esc}} \cdot \sigma^{\text{ext}}^{-1} \) and scattered otherwise. If the ray is scattered, a new direction is computed in accordance with the scattering angle \( \theta \), as shown in Figure 2, provided by the scattering phase function of a single fibre. Scattering angles are generated following several successive steps. The first one consists in computing the incident angle \( \Phi \) based on the former direction of the ray and the orientation of the fibre, randomly chosen in accordance with the orientation distribution function. Then, the scattering angle \( \theta \) is obtained from the following equation that involves the normalized cumulated phase function defined as:

\[
P(\theta, \Phi) = \frac{\int_0^\theta s_{11}(x, \Phi) dx}{\int_0^\theta s_{11}(x, \Phi) dx} = \text{Rand}
\]

In Eq. (5) \( s_{11} \) is the first element of the amplitude scattering matrix that can be estimated by Mie theory as detailed in Ref. [6]. If the ray is absorbed, the radiative distribution factor \( D_v^{\text{dir}}(u) \) is updated. It is defined as the fraction of the total radiation emitted in the emission direction \( u \) from the detector and absorbed by a volume element \( j \) within the fibrous medium. Then, in the inverse procedure absorption sites \( j \) become emission sites and \( u \) become the direction in which the emission factor is
computed. The radiative spectral intensity in the direction \( \mathbf{u} \) is the sum of all the radiative distribution factor \( D^j_{\nu}(\mathbf{u}) \) times the radiative intensity of the black body \( I^B_{\nu}(T_j) \):

\[
I_{\nu}(\mathbf{u}) = \sum_{j=0}^{N} D^j_{\nu}(\mathbf{u}) \times I^B_{\nu}(T_j)
\]  

(6)

The apparent spectral directional emission factor based on a temperature \( T_0 \) can then be calculated as

\[
F_{\nu}(\mathbf{u}) = \frac{I_{\nu}(\mathbf{u})}{I^B_{\nu}(T_0)}
\]

(7)

The Monte Carlo model requires estimating the scattering and extinction coefficients of the medium as well as the scattering phase function of a single fibre. Radiative properties are obtained by homogenisation of those of single fibres assumed to be infinite cylinders and estimated with Mie theory. Homogenisation is based on the method described in Lee [7]. This method uses the orientation of fibres in the medium, as shown in Figure 2.

![Figure 2. Orientation of fibres in the medium (adapted from [6]).](image)

The scattering/absorption coefficient for fibres randomly oriented in space (see Eq. 8 below) or randomly oriented in a plane (Eq. 9) for media composed of fibres of same diameters are given as

\[
\sigma_{(ext,sca)} = \frac{f_w}{\pi R} \int_0^\pi Q_{(ext,sca)}(\Phi) \sin(\Phi) \, d\Phi
\]

(8)

\[
\sigma_{(ext,sca)} = \frac{f_w}{2\pi^2 R} \int_0^{2\pi} \int_0^\pi Q_{(ext,sca)}(\Phi) \sin(\xi_f)d\xi_f \, d\omega
\]

(9)

For configuration involving fibres in specific directions \( \omega_{fi} \) and \( \xi_{fi} \), we obtain:

\[
\sigma_{(ext,sca)} = \sum_{i=1}^{N} \sigma_{(ext,sca)}(\omega_{fi}, \xi_{fi})p(\omega_{fi}, \xi_{fi}) \delta(\omega_f - \omega_{fi}) \delta(\xi_f - \xi_{fi})
\]

(10)

Where \( \sigma_{(ext,sca)} \) are the extinction/scattering coefficients of single fibres and \( Q_{(ext,sca)} \) their corresponding efficiencies \( f_w \) is the volume fraction and \( R \) is the radius of a fibre assumed to be the same for all fibres. The incident angle is estimated as:

\[
\text{incident angle}
\]
\[
\cos \Phi = \sin(\xi_i) \sin(\xi_f) \cos(\omega_i - \omega_f) + \cos(\xi_i) \cos(\xi_f)
\]  
(11)

The main parameters for Mie computations are the size factor \( x = 2\pi Rv \) (\( v \) is the wavenumber) and the complex refractive index of the material fibres are made of. This quantity can be modelled by the Drude-Lorenz formula for the dielectric function with two bound electron \( j \) and one free one \( q \):

\[
\varepsilon = 1 - \frac{\omega_{p,j}^2}{\omega_0^2 + i\gamma_j \omega_0} + \sum_{j=1}^{2} \frac{\omega_{p,j}^2}{\omega_{r,j}^2 - \omega_0^2 + i\gamma_j \omega_0}
\]

(12)

with

\[
\omega_{p,j}^2 = \frac{e^2 N \bar{e}_j}{m_e \varepsilon_0}, \quad \omega_0 = 2\pi c_0 v \quad \text{and} \quad m = n + ik = \sqrt{\varepsilon}
\]

In Eq. (12) \( m_e, \omega_{r,j}^2, N \bar{e}_j \) and \( \gamma_j \) are respectively the mass of the electron \( [9.1096 \times 10^{-31} \text{kg}] \), the resonant frequency \( (0 \text{ for free electrons, } \omega_{r,1} = 1.25 \times 10^{15} \text{ [rad/s] and } \omega_{r,2} = 7.25 \times 10^{15} \text{ [rad/s]} \) [10,11]), the electron number density \([\#/\text{m}^3]\) and the damping constant [rad/s]. \( e \) is the charge of an electron \( [1.6022 \times 10^{-19} \text{C}] \) and \( \varepsilon_0 \) is the dielectric constant in vacuum \( [8.8542 \times 10^{-12} \text{F.m}^{-1}] \).

Computation took up to 902 seconds on an Intel Xeon E5620 CPU dual core at 2.40 GHz to calculate the 2.26 milliard bundles required to achieve a standard deviation lower than 0.1% with the Monte Carlo method (see Table 1). The code is parallelized on 8 different processors. Computation made with 113 and 226 wavelengths taken uniformly in the 0.25-2.5 \( \mu \text{m} \) spectral range provided the results given in Table 1 in terms of computation time and standard deviation. For each calculation, 4 different samples (4 computation sets with the same parameters) are simulated and the mean value is taken as solution in order to reduce the impact of statistical noise on the results.

### Table 1. Monte Carlo method computation times for two different numbers of computed wavelengths.

| Number of bundles | Mie theory computation time | Monte Carlo computation time |
|-------------------|-----------------------------|------------------------------|
|                   | 113 wavelengths             | 226 wavelengths              | 113 wavelengths             | 226 wavelengths |
| 1000000           | 8 sec.                      | 16 sec.                      | 4 sec.                      | 9 sec.          | 1.18 %          |
| 5000000           | 8 sec.                      | 16 sec.                      | 22 sec.                     | 44 sec.         | 0.74 %          |
| 10000000          | 8 sec.                      | 16 sec.                      | 44 sec.                     | 88 sec.         | 0.44 %          |
| 50000000          | 8 sec.                      | 16 sec.                      | 224 sec.                    | 443 sec.        | 0.17 %          |
| 100000000         | 8 sec.                      | 16 sec.                      | 445 sec.                    | 891 sec.        | 0.10 %          |

Standard deviation values given in Table 1 are the maximum values of the mean deviation between each sample and their mean value calculated for each wavelength as

\[
\text{stddev} = \max \left( \text{stddev}(v) \right)
\]

(13)

With

\[
\text{stddev}(v) = \sum_{i=0}^{N_{\text{sample}}} \frac{|F_i - \bar{F}_v|}{F_v} \times N_{\text{sample}}^{-1}
\]

(14)

The Monte Carlo computation can be quite computationally expensive for identification purpose. As one of the goals of this study is to estimate refractive indexes from experimental emittance data, a simplified model is required. Coupling conduction and radiative heat transfers will be considered as future work to treat non isothermal configurations and may also benefits from such a simplified model.

The modifications made on a standard Backward Monte Carlo method using radiation distribution factor are summarized in the flowcharts shown in Figure 4.
2.3. Multi-Linear Model (MLM) from sensitivity analyses

As shown in Eq. (12) six main parameters are used in the Drude-Lorenz model for the dielectric function, \( N_{efr}, N_{e1}, N_{e2}, \gamma_{fr}, \gamma_1 \) and \( \gamma_2 \) chosen in this work. Using a multi-linear approximation of the emission function we can obtain a simple model for the emission factor that takes into account the complex refractive index of the bulk material:

\[
\tilde{R}_v = F_{v0} + \left( \frac{\partial F_v}{\partial \log N_{efr}} \left( \frac{N_{efr}}{N_{efr}} - 1 \right) \right) + \left( \frac{\partial F_v}{\partial \log N_{e1}} \left( \frac{N_{e1}}{N_{e1}} - 1 \right) \right) + \left( \frac{\partial F_v}{\partial \log N_{e2}} \left( \frac{N_{e2}}{N_{e2}} - 1 \right) \right) + \left( \frac{\partial F_v}{\partial \log \gamma_{fr}} \left( \frac{\gamma_{fr}}{\gamma_{fr}} - 1 \right) \right) + \left( \frac{\partial F_v}{\partial \log \gamma_1} \left( \frac{\gamma_1}{\gamma_1} - 1 \right) \right) + \left( \frac{\partial F_v}{\partial \log \gamma_2} \left( \frac{\gamma_2}{\gamma_2} - 1 \right) \right)
\]

(15)

In Eq. (15) \( N_{efr}, N_{e1}, N_{e2}, \gamma_{fr}, \gamma_1 \) and \( \gamma_2 \) are the mean value between those given in Table 2 and \( \bar{N}_{efr}, \bar{N}_{e1}, \bar{N}_{e2}, \bar{\gamma}_{fr}, \bar{\gamma}_1 \) and \( \bar{\gamma}_2 \) are the estimated parameters. \( F_{v0} \) is the emission factor computed with the mean values for all parameters. The influence of each parameter on this model sensitivity analyses have been studied on the Monte Carlo method based on values given in Table 2. These sensitivity analyses have allowed us to calculate sensitivity spectra as:

\[
\frac{\partial F_v}{\partial \log x} = \frac{F_v(x + dx) - F_v(x - dx)}{2dx}
\]

(16)
where \( X \) represent either \( N_{e_{fr}}, N_{e_1}, N_{e_2}, \gamma_{fr}, \gamma_1 \) or \( \gamma_2 \). Those spectra are required to use Eq. (15).

**Table 2.** Range of the parameters used for the sensitivity analysis.

| Parameter               | Min       | Max       |
|-------------------------|-----------|-----------|
| Electron number density | \( 1.00 \times 10^{24} \) | \( 6.40 \times 10^{25} \) |
| \( N_{e_{fr}} \)        | \( 5.00 \times 10^{26} \) | \( 5.00 \times 10^{27} \) |
| \( N_{e_1} \)           | \( 5.00 \times 10^{27} \) | \( 1.00 \times 10^{29} \) |
| \( N_{e_2} \)           | \( 5.00 \times 10^{27} \) | \( 1.00 \times 10^{29} \) |
| Damping constant [rad/s] | \( 5.00 \times 10^{14} \) | \( 3.00 \times 10^{15} \) |
| \( \gamma_{fr} \)       | \( 1.00 \times 10^{15} \) | \( 1.00 \times 10^{16} \) |
| \( \gamma_1 \)          | \( 1.00 \times 10^{16} \) | \( 1.00 \times 10^{16} \) |
| \( \gamma_2 \)          | \( 1.00 \times 10^{16} \) | \( 1.00 \times 10^{16} \) |

Several sensitivity spectra are provided in Figure 5 as examples.

**Figure 5.** Sensitivity spectra for \( \frac{\partial F_y}{\partial \log N_{e_{fr}}} \) (a), \( \frac{\partial F_y}{\partial \log N_{e_1}} \) (b) \( \frac{\partial F_y}{\partial \log \gamma_{fr}} \) (c) and \( \frac{\partial F_y}{\partial \log \gamma_1} \) (d).
As shown in Figure 5, each parameter has a more or less predominant effect on the calculated emission factor depending on the spectral range that is considered. Consequently an analysis of the sensitivity spectra will enable to define the most relevant spectral regions for identification of given spectral properties. It is important to notice that as a Taylor development was used, this method will only work for properties close to those of the reference state $F_{v0}$. In our case, the MLM model will be used to identify those parameters for our carbon TPS sample. Following results found in the literature for different carbonaceous compounds (soot, amorphous carbon, and pyrolytic graphite) it seems safe to assume that the variation of the parameters will not be too large to use this model.

3. Results and discussion
The Monte Carlo model is used as a reference for the modelling of the spectral directional emission factor of the fibrous medium. For each case, computations were made for a 3 mm thick medium composed of fibres randomly oriented in space. Fibres radius is 5 µm and the volume fraction is 11%. The medium is isothermal. Results presented here are for the direction normal to the surface. Results are shown in Figures 6 to 8 for refractive index estimated with the parameters from Habib and Vervisch [11] for soot obtained from ethylene and acetylene flames or from Charalampopoulos and Chang [12]. Results from the MLM approximation and for surface emissivity assuming an opaque body are also provided.

The MLM is in good agreement with the Monte Carlo method for most of the studied cases, whereas the assumption of surface emissivity is not satisfactory in any of them. The maximal error is 3% for the MLM and reaches 25% for the surface emissivity model. It should be kept in mind that the surface emissivity model is for specular reflection which underestimates the emission factor but the spectral behaviour should not be affected anyhow. Higher order derivation should improve the MLM approximation quite a bit without involving prohibitive computation costs. Other parameters such as the fibre orientation could also be taken into account using other coefficients.

![Figure 6.](image_url)

**Figure 6.** Spectral normal emission factor computed with the Monte Carlo method, the opaque surface model and MLM. Refractive index parameters are from Habib and Vervisch [11] for soot particles produced by ethylene flames.
Figure 7. Spectral normal emission factor computed with the Monte Carlo method, the opaque surface model and MLM. Refractive index parameters are from Habib and Vervisch [11] for soot particles produced by acetylene flames.

Figure 8. Spectral normal emission factor computed with the Monte Carlo method, the opaque surface model and MLM. Refractive index parameters are from Charalampopoulos and Chang [12].
4. Conclusion
Several models have been developed to study the possibility to derive a simplified model to identify the complex refractive index required to estimate the radiative transfer inside fibrous media at high temperature.

A backward Monte Carlo method for spectral directional emittance of fibrous media has been presented in this paper. Radiative properties of the fibres have been obtained from Mie theory with the complex refractive index computed from the Drude-Lorenz model for the dielectric function. Radiative properties are homogenised over ensembles of fibres whereas the direction of the radiation after scattering events is determined by the phase function of a single one.

This method is computationally expensive and unsuitable for inversion process. For identification purpose, a quicker but accurate model is required. As expected, the simplest model assuming an opaque body is not relevant for the studied material, so the MLM was proposed. Calculations of the normal spectral emission factor performed with the different methods have been compared for four different sets of parameters for Drude-Lorenz model for the dielectric function.

Sensitivity analysis of the refractive index on the spectral directional emission factor was performed on the Monte Carlo model to derive a multi-linear model. This model can be improved furthermore with higher order derivation without significant influence in computation time. Other parameters such as the fibre orientation may also be taken into account using other coefficients. This model will be used for identification purpose of refractive indexes from experimental radiative emission spectra of samples of carbon felt obtained by FTIR spectroscopy. Another interesting point of this Monte Carlo method is the ability to compute the emission factor of a fibrous medium filled with a participating gas. This will later be used to study the impact of the pyrolytic gazes on the radiative transfer inside low density carbon TPS.

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