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Hybrid method – the case of arbitrary particle size distribution

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The aim of the paper is to present the principles of a hybrid method to predict light transmittances through dense 3D layered media in the case of arbitrary particle size distribution. In our previous paper, the hybrid method has been introduced as a combination of 4-flux method with coefficients predicted from a Monte Carlo statistical model to take into account the actual 3D geometry of the problem under study. In this paper, we present the evaluation of the method, the results of numerical simulations and their comparison with results obtained from Bouguer–Lambert–Beer law and from Monte Carlo simulations for polydisperse particle size distributions.

1. Introduction

In our previous paper [1], we presented the evaluation of the hybrid method to predict light transmittances in optically dense media.

The hybrid method have been elaborated to take advantage of the Monte Carlo technique and the 4-flux model properties, yet getting rid of their limitations [2], [3]. More precisely, it is based on the 4-flux model, it offers such advantages as simplicity, computational efficiency and analytical form, and, owing to a series of coefficients calculated from the Monte Carlo simulations, it takes under consideration the actual characteristics of the system under study. In this paper, we describe application of the hybrid method in the case of arbitrary polydisperse particle distributions.

2. Simulation

The next step is to evaluate how the hybrid methods behave in the presence of arbitrary particle size distributions. To examine this issue, we use the coefficients A and B previously estimated to determine light transmittances for clouds containing particles of different diameters [4]. Obviously, as the coefficients were only calculated for discrete values of particle diameters, the particle size distribution has to be presented in the form of a histogram.

In this paper, we consider the case of symmetric unimodal distribution defined in Tab. 1 [5] as well as asymmetric bimodal distributions presented in Tabs. 2 and 3.

For the distributions under examination, transmittances were computed for three wavelengths $\lambda = 0.4\times10^{-6}$ m, $\lambda = 0.75\times10^{-6}$ m and $\lambda = 0.9\times10^{-6}$ m. For each

Table 1. Particle size distribution (polydispersion 1).

Diameter [$\times 10^{-6}$ m]	Concentration in numbers [%]	Volume concentration [%]
0.1	10	0.264
0.2	20	4.233
0.3	40	28.571
0.4	20	33.862
0.5	10	33.069

Table 2. Particle size distribution (polydispersion 2).

Diameter [$\times 10^{-6}$ m]	Concentration in numbers [%]	Volume concentration [%]
0.1	10.0	0.13
0.2	20.0	2.06
0.3	39.5	13.73
0.4	20.0	16.48
0.5	10.0	16.10
2.0	0.5	51.50

Table 3. Particle size distribution (polydispersion 3).

Diameter [$\times 10^{-6}$ m]	Concentration in numbers [%]	Volume concentration [%]
0.1	10.0	0.22
0.2	20.0	3.50
0.3	39.9	23.53
0.4	20.0	27.96
0.5	10.0	27.31
2.0	0.1	17.48

Table 4. Constant coefficients E and F.

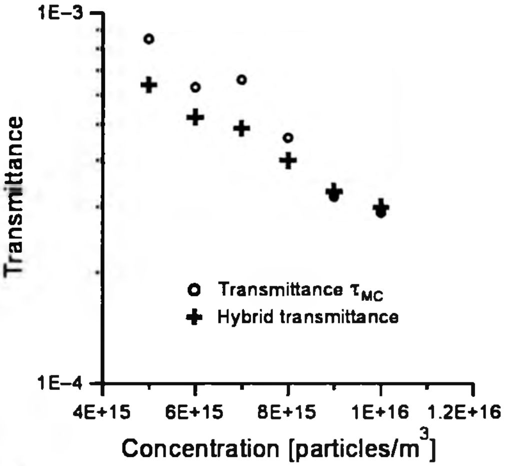
Wavelength [$\times 10^{-6}$ m]	E	F
0.4	0.3	0.0008
0.75	0.3	0.0015
0.9	0.3	0.001

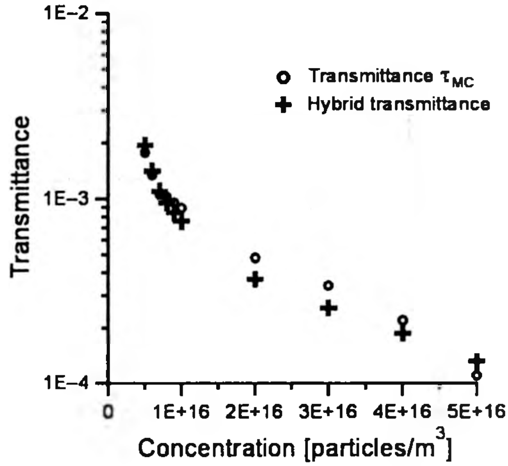
number-density we calculated the partial number-density of each class of particle diameter and for these partial number-densities we calculated the partial transmittances τ_{hyb_i} associated with the corresponding class. The total transmittance τ_{tot} is then evaluated from the partial transmittances τ_{hyb_i} by using

$$\tau_{\mathrm{tot}} = \left(1 / \sum_{i=1}^{N} \tau_{\mathrm{hyb}_i} \right)^{1-E} F^{E} \tag{1}$$

in which N is the number of classes. Table 4 presents the obtained values of the parameters E and F for particular wavelengths.

The following set of figures presents comparisons of the total transmittances calculated according to the hybrid method supplemented with Eq. (1) and the Monte

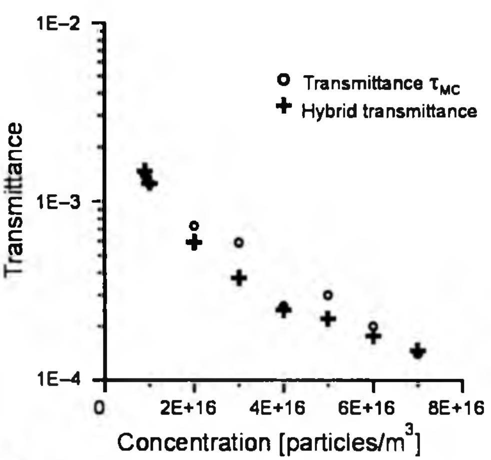




▲

Fig. 1. Comparison of transmittances calculated with the hybrid and Monte Carlo methods for $\lambda = 0.4\times10^{-6}$ m (polydispersion 1).

Fig. 2. Comparison of transmittances calculated with the hybrid and Monte Carlo methods for $\lambda = 0.75\times10^{-6}$ m (polydispersion 1).



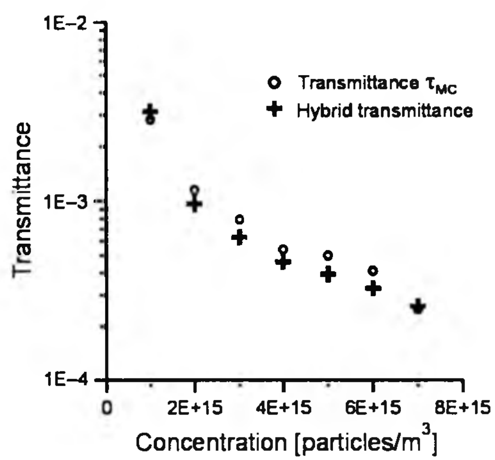


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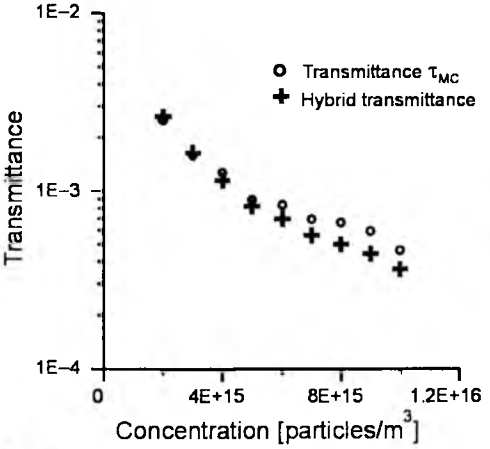
Fig. 3. Comparison of transmittances calculated with the hybrid and Monte Carlo methods for $\lambda = 0.9\times10^{-6}$ m (polydispersion 1).

Fig. 4. Comparison of transmittances calculated with the hybrid and Monte Carlo methods for $\lambda = 0.4\times10^{-6}$ m (polydispersion 2).



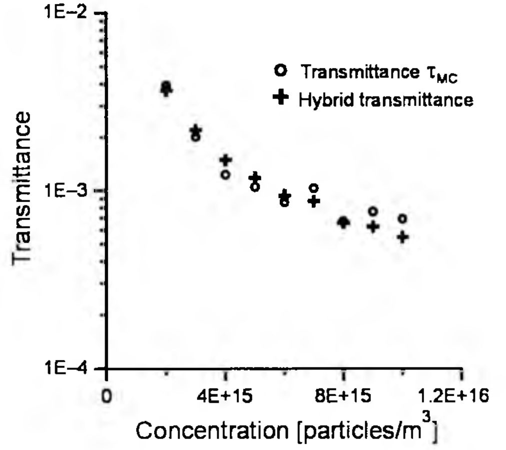
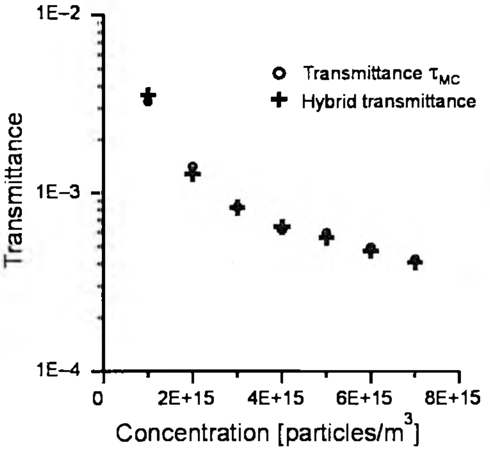


Fig. 5. Comparison of transmittances calculated with the hybrid and Monte Carlo methods for $\lambda = 0.75\times10^{-6}$ m (polydispersion 2).

Fig. 6. Comparison of transmittances calculated with the hybrid and Monte Carlo methods for $\lambda = 0.9\times10^{-6}$ m (polydispersion 2).



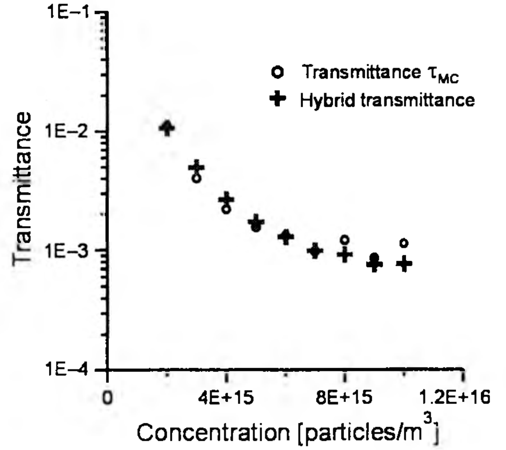


Fig. 7. Comparison of transmittances calculated with the hybrid and Monte Carlo methods for $\lambda = 0.4\times10^{-6}$ m (polydispersion 3).

Fig. 8. Comparison of transmittances calculated from with the and Monte Carlo methods for $\lambda = 0.75\times10^{-6}$ m (polydispersion 3).

Carlo method (τ_{MC}) for $\lambda = 0.4\times10^{-6}$ m, $\lambda = 0.75\times10^{-6}$ m and $\lambda = 0.9\times10^{-6}$ m. The figures do not present the classical Bouguer–Lambert–Beer results because, for the concentrations under study, the associated values differ too much from the presented

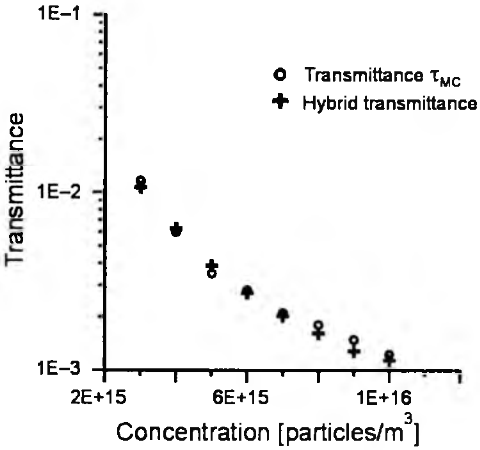


Fig. 9. Comparison of transmittances calculated with the hybrid and Monte Carlo methods for $\lambda = 0.9\times10^{-6}$ m (polydispersion 3).

ones. For example, in the case of polydispersion 1 for $\lambda = 0.4\times10^{-6}$ m the transmittances computed according to Bouguer–Lambert–Beer law varied from 0.16×10^{-30} down to 0.27×10^{-61} for 10^{16} particles/m^3.

Transmittance predictions from hybrid method are not in perfect agreement with Monte Carlo predictions. Nevertheless, the slope behaviour of the dependence between the transmittance and the concentration is retrieved, and the absolute values of the transmittances are close enough. The maximal difference between Monte Carlo results and hybrid method predictions is smaller than by a factor equal to 5, while the values calculated according to Bouguer–Lambert–Beer law typically differ by a factor of about 10^{65} representing in any case a dramatic improvement.

Moreover, once the proportionality coefficients K, (*eg*. [5]), are established for the experimental geometry under study, a hybrid method computes the transmittances in real time when compared to Monte Carlo simulations.

3. Conclusions

The hybrid method, based on the 4-flux model with empirical coefficients evaluated from a finite number of Monte Carlo computations has proved to be a computationally efficient and accurate tool for predicting light transmittances for arbitrary particle size distributions, especially when compared to the classical Bouguer–Lambert–Beer law. The hybrid method provides a solution to the direct problem, *i.e.*, it allows one to estimate light transmittances versus particle properties and wavelength for the given source-slab-detector geometrical set-up.

Numerical results demonstrate that the hybrid methods converge to the results obtained from Monte Carlo simulations in a wide range of concentrations.

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