New concept of hybrid method to describe the light transmittances in terms of multiple light scattering — monodisperse distribution approximation

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The aim of this paper is to present a new concept of the hybrid method that 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 recall the evaluation of the method, estimation of the coefficients and the results of numerical simulations. We also present a comparison of the hybrid method with the results obtained from Bouguer-Lambert -Beer law and from the Monte Carlo simulations for a wide range of monodisperse particle size distributions.

1. Introduction

Although the principles of multiple scattering of electromagnetic radiation were first established on a firm theoretical basis almost 50 years ago [1], it still remains a complex phenomenon. In certain media such as multiphase flows, suspensions in liquids, fuel injectors, etc., multiple scattering may be the predominant process of radiative transfer and one of the most relevant physical phenomena to be used for diagnostic purposes.

The phenomenon of multiple light scattering may be approached in different ways. Among them, the statistical Monte Carlo method relies on recording the behaviour of the light emitted from a source viewed as small light pencils (here called photons, but it is essential to notice that the name photon has little to do with the quantum light theory), characterised by their direction and intensity. The method is accurate but time consuming, because its validity crucially depends on the number of photons emitted by the light source. Also, due to its statistical formulation it is hardly possible to apply any method of inversion to the Monte Carlo approach. Conversely, the 4-flux method views the cloud of particles as a continuous and isotropic medium possessing average scattering and absorption properties determined by the particles. It is a fast analytical method but the scattering media have to be monodimensional (the cloud is considered as a medium of infinite lateral

extension limited by two infinite and parallel planes). These assumptions make it impossible to use the method directly to simulate actual complex geometries.

The hybrid method has been elaborated to take advantage of the Monte Carlo technique and the properties of 4-flux models, yet getting rid of their limitations. More precisely, it is based on the 4-flux model, possesses its advantages of simplicity, computational efficiency and analytical form and, owing to the series of coefficients calculated from the Monte Carlo simulations it takes under consideration actual characteristics of the system under study.

2. The 4-flux method

This model is based on the solution of the radiative transfer equation through the slab under study. It allows to calculate the transmittances of the light through the scattering cloud irradiated by a plane wave [2]-[5]. The cloud is assumed to be limited by two parallel surfaces I and O. The detector is represented by a surface parallel to I and O. The plane surface S placed between the slab and the detector is used to take into account the reflectances of the detection system (Fig. 1). The purpose of this model is to relate the total light transmittances and reflectances to the optical properties of the disperse medium contained between the planes I and O.

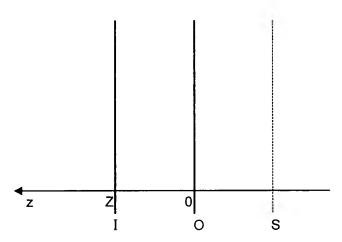


Fig. 1. Geometry of the 4-flux model

In the general model, the incident light is composed of a collimated beam with infinite lateral extension hitting perpendicularly the slab and of semi-isotropic radiation (semi-isotropic means isotropy in hemisphere). Without any loss of generality it is assumed that the incident light is monochromatic and the polarisation of light is not taken into account.

The whole radiation field inside the medium is decomposed into four beams (4-flux):

- a collimated beam of intensity $I_c(Z)$ propagating towards negative z (intensity means the amount of energy flowing per unit of time and per unit of area through a surface perpendicular to the z axis,
 - collimated beam of intensity $J_c(Z)$ propagating towards positive z,
 - diffuse radiation of intensity $I_d(Z)$, propagating towards negative z,
 - diffuse radiation of intensity $J_d(Z)$ propagating towards positive z.

Let us note that we use here the word "intensity" according to a common practice in the field but the quantities $I_c(Z)$, $J_c(Z)$, $I_d(Z)$ and $J_d(Z)$ may actually also be called fluxes, i.e., the 4-flux model is written in terms of energy balances obtained from integration of the corresponding intensities over appropriate hemispheres.

The planes I, O and S can be characterised by the coefficients of reflection for the collimated and diffused beams. For the sake of simplicity in this study, we assumed that the coefficients of reflection are equal to zero for both the diffused and collimated beams. This assumption, for I and O, is perfectly valid when no solid walls confine the medium under study. This assumption, for S, defines what we could call an ideal detector. We expect that the relaxation of these assumptions would not modify the essential results of this paper, but could affect the numerical values of empirical coefficients defined later on. It is also assumed that no diffuse radiation enters the slab.

A complete description of the 4-flux model can be found elsewhere [2], here we present only the final solution of the model.

The total transmittance calculated from the 4-flux method in general consists of three components:

- collimated collimated transmittance, corresponding to the transmittance of light entering and leaving the medium in collimated form (τ_{CC}),
- collimated diffused transmittance, corresponding to the transmittance of the light entering the slab under collimated form and leaving it as diffuse radiation (τ_{CD}),
- diffused diffused transmittance, corresponding to the transmittance of the light entering and leaving the media in diffused form (τ_{DD}) .

As it is assumed that the only radiation entering the medium under study is the collimated radiation, the third contribution is zero. Therefore, the total light transmittance reads as follows:

$$\tau_{\text{tot}} = \tau_{\text{CC}} + \tau_{\text{CD}}.\tag{1}$$

The transmittance $\tau_{\rm CD}$ corresponds to the radiation that interacted with particles inside the slab and reached the plane detector. The $\tau_{\rm CD}$ is a theoretical transmittance that does not depend on the geometry of the detection system since, according to its definition, all the flux of the emerging radiation is collected when integrating over the forward hemisphere. However, this transmittance crucially depends on the dimensions of the measuring system in an actual experiment since a certain amount of diffuse radiation does not reach the detector. Conversely, the transmittance $\tau_{\rm CC}$ does not depend on the geometry of the measuring system. It depends only on the

physical properties of the dispersed medium and on the width of the slab. Assuming that the reflectances of the enclosing planes are equal to 0, it is equal to the transmittance evaluated from the Bouguer-Lambert-Beer law.

3. Monte Carlo method

In this paper, the Monte Carlo method is implemented under the following light scattering assumptions [6], [7]:

- steady-state,
- quasi-elastic scattering,
- no multiple scattering in an infinitesimal slab,
- the light is described by its scalar intensity (no account for polarisation, no interference),
 - the medium under study is considered as homogenous and isotropic.

Processing multiple light scattering in terms of single scattering relies on the description of the volume element by using three parameters: its single scattering albedo a, its extinction coefficient $k_{\rm ext}$ and its phase function $P(\theta)$ using the Lorenz-Mie scattering theory [8], [9].

The basic idea of the model is to track the trajectory of what we call photons. The trajectory of each photon from the moment it leaves the light source until being captured by the detector or lost (either by absorption or by leaving out the medium without reaching the detector), is stochastically reconstructed in accordance with a set of probability densities. As the number of photons increases the statistical description of the physical problem approaches the exact deterministic solution.

The computing program allows one to take into account any arbitrary design of the measuring system, different media, various optical characteristics of obstacles (walls can be reflective or absorbant), sources and detectors (locations, sizes and apertures).

Moreover, the program records the number of collisions of each collected photon. This allows the computation of the following transmittances:

- $-\tau_{MC0}$ corresponding to the ratio of the number of photons traversing the medium without any collision over the total number of launched photons (this transmittance directly corresponds to the Bouguer-Lambert-Beer law), and
- $-\tau_{MCm}$ corresponding to the ratio of the number of photons captured by the detector after one or more collisions inside the medium over the total number of launched photons.

The total transmittance calculated by the Monte Carlo approach reads as

$$\tau_{MC} = \tau_{MC0} + \tau_{MCm}. \tag{2}$$

4. Hybrid method

To match the advantages of the previously presented approaches, we have elaborated a hybrid method which assembles the advantages of simplicity and computational efficiency of the 4-flux model together with the accuracy and generality of the Monte Carlo approach [10].

We then remark that the total transmittances calculated from the 4-flux model or from the Monte Carlo approach are expressed as the summation of two contributions:

- from collimated-collimated transmittance (τ_{CC}) and collimated-diffused transmittance (τ_{CD}) in the 4-flux model, and
 - τ_{MC0} and τ_{MCm} in the Monte Carlo approach.

One can easily note that the first contribution actually identifies and does not depend on the geometric properties of the measuring set-up, both directly corresponding to the transmittance of the Bouguer-Lambert-Beer law [11], [12].

The second kind of contributions (τ_{CD} and τ_{MCm}) corresponds to the photons that experienced at least one interaction with the particles. However, τ_{MCm} , contrary to τ_{CD} , takes into account the effects associated with the full 3D geometry of the problem under study.

The principle of the hybrid method is then to assume that τ_{MCm} is proportional to τ_{CD} , which can be well understood when we consider that both factors depend on the geometry of the measuring system. The challenge is then to evaluate the proportionality coefficients, which depend on wavelength, the 3D geometry of the light source, the properties of the cloud of particles, and the detector.

We also assume that the validity range of these coefficients is large enough in such a way that only a few of them have to be evaluated for practical applications. We then have the following assumption:

$$\tau_{\rm MC} = \tau_{\rm CC} + K \tau_{\rm CD}. \tag{3}$$

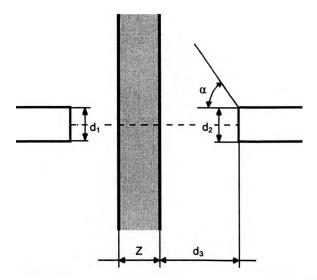


Fig. 2. Experimental geometry for the Monte Carlo simulations.

Many numerical experiments have been carried out for different wavelengths (ranging from $4\cdot10^{-7}$ m to $9\cdot10^{-7}$ m) for different diameters of particles (ranging from 10^{-7} m to $3\cdot10^{-6}$ m) and for various number-densities. We could then exhibit certain dependences between the values of the coefficient K versus transmittance $\tau_{\rm CD}$.

All the calculations included in this paper were made for water particles in the air and the following geometrical parameters of the system (Fig. 2):

- light source diameter d = 0.002 m.
- thickness of the medium examined Z = 0.1 m,
- distance between the outer plane of the slab and the detector $d_3 = 0.01$ m,
- diameter of the detector $d_2 = 0.02$ m,
- half-angle of aperture of the detector $\alpha = 30^{\circ}$.

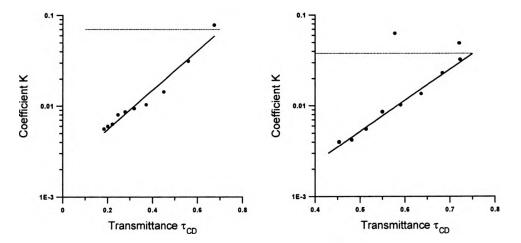


Fig. 3. Relationship between the coefficient K and the transmittance τ_{CD} ($\lambda = 0.4 \cdot 10^{-6}$ m, $d = 0.4 \cdot 10^{-6}$ m). Fig. 4. Relationship between the coefficient K and the transmittance τ_{CD} ($\lambda = 0.6 \cdot 10^{-6}$ m, $d = 0.4 \cdot 10^{-6}$ m).

In the hybrid method, where the coefficient K depends on $\tau_{\rm CD}$ ($K=h(\tau_{\rm CD})$), one calculates the value of $\tau_{\rm CD}$ for the given wavelength, particle diameter and concentration. Figures 3–10 then exemplify the relationship between K and $\tau_{\rm CD}$ for the particle diameters ranging from $0.4\cdot 10^{-6}$ m to $2.0\cdot 10^{-6}$ m and for wavelengths $\lambda=0.4\cdot 10^{-6}$ m and $\lambda=0.6\cdot 10^{-6}$ m.

In these figures, multiple scattering situations are represented by the linear parts of the graphs below the dotted lines. For these data, the ratio of τ_{CC} over τ_{CD} is smaller than 0.15. It means that the associated particle concentrations are rather large and that the beam entering the cloud of particles in collimated form essentially reaches the detector as a diffuse radiation. Points above the dotted line correspond to relatively weak concentrations of particles with the consequence that the influence of τ_{CD} on the total light transmittance is negligible enough when compared to τ_{CC} .

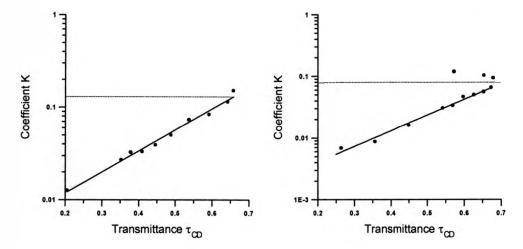


Fig. 5. Relationship between the coefficient K and the transmittance τ_{CD} ($\lambda = 0.4 \cdot 10^{-6}$ m, $d = 0.6 \cdot 10^{-6}$ m). Fig. 6. Relationship between the coefficient K and the transmittance τ_{CD} ($\lambda = 0.6 \cdot 10^{-6}$ m, $d = 0.6 \cdot 10^{-6}$ m).

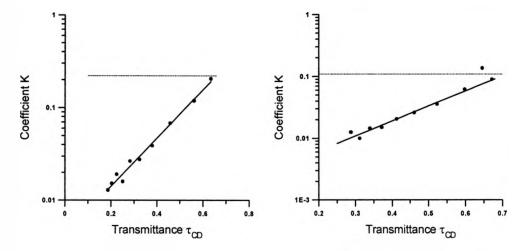


Fig. 7. Relationship between the coefficient K and the transmittance τ_{CD} ($\lambda = 0.4 \cdot 10^{-6}$ m, $d = 0.8 \cdot 10^{-6}$ m). Fig. 8. Relationship between the coefficient K and the transmittance τ_{CD} ($\lambda = 0.6 \cdot 10^{-6}$ m, $d = 0.8 \cdot 10^{-6}$ m).

Equation (3) then shows that, for the data, the value K has little influence. Using the points below the dotted line, we then obtained the following mathematical correlation that is valid for all the concentrations in the range examined

$$K = B \exp\left(\tau_{\rm CD} A\right) \tag{4}$$

where A and B are constants for λ and d given.

Particle diameter [m·16 ⁻⁶]	Wavelength [m·10 ⁻⁶]					
	A	В	A	В	A	В
	0.4	3.2104	0.003163	4.5643	0.001293	5.979
0.5	2.8817	0.004528	4.4125	0.002193	5.9392	0.0007837
0.6	3.7393	0.005794	3.603	0.00389	4.2694	0.002536
0.7	2.8492	0.00797	3.5145	0.004791	4.6141	0.002393
0.8	3.8781	0.006528	2.1367	0.008175	3.0566	0.0045
1.0	7.2711	0.002607	6.189	0.00404	6.2148	0.003129
1.6	7.8028	0.0022	7.849	0.001602	7.5168	0.00251
2.0	8.85	0.004343	8.8776	0.003084	7.8198	0.002126

Table. Example values of the coefficients A and B (hybrid method).

The Table presents exemple values of the coefficients A and B for the particle diameters in the range from $0.4 \cdot 10^{-6}$ m to $2.0 \cdot 10^{-6}$ m and wavelengths from $0.4 \cdot 10^{-6}$ m to $0.6 \cdot 10^{-6}$ m.

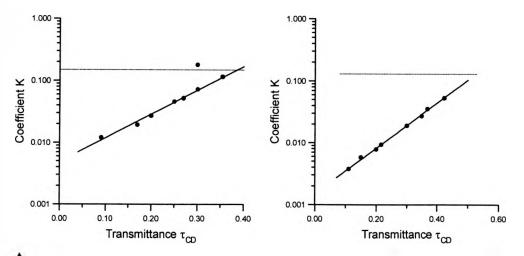


Fig. 9. Relationship between coefficient K and transmittance τ_{CD} ($\lambda = 0.4 \cdot 10^{-6}$ m, and $d = 2.0 \cdot 10^{-6}$ m). Fig. 10. Relationship between coefficient K and transmittance τ_{CD} ($\lambda = 0.6 \cdot 10^{-6}$ m, $d = 2.0 \cdot 10^{-6}$ m).

5. Comparisons

Figures 11-16 present comparisons between the transmittances calculated by different methods: Monte Carlo method, classical method based on Bouguer –Lambert–Beer law, classical 4-flux and hybrid method.

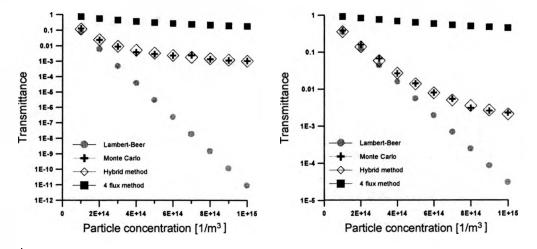


Fig. 11. Transmittance as a function of particle concentration $d = 0.4 \cdot 10^{-6}$ m, $\lambda = 0.4 \cdot 10^{-6}$ m. Fig. 12. Transmittance as a function of particle concentration $d = 0.4 \cdot 10^{-6}$ m, $\lambda = 0.6 \cdot 10^{-6}$ m.

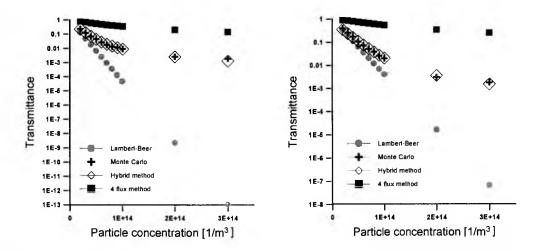


Fig. 13. Transmittance as a function of particle concentration $d = 0.6 \cdot 10^{-6}$ m, $\lambda = 0.4 \cdot 10^{-6}$ m. Fig. 14. Transmittance as a function of particle concentration $d = 0.6 \cdot 10^{-6}$ m, $\lambda = 0.6 \cdot 10^{-6}$ m.

The hybrid method therefore provides correct values of transmittances as one can see from its agreement with the Monte Carlo method. Once the values of A and B are obtained, the accuracy of the method is advantageously complemented by its extreme computational efficiency, allowing one to use it as a routine technique.

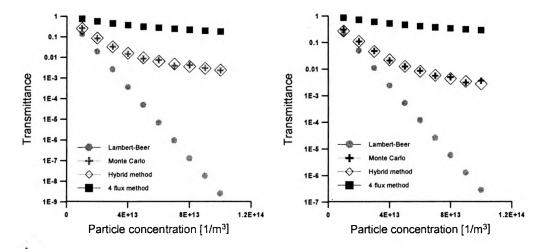


Fig. 15. Transmittance as a function of particle concentration $d = 0.8 \cdot 10^{-6}$ m, $\lambda = 0.4 \cdot 10^{-6}$ m. Fig. 16. Transmittance as a function of particle concentration $d = 0.8 \cdot 10^{-6}$ m, $\lambda = 0.6 \cdot 10^{-6}$ m.

Of course, the Bouguer-Lambert-Beer law is not valid for large particle concentrations (for instance, in Fig. 13, the discrepancy may reach 10 orders of magnitude).

Moreover, once the coefficients K are established for the experimental geometry under study, the hybrid method computes the transmittances in real time while compared to Monte Carlo simulations. For example, the computations of the results presented in this paper require about 0.1 s using a typical PC Pentium 100, compared to about 8 hours of Monte Carlo computations using HP 9000 series 700. Furthermore, the capability of the hybrid methods to be applied to the case of arbitrary particle size distributions has been successfully tested [13].

6. Conclusion

The purpose of this paper was to present an original method for predicting light transmittances through clouds of particles, where multiple light scattering might be a dominant phenomenon, taking into account the 3D geometry of source, the cloud and detector.

The hybrid method, based on a 4-flux method with empirical coefficients evaluated from a finite number of Monte-Carlo computations has been demonstrated as the computationally efficient and accurate tool to predict light transmittances for monodisperse particle size distributions, especially when compared with 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. In a companion paper, we shall demonstrate that the hybrid methods are well suited to the solution of the direct problem for arbitrary polydisperse particle size distribution.

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