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Technical Note

An efficient procedure to evaluate asymptotic limits of particles scattering efficiency and asymmetry factor

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Abstract

Radiative properties of particulate matter must be calculated accurately and in an expeditious way, in order to ensure both correct radiative transfer predictions and computational efficiency, requiring practicable computation time expenditure. The influence of large particles in radiative transfer is of major importance, placing an increased emphasis on the asymptotic solutions applicable to those particles. For large particles the scattering is highly anisotropic, causing the asymmetry factor to assume a very significant role. In the present work, an efficient method for the calculation of the asymptotic limits of both scattering efficiency and asymmetry factor for spherical particles is presented. The results are presented in simple and closed form expressions that exhibit a high degree of accuracy. This allows for a simultaneously accurate and expeditious evaluation of the referred parameters for large particles.

1. Introduction

When performing radiative transfer calculations in participative and anisotropically scattering media, one of the fundamental parameters that must be known, besides the extinction and scattering efficiencies, is the asymmetry factor. The influence of this parameter becomes more striking as the scattering anisotropy of the medium increases.

As it is well known, the scattering properties of the media found in combustion environments stem from the presence of solid particles, since the gaseous phase has a negligible influence in this phenomenon. Moreover, the scattering anisotropy of solid particles is strongly influenced by their size, since small particles like soot (small diameter when compared with the radiation wavelength) behave nearly isotropically, while large particles exhibit a marked anisotropic forward scattering.

Recalling that large particles have a much more important contribution for the radiative heat transfer mechanism than small ones [1], it can be concluded that the correct evaluation of the radiative properties of large particles is mandatory for accurate predictions of radiative heat transfer in combustion equipments, and that, within these properties, the asymmetry factor plays a major role.

Care must be taken so that the evaluation of the radiative properties of participating media is performed in an efficient fashion, particularly if radiative transfer calculations are to be coupled with CFD and combustion calculation, as previously referred by the authors (e.g., [2,3]).

Within this scope, the asymptotic limit values of the radiative properties of particulate matter constitute an extremely useful result, since they apply to large particles, the most important contributors to radiative transfer, and can be used as an input to more general models, see e.g., [2,3].

Therefore, an efficient method for the calculation of the asymptotic limits of particulate matter radiative properties appears to be mandatory. In the present note,

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such a method is presented and discussed. More precisely, recourse is made to an approximation previously used by [4] for the calculation of the hemispherical emissivity of surfaces to derive herein simple and closed form expressions that allow for a very accurate evaluation of the referred parameters, particularly if the refractive index of the particles presents a high value.

2. Analysis and results

As known from the general theory of scattering by a sphere (e.g., [5] or [6]) the scattering efficiency (Q_s) and the asymmetry factor (g) of an isolated particle are given by Eqs. (1) and (2), respectively, where μ is the cosine of the scattering angle ($\mu = \cos\theta$), x represents the particles size parameter given by $x = \pi D/\lambda$, D being the particle diameter and λ being the radiation wavelength, and $i(\mu)$ is the dimensionless unpolarised scattering intensity.

$$Q_s = \frac{2}{x^2}\int_{-1}^{1} i(\mu)\,d\mu, \tag{1}$$

$$g = \frac{1}{Q_s}\frac{2}{x^2}\int_{-1}^{1} i(\mu)\mu\,d\mu. \tag{2}$$

In the limit of large particles (large diameters when compared to the radiation wavelength) these factors can be expressed as in Eqs. (3) and (4), see [5] or [6] for details, where v and w are parameters discussed below.

$$Q_s = 1 + w, \tag{3}$$

$$g = \frac{1+v}{1+w}. \tag{4}$$

Notice that in these equations the diffraction effects are included. In fact, although diffraction is commonly neglected for large particles since it is essentially in the forward direction, the authors believe that it should be included for compatibility with more general theories applicable to smaller particles, like Mie theory, where diffraction and reflection cannot be separated. Should diffraction effects not be considered Eqs. (3) and (4) would read: $Q_s = w$ and $g = v/w$.

It is convenient to separate the contribution to the w and v parameters into those resulting from perpendicularly and parallel polarised intensity components, as in Eqs. (5) and (6), where subscripts 1 and 2 represent the perpendicularly polarised intensity component and the parallel polarised intensity component, respectively.

$$w = \frac{1}{2}(w_1 + w_2), \tag{5}$$

$$v = \frac{1}{2}(v_1 + v_2) \tag{6}$$

The expressions for the evaluation of each of these components are given by Eqs. (7) and (8) (see e.g., [5]).

$$w_i = \frac{1}{2}\int_{-1}^{1} |r_i|^2\,d\mu, \tag{7}$$

$$v_i = \frac{1}{2}\int_{-1}^{1} |r_i|^2\mu\,d\mu. \tag{8}$$

In the previous equations r_1 and r_2 represent the Fresnel reflection coefficients given by Eqs. (9a) and (9b) (see e.g., [5,6] or [7]), where τ is the angle of incidence and m is the complex refractive index ($m = n - ik$).

$$r_1 = \frac{\sqrt{1-\sin^2\tau} - \sqrt{m^2-\sin^2\tau}}{\sqrt{1-\sin^2\tau} + \sqrt{m^2-\sin^2\tau}}, \tag{9a}$$

$$r_2 = -\frac{m^2\sqrt{1-\sin^2\tau} - \sqrt{m^2-\sin^2\tau}}{m^2\sqrt{1-\sin^2\tau} + \sqrt{m^2-\sin^2\tau}}. \tag{9b}$$

The square of the moduli of the Fresnel reflection coefficients can be expressed, after some algebraic manipulation, by Eqs. (10a) and (10b) (see e.g., [5] or [7]).

$$|r_1|^2 = \frac{(\cos\tau - p)^2 + q^2}{(\cos\tau + p)^2 + q^2}, \tag{10a}$$

$$|r_2|^2 = \frac{(p - \sin\tau\,\mathrm{tg}\,\tau)^2 + q^2}{(p + \sin\tau\,\mathrm{tg}\,\tau)^2 + q^2}|r_1|^2. \tag{10b}$$

In the above equations, p and q are parameters that depend both on m and τ, and are defined by Eq. (11).

$$p - iq = \sqrt{m^2 - \sin^2\tau} \tag{11}$$

Notice that the integration indicated on Eqs. (7) and (8) is performed on μ, while the Fresnel reflection coefficients – Eqs. (10a) and (10b) – are expressed in terms of the angle of incidence, τ. However, in the case of very large particles there is a simple relation between μ and τ, since it is assumed that all the radiation that enters the particle is absorbed and only external reflections are considered. This relation is expressed by Eq. (12).

$$\theta = \pi - 2\tau. \tag{12}$$

The relations that allow for an immediate evaluation of the Fresnel reflection coefficients in terms of μ are given by Eqs. (13a), (13b), and (13c).

$$\cos\tau = \left(\frac{1-\mu}{2}\right)^{1/2}, \tag{13a}$$

$$\sin\tau\,\mathrm{tg}\,\tau = \frac{1+\mu}{1-\mu}\left(\frac{1-\mu}{2}\right)^{1/2}, \tag{13b}$$

$$\sin^2\tau = \frac{1+\mu}{2}. \tag{13c}$$

After performing the change in variable indicated before, from τ to μ, the resulting expressions for the Fresnel reflection coefficients are much involved to allow for their analytical integration. Therefore, the evaluation of the scattering efficiency and of the asymmetry factor would require a numerical integration, fact that would jeopardise the efficiency of their calculation.

However, if the values of n and k are high, the term $\sin^2 \tau$ can be neglected in Eq. (11) – resulting in $p = n$ and $q = k$. Therefore, the squares of the moduli of the Fresnel reflection coefficients given by Eqs. (10a) and (10b) assume simpler forms, as expressed by Eqs. (14a) and (14b) (see e.g., [7]).

$$|r_1|^2 = \frac{(n - \cos\tau)^2 + k^2}{(n + \cos\tau)^2 + k^2}, \tag{14a}$$

$$|r_2|^2 = \frac{(n\cos\tau - 1)^2 + (k\cos\tau)^2}{(n\cos\tau + 1)^2 + (k\cos\tau)^2}. \tag{14b}$$

Using this approximation, the integrals of equations (7) and (8) can be performed analytically, yielding for the scattering efficiency the result presented in Eqs. (15a) and (15b), where the nomenclature presented in Eqs. (16a)–(16c) is used.

$$w_1 = \left[8n^2 \ln\left(\frac{C}{A}\right) - 8n\frac{B}{k}\mathrm{tg}^{-1}\left(\frac{k}{n+A}\right) + (1 - 8n)\right], \tag{15a}$$

$$w_2 = \frac{1}{A^2}\left[8n^2 \ln(C) - 8n\frac{B}{k}\mathrm{tg}^{-1}\left(\frac{k}{n+1}\right) + A(A - 8n)\right], \tag{15b}$$

$$A = n^2 + k^2, \tag{16a}$$

$$B = n^2 - k^2, \tag{16b}$$

$$C = (n+1)^2 + k^2. \tag{16c}$$

Notice that [4] has used this approximation to determine the hemispherical emissivity of surfaces and that Eqs. (15a) and (15b) can be directly derived from his work, since $w_i = 1 - \varepsilon_i$ and $w = 1 - \varepsilon$. However, the result of the integration of equation (8) under the same approximation has never been presented elsewhere, to the extent of the authors knowledge, that result being expressed by Eqs. (17a) and (17b).

$$v_1 = \left[8n^2(1 - 4B)\ln\left(\frac{C}{A}\right) - 8n\frac{B - 2B^2 + 8n^2k^2}{k} \times \mathrm{tg}^{-1}\left(\frac{k}{n+A}\right) - \frac{8}{3}n\left[1 + 6n - 6\left(B + 2n^2\right)\right]\right], \tag{17a}$$

$$v_2 = \frac{1}{A^4}\left[8n^2\left(A^2 - 4B\right)\ln(C) - 8n\frac{BA^2 - 2B^2 + 8n^2k^2}{k} \times \mathrm{tg}^{-1}\left(\frac{k}{n+1}\right) - \frac{8}{3}n\left[A^3 + 6nA^2 - 6A\left(B + 2n^2\right)\right]\right]. \tag{17b}$$

Fig. 1 shows the relative error contours of the scattering efficiency calculated through Eqs. (15a) and (15b) when compared with the numerical integration of equation (7). It can be noticed that the isolines of the relative error follow a roughly circular pattern centred about $n = 1.0, k = 0.0$, where the maximum error (9.0%) occurs. It is also perceivable that the relative error of the solution is inferior to 2.0% if $(n-1)^2 + k^2 \geqslant 0.43$, and if $(n-1)^2 + k^2 \geqslant 1.02$ the relative error is always inferior to 1.0%.

Fig. 2 displays the relative error contours of the asymmetry factor calculated through Eqs. (17a) and (17b) when compared with the numerical integration of equation (8). Observing that figure, it becomes quite evident that the relative error associated with Eqs. (17a) and (17b), is much lower than that associated with Eqs. (15a) and (15b). In fact, the maximum error presented

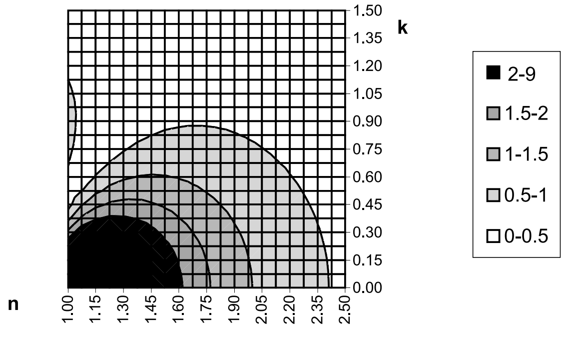

Fig. 1. Relative error (%) produced by Eqs. (15a) and (15b) for the evaluation of the scattering efficiency.

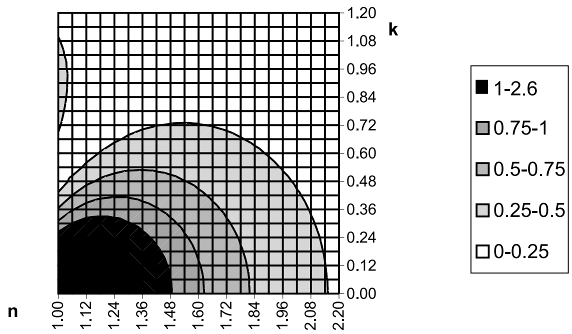

Fig. 2. Relative error (%) produced by Eqs. (17a) and (17b) for the evaluation of the asymmetry factor.

by this approximation is of 2.6%, occurring also at $n = 1.0$, $k = 0.0$. Again a circular pattern in the relative error isolines is clearly discernible, although their magnitude is much lower than in the previous case. It can be noticed that for $(n-1)^2 + k^2 \geqslant 0.23$ the relative error is always inferior to 1.0%, and that if $(n-1)^2 + k^2 \geqslant 0.71$ than, the relative error does not go beyond 0.5%.

3. Conclusions

For the first time, a known approximation was applied to the calculation of the asymmetry factor and scattering efficiency of large spherical solid particles.

For the case of the scattering efficiency evaluation this approximation provides a simple and closed form expression that yields very accurate results, particularly if the refractive index presents high values, $(n-1)^2 + k^2 \geqslant 1.02$.

For the case of the asymmetry factor evaluation, where this approximation was used, the results achieved, also presented in closed form expressions, display an even greater accuracy than in the previous case.

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