Mathematical modelling of the heat-protection properties of the composite coating consisted of hollow ceramic microspheres

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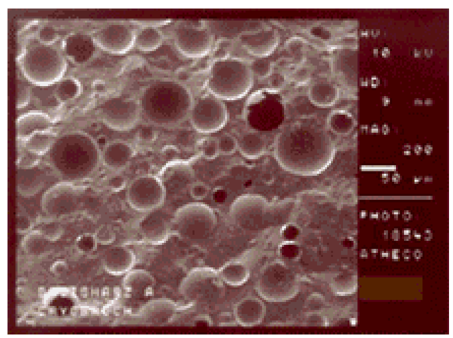

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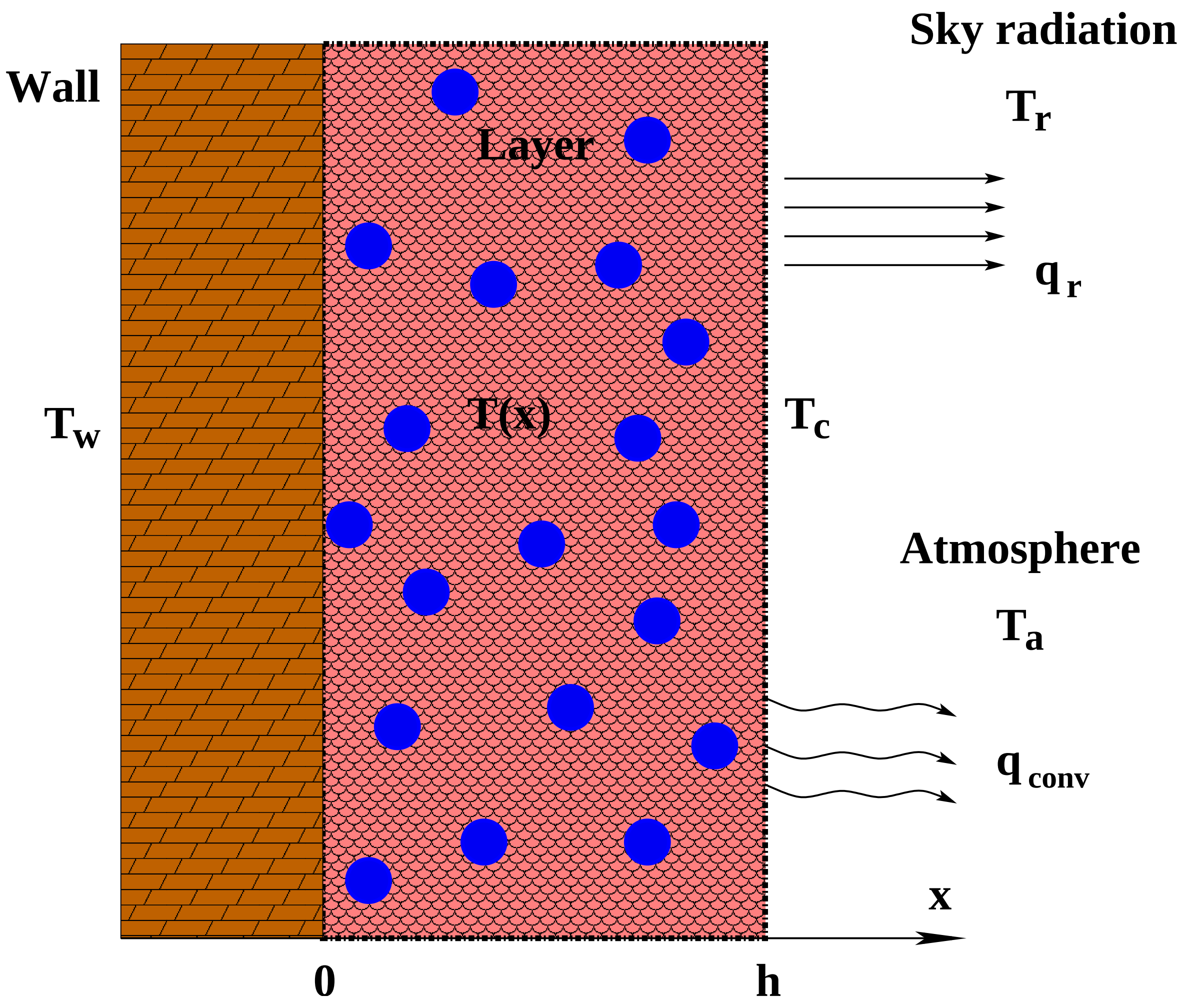
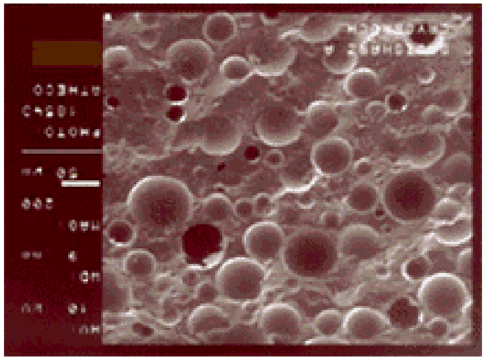


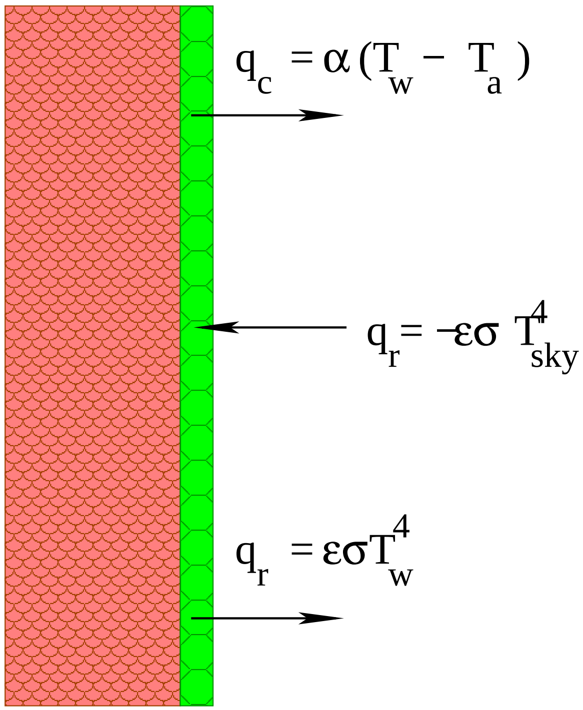
Polydisperse coating,
a layer of hollow
ceramic microsperes;
Size: 20-100 μm;
Thickness: 0.3-0.5 mm



Heat transfer equation

The problem: to define the temperature profile within a body.

There are three mechanisms by which thermal energy is transported
1. Convection   2. Conduction   3. Radiation



Fourier's Law: *When there exists a temperature gradient within a body, heat energy will flow from the region of high temperature to the region of low temperature:* $\vec{q}_c = \alpha \nabla T$, where $\vec{q}_c$ is the convection heat flux vector and α is the heat transfer coefficient.

Heat Conduction Equation: $\frac{\partial T}{\partial t} = \alpha \nabla^2 T - \nabla \vec{Q}$

Steady State problem: $\alpha \frac{d^2 T}{dx^2} = \nabla \vec{Q}$

In the case under consideration $Q = q_c = \alpha[T(h) - T(0)]$.

However the energy can also be carried out by radiation: $\vec{Q} = \vec{g}_c + \vec{q}_r$.

Radiative transfer equation

Raduative flux: *radiative flux vector can be calculated from the radiative intensity $I(\vec{x}, \mu)$ by solving the radiative transfer equation:*

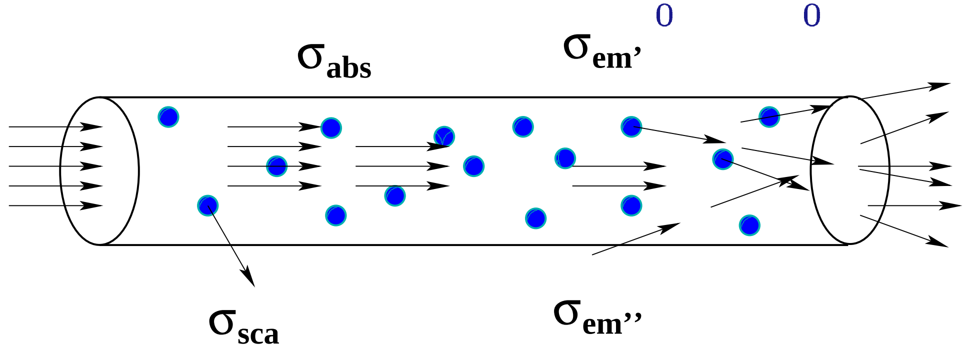
$$\cos\theta \frac{dI}{dx} = -\sigma_{ext} \cdot I + \sigma_{em}$$

The intensivuty I is decreasing due to extinction σ_{ext} and increasing due to emission σ_{em}.

$$\sigma_{ext} = \sigma_{abs} + \sigma_{sca} \qquad \sigma_{em} = \sigma'_{em} + \sigma''_{em}$$

Internal sources: $\sigma'_{em} = \sigma_{abs} B(T) = \sigma_{abs} \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1}$, external sources: $\sigma''_{em} = \frac{\sigma_{sca}}{4\pi} \int\limits_{4\pi} p(\Omega, \Omega')\ I(\Omega') d\Omega'$ where the phase function $p(\Omega, \Omega')$ defines a probability of scattering in a given direction. Thus, the radiative transfer equation is written as

$$\cos\theta \frac{dI(\theta,\varphi)}{dx} = -\sigma_{ext} \cdot I(\theta,\varphi) + \sigma_{abs} B(T) + \frac{\sigma_{sca}}{4\pi} \int\limits_0^{2\pi} d\varphi' \int\limits_0^{\pi} d\theta'\ \sin\theta' p(\theta,\theta',\varphi,\varphi') I(\theta',\varphi')$$



Formulation of the problem

- *Calculate the absorbtion and scattering coefficients* σ_{abs} *and* σ_{sca}*;*
- *Calculate the differential cross section (or probability of scattering in a given direction)* $p(\Omega, \Omega')$*;*
- *Set up the boundary conditions* T_w, T_a, T_r*;*
- *Implement the numerical procedure to define the density of the conductive heat flux, an initial approximation is set as there is no compound layer and* $T(x) = T_w$*;*
- *To find a solution of the heat conduction equation for a temperature field* $T(x)$*;*
- *Implement the information about the temperature distribution to calculate the effect of the radiation sources* $\nabla q_r(x)$ *within the compound layer, i.e. to solve the radiation transfer equation. That yields*

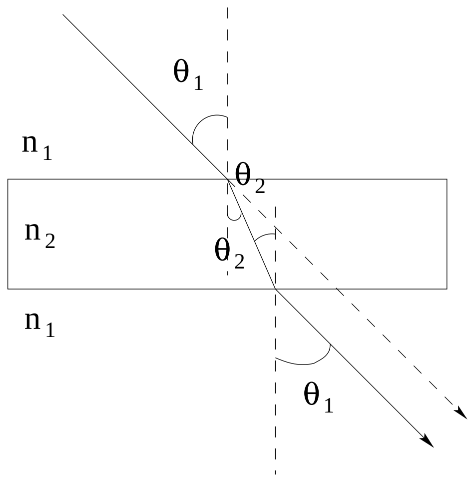
$$\nabla q_r(x) = \int d\nu \, \left(B(T) - \int I(x, \Omega) d\Omega \right) \approx \sigma T^4 - \int d\nu d\Omega \; I(x, \Omega)$$

- *Solve the heat transfer equation with given field of* $q_r(x)$*.*

Electromagnetic light scattering in disperse media

(i) Snell's Law of refraction: $n_1 \sin\theta_1 = n_2 \sin\theta_2$

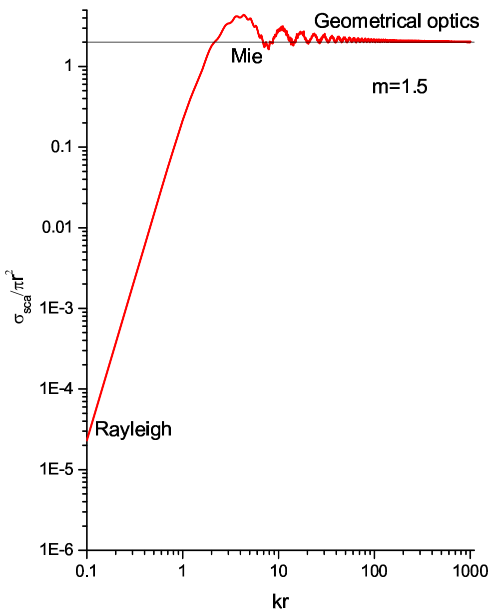
A complex index of refraction can be defined for substances which absorb as well as refract: $m = n' - in''$

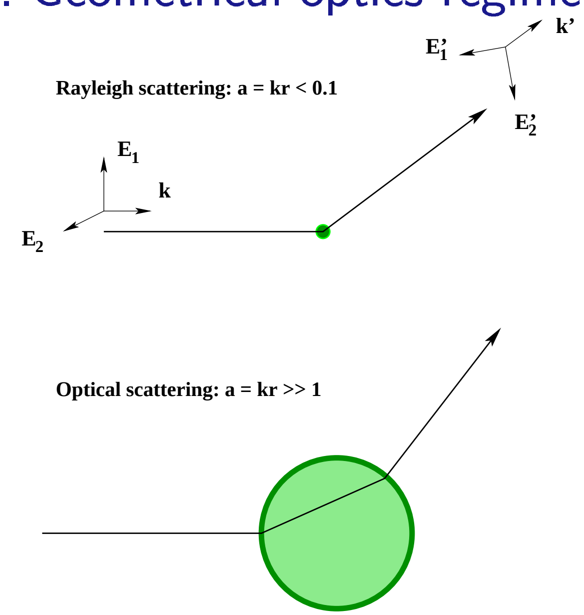


(ii) Light scattering on a sphere

There are three different regimes depending from the ratio of the size of the particle and the wavelength:

1. Rayleight Scattering 2. Mie scattering 3. Geometrical optics regime





For ‘ThermoShield’ coating we have IR $\lambda \in [1 - 75] \ \ \mu m$ and $r \in [20 - 100] \ \ \mu m$

Mie scattering

The wave equation for two homogeneous media, one of which is spherical and imbedded in the other:

$$\Delta \vec{E} + k^2 \vec{E} = 0, \quad \Delta \vec{H} + k^2 \vec{H} = 0$$

where $\vec{E}$ and $\vec{H}$ are the electric and magnetic fields of a planar electromagnetic wave.

It has the solutions in terms of orthogonal polynomials (spherical surface functions):

$$E(r,\theta,\varphi) = \left.\begin{matrix} \cos(m\varphi) \\ \sin(m\varphi) \end{matrix}\right\} P_n^m(\cos\theta) H_n(kr); \quad H(r,\theta,\varphi) = \left.\begin{matrix} \sin(m\varphi) \\ \cos(m\varphi) \end{matrix}\right\} P_n^m(\cos\theta) H_n(kr),$$

where $P_n^m(\cos\theta)$ is the Legendge function and $H_n(kr)$ is the Hankel function.

Jones light scattering matrix yields the complex scattering amplitudes:

$$\begin{pmatrix} E_\perp^{out} \\ E_\parallel^{out} \end{pmatrix} = \frac{e^{ik(r-z)}}{ikr} \begin{pmatrix} S_2 & 0 \\ 0 & S_1 \end{pmatrix} \begin{pmatrix} E_\perp^{in} \\ E_\parallel^{in} \end{pmatrix}$$

Mie solution for a scattered wave

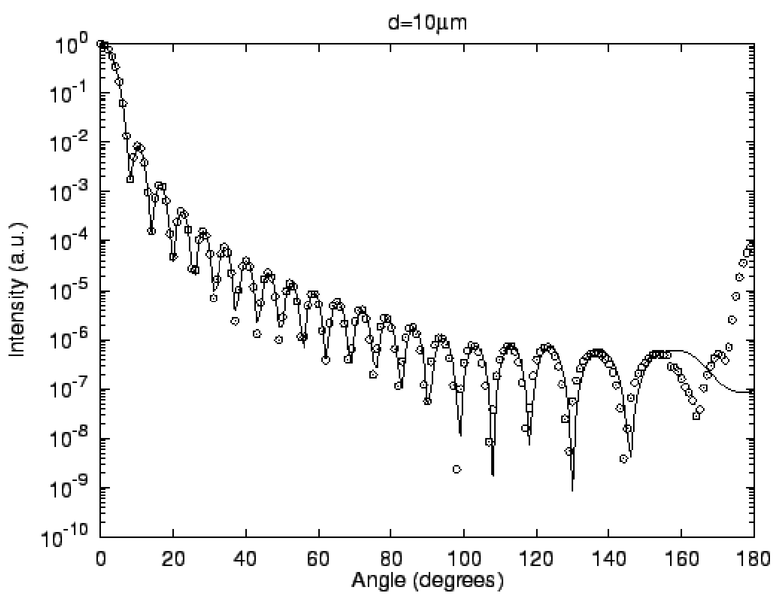
Scattering amplitudes:

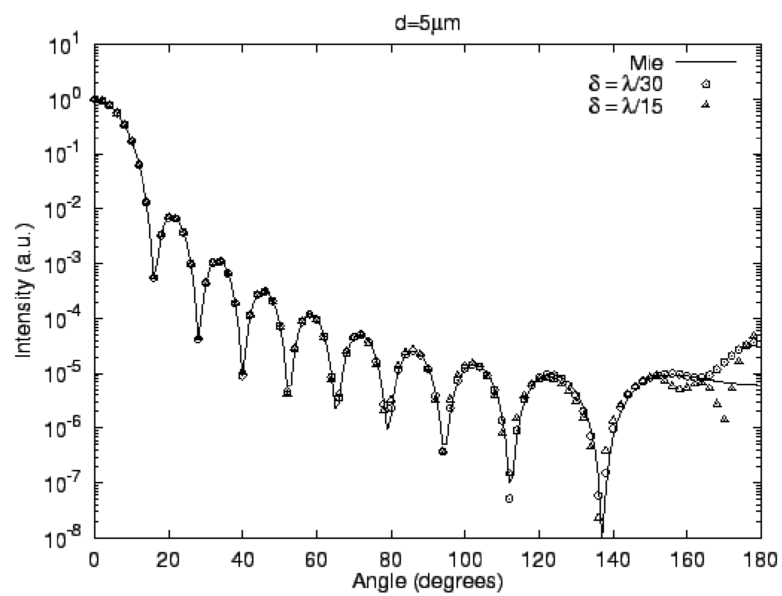
$$S_2 = \sum_n^{\infty} C(n) \left(a_n \frac{dP_n(\cos\theta)}{d\theta} + b_n \frac{P_n(\cos\theta)}{\sin\theta} \right); \quad S_1 = \sum_n^{\infty} C(n) \left(a_n \frac{P_n(\cos\theta)}{\sin\theta} + b_n \frac{dP_n(\cos\theta)}{d\theta} \right)$$

where $C(n) = \frac{2n+1}{n(n+1)}$ and

$$a_n = \frac{\psi_n(kr)\psi_n'(mkr) - m\psi_n(mkr)\psi_n'(kr)}{\xi(kr)\psi_n'(mkr) - m\psi(mkr)\xi_n'(kr)}; \quad b_n = \frac{m\psi_n(kr)\psi_n'(mkr) - \psi_n(mka)\psi_n'(kr)}{m\xi_n(kr)\psi_n'(mkr) - \psi_n(mkr)\xi_n'(kr)}$$

where $m = n - i\chi$ is a complex index of refraction, $kr = 2\pi a/\lambda$.





Modelling the 'Thermoshield'

- *An approximation of a mono-disperse system of separated spherically symmetric particles with an equivalent radius* r_{eff} *and an effective concentration* n_0*; classical Mie theory* – Oversimplified*;*

- *An approximation of a mono-disperse system of randomly oriented axially symmetric particles with relatively low volumetric concentration; modified Mie theory* – May be used as a zero-order approximation*;*

- *Model of spherical 2-layered polydispersed particles having the same fixed ratio* $s = \frac{r_2}{r_1}$ *with a given bubble size distribution* – Work in progress*;*

- *'Averaging' approximation: to replace the optical characteristics of an elementary volume of the layer by the corresponding characteristics of a single 'average' particle whose shape yields the light scattering and absorbtion characteristics of an ensemble of scatterers* – Works well for a polydisperse system*;*

- *Random walks model: photons are performing random walks in a complex, randomly inhomogeneous media - beyond the conventional radiative transfer theory* – Works very well, needs extensive use of Monte Carlo techniques

Calculation of optical characteristics

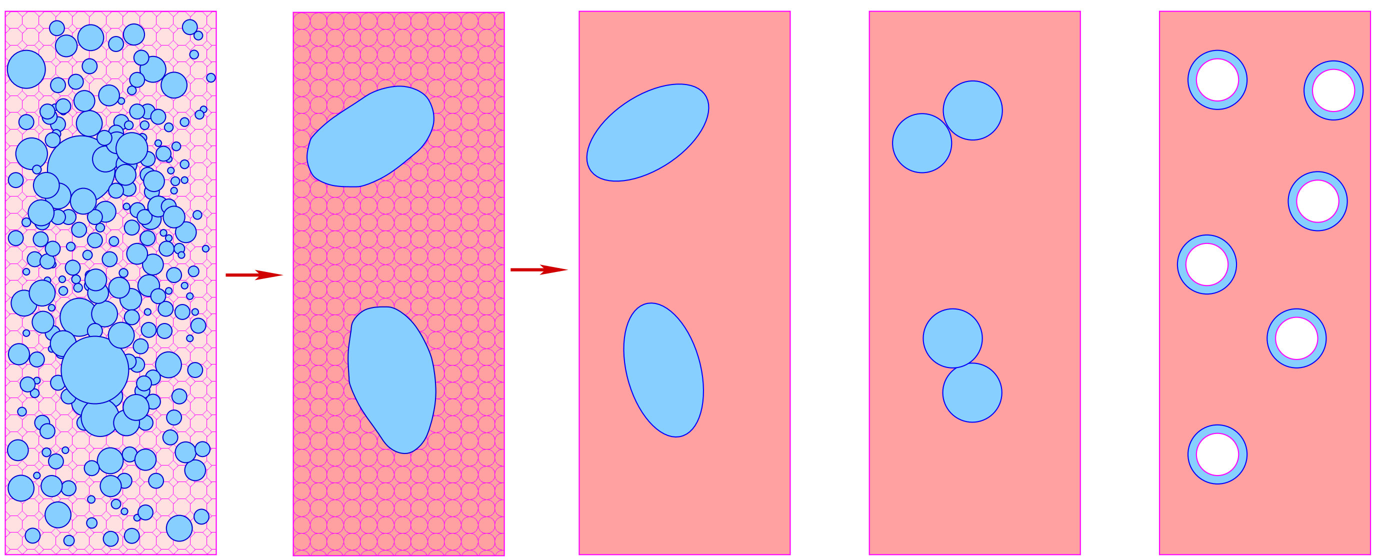
Condition of applicability of the RTE: an average distance between the scatterers d is larger than $a \sim \lambda$.

- The monodisperse system. The absorbtion and scattering coefficients are

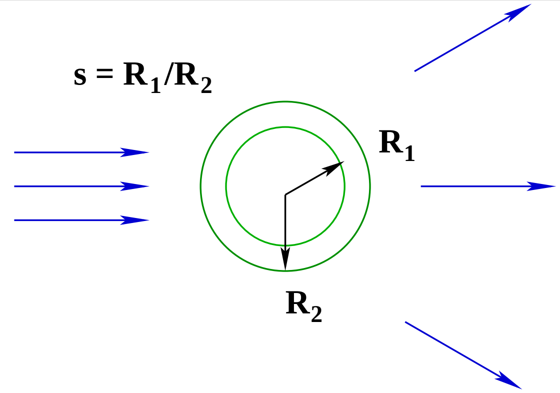
$$\sigma_{abs} = n_0 < \Sigma_{abs} >; \quad \sigma_{sca} = n_0 < \Sigma_{sca} >,$$

$$where \quad < \Sigma_{abs} >= \int f(r)\Sigma_{abs} dr, \quad < \Sigma_{sca} >= \int f(r)\Sigma_{sca} dr.$$

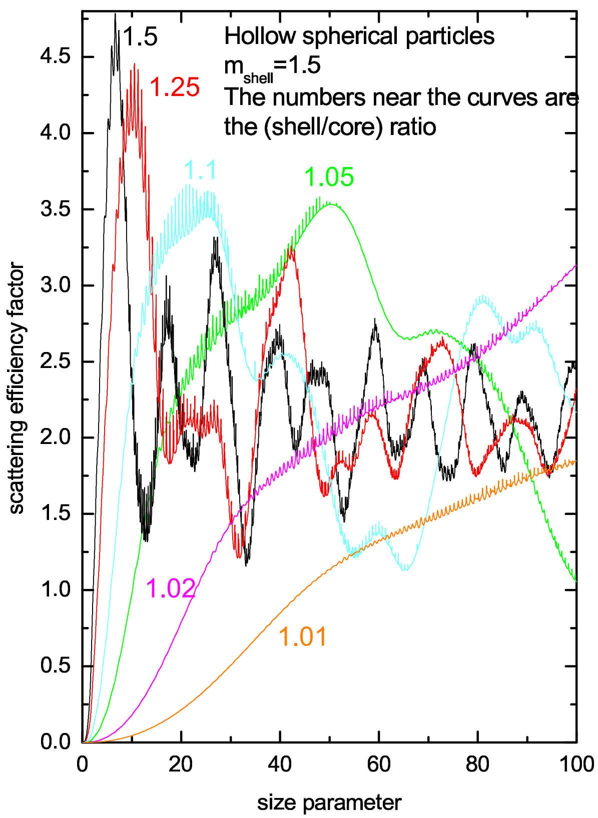
- The polydisperse composite coating is approximated by an effective model of a monodisperse media with relatively low volumetric concentration. The modified Mie theory may be applied.

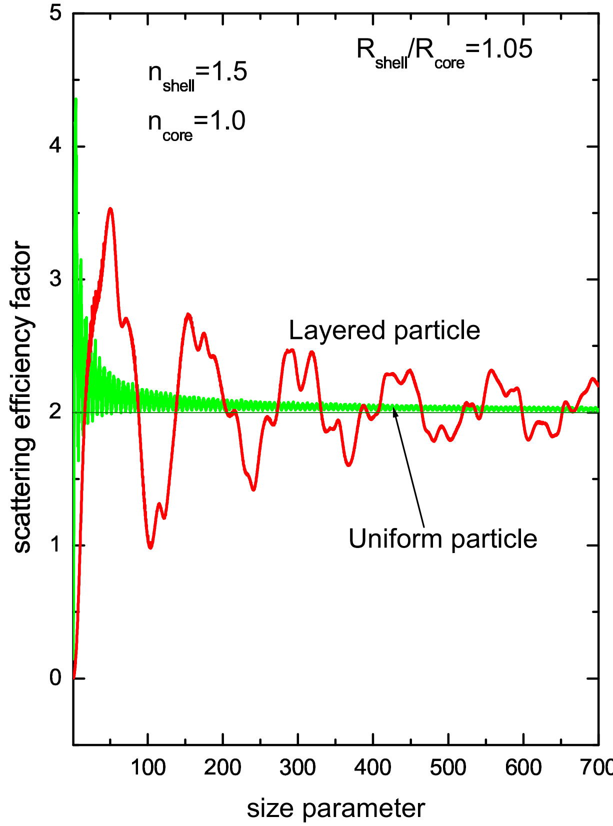


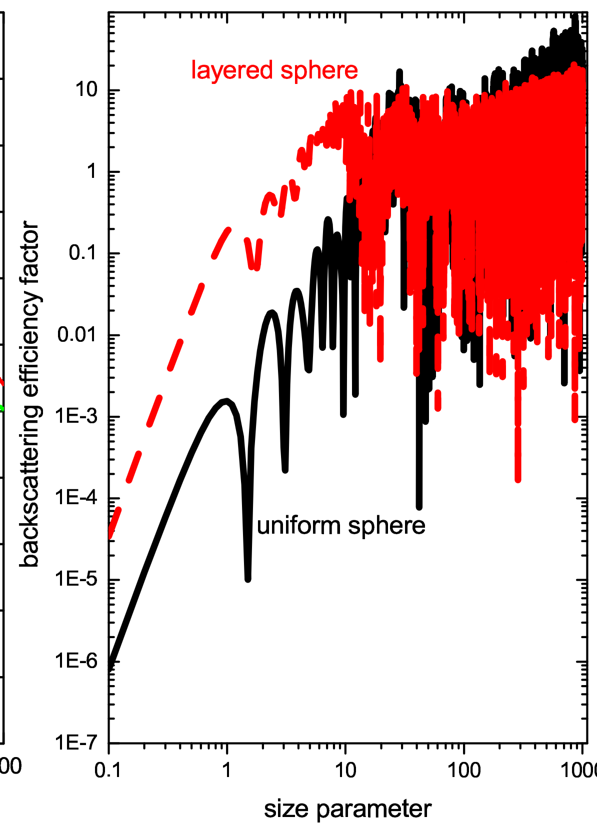
Light scattering on a layered sphere



Efficiency of scattering depends on the thickness of the layer and the size of the particles: Optimization is possible.







Numerical solution of RTE

A goal of any algorithm that solves the integral-differential RTE equation is to determine the energy fluence rate $\int I(\Omega)d\Omega$. A variety of methods has been proposed:

- Asymptotic analyse, for example the Rosseland approximation;
- Monte Carlo calculations;
- Iterative methods;
- Discretisation methods, e.g. ray tracing method or discrete-ordinates methods (e.g. DANTSYS code);
- Expansion of the angular dependence of scattering in special functions, e.g. spherical harmonics (Galerkin approach);
- Hybride models etc...

Imput parameters of the model are the absorption coefficient σ_{abs}, the scattering coefficient σ_{sca} and the phase function $p(\Omega, \Omega')$. The boundary conditions are set for incident radiation fluxes.

Numerical algorithm:

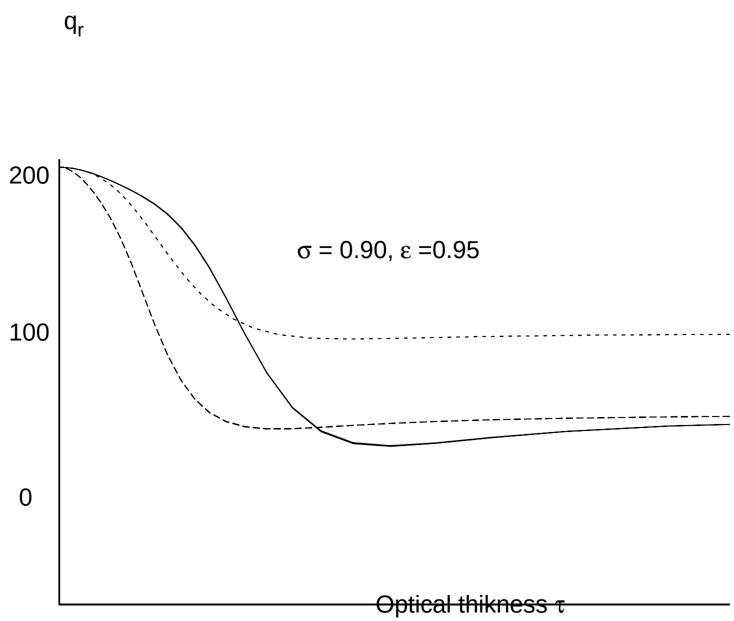
- Discretize the calculation region both for spacial variable x and the directional variable Ω;
- Evaluate the radiative intensivities at the nodes;
- Calculate the radiation field in discrete set of direction $\cos\theta_i$, for each of these direction, thus the RTE is transformed into a set of coupled integro-differential equations;
- Transform each of these equations into a linear differential equation by expansion of the phase function in a series of orthogonal polinomials; a simplified approximation is to make use of the phenomenological Heney-Greenstein phase function

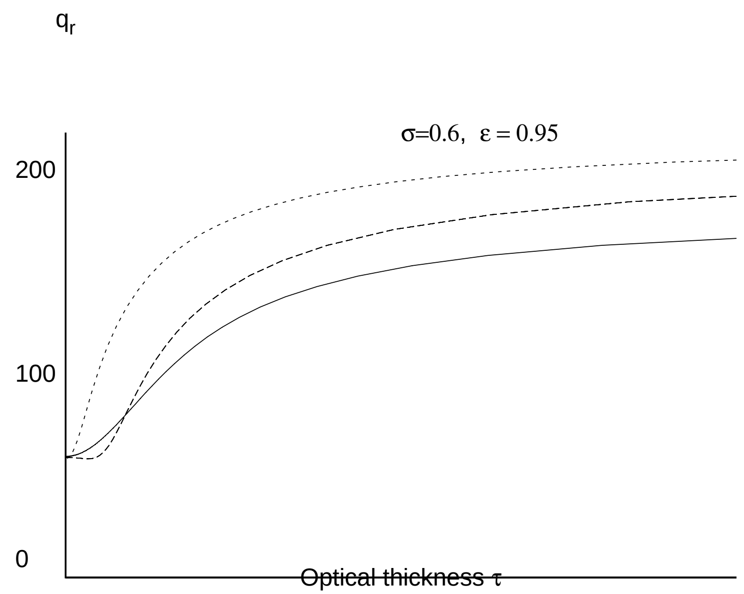
$$p(\cos\theta) = \frac{1-b^2}{[1+b^2-2b\ \cos\theta]^{3/2}}, \text{ where asymmetry parameter } b \in [-1, 1]$$

- Replace the scattering integral by a quadrature (e.g. Gauss-Legendge);
- Evaluate the total flux intergrated over the frequencies (wavelengths) and angles.

Numerical results:

Flux density from the compound surface; $T_w = 0°C$, $T_a = -10°C$, $b = -0.3, 0, 0.3$



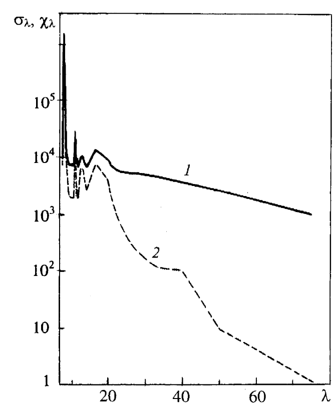


- Scattering anisotropy affects the radiation flux: it increases for a forward directed scattering $(b < 0)$ and decreases for a spherically symmetric $(b = 0)$ and backward directed indicatrice $(b > 0)$ respectively;
- If the emission from the wall is very high, the radiation flux is decreasing exponentially;
- If the emission from the wall is relatively low, the radiation flux is increasing;

Spectral characteristics

It has been shown that the optical properties of the compound depend from wavelength λ. Spectral coefficients of absorption and scattering for were evaluated by M.German, P.Grinchuk and V.P.Nekrasov for the following set of parameters:

- Mean diameter of microspheres: 35 μm;
- Concentration of the microspheres in the compound layer: $N_0 = 2.5 \cdot 10^{12}\ m^{-3}$;
- Mean distance between the microspheres: $d = 40\ \mu$m;
- Temperature $T_r = 250$ K (cloudy weather, or at the night time);
- Temperature $T_r = 100$ K (clear sky).



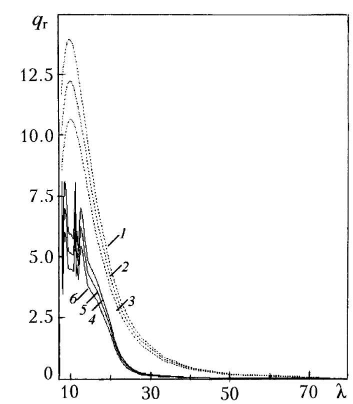
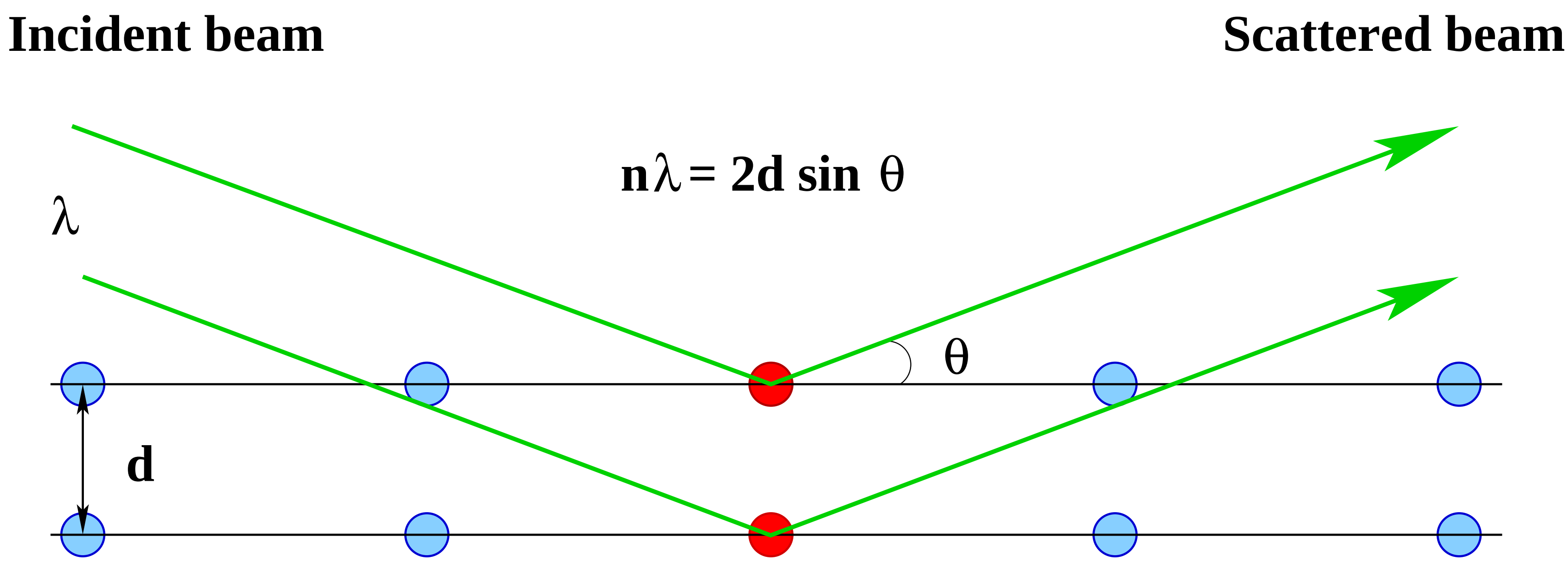


Fig. 4. Spectral coefficients of absorption $\sigma\lambda$ (1) and scattering $\chi\lambda$ (2) of the "ceramic microspheres–binder" compound. $\sigma\lambda$, m^{-1}; $\chi\lambda$, m^{-1}; λ, µm.

Fig. 5. Spectral densities of the radiation flux from the surface of the "bare" wall (1–3) and the wall coated with the compound (4–6) on a clear windless night for Ta = −20°C and Tw = 0°C (1 and 4); −5°C (2 and 5); −10°C (3 and 6). q_r, $W/(m^2 \cdot \mu m)$; λ, µm.

Close-Packed media

RTE approach is no longer valid for a close-packed media. For an ordered structure collective effects appear (Bragg scattering, coherent radiation etc).



Summary and outlook

- *"ThermoShield" coating, which is a compound of a binder and hollow ceramic microspheres, is an efficient means of additional heat protection of enclosing structures;*
- *Physical mechanism of the heat protection of the "Thermo-Shield" coating is related to the suppression of the flux density of the radiative component of the heat transfer due to effects of the light scattering on the microspheres;*
- *The heat-protection effect of the composite "ThermoShield" coating substantially depends on the optical properties of the substrate (wall), the environment and on the temperature regime of operation. In some situations, the heat-protection effect can be even inverted;*
- *One have to avoid homogeneity of the microspheres, the Bragg scattering may open a straight way to the outward radiation transfer;*
- *Consistent mathematical description of the compound is based on the correct description of microscopic optical characteristics.*
- *Constructed mathematical model and the corresponding computer codes nicely describe the heat-protecting properties of the "ThermoShield" coating.*