The modeling of radiation transfer in highly-porous composite materials with strong scattering

O.M. Alifanov, V.V. Cherepanov and A.V. Zaytseva
Moscow Aviation Institute,
Volokolamskoe Hgw. 4, 125993, Moscow, Russia
Email: o.alifanov@yandex.ru

Abstract. In this report the problems, which arise during the radiative transfer of highly-porous thermal protective material with high spectral albedo of scattering, were studied. A three-step iterative numerical method based on splitting the problem operator by "physical processes" was developed. The method is useful and does not need any restrictions in initial approach and optical thickness of a layer. Results of computational modeling are given below.

1. Introduction
There are usually [1-4] the diffusion and transport-diffusion approximations, radiative thermal conductivity approximation or their combination for estimation of values integrated by radiative spectrum such as radiation component of thermal conductivity. However, if the material fragments are anisotropic and their sizes are comparable to the wavelength, such as the fragments of highly-porous thermal protective materials or the material layer is optically thin in the spectral range, then the radiations for these wavelengths can be far different from isotropic radiation. So it is necessary to describe the radiation by means of kinetic theory. For example, in the case of flat layer with thickness \( d \) we come to the known integral-differential boundary problem [3]

\[
\frac{d}{dz} I(z, \mu) + \gamma(z) I(z, \mu) = \alpha(z) I_{in}(z) + \beta(z) \int_{\Omega} \sigma(z, \mu, \mu_s) I_s(z, \mu_s) d \mu_s ,
\]

(1)

\[
I_s(0, \mu) = I_{in}(0) , \mu > 0 , \quad I_s(d, \mu) = I_{in}(d) , \mu < 0 ,
\]

(2)

in which \( I \) - the spectral intensity of radiation \( \sigma(z, \mu, \mu_s) = \frac{1}{4\pi^2} \int \int_{0}^{2\pi} p(\Omega, \Omega_s) d\phi d\phi_s \) - is an average phase function for which the normalization requirement is met, \( p(\Omega, \Omega_s) d\Omega d\Omega_s = 1 \), \( n, a, \beta, \gamma = \alpha + \beta, \rho \) - the local spectral coefficients of absorption, scattering and extinction respectively, \( \Omega \) - the direction unitary vector, \( d\Omega = \sin\theta d\theta d\phi \) - an elementary solid angle (\( \theta, \phi \) - polar and azimuth angles of spherical coordinate system with the polar axis \( Oz \) directed across layer), \( \mu = \cos\theta \), \( I_0 \) - the intensity of equilibrium radiation defined by the Planck formula.

There are various methods for the numerical solution to the problems, which are similar to (1-2) [4-9]. The Monte-Carlo and «ray tracing» methods are time-consuming; they have a set of peculiarities, which are connected to their practical realization. These methods are not considered in this report as well as the semianalytic methods, which use different approximations of phase function and scattering intensity (moments methods, spherical harmonic methods and etc.)
It is very simple to solve the problem (1-2) if we introduce the “dummy” time so that we can determine the stationary solution during stabilization of the non-stationary solution, which was received with the help of the discrete ordinates method (DOM). However, the use of stable implicit finite difference approximations in the equations with integral operator leads to the linear systems with high dimension. It is difficult enough to make the explicit and comparatively low-cost DOM variants stable. Hereafter we will show that the intense scattering in media exacerbates this problem by making the one- and two-step methods unstable. It will also be demonstrated that problem is easily solvable in the frame of three-step method.

2. Scaling and the explicit one-step method of stabilization

Let us introduce the “dummy” time and use the scale natural system for realization of the residual methods during the stationary problem (1-2) solution

$$M_\gamma = M_\alpha = M_\beta = M_z^{-1} = a \gamma_{\max} , c_M M_\gamma l n_{st} = 1, a \in (0,1).$$

As a result we come to the equation

$$\frac{\partial}{\partial t} M_\gamma I(z,\mu) + \frac{\partial}{\partial z} [V(z,\mu,t) I(z,\mu,t)] = 0, V(z,\mu,t) = \mu + W(z,\mu,t) I^z(z,\mu,t),$$

$$W(z,\mu,t) = \int f(z,\mu,t) dz, \mu > 0, W(z,\mu,t) = \int f(z,\mu,t) dz, \mu < 0$$

For the approximation of equation (5) we use the «upstream» scheme [10]. This scheme is very simple, conservative, conditionally stable and has accuracy of the first order of approximation, which leads to the appearance of the numerical diffusion. In order to decrease the diffusion influence on solution quality it is possible to introduce the additional step realizing the Flax Corrected Transport method (FCT) [11,12]. Such an approach slightly increases the amount of calculations and practically raises the approximation order in $\Delta z$ of equation (5) to the second one. Also, it is possible to realize the scheme [13].

During the use of scheme [10] the most serious problems arise near to the intensity sharp changes and areas, where the intensity values are relatively close zero. It essentially increases the effective "speeds" $V_z$ that leads to the time step reduction in this method up to the unacceptably small values.

Besides, the integral character of potential function (5) can have the great influence on the method stability. That’s why we will carry out the detailed research in approximation. For simplicity we will consider a homogeneous media case $\alpha, \sigma = const$ and assume $\mu > 0$ for clarity. Because the effective speeds are positive in this case, then the approximation (5) becomes

$$I_{n-1}^{n+1} = I_{n-1}^{n} + \frac{\Delta t}{\Delta z} \frac{\mu_{j}}{\gamma} \left( I_{k-1}^{n} - I_{k+1}^{n} \right) - \int_{k-1}^{k+1} I_{j}^{n} (z) dz + o(\Delta t^2, \Delta z^2)$$

$$\rho_{k,j} = \rho(\gamma_{k}, \mu_{j}, \mu_{k}) , \ t_{n} = t_{n-1} + \Delta t_{n} , n \geq 1 , t_{0} = 0 , \Delta t_{n} < \Delta z / \max |V_{n,n}^{n+1}| ,$$

$$\mu_{j} = \cos((j-0.5)\pi/n_{\mu}), j = 1...n_{\mu}, n_{\mu} = 2m, \gamma_{k} = (k-1)\Delta z , \Delta z = d / (n_{z} - 1)$$

It is received after uncomplicated transformations and removals of subscripts and superscripts from functions:
\[
\frac{\partial l}{\partial t} + \left( \frac{\mu - \Delta z}{\gamma} \right) \frac{\partial l}{\partial z} + \frac{\Delta t^2}{2} \frac{\partial^2 l}{\partial t^2} + o(\Delta t^2) = \frac{\mu \Delta z}{2\gamma} \frac{\partial^2 l}{\partial z^2} - l + o(\Delta z^2), \quad \mu > 0.
\] (6)

Thus, in the members of the first order grid steps of the approximating equation (6) we can see three additional effects in comparison with the equations (5):

1. The «convectional» speed changes and this change can be meaningful in case of big \(\gamma\).
2. The additional “diffusive” component appears and its influence on the solution increases with reduction of \(\gamma\) and with the increase of \(\mu\) (the instabilities process spreads over from areas with intense scattering and small \(\mu\) magnitude).

![Figure 1](image1)

(a) (b)

Figure 1: (a) - the exact solution to (1), (b) - the intermediate solution to (5).

\[d = 0.026, \quad \alpha = \sigma = 0, \quad \gamma = 130, \quad n_x \times n_y = 10 \times 8, \quad T(C) \in [800, 1200].\]

3. The additional wave disturbances of solution appear. And it is easy to show that the unstable components are always contained in them (see fig.1)

The reason for such unstable behavior of scheme [10] in the range of its «traditional stability», which is determined by Courant condition, is the presence of small multiplier \(\mu\) near the spatial derivative of intensity. The equations with such structure usually «behave badly» during the numerical solution and it is necessary to take special steps for increasing the computing procedure stability.

The research on steady approximation of the problem can be organized in different ways. As it has been marked above such problems arise during the implicit approximation of the equations with the integral operator. At the same time it is possible to decrease their influence if we use the problem operator splitting and construct a multistage algorithm [14,15].

3. Two-stage scheme “predictor-corrector”

Let us write equation (1) in the form

\[
\frac{\partial l}{\partial t} + L_1 l = \alpha I_b + L_2 I, \quad L_2 I(z, \mu, t) = (\mu \frac{\partial}{\partial z} + \gamma(z)I(z, \mu, t),
\]

\[L_1 I(z, \mu, t) = \beta(z) \int_{-1}^{1} \sigma(z, \mu, \mu_i) I(z, \mu_i, t) d\mu_i.
\] (7)

and use the following “predictor-corrector” scheme

\[
\frac{I^{n+1/2} - I^n}{\tau} + L_1 I^{n+1/2} = \alpha I_b, \quad \frac{I^{n+1} - I^{n+1/2}}{\tau} = L_2 I^{n+1},
\] (8)

which is implicit on each “fractional” step. However, the scheme (8) approximates the equation (7) explicitly and with the first order of accuracy. Let us investigate the (8) more clearly.
2.1 The analysis of “predictor” work

The first out of the equations (8) is not complicated for exact solution and we calculated the follows result:

\[
I^{n+1/2}(z, \mu) = I_b(0) e^{-\int_{z_1}^{z_2} \frac{f(z, \mu)}{1 + \tau^2(z)}} + \int_{z_1}^{z_2} dz_1 g(z_1, \mu) e^{-\int_{z_1}^{z_2} \frac{f(z, \mu)}{1 + \tau^2(z)}}, \quad \mu > 0,
\]

\[
I^{n+1/2}(z, \mu) = I_b(d) e^{-\int_{z_1}^{z_2} \frac{f(z, \mu)}{1 + \tau^2(z)}} - \int_{z_1}^{z_2} dz_1 g(z_1, \mu) e^{-\int_{z_1}^{z_2} \frac{f(z, \mu)}{1 + \tau^2(z)}}, \quad \mu < 0,
\]

\[
f(z, \mu) = \frac{1}{\mu(1 + \tau^2(z))}, \quad g(z, \mu) = \frac{1}{\mu(1 + \tau \alpha I_b)}.
\]

Let us note, that functions \( f(z, \mu) \) and \( g(z, \mu) \) always coincide with sign of \( \mu \) and that’s why in exponent dimension there are always negative values. Functions \( f(z, \mu) \) and \( g(z, \mu) \) hyperbolically increase with decreasing of \( \tau, \mu \) so that the question about boundedness appears. Let us note that the fulfillment of the continuity condition

\[
I^{n+1/2} \rightarrow I^n, \quad \tau \rightarrow 0,
\]

contains, in particular, the answer to boundedness question. Let’s investigate the question on solutions boundedness, assuming that the layer is optically homogeneous, i.e. setting \( \alpha, \gamma = \text{const} \) and suppressing the inappreciable dependences from \( \mu \). Because of

\[
\frac{1}{\mu} \int_0^z dz_1 \rho(z_1, \tau) e^{-\frac{z_1^2 + \gamma^2}{4(1 + \tau^2)}} = \frac{1}{1 + \tau^2} \int_0^z \rho(z - \mu \cdot \frac{u \tau}{1 + \gamma^2}, \tau) e^{-\mu} du \rightarrow \rho(z, 0),
\]

then from this as \( \rho(z, \tau) = I^n(z) + \tau \alpha I_b(z) \) the condition (10) follows.

Besides it is possible to be confirmed in this equation

\[
I^{n+1/2}(z, \mu) \rightarrow I_b(0) e^{-\int_{z_1}^{z_2} \frac{f(z, \mu)}{1 + \tau^2(z)}} + \int_{z_1}^{z_2} dz_1 I_b(z_1) e^{-\int_{z_1}^{z_2} \frac{f(z, \mu)}{1 + \tau^2(z)}}, \quad \tau \rightarrow \infty, \quad \mu > 0,
\]

in which the solution to stationary equation (1) for scattering media is contained in right part. Analogical equations are realized for \( \mu < 0 \). And it is possible to generalize these limitary equations in case of heterogeneous media.

It is clearly shown that in analytic realization the “predictor” step of scheme (8) works normally and leads to the necessary limitary consequences. Moreover the computing realization of equations (9) is associated with major problems.
In Figure 2 the results of step-predictor exposure on equilibrium intensity at \( \tau = 0.1 \) and \( \tau = 1 \) for the same set of parameters as for Figure 1 are shown. The numerical integration was carried out by Romberg method with different accuracies. The order of main inaccuracy component is also given in figures. It is obvious from figures, that at the “predictor" step the meaningful errors of integration arise, which appear and spread over from small \( \mu \) magnitude range. They can be reduced only with the rise in integration accuracy. With the small \( \tau \) the accuracy conditions arise so that it excludes the practical use of method. On the whole, the continuity condition (10) violates at the "predictor" step of scheme (8) because of current integration errors with small \( \tau \mu \).

With \( \tau \mu \approx 1 \) and above such problems don’t arise or they are easy to reduce. However, the condition of \( \tau \mu > 1 \) leads to such high values of \( \tau \), that it violates the approximation of (1) by scheme (8). And arising problems in this method are not limited only by this.

2.2 Analysis of “corrector” work. Unremovable problems of two-step method

The equation of “corrector"(8) step has the form

\[
I^{n+1}(z, \mu) = I^{n+1/2}(z, \mu) + \tau \beta(z) \int_{-1}^{1} \sigma(z, \mu, \mu_{i}) I^{n+1}_{\nu}(z, \mu_{i}) d \mu_{i}. \tag{11}
\]

Let us use the iterative process for its solution

\[
I^{n+1,p+1}(z, \mu) = I^{n+1/2}(z, \mu) + \tau \beta(z) \int_{-1}^{1} \sigma(z, \mu, \mu_{i}) I^{n+1,p}_{\nu}(z, \mu_{i}) d \mu_{i}, \quad p = 0, 1, \ldots, \tag{12}
\]

Iteration convergence of “corrector" step is valid only with the small time steps submitting to \( \tau \mu_{\max} < 1 \) condition, because

\[
\| \delta^{p+1} \| = \max_{\tau, \mu} \left| I^{n+1, p+1}_{\nu}(z, \mu) - I^{n+1, p}_{\nu}(z, \mu) \right| \leq \tau \max_{\tau, \mu} \beta(z) \int_{-1}^{1} \sigma(z, \mu, \mu_{i}) \| \delta^{p} \| d \mu_{i} = \tau \beta_{\max} \| \delta^{p} \|. \tag{13}
\]

The main problem of two-step method is existence of contradictory conditions: \( \tau \mu > 1 \) for “predictor" and \( \tau \mu_{\max} < 1 \) for “corrector". These conditions are not consistent during the extension of scattering effects. At this step in case of decisive “predictor” we face with the unremovable problems, which were discussed in part 2.

It turns out that the problem of ill-posed condition can be removed with the help of right organization of “fractional" steps.

4. Three-stage splitting «by physical processes»

Results from part 2 and 3 show, that the problems of the numerical solution to the equation (1) are connected with the presence of small-value coefficient near to the spatial derivative. They arise when the hard component of the equation (1) is included into any equations for “fractional steps” along with
the other components of the original equation (perhaps, except the time derivative). The following algorithm of splitting by «physical processes» is offered:

1. First of all the “fractional” step of “convection” is carried out and it only processes the hard component of the equation (1). At this step the «upstream» scheme is used. The condition of stability, which defines a method time step, is formed and spatial boundary conditions are considered:

\[ I^{n+1/3}(z, \mu) - I^n(z, \mu) + \tau \frac{\partial}{\partial z}(\mu I^n(z, \mu)) = 0, \quad \tau \Delta z / \max \mu_j \]  \hspace{1cm} (13)

Let us note that if the following step of similar explicit algorithm considers other not integrated components of the equation (1), in other words it will be connected with the consideration of physical effects of radiation extinction and secondary radiation after absorption, then as a result there is two-step method, whose first step is similar to (8).

2. That’s why for the second step it is necessary to consider the action of equation (1) integrated components, with the help of connection of this step in the process of unusual “hashing” of the radiation generated by scattering:

\[ I^{n+2/3}(z, \mu) = I^{n+1/3}(z, \mu) + \frac{\tau}{1} \int \sigma(z, \mu, \mu_j) I^{n+1/3}(z, \mu_j) d\mu_j, \]  \hspace{1cm} (14)

3. The step of taking into account secondary radiation effects and attenuation:

\[ I^{n+1}_\nu(z, \mu) = I^{n+2/3}_\nu(z, \mu) + \tau(\alpha(z) I^\nu_{\nu}(z) - \gamma(z) I^{n+2/3}_\nu(z, \mu)) . \]  \hspace{1cm} (15)

Practical use shows the simplicity and efficiency of this method. The iterations (13-15) converge at performance of the stability condition (13). The method convergence practically does not depend on the choice of an initial condition, as well as the structure of the stationary solution, which, how it must be for these problems, is attractor state dependent only on problem parameters. Naturally, in similar calculations the continuous control of stationary equation discrepancy in the knots of finite-difference grids should be also carried out.

5. Some modeling results

As the example of practical use of developed method we consider the radiation transfer with wavelength \( \lambda = 2.4 \, \mu m \) in foamed glassy carbon RVC ETTI-CF-ERG with the following parameters: thickness \( d = 26 \) mm, temperature of boundaries \( T_{\min} = 800^\circ C, \ T_{\max} = 1200^\circ C \). The temperature profile in the layer of material is needed for solution to problems (1) and (2). This profile defines the local values of Planck’s component in equation (1), the values of spectral coefficients of scattering and attenuation, and phase function of the material. Before [16] the temperature dependencies of full thermal conductivity \( \lambda(T) \) and volumetric heat capacity \( C(T) \) were experimentally determined (see Figure3).

As the full thermal conductivity contained radiation component, the energy equation in the problem of radiation-conductive heat transfer for flat layer with known dependences of \( C(T) \) and \( \lambda(T) \) had the divergence form, closed under temperature and its stationary solution determine the necessity temperature profile in the material layer:

\[ C(T) \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \lambda(T) \frac{\partial T}{\partial z} , \ T(0, z) = T_{\max} + \frac{T_{\min} - T_{\max}}{d} z , \ T(t, 0) = T_{\max} , \ T(t, d) = T_{\min} . \]  \hspace{1cm} (16)
The one-dimensional variant of implicit scheme [17] was used for solution to non-linear problem (16). There were organized additions inner iterations at each time step for account of nonlinearity in coefficients of “predictor-corrector” scheme.

The spectral dependencies of the absorption coefficient $\alpha_\lambda$ and the scattering coefficient $\beta_\lambda$, which were calculated for one of the representative elements [18] of carbon foam ETTI-CF-ERG shone in the direction of axis Oz, are shown on Figure 4. Values of wavelength on horizontal axes are specified in meters. The scanning of area on Figure 4 (a) was spent with step $\Delta \lambda = 2 \times 10^{-6}$ m, on Figure 4 (b) with step $\Delta \lambda = 2 \times 10^{-8}$ m. Diameters of knot and crosspieces are noted on horizontal axes. A smooth line, which is the best visible on Figure 4 (b), corresponds to the spectral weight function at $T=500$K multiplied by 0.03, which enters into expression [1] for radiating heat conductivity in a diffusive approach

$$
\psi(\tau) = \tau^3 e^{-\tau^3} (1 - e^{-\tau^3})^{-3}, \quad \tau = \lambda kT / \hbar c = 10^3 \lambda T / 14.39.
$$

The bottom pulsing line, which has narrow and relatively high peaks of a resonance, corresponds to the spectral coefficient of absorption $\alpha_\lambda$ in all pictures. The pulsing line located above displays the spectral scattering coefficient $\beta_\lambda$, which is reduced in $10^3$ times.

The calculations show, that the highest resonance peaks of absorption are located in the spectral area, which ingeniously contains the values of diameters of knot and crosspieces. The width of resonant peaks increases and the height, especially in absorption resonances, decreases in a long-wave part of a spectrum (Figure 4(a)). The especial coherency of resonant effect arises in the processes of absorption and scattering. The coherency was observed in the spectrums, which are shone on a normal of homogeneous flat layers and this coherency is well-known [19]. In this spectral range the representative element (as well as the material) starts to behave itself like a homogeneous media, because the scales of its spatial heterogeneity become insignificant in comparison with wavelength.

The resonant effects weaken in the process of the further increase in wavelength. Absorption and scattering become neglectfully small, the material becomes optically transparent. The resonant effects in the absorption are not so significant in the short wavelengths range, containing the carrier of weight function at temperature $T=500$K. In this range the change of spectral coefficients has a character of small fluctuations in amplitude near some average values, the absorption has little significant and the considered material behaves itself practically like the conservative media with constant properties in spectrum. Values of similar characteristics of a material can be received with the help of averaging corresponding values for representative elements. However, the scattering and absorption spectrums of representative elements of carbon foam in the temperatures range between 500 and 1000C practically do not vary [2]. It is not right for the weight function $\psi$, whose carrier displaces the area of shorter wavelengths in the process of temperature rising. Thus, the accuracy of the description with use of average radiating characteristics at a considered material with temperature growth rises.

![Figure 4](image.png)
Scattering by foam glass carbon is practically isotropic and its phase function was practically constant. The grid with dimension $n_z \times n_{\mu} = 17 \times 8$ and $M = 130$ was used in calculations. The structure of intensity at the first and last iterations is shown in Figure 5. The evolution of equation (1) residual during the iterations (13)-(15) is shown in Figure 6. The modulus of difference between left and right parts is regarded as residual. The $z$-variable initial approach was parabolic and hard enough. Numbers of corresponding iterations are specified in pictures. As it is visible from Figure 6, at separate stages of solution the maximum of residual can rise. But it is always accompanied by cardinal reorganization of the solution form to residual. After the finish of “sweeping changes” process the relaxation to a stationary stage with minimum residual becomes monotonous. In conclusion the convergence is obtained only in three-step method for such high values of scattering coefficient.
6. Conclusion

The method, which has great stability factor in comparison to traditional two-step method, was developed. The method is quick enough, is easily realized and doesn’t lead to any restrictions on optical thickness of a layer, scattering character, etc.

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8. References

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