NUMERICAL METHODS FOR RADIATIVE HEAT TRANSFER IN DIFFUSIVE REGIMES AND APPLICATIONS TO GLASS MANUFACTURING*

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Abstract. In this paper, different approaches for the numerical solution of radiative heat transfer problems in diffusive regimes are considered. We discuss asymptotic preserving schemes, domain decomposition methods and the development of improved diffusion approximations. Problems related to glass manufacturing processes are numerically investigated.

Key words. Radiative heat transfer, glass manufacturing, diffusion approximations

AMS(MOS) subject classifications.

1. Introduction. Simulation of heat transfer in semitransparent materials such as glass are usually done on the basis of the radiative transfer equations or, using a diffusion approximation, on the basis of a nonlinear diffusion equation. We refer to [15], [18], [19], [22], [24], [25] for a detailed description of the equations and further references.

The diffusion approximation of radiative transfer models is obtained by an asymptotic analysis using the diffusion scaling and letting the scaled mean free path tend to zero. If standard numerical methods are used to solve the radiative transfer equations in regimes with small mean free path, usually, a very fine and expensive discretization depending on the mean free path is required due to the stiffness of the equations near the diffusion limit. This makes these schemes extremely time consuming. To deal with this problem different approaches have been used. Examples will be surveyed in the following:

The first approach is to develop numerical schemes for the transport equation working uniformly for different regimes. In particular, it should be possible to chose the discretization size independent of the mean free path. In recent years there has been a lot of work on numerical methods for transport equations working uniformly for a large range of parameters,see [4, 14, 13, 17, 2, 6, 5, 21, 20, 7, 8]. These schemes are usually based an semiimplicit time discretizations. In section 3 such a scheme will be presented for the radiative transfer equations, see [10].

The second approach is based on the following observation: In many applications it is not necessary to model the whole computational region

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by the computationally expensive radiative transfer equation. Only in particularly sensitive regions, where the solution is far from equilibrium, as for example in boundary layers, these equations have to be employed. In the remaining regions of the domain the diffusion approximation is valid, and will lead to sufficiently accurate results. Domain decomposition methods are thus a natural design tool in this case leading to accurate numerical codes with reasonable computation times. One major problem is to obtain the correct coupling conditions at the interface between the two regions, see [10]. This is discussed in section 4.

The third approach is to use improved diffusion approximations. As mentioned above diffusion theory is not capable of describing boundary layers, and the question arises whether some more sophisticated diffusion type approximations can suitably model the boundary layer effects. Such higher–order asymptotic corrections to diffusion theory exist: they are the so–called simplified P_N (SP_N) theories, see [23, 1]. These SP_N theories are, in fact, diffusion in nature. That is, they employ diffusion equations, or coupled systems of diffusion equations. They contain boundary layer effects and can be remarkably accurate – much more accurate than standard diffusion theory. In practice, one views these equations as an extended form of diffusion theory. No separate boundary–layer treatment is necessary because the boundary layers are included in the SP_N equations. For other approximate theories for the above equations and applications, see for example [3, 16]. In these papers approximations based on the Levermore moment expansion and improved diffusion equations are derived.

2. The equations. In a domain $D \in \mathbb{R}^3$ we consider the radiative transfer equations including conductive heat transfer but without photon scattering. The space variable is dentoted by $x \in D$, the direction by the unit vector $\Omega \in S$, S the unit sphere, $\nu \in \mathbb{R}^+$ denotes the frequency, $t \in \mathbb{R}^+$ the time and M the number of spectral bands. For the absorption cross-section $\tilde{\kappa} = \tilde{\kappa}(\nu)$ we assume $\tilde{\kappa}(\nu) = \kappa(k) = \text{const}, k = 1, \cdots, M$ for $\nu \in [\nu_k, \nu_{k+1})$, where $\kappa(k)$ is the absorption cross-section for band k. This assumption is justified in many cases, for example, in the case of radiative heat transfer in glass. The interval $[\nu_1, \infty)$ is called the transparent region and $[0, \nu_1)$ the opaque region of the frequency. We denote by $I = I(x, \Omega, t, k)$ the radiative intensities at x in the direction Ω in band k and by $T(x, t)$ the temperature. We consider the transport equation for the radiative intensity

$$\Omega \cdot \nabla_x I(x, \Omega, t, k) = \kappa(k)[B(T(x, t), k) - I(x, \Omega, t, k)], \tag{2.1}$$

where the spectral black body intensity for the k-th band is defined by

$$B(T(x, t), k) = \int_{\nu_k}^{\nu_{k+1}} \tilde{B}(T(x, t), \nu))d\nu$$

with the spectral black body intensity

$$\tilde{B}(T,\nu) = \frac{2h_p\nu^3}{c^2}(e^{\frac{h_p\nu}{k_BT}} - 1)^{-1},$$

where h_p, c, k_B are Planck's constant, the speed of light and the Boltzmann constant, respectively.

This equation is considered together with the temperature equation

$$(2.2)\quad c_m\rho_m\partial_t T(x,t) = \nabla_x \cdot (k_h \nabla_x T(x,t)) - \sum_k \kappa(k) \int_S [B(T(x,t),k) - I(x,\Omega,t,k)]d\Omega.$$

Here c_m, ρ_m, k_h are the specific heat, the density and the thermal conductivity, respectively. Initial conditions have to be imposed on the temperature:

$$(2.3)\qquad T(x,0) = T_0(x), x \in D.$$

Boundary conditions for I can be of absorbing, reflecting or mixed type. For example, for $\hat{x} \in \partial D$, whose inward–pointing normal is n, one can use the semi–transparent boundary condition

$$(2.4)\qquad I(\hat{x},\Omega,t,k) = \rho(\Omega)I(\hat{x},\Omega',t,k) + [1-\rho(\Omega)]R(\hat{x},\Omega,k),$$

where $\Omega \cdot n > 0$. Here Ω' is the reflection of Ω in the tangent plane to ∂D:

$$\Omega' = \Omega - 2n(n\cdot\Omega),$$

and ρ is the reflectivity and R denotes the radiative intensity transmitted into the medium from the outside. The reflectivity ρ is given by the Fresnel and Snell law. This means for incident angle Θ_1 with $cos\Theta_1 = n \cdot \Omega$ we have

$$\rho = \frac{1}{2}[\frac{tan^2(\Theta_1 - \Theta_2)}{tan^2(\Theta_1 + \Theta_2)} + \frac{sin^2(\Theta_1 - \Theta_2)}{sin^2(\Theta_1 + \Theta_2)}]$$

with

$$n_2 sin\Theta_2 = n_1 sin\Theta_1,$$

if $|sin(\Theta_1)| \leq \frac{n_2}{n_1}$ and $\rho = 1$ otherwise. Here n_1 is the refractive index for the material and n_2 the coefficient for the surroundings. We assume $n_1 \geq n_2$.

Boundary conditions for the heat transfer equation (2.2) are needed as well. One can prescribe either the temperature or the heat flux at the boundary. The heat flux is given by the total (convective plus radiative)

heat input at the boundary. For example, the following conditions can be imposed at $\hat{x} \in \partial D$, see [25]:

$$k_h n \cdot \nabla_x T(\hat{x}, t) = -q(T(\hat{x}, t)) \tag{2.5}$$

with q given by

$$\begin{aligned} q(T(\hat{x}, t)) &= h(T_{ext}(\hat{x}, t) - T(\hat{x}, t)) \\ &\quad + \alpha\pi \int_0^{\nu_1} [\tilde{B}(T_{ext}(\hat{x}, t), \nu) - \tilde{B}(T(\hat{x}, t), \nu)] d\nu, \end{aligned}$$

where T_{ext} is a fixed exterior temperature. The last equation models the heat transfer at the boundary resulting from a convective term due to the temperature difference at the boundary and a term due to the surface radiation of the body, h denoting the convective heat transfer coefficient and α the emissivity depending on the refractive indizes. The integration is only over the opaque frequencies, $\nu \in [0, \nu_1)$.

To simplify the notation we restrict in the following to the case of only one frequency band $\tilde{\kappa} = \kappa$ for $\nu \in [\nu_1, \infty)$. We use the notation

$$< f >= \int_S f(\Omega) d\Omega.$$

We introduce the diffusion scaling, see [12, 15]. If $l_{ref}, t_{ref}, \kappa_{ref}, k_{h\,ref}$ denote the reference scales for length, time, absorption and conduction, the quantity

$$\epsilon = \frac{1}{\kappa_{ref} l_{ref}}$$

is assumed to be small. Moreover we have the relations

$$\begin{aligned} t_{ref} &= c_m \rho_m \kappa_{ref} l_{ref}^2 \\ k_{h\,ref} \kappa_{ref} &= 1 \end{aligned}$$

This gives the nondimensionalized equations

$$\epsilon \Omega \cdot \nabla_x I = \kappa (B(T) - I) \tag{2.6}$$

$$\epsilon^2 \partial_t T = \epsilon^2 \nabla_x \cdot (k_h \nabla_x T) - \kappa < B(T) - I > . \tag{2.7}$$

We investigate equations (2.6), (2.7) as ϵ tends to 0 using an ansatz of the form

$$\begin{aligned} I &= I^0 + \epsilon I^1 + \epsilon^2 I^2 + \dots \\ T &= T^0 + \epsilon^2 T^2 + \dots . \end{aligned}$$

Collecting terms of the same order in ϵ one obtains:

$$\begin{aligned} I^0 &= B(T^0) \\ I^1 &= -\frac{1}{\kappa} \Omega \cdot \nabla_x I^0 \end{aligned}$$

and the limiting diffusion equation for T^0:

$$\partial_t T^0 = \nabla_x \cdot [(k_h + k_r(T^0))\nabla_x T^0], \tag{2.8}$$
$$k_r(T) = \frac{4\pi}{3}\frac{1}{\kappa}\frac{\partial B}{\partial T}(T).$$

Boundary conditions for (2.8) are given by (2.5).

3. Asymptotic preserving schemes. For small values of ϵ, problem (2.6), (2.7) is stiff. In this section we are interested in developing a numerical scheme which is suitable for simulations of the equations in the small mean free path limit. The algorithm should work uniformly for all ϵ and tend to a suitable scheme for the diffusion equation as ϵ tends to 0. In particular, it should not be necessary to adapt the stepsize as $\epsilon \to 0$. These points are obviously not satisfied for a straightforward explicit discretization of the equations. However, they can be achieved by a semi–implicit discretization. For $\epsilon \to 0$ the discretization presented below tends to a standard linear implicit method for the nonlinear diffusion equation (2.8). To obtain a suitable discretization of (2.6), (2.7) we start by rewriting the problem.

The asymptotic procedure suggests writing the radiative intensity in the form $I(x,\Omega,t) = B(T(x,t)) + \epsilon\hat{I}(x,\Omega,t) + \epsilon^2 Z(x,t)$, with $\langle\hat{I}\rangle = 0$. This is a decomposition of I into its mean value $\langle I\rangle = 4\pi B(T) + \epsilon^2 Z$ with respect to Ω and the remainder $\epsilon\hat{I}$. Instead of I, we use the new unknowns $\hat{I}$ and Z.

Equations (2.6) are now rewritten as a system for $\hat{I}$, Z and T determining an equation for the mean value of (2.6), and the deviation from the mean value:

$$\nabla_x \cdot \langle\Omega\hat{I}\rangle = -4\pi\kappa Z\,, \tag{3.1}$$

$$\Omega \cdot \nabla_x B(T) + \epsilon\nabla_x \cdot (\Omega\hat{I} - \frac{1}{4\pi}\langle\Omega\hat{I}\rangle) + \epsilon^2\Omega\cdot\nabla_x Z = -\kappa\hat{I}\,, \tag{3.2}$$

$$\partial_t T = k_h\Delta_x T + 4\pi\kappa Z\,. \tag{3.3}$$

The transformed system consists of the the kinetic equation (3.2) for $\hat{I}$, and the parabolic equation (3.3) for T. Therefore, boundary conditions for $\hat{I}$ and T are needed. We refer to [10] for details.

In the following the problem in the form (3.1)–(3.3) will be discretized. First the time discretization is discussed. We introduce a time step $\tau > 0$ and approximations of the solution at time $t^n = n\tau$, denoted by the superscript n. We use a semi-implicit discretization of (3.1)–(3.3) where backward differences are used for the zeroth order terms (as $\epsilon \to 0$) and forward differences for higher order terms:

$$\nabla_x \cdot \langle\Omega\hat{I}^{n+1}\rangle = -4\pi Z^{n+1}\,, \tag{3.4}$$

$$B'(T^n)\Omega\cdot\nabla_x T^{n+1} + \epsilon\nabla_x\cdot(\Omega\hat{I}^n - \frac{1}{4\pi}\langle\Omega\hat{I}^n\rangle) \tag{3.5}$$

$$+\epsilon^2 \nabla_x \cdot (\Omega Z^n) = -\kappa \hat{I}^{n+1} ,$$

$$\frac{1}{\tau}(T^{n+1} - T^n) = k_h \Delta_x T^{n+1} + 4\pi\kappa Z^{n+1} . \tag{3.6}$$

Note that linearization about the old time step has been used to make the problem at the new time step linear. From the equations (3.4), (3.5), Z^{n+1} and $\hat{I}^{n+1}$ can be computed explicitly in terms of T^{n+1}. Using the expressions for Z^{n+1} and $\hat{I}^{n+1}$ in (3.6) we obtain

$$\kappa \hat{I}^{n+1} = -B'(T^n)\Omega \cdot \nabla_x T^{n+1} + \epsilon G^n , \tag{3.7}$$

$$\text{with } G^n = -\nabla_x \cdot (\Omega \hat{I}^n - \frac{1}{4\pi}\langle \Omega \hat{I}^n \rangle) - \epsilon \nabla_x \cdot (\Omega Z^n) ,$$

$$\kappa Z^{n+1} = \nabla_x \cdot \left(\frac{1}{3\kappa} B'(T^n) \nabla_x T^{n+1} \right) + \epsilon H^n , \tag{3.8}$$

$$\text{with } H^n = -\frac{1}{4\pi\kappa} \nabla_x \cdot \langle \Omega G^n \rangle ,$$

$$\frac{1}{\tau}(T^{n+1} - T^n) = \nabla_x \cdot \left[\left(k_h + \frac{4\pi}{3\kappa} B'(T^n) \right) \nabla_x T^{n+1} \right] + \epsilon 4\pi H^n . \tag{3.9}$$

Thus, an elliptic equation for T^{n+1} remains to be solved. For $\epsilon = 0$, the last equation becomes a stable, linear-implicit discretization of the diffusion equation (2.8).

To state the spatial discretization we consider for simplicity a one-dimensional problem $x \in [0,1]$ and denote the component of Ω in this direction by the one-dimensional variable μ, $\mu \in [-1,1]$.

We discretize space using staggered grids with $h = 1/\text{imax}$:

$$x_i = ih, \qquad i = 0, \ldots, \text{imax}$$

and

$$x_{i-1/2} = (i - 1/2)h, \qquad i = 0, \ldots, \text{imax} + 1.$$

The variables T, and Z are discretized at the full grid points x_i, and $\hat{I}$ is discretized at the points $x_{i-1/2}$. The approximations at time t^n are denoted by T_i^n, Z_i^n, and $\hat{I}_{i-1/2}^n$. Defining

$$(B')_i^n = B'(T_i^n) , \qquad (B')_{i-1/2}^n = \frac{1}{2} \left(B'(T_i^n) + B'(T_{i-1}^n) \right) ,$$

the one-dimensional, space-discretized version of (3.7)–(3.9) reads

$$\kappa \hat{I}_{i-1/2}^{n+1} = -(B')_{i-1/2}^n \mu \frac{T_i^{n+1} - T_{i-1}^{n+1}}{h} + \epsilon G_{i-1/2}^n , \tag{3.10}$$

with

$$G_{i-1/2}^n = -\frac{\mu}{h}(\hat{I}_i^n - \hat{I}_{i-1}^n) + \frac{1}{4\pi} \left\langle \frac{\mu}{h}(\hat{I}_i^n - \hat{I}_{i-1}^n) \right\rangle - \frac{\epsilon\mu}{h}(Z_i^n - Z_{i-1}^n) \tag{3.11}$$

$$\kappa Z_i^{n+1} = \epsilon H_i^n + \frac{1}{3h\kappa}\left((B')_{i+1/2}^n \frac{T_{i+1}^{n+1} - T_i^{n+1}}{h} - (B')_{i-1/2}^n \frac{T_i^{n+1} - T_{i-1}^{n+1}}{h} \right) \tag{3.12}$$

with

$$H_i^n = -\frac{1}{4\pi\kappa}\left\langle \frac{\mu}{h}(G_{i+1/2}^n - G_{i-1/2}^n) \right\rangle , \tag{3.13}$$

$$\frac{1}{\tau}(T_i^{n+1} - T_i^n) = \frac{1}{h}\left[\left(k_h + \frac{4\pi}{3\kappa}(B')_{i+1/2}^n \right) \frac{T_{i+1}^{n+1} - T_i^{n+1}}{h} - \left(k_h + \frac{4\pi}{3\kappa}(B')_{i-1/2}^n \right) \frac{T_i^{n+1} - T_{i-1}^{n+1}}{h} \right] + \epsilon 4\pi H_i^n \tag{3.14}$$

The free streaming operator in (3.11) is discretized by an upwinding procedure:

$$\hat{I}_i^n = \begin{cases} \hat{I}_{i-1/2}^n , & \text{for } \mu > 0 , \\ \hat{I}_{i+1/2}^n , & \text{for } \mu < 0 . \end{cases}$$

For $\epsilon = 0$, (3.14) becomes a standard linear-implicit discretization of (2.8).

For the discretization of the boundary conditions we refer to [10]. The following algorithm needs to be carried out for each time step:

Step 1: Compute $G_{i-1/2}^n$, $i = 1, \ldots$,imax, from (3.11).
Step 2: Compute H_i^n, $i = 1, \ldots$,imax-1, from (3.13).
Step 3: Compute T_i^{n+1}, $i = 0, \ldots$,imax, from (3.14) subject to boundary conditions.
Step 4: Compute Z_i^{n+1}, $i = 1, \ldots$,imax-1, from (3.12).
Step 5: Compute $\hat{I}_{i-1/2}^{n+1}$, $i = 1, \ldots$,imax, from (3.10) subject to boundary conditions.

Note that only Step 3 is implicit. A tridiagonal system resulting from the implicit discretization of a parabolic equation needs to be solved there. finally, we mention that for the velocity discretization standard methods are used.

4. Domain decomposition methods. By solving radiative transfer and diffusion equations simultanously in different domains, a good approximation of the full radiative transfer solution may be obtained. Moreover, the computational complexity is in general considerably below the one needed for the full radiative transfer solution, in particular, if the diffusion approximation is valid in the main part of the domain as it is the case in diffusive regimes. We assume that the computational domain is separated into a subdomain where the radiative transfer equation is solved and another subdomain where the diffusion approximation is used. That

means we consider the domain D divided into two non-overlapping subdomains D_A and D_B, $D_A \cup D_B = D$ with boundaries $\partial D_A, \partial D_B$ and the interface $F = \partial D_A \cap \partial D_B$.

The global radiative transfer solution is approximated by the solution of the following coupling problem: in D_A the radiative transfer equation (2.6) is solved and in D_B the diffusion equation (2.8). Providing these equations with coupling conditions at the interface F will lead to a properly-stated problem. This is solved by an iterative procedure solving in turn the two equations, see [11]. In the following I_A, T_A and I_B, T_B denote the solution of (2.6) in D_A and D_B, respectively. T_B^0 denotes the solution of the diffusion equation (2.8) in D_B.

These coupling conditions can be found by using an additional rescaling of the normal component of the space variable in an interface layer between the two domains. Equations for interface layer terms can be derived. Coupling conditions can be found using an appropriate matching of the radiative transfer domain, the layer and the diffusion domain, see [11]. Here we state suitable approximations of these conditions. They are based on equalizing fluxes and the fact that the intensity I_B in the diffusion domain can be approximated by

$$I_B(x,\Omega) \sim B(T_B^0(x)) - \epsilon \frac{1}{\kappa} \Omega \cdot \nabla_x B(T_B^0(x)) + O(\epsilon^2). \tag{4.1}$$

Assuming T_A in the radiative transfer domain to be known a straightforward coupling condition for T_B^0, the diffusion solution, would be $T_B^0(\hat{x}) = T_A(\hat{x}), \hat{x} \in F$. T_B^0 is however only a first order approximation of T_B. A much better condition can be found by the analysis of the interface layer. An approximation is

$$T_B^0(\hat{x}) - \epsilon \alpha(\hat{x}) n \cdot \nabla_x T_B^0(\hat{x}) = T_A(\hat{x}), \tag{4.2}$$

where n is the normal to the interface pointing into D_B and α is determined by

$$< \frac{1}{\kappa} \int_{\mu>0} \mu^2 d\Omega > = < \int_{\mu>0} \mu \alpha(\hat{x}) d\Omega > \tag{4.3}$$

with $\mu = n \cdot \Omega$. (4.3) is found by comparing the positive halffluxes of $\frac{\mu}{\kappa}$ and α.

The condition for the radiative transfer solution in D_A assuming T_B^0 to be known are found using (4.1) as an approximation of the ingoing function. I.e.

$$I_A(\hat{x},\Omega) = B(T_B^0(\hat{x})) - \epsilon \frac{1}{\kappa} \Omega \cdot \nabla_x B(T_B^0(\hat{x})), \mu < 0. \tag{4.4}$$

The condition for T_A is found by equalizing the total flux (radiative transfer and heat flux) in the direction of the normal to the interface, i.e.

$$\epsilon^2 k_h n \cdot \nabla_x T(x) - \epsilon < n \cdot \Omega I(x,\Omega) > .$$

We obtain the additional coupling condition by requiring the continuity of these fluxes at the interface, i.e.

$$\begin{aligned}(4.5)\qquad &\epsilon k_h n\cdot\nabla_x T_A(\hat{x})- < n\cdot\Omega I_A(\hat{x},\Omega) >\\ &= \epsilon k_h n\cdot\nabla_x T_B(\hat{x})- < n\cdot\Omega I_B(\hat{x},\Omega) > .\end{aligned}$$

Using (4.1) and approximating T_B by T_B^0 one obtains

$$\begin{aligned}(4.6)\qquad &\epsilon k_h n\cdot\nabla_x T_A(\hat{x})- < n\cdot\Omega I_A(\hat{x},\Omega) >\\ &= \epsilon k_h n\cdot\nabla_x T_B^0(\hat{x}) + \epsilon < \frac{1}{\kappa} n\cdot\Omega\Omega\cdot\nabla_x B(T_B^0(\hat{x})) >\\ &= \epsilon k_h n\cdot\nabla_x T_B^0(\hat{x}) + \epsilon\frac{1}{\kappa}\frac{4\pi}{3}B'(T_B^0(\hat{x}))n\cdot\nabla_x T_B^0(\hat{x})\\ &= \epsilon[k_h + k_r(T_B^0(\hat{x}))]n\cdot\nabla_x T_B^0(\hat{x}).\end{aligned}$$

Equation (4.6) gives a second straightforward coupling condition.

The coupled solution is now obtained by an iterative procedure solving in turn radiative transfer and diffusion equations. A numerical example using the above coupling conditions is found in the last section.

5. Approximate equations. In this section we derive improved diffusion approximations, the SP_N equations for radiative transfer see [9]. In order to formally "solve" equation (2.6), we write it in the form

$$\Big(1+\frac{\varepsilon}{\kappa}\Omega\cdot\nabla\Big)I = B(T).$$

and invert the operator on the left using Neumann's series

$$\begin{aligned}(5.1)\qquad I &= \Big(1+\frac{\varepsilon}{\kappa}\Omega\cdot\nabla\Big)^{-1}B\\ &= \Big[1-\frac{\varepsilon}{\kappa}\Omega\cdot\nabla+\frac{\varepsilon^2}{\kappa^2}(\Omega\cdot\nabla)^2-\frac{\varepsilon^3}{\kappa^3}(\Omega\cdot\nabla)^3+\cdots\Big]B.\end{aligned}$$

Integrating with respect to Ω and using the result

$$< (\Omega\cdot\nabla)^n >= [1+(-1)^n]\,\frac{2\pi}{n+1}\nabla^n,$$

we get

$$\begin{aligned}\phi &= < I >\\ (5.2)\qquad &= 4\pi\Big[1+\frac{\varepsilon^2}{3\kappa^2}\nabla^2+\frac{\varepsilon^4}{5\kappa^4}\nabla^4+\frac{\varepsilon^6}{7\kappa^6}\nabla^6\cdots\Big]B+\mathcal{O}(\varepsilon^8).\end{aligned}$$

Hence

$$4\pi B = \Big[1+\frac{\varepsilon^2}{3\kappa^2}\nabla^2+\frac{\varepsilon^4}{5\kappa^4}\nabla^4+\frac{\varepsilon^6}{5\kappa^6}\nabla^6\Big]^{-1}\phi+\mathcal{O}(\varepsilon^8)$$

$$
\begin{aligned}
&= \Big\{ 1 - \Big[\frac{\varepsilon^2}{3\kappa^2}\nabla^2 + \frac{\varepsilon^4}{5\kappa^4}\nabla^4 + \frac{\varepsilon^6}{5\kappa^6}\nabla^6\Big] \\
&\quad + \Big[\frac{\varepsilon^2}{3\kappa^2}\nabla^2 + \frac{\varepsilon^4}{5\kappa^4}\nabla^4 + \frac{\varepsilon^6}{5\kappa^6}\nabla^6\Big]^2 \\
&\quad - \Big[\frac{\varepsilon^2}{3\kappa^2}\nabla^2 + \frac{\varepsilon^4}{5\kappa^4}\nabla^4 + \frac{\varepsilon^6}{5\kappa^6}\nabla^6\Big]^3 \cdots \Big\}\phi + \mathcal{O}(\varepsilon^8) \\
&= \Big[1 - \frac{\varepsilon^2}{3\kappa^2}\nabla^2 - \frac{4\varepsilon^4}{45\kappa^4}\nabla^4 - \frac{44\varepsilon^6}{945\kappa^6}\nabla^6\Big]\phi + \mathcal{O}(\varepsilon^8),
\end{aligned}
$$

so

$$
4\pi B = \Big[1 - \frac{\varepsilon^2}{3\kappa^2}\nabla^2 - \frac{4\varepsilon^4}{45\kappa^4}\nabla^4 - \frac{44\varepsilon^6}{945\kappa^6}\nabla^6\Big]\phi + \mathcal{O}(\varepsilon^8). \tag{5.3}
$$

If we discard terms of $\mathcal{O}(\varepsilon^4)$,$\mathcal{O}(\varepsilon^6)$ or $\mathcal{O}(\varepsilon^8)$ we obtain the P_1, SP_2 and SP_3 approximations, respectively. The above approximation (5.2) for ϕ is then used in the temperature equation (2.6). In the following we state the different approximate equations and suitable boundary conditions, see [9] for details. Let us define for $m = 1, 3$ integrals of the influx of radiation on the boundary, $\hat{x} \in \partial D$

$$
I_m(\hat{x}) = \int\limits_{n\cdot\Omega>0} \big(1 - \rho(n\cdot\Omega)\big) P_m(|n\cdot\Omega|) R(\hat{x},\Omega)\; d\Omega
$$

where P_1 and P_3 are the Legendre polynomials of order 1 and 3, respectively: $P_1(\mu) = \mu$ and $P_3(\mu) = (5\mu^3 - 3\mu)/2$. Furthermore, it will be convenient for the statement of the boundary conditions below to have the following integrals with respect to the weight ρ at hand:

$$
\begin{aligned}
r_1 &= 2\pi\textstyle\int_0^1 \mu\rho(\mu)\; d\mu, & r_5 &= 2\pi\textstyle\int_0^1 P_3(\mu)\rho(\mu)\; d\mu, \\
r_2 &= 2\pi\textstyle\int_0^1 \mu^2\rho(\mu)\; d\mu, & r_6 &= 2\pi\textstyle\int_0^1 P_2(\mu)P_3(\mu)\rho(\mu)\; d\mu, \\
r_3 &= 2\pi\textstyle\int_0^1 \mu^2\rho(\mu)\; d\mu, & r_7 &= 2\pi\textstyle\int_0^1 P_3(\mu)P_3(\mu)\rho(\mu)\; d\mu, \\
r_4 &= 2\pi\textstyle\int_0^1 \mu P_3(\mu)\rho(\mu)\; d\mu,
\end{aligned}
$$

The $O(\epsilon^2)$ or P_1 *approximation* is given by the approximate flux equation

$$
-\frac{\varepsilon^2}{3\kappa^2}\nabla^2\phi + \kappa\phi = \kappa(4\pi B) \tag{5.4}
$$

together with the energy equation

$$
\frac{\partial T}{\partial t} = \nabla\cdot(k_h\nabla T) + \nabla^2\frac{\phi}{3\kappa} \tag{5.5}
$$

and the flux boundary condition

$$
(1 - 2r_1)\phi(\hat{x}) - (1 + 3r_2)\frac{2\varepsilon}{3\kappa} n\cdot\nabla\phi(\hat{x}) = 4I_1(\hat{x}). \tag{5.6}
$$

where n is the normal to the boundary pointing into the domain. The boundary condition for the temperature is in all cases given by (2.5). Condition (5.6) is found by equating half–fluxes and expanding the radiative intensity similar to (4.1) in section 4. Introducing the variable

$$\xi = \phi + \frac{4}{5}(\phi - 4\pi B),$$

the SP_2 *approximation* is

$$-\frac{3\varepsilon^2}{5\kappa}\nabla^2\xi + \kappa\xi = \kappa(4\pi B), \tag{5.7}$$

and again

$$\frac{\partial T}{\partial t} = \nabla\cdot(k_h\nabla T) + \nabla^2\frac{\xi}{3\kappa}, \tag{5.8}$$

with boundary condition

$$\alpha_1\xi(\hat{x}) - (1+3r_2)\frac{2\varepsilon}{3\kappa}n\cdot\nabla\xi(\hat{x}) = \alpha_2 4\pi B(T_b(\hat{x})) + 4I_1(\hat{x}), \tag{5.9}$$

where we use the short notation

$$\begin{aligned}\alpha_1 &= \frac{5}{9}\Big(1 - 2r_1 + \frac{1}{2}(1 - 4\big(3r_3 - r_1)\big)\Big)\\ \alpha_2 &= \frac{1}{2}\big(1 - 4(3r_3 - r_1)\big) - \frac{4}{5}\alpha_1.\end{aligned}$$

The SP_3 approximation is given by the following: Let

$$\psi_n = \phi + \gamma_n\phi_2, \quad n = 1,2 \tag{5.10}$$

where ϕ_2 is given by

$$\phi_2 = (1 - \frac{11}{21}\frac{\epsilon^2}{\kappa^2}\nabla^2)^{-1}\frac{2\epsilon^2}{15\kappa^2}\phi$$

and

$$\gamma_n = \frac{5}{7}\Big[1 + (-1)^n\sqrt[3]{\frac{6}{5}}\Big].$$

If we define constants

$$a_n = \frac{1}{30}\Big(5 \mp 3\sqrt{\frac{5}{6}}\Big), n = 1,2,$$

and

$$\mu_n^2 = \frac{3}{7} \pm \frac{2}{7}\sqrt{\frac{6}{5}}, n = 1,2,$$

then the SP_3 *approximation* consists of the flux equations

$$-\varepsilon^2\nabla\cdot\frac{1}{\kappa}\nabla\mu_1^2\psi_1+\kappa\psi_1=\kappa(4\pi B), \tag{5.11}$$

$$-\varepsilon^2\nabla\cdot\frac{1}{\kappa}\nabla\mu_2^2\psi_2+\kappa\psi_2=\kappa(4\pi B), \tag{5.12}$$

together with the energy equation

$$\frac{\partial T}{\partial t}=\nabla\cdot(k_h\nabla T)+\nabla^2\frac{a_1\psi_1+a_2\psi_2}{\kappa}. \tag{5.13}$$

The SP_3 boundary conditions for ϕ and ϕ_2 are originally

$$\begin{aligned}(1-2r_1)\frac{1}{4}\phi(x)+(1-8r_3)\frac{5}{16}\phi_2(x)+(1+3r_2)\frac{\varepsilon}{6\kappa}n\cdot\nabla\phi(x)&\\ -\Big(\frac{1+3r_2}{3}+\frac{3r_4}{2}\Big)\frac{2\varepsilon}{3\kappa}n\cdot\nabla\phi_2(x)=\ I_1(x),&\\ -(1+8r_5)\frac{1}{16}\phi(x)+(1-8r_6)\frac{5}{16}\phi_2(x)+3r_4\frac{\varepsilon}{6\kappa}n\cdot\nabla\phi(x)&\\ -\Big(r_4+\frac{3}{14}(1+7r_7)\Big)\frac{\varepsilon}{\kappa}n\cdot\nabla\phi_2(x)=I_3(x).&\end{aligned}$$

or formally

$$\begin{aligned}A_1\phi(x)+A_2\phi_2(x)+A_3\frac{\varepsilon}{\kappa}n\cdot\nabla\phi(x)+A_4\frac{\varepsilon}{\kappa}n\cdot\nabla\phi_2(x)\ &=I_1(x)\\ B_1\phi(x)+B_2\phi_2(x)+B_3\frac{\varepsilon}{\kappa}n\cdot\nabla\phi(x)+B_4\frac{\varepsilon}{\kappa}n\cdot\nabla\phi_2(x)&=I_3(x).\end{aligned}$$

We have to derive boundary conditions for ψ_1 and ψ_2. Using the formulae in (5.10), we can transform the boundary conditions for ϕ and ϕ_2 into boundary conditions for ψ_1 and ψ_2. Defining $w_0=1/(\gamma_2-\gamma_1)$ we have

$$\phi=w_0\gamma_2\psi_1-w_0\gamma_1\psi_2,\qquad \phi_2=-w_0\psi_1+w_0\psi_2,$$

such that the boundary equations above become

$$\begin{aligned}&(A_1\gamma_2w_0-A_2w_0)\psi_1+(-A_1\gamma_1w_0+A_2w_0)\psi_2\\ &\quad+(A_3\gamma_2w_0-A_4w_0)\frac{\varepsilon}{\kappa}n\cdot\nabla\psi_1+(-A_3\gamma_2w_0+A_2w_0)\frac{\varepsilon}{\kappa}n\cdot\nabla\psi_2=I_1\\ &(B_1\gamma_2w_0-B_2w_0)\psi_1+(-B_1\gamma_1w_0+B_2w_0)\psi_2\\ &\quad+(B_3\gamma_2w_0-B_4w_0)\frac{\varepsilon}{\kappa}n\cdot\nabla\psi_1+(-B_3\gamma_2w_0+B_2w_0)\frac{\varepsilon}{\kappa}n\cdot\nabla\psi_2=I_3\end{aligned}$$

or, again formally rewritten for writing convenience,

$$\begin{aligned}C_1\psi+C_2\psi_2+C_3\frac{\varepsilon}{\kappa}n\cdot\nabla\psi+C_4\frac{\varepsilon}{\kappa}n\cdot\nabla\psi_2\ &=I_1\\ D_1\psi+D_2\psi_2+D_3\frac{\varepsilon}{\kappa}n\cdot\nabla\psi+D_4\frac{\varepsilon}{\kappa}n\cdot\nabla\psi_2&=I_3.\end{aligned}$$

We eliminate the gradient term $n \cdot \nabla\psi_2$ in the first equation and $n \cdot \nabla\psi_1$ in the second in order to get boundary conditions for the ψ_1 and ψ_2 equations, respectively, such that ψ_1 and ψ_2 are only weekly coupled. We find

$$\begin{aligned}(C_1D_4 - D_1C_4)\psi_1 + (C_3D_4 - D_3C_4)\frac{\varepsilon}{\kappa}n \cdot \nabla\psi_1 \\ = -(C_2D_4 - D_2C_4)\psi_2 + (D_4\ I_1 - C_4\ I_3) \\ -(C_2D_3 - D_2C_3)\psi_2 + (C_3D_4 - D_3C_4)\frac{\varepsilon}{\kappa}n \cdot \nabla\psi_2 \\ = (C_2D_3 - D_2C_3)\psi_1 - (D_3\ I_1 - C_3\ I_3)\end{aligned}$$

so, if we set $D = C_3D_4 - D_3C_4$ and define constants

$$\begin{array}{rclcrcl}\alpha_1 & = & (C_1D_4 - D_1C_4)/D, & \qquad & \alpha_2 & = & -(C_2D_3 - D_2C_3)/D, \\ \beta_1 & = & (C_2D_4 - D_2C_4)/D & & \beta_2 & = & -(C_2D_3 - D_2C_3)/D,\end{array}$$

then we end up with SP_3 boundary conditions for (5.11) and (5.12) in the following form:

$$\alpha_1\psi_1(x) + \frac{\varepsilon}{\kappa}\psi_1(x) = -\beta_2\psi_2(x) + (D_4\ I_1(x) - C_4\ I_3(x))/D, \tag{5.14}$$

$$\alpha_2\psi_2(x) + \frac{\varepsilon}{\kappa}\psi_2(x) = -\beta_1\psi_1(x) - (D_3\ I_1(x) - C_3\ I_3(x))/D. \tag{5.15}$$

6. Numerical Results. We investigated the approximation of the radiative transfer solution by the coupling approach from section 4 and the approximations using improved diffusion equations in section 5. In our first example we consider domain decomposition, see [11]. 3D–multiband equations were studied for a typical example in glass manufacturing. We simulated the annealing of a cylindrical glass slab with radius $1cm$ and height $2cm$. The number of frequency bands was $M = 18$ and the absorption coefficients $\kappa(k)$ ranged in magnitude from $1m^{-1}$ to 10^5m^{-1} for the different bands. We started with an initial temperature $T_0 = 873K$ of the glass and used (2.5) as boundary condition for the heat transfer equation. We assumed room temperature $T_{ext} = 293K$ in the exterior and the outside radiation is accordingly assumed to be a Planckian i.e. isotropic $R(\Omega, \nu) = B(T_{ext}, \nu)$. In our case, the refractive coefficients n_1 and n_2 were chosen for glass with surrounding air: we set $n_1 = 1.46$ and $n_2 = 1$. Therefore, the corresponding hemispheric emissivity was set $\alpha = 0.92$. The edge of of the opaque part of the spectrum was located at the wavelength $\lambda_1 = 7\mu m$ thus giving $\nu_1 = c/\lambda_1 = 4.28 \cdot 10^{13}s^{-1}$. Furthermore, we used the density $\rho_m = 3000kg/m^3$, the specific heat $c_m = 1000J/kgK$, the thermal heat conductivity $k_h = 1.6W/mK$ and a vanishing convective heat transfer coefficient $h = 0W/m^2K$. Figure 1 shows a comparison of the domain decomposition approach, the global radiative transfer solution and the diffusion approximation for the above data. The temperature is plotted at a fixed time considering a horizontal section in the middle of the cylinder. The radiative transfer solution and the coupled solution show good agreement in contrast to the diffusion solution.

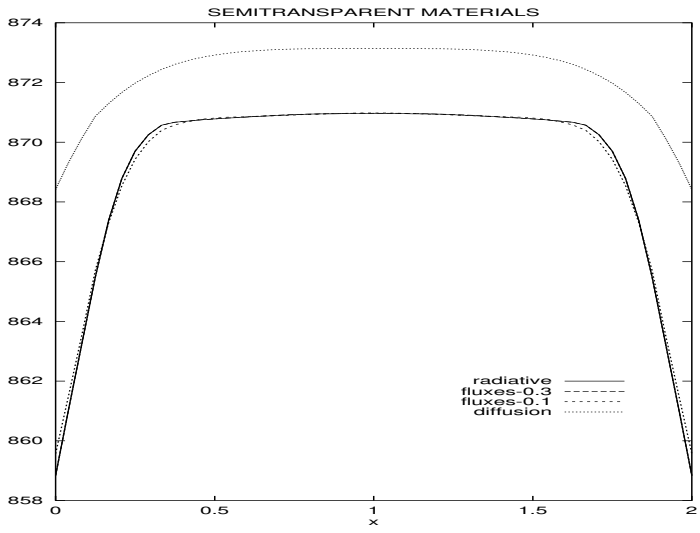

FIG. 1. *Domain decomposition approach. The classical diffusion (Rosseland) approximation used in the interior domain while the radiative transfer equations solved in the boundary layer. Two decompositions with layers of size* 0.1 *and* 0.3*, respectively, were investigated.*

The investigation of the diffusion approximations was done for the 1D model in so–called *slab geometry*. Temperature and radiation only depend on the x–coordinate in space but not on y and z and, moreover, the radiation is symmetric with respect to the x–axis. Simulations were done for the single band case as described above. Standard finite differences were applied to discretize the diffusion equations and uniform space and time grids were used. We chose a grid size 0.01 for the scaled interval $[0, 1]$ and the time step 0.0001. The initial temperature is $T_0 = 1000K$ while the exterior temperature is $T_{ext} = 300K$. We assume the scaled physical parameters in the equations to have the values $\kappa = 1$, $k_h = 1$ and $h = 1$. The rest of the parameters were the same as in the previous example. Different optical regimes were considered corresponding to different values of the parameter ϵ. Figures 2 and 3 show the three improved SP_N diffusion approximations explained in section 5 in comparison with the radiative transfer solution and the Rosseland approximation at time $t = 0.01$. As can be observed, the improved approximations, in particular the SP_3 approximation, give better results than the conventional diffusion approximation. Furthermore, owing to the asymptotic analysis leading to the classical diffusion approximation and the SP_N approximations, one expects that all of them become the more accurate the smaller ε is i.e. the more optically thick and diffusive the regime is. The results confirm this asymptotic behaviour which is particularly distinctive in the Rosseland approximation. We mention

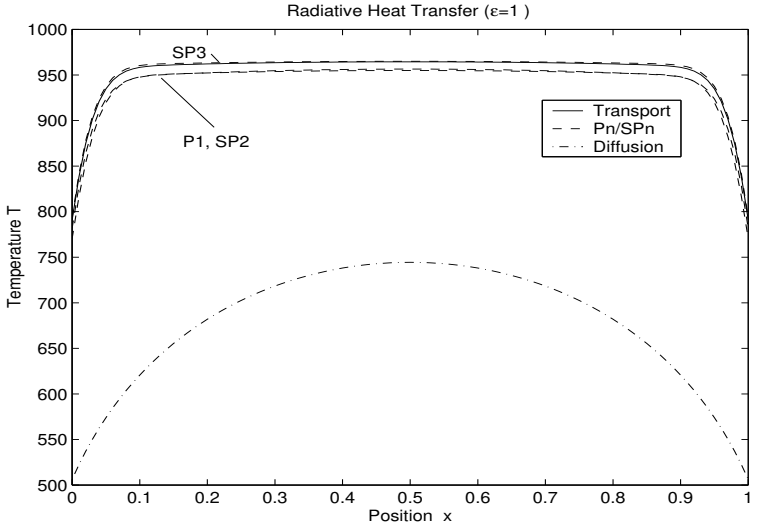

FIG. 2. *The SP_N approximations for large parameter $\varepsilon = 1$.*

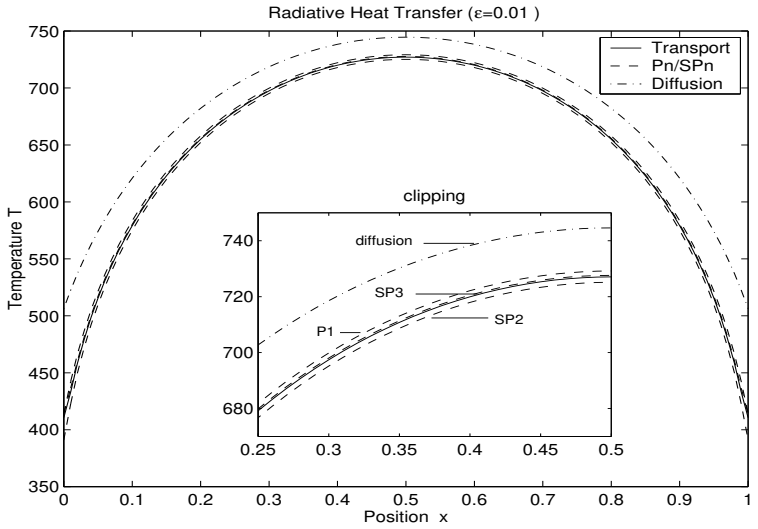

FIG. 3. *The SP_N approximations in the optically thick, diffusive regime corresponding to the small parameter $\varepsilon = 0.01$.*

that the Levermore moment method [3] for radiative transfer mentioned in the introduction gives, in this simple case, the same result as the P_1 approximation. However, this behaviour can change drastically for more complicated problems with strong anisotropies, see [3].

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