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Time-dependent simplified P_N approximation to the equations of radiative transfer

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Abstract

The steady-state simplified P_N approximation to the radiative transport equation has been successfully applied to many problems involving radiation. This paper presents the derivation of time-dependent simplified P_N (SP_N) equations (up to $N = 3$) via two different approaches. First, we use an asymptotic analysis, similar to the asymptotic derivation of the steady-state SP_N equations. Second, we use an approach similar to the original derivation of the steady-state SP_N equations and we show that both approaches lead to similar results. Special focus is put on the well-posedness of the equations and the question whether it can be guaranteed that the solution satisfies the correct physical bounds. Several numerical test cases are shown, including an analytical benchmark due to Su and Olson [B. Su, G.L. Olson, An analytical benchmark for non-equilibrium radiative transfer in an isotropically scattering medium, Ann. Nucl. Energy 24 (1997) 1035–1055.].

Keywords: Radiative transfer; Asymptotic analysis; Simplified P_N equations

1. Introduction

The transport of charged and uncharged particles in scattering and absorbing media is challenging from both a theoretical and a computational point of view. The up-to seven-dimensional phase space (space, time, velocity) of the Boltzmann transport equation combined with the necessity of a fine resolution still poses major problems. Time-dependent radiative transfer plays a role in astrophysics (supernova explosions), in the interaction of short-pulsed lasers with plasmas, or in LIDAR (light detection and ranging) technology, to name a few. In the past, many sophisticated discretization schemes and approximate models have been developed. But still in many fields, deterministic particle transport calculations are hardly used.

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In this paper, we consider a new approximation to the time-dependent Boltzmann transport equation. The simplified P_N (SP_N) equations were originally developed for steady-state problems in nuclear engineering [4–6] and have subsequently been generalized and successfully applied in several other fields, including radiative transfer [9,8]. The first formal derivation by Gelbard [4–6] started with the one-dimensional P_N equations, which contain only first-order space derivatives, and used substitutions to obtain a system of elliptic partial differential equations. To obtain equations in three space dimensions, even-order moments are interpreted as scalars, odd-order moments are interpreted as vectors, and one-dimensional derivatives ∂_x are replaced by divergence operators and gradients, respectively. In three space dimensions, compared to the $(N+1)^2$ independent unknowns in the spherical harmonics P_N equations, the number of unknowns in the SP_N equations increases only linearly as N. Because of the derivation via the one-dimensional P_N equations, the SP_N method was at first not widely accepted. But alternative derivations via asymptotic expansion [7] and via a variational approach [2,14] have substantiated the validity of the SP_N hierarchy.

The SP_N equations are accurate if the medium is optically thick, the scattering rate is comparable to the collision rate, and scattering is not highly forward-peaked [7]. In addition, numerical experiments (cf. [9] and references therein) have shown that the SP_N equations give good results even when the regime is not so diffusive, and even in the presence of a discontinuity in the opacities. This means that in the diffusive regime a higher accuracy is obtained and at the same time the range of applicability is increased.

Until now, the SP_N method was almost exclusively applied to steady-state transport equations, i.e. no time-dependence was assumed. Only then can the P_N equations be substituted into each other to give a second-order system. To our knowledge, there is only one attempt in the literature [12] to apply the SP_N method to a time-dependent problem. Here, the authors use a semi-discretization in time (i.e. the time variable is discretized whereas the other variables are treated as being continuous) and apply the SP_N approximation to the then steady system.

In this paper, we systematically derive a SP_N hierarchy for time-dependent problems on the continuous level via a formal asymptotic analysis of the Boltzmann transport equation. We explicitly derive time-dependent SP_N equations up to $N=3$ (Section 2). We put special focus on the question whether the approximation preserves the positivity of the radiative energy. Many approximations lack this property. For instance, the time-dependent P_N equations are not positivity-preserving and have unphysical oscillatory behavior [3]. We demonstrate that the time-dependent SP_N equations, which are simpler than the time-dependent P_N equations, also lose positivity and monotonicity. An analysis of the diffusion matrix of the time-dependent SP_N equations shows that a necessary criterion for positivity is violated. A simplified system of equations is derived which satisfies this criterion. In Section 3, we try to obtain the SP_3 equations by algebraic manipulations of the P_3 equations. In the steady-state case, this leads to the same result as the asymptotic analysis, but in the time-dependent case, the results are different. Boundary and initial conditions are derived in Section 4. The numerical results in Section 5 demonstrate the validity of the SP_N approach for time-dependent problems. Furthermore, the positivity of the energy in the different models is investigated numerically. Finally, the SP_3 equations are tested in an analytical benchmark for non-equilibrium radiative transfer [13].

1.1. The transport equation

We consider a convex, open, bounded domain Z in $\mathbb{R}^3$, and we assume that Z has a smooth boundary with outward normal vector n. The direction of particle motion is given by $\Omega \in S^2$, where S^2 is the unit sphere in three dimensions. Moreover, we let

$$\Gamma = \partial Z \times S^2 \quad \text{and} \quad \Gamma^- = \{(x,\Omega) \in \Gamma : n(x)\cdot\Omega < 0\}.$$

The transport of mono-energetic particles that undergo isotropic scattering in a medium is modeled by the linear Boltzmann equation

$$\frac{1}{v}\partial_t\psi(t,x,\Omega) + \Omega\cdot\nabla_x\psi(t,x,\Omega) + \sigma_t(x)\psi(t,x,\Omega) = \frac{\sigma_s(x)}{4\pi}\int_{S^2}\psi(t,x,\Omega')\mathrm{d}\Omega' + \frac{q(t,x)}{4\pi}, \tag{1.1}$$

where q is an isotropic source term. At the boundary, we prescribe the ingoing radiation

$$\psi(t,x,\Omega)=\psi_b(t,x,\Omega)\quad \text{on } \Gamma^-, \tag{1.2}$$

and as the initial condition, we prescribe

$$\psi(0,x,\Omega)=\psi_0(x,\Omega). \tag{1.3}$$

Here, $\psi(t,x,\Omega)\cos\theta\,\mathrm{d}A\,\mathrm{d}t\,\mathrm{d}\Omega$ is the number of particles at point x and time t that move with velocity v during $\mathrm{d}t$ through an area $\mathrm{d}A$ into a solid angle $\mathrm{d}\Omega$ around Ω, and θ is the angle between Ω and $\mathrm{d}A$. The total cross section $\sigma_t(x)$ is the sum of the absorption cross section $\sigma_a(x)$ and the total scattering cross section $\sigma_s(x)$.

1.2. The steady-state SP_N equations

In one-dimensional slab geometry, the steady-state transfer equation simplifies to

$$\mu\partial_z\psi(z,\mu)+\sigma_t(z)\psi(z,\mu)-\frac{\sigma_s(z)}{2}\int_{-1}^{1}\psi(z,\mu')\mathrm{d}\mu'=\frac{q(z)}{2}. \tag{1.4}$$

Here, ψ depends only on z, which is the spatial coordinate perpendicular to the surfaces of the slab, and on $\mu\in[-1,1]$, which is the cosine of the angle between direction and z-axis. Let P_l denote the lth Legendre polynomial on $[-1,1]$. The P_N approximation assumes a decomposition of the intensity ψ into a finite number of Legendre moments ψ_l, $l=0,\ldots,N$

$$\psi(z,\mu)=\sum_{l=0}^{N}\psi_l(z)\frac{2l+1}{2}P_l(\mu). \tag{1.5}$$

Furthermore, we make the usual assumption that N is odd. If we apply the P_N approximation (1.5) to (1.4) we obtain for $l=0,\ldots,N$

$$\partial_z\left(\frac{l+1}{2l+1}\psi_{l+1}+\frac{l}{2l+1}\psi_{l-1}\right)+\sigma_t\psi_l=\sigma_s\delta_{0,l}\psi_l+\delta_{0,l}q, \tag{1.6}$$

with $\psi_{-1}=\psi_{N+1}=0$.

The SP_N equations can be formally obtained from any 1-D P_N approximation by algebraically solving every second equation for the odd-order moment and inserting the result into the equations above and below to obtain a system of second-order partial differential equations. (These are the second-order form of the 1-D P_N equations.) Then, the one-dimensional diffusion operators are formally replaced by three-dimensional diffusion operators. For example, the second-order form of the P_1 equations reads

$$-\partial_z\frac{1}{3\sigma_t}\partial_z\psi_0=q-\sigma_a\psi_0. \tag{1.7}$$

The three-dimensional version is

$$-\mathrm{div}_x\frac{1}{3\sigma_t}\nabla_x\psi_0=q-\sigma_a\psi_0. \tag{1.8}$$

Eq. (1.8) is the familiar 3-D P_1 approximation. If one follows this procedure starting with the 1-D P_N equations with $N>1$, one does not obtain the 3-D P_N equations; instead, one gets the 3-D SP_N equations.

On the other hand, the derivation of the steady-state SP_N equations via asymptotic analysis starts from the scaled equations [7]

$$\Omega\cdot\nabla_x\psi(x,\Omega)+\frac{1}{\varepsilon}\sigma_t(x)\psi(x,\Omega)=\left(\frac{\sigma_t}{\varepsilon}-\varepsilon\sigma_a\right)\frac{1}{\varepsilon}\int_{S^2}\psi(x,\Omega')\mathrm{d}\Omega'+\varepsilon\frac{q(x)}{4\pi}. \tag{1.9}$$

All quantities are now assumed to be $\mathcal{O}(1)$ except for the scalar parameter ε, which is assumed to be small. The asymptotic analysis of this steady-state equation emerges as a special case of the time-dependent equations considered below.

2. Time-dependent SP_N equations via asymptotic analysis

The steady-state diffusion equation is an elliptic PDE. Time-dependent diffusion theory is governed by a parabolic PDE. To obtain higher-order corrections to diffusion theory, we write the transport equation in a parabolic scaling. As before, space-derivatives are scaled by a small parameter ε. The additional time-derivative is scaled by ε^2. This is called a parabolic scaling, since a differential operator that is first-order in time and second-order in space is invariant under this scaling. The transport equation is therefore written as

$$\varepsilon^2 \frac{1}{v}\partial_t\psi + \varepsilon\Omega\cdot\nabla_x\psi + \sigma_t\psi = \left(\sigma_t - \varepsilon^2\sigma_a\right)\frac{1}{4\pi}\phi + \varepsilon^2\frac{q}{4\pi}, \tag{2.1}$$

where $\psi = \psi(t,x,\Omega)$, $\phi(t,x) = \int_{S^2}\psi(t,x,\Omega)\mathrm{d}\Omega$ and $q = q(t,x)$.

The asymptotic analysis in the following is guided by two main properties that we want the equations to preserve.

Integrating (2.1) over Ω and dividing by ε^2, we obtain the ‘‘balance’’ equation

$$\frac{1}{v}\partial_t\phi + \frac{1}{\varepsilon}\nabla_x\cdot\int_{S^2}\Omega\psi\mathrm{d}\Omega + \sigma_a\phi = q, \tag{2.2}$$

which states a basic physical principle: changes in the scalar flux ϕ are either due to leakage (the spatial derivative term), absorption, or sources. We require that this ‘‘balance’’ equation be contained in the final choice of SP_N equations.

Second, our aim is to obtain a well-posed system of parabolic PDEs that have a positive solution ϕ. These questions are related to the diffusion matrix of the system. The linear systems that we obtain can be written in the general form

$$u_t + A\Delta u = B(u_e - u), \tag{2.3}$$

where the functions u and u_e have values in $\mathbb{R}^n$, and the matrices A and B have dimension $n\times n$. The properties (e.g. boundedness, positivity) of the solutions of the system depend on the eigenvalues of the diffusion matrix A. Such properties are standard in the case $n = 1$. There exists no general result on conditions that ensure boundedness, positivity or maximum principles for systems of parabolic (i.e. first-order time, second-order space derivatives) equations [1]. However, we argue in the following that the non-negativity of all eigenvalues of A is a necessary condition for that. It is well-known that if one eigenvalue of the diffusion matrix is negative, then we have an ill-posed problem, similar to inverse heat conduction. If we have a pair of complex eigenvalues, then we do not have a maximum principle (cf. Appendix A for a counterexample). The solution might have an oscillatory behavior, and we cannot expect the positivity of the solution. Thus we try to derive time-dependent SP_N equations with non-negative diffusion matrices.

We write (2.1) as

$$(1 + \varepsilon\Omega\cdot X + \varepsilon^2 T)\psi = S, \tag{2.4}$$

where

$$X = \frac{1}{\sigma_t}\nabla_x, \quad T = \frac{1}{v\sigma_t}\partial_t, \quad \text{and} \quad S = \left(1 - \varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\frac{\phi}{4\pi} + \varepsilon^2\frac{q}{4\pi\sigma_t}. \tag{2.5}$$

We start by expanding the inverse of the operator in (2.4) in powers of ε

$$\begin{aligned}\psi &= (1 + \varepsilon\Omega\cdot X + \varepsilon^2 T)^{-1}S \\ &= \Big\{1 - (\Omega\cdot X)\varepsilon + \left[-T + (\Omega\cdot X)^2\right]\varepsilon^2 + \left[(\Omega\cdot X)T + (T - (\Omega\cdot X)^2)(\Omega\cdot X)\right]\varepsilon^3 \\ &\quad + \left[(T - (\Omega\cdot X)^2)T + (-2(\Omega\cdot X)T + (\Omega\cdot X)^3)(\Omega\cdot X)\right]\varepsilon^4 + \cdots\Big\}S + \mathcal{O}(\varepsilon^5).\end{aligned} \tag{2.6}$$

In the following we assume that the system is homogeneous, i.e. σ_a and σ_t are constant. This assumption is crucial for the validity of the following analysis. For a discussion of the non-homogeneous case we refer the reader to Section 6. Integrating (2.6) with respect to Ω and using

$$\int_{S^2}(\Omega\cdot X)^n \mathrm{d}\Omega = [1+(-1)^n]\frac{2\pi}{n+1}X^n = [1+(-1)^n]\frac{2\pi}{n+1}(X\cdot X)^{\frac{n}{2}}, \tag{2.7}$$

we obtain

$$\begin{aligned}\phi &= \int_{S_2}\psi\,\mathrm{d}\Omega\\ &= 4\pi\left\{1+\left(\frac{1}{3}X^2-T\right)\varepsilon^2+\left(T^2+\frac{1}{5}X^4-TX^2\right)\varepsilon^4+\left(\frac{1}{7}X^6+2T^2X^2-T^3-TX^4\right)\varepsilon^6\right\}S+\mathcal{O}(\varepsilon^8).\end{aligned} \tag{2.8}$$

Hence,

$$\begin{aligned}4\pi S &= \left\{1+\left(\frac{1}{3}X^2-T\right)\varepsilon^2+\left(T^2+\frac{1}{5}X^4-TX^2\right)\varepsilon^4+\left(\frac{1}{7}X^6+2T^2X^2-T^3-TX^4\right)\varepsilon^6\right\}^{-1}\phi+\mathcal{O}(\varepsilon^8)\\ &= \left\{1+\left(-\frac{1}{3}X^2+T\right)\varepsilon^2+\left(-\frac{4}{45}X^4+\frac{1}{3}TX^2\right)\varepsilon^4+\left(-\frac{44}{945}X^6-\frac{1}{3}T^2X^2+\frac{4}{15}TX^4\right)\varepsilon^6\right\}\phi+\mathcal{O}(\varepsilon^8).\end{aligned} \tag{2.9}$$

Inserting the definition of the source term S from (2.5), we get

$$\begin{aligned}&\left(1-\varepsilon^2\frac{\sigma_a}{\sigma_t}\right)\phi+\varepsilon^2\frac{q}{\sigma_t}\\ &\quad=\left\{1+\left(-\frac{1}{3}X^2+T\right)\varepsilon^2+\left(-\frac{4}{45}X^4+\frac{1}{3}TX^2\right)\varepsilon^4+\left(-\frac{44}{945}X^6-\frac{1}{3}T^2X^2+\frac{4}{15}TX^4\right)\varepsilon^6\right\}\phi+\mathcal{O}(\varepsilon^8).\end{aligned} \tag{2.10}$$

Deleting ϕ on both sides and multiplying by σ_t/ε^2, we obtain

$$-\sigma_a\phi+q=\sigma_tT\phi-\frac{\sigma_t}{3}X^2\left[\phi-\varepsilon^2T\phi+\frac{4}{15}\varepsilon^2X^2\phi+\frac{44}{315}\varepsilon^4X^4\phi+\varepsilon^4T^2\phi-\frac{4}{5}\varepsilon^4TX^2\phi\right]+\mathcal{O}(\varepsilon^6). \tag{2.11}$$

We note that this equation has the form of the balance equation (2.2). Since we want to keep this form, in the subsequent approximations we only manipulate the terms within the brackets.

2.1. SP_1 approximation

For the lowest-order approximation, we neglect terms of order $\mathcal{O}(\varepsilon^2)$. Then (2.11) can be written as

$$-\sigma_a\phi+q=\sigma_tT\phi-\frac{\sigma_t}{3}X^2\phi. \tag{2.12}$$

This gives the classical diffusion (SP_1) equation

$$\frac{1}{v}\partial_t\phi=\frac{1}{3\sigma_t}\nabla_x^2\phi-\sigma_a\phi+q. \tag{2.13}$$

Remark 1. The SP_1 equation is a parabolic PDE. It is well-known that, with the boundary conditions derived in Section 4, the radiative energy ϕ is always positive.

2.2. SP_2 approximation

For the SP_2 approximation, we neglect terms of order $\mathcal{O}(\varepsilon^4)$. Using Neumann's series, we write (2.11) as

$$-\sigma_a\phi+q=\sigma_tT\phi-\left(1-\epsilon^2T+\frac{4}{15}\epsilon^2X^2\right)\frac{\sigma_t}{3}X^2\phi+\mathcal{O}(\varepsilon^4) \tag{2.14}$$

$$= \sigma_t T\phi - \left(1 + \epsilon^2 T - \frac{4}{15}\epsilon^2 X^2\right)^{-1} \frac{\sigma_t}{3} X^2 \phi + \mathcal{O}(\epsilon^4). \tag{2.15}$$

If we define

$$\xi = \left(1 + \epsilon^2 T - \frac{4}{15}\epsilon^2 X^2\right)^{-1} \frac{\varepsilon^2}{3} X^2 \phi, \tag{2.16}$$

we obtain a system of equations with first-order time and second-order space derivatives

$$\sigma_t T\phi = -\sigma_a \phi + \frac{\sigma_t}{\varepsilon^2}\xi + q, \tag{2.17a}$$

$$\sigma_t T\xi = \frac{\sigma_t}{3} X^2 \left(\phi + \frac{4}{5}\xi\right) - \frac{\sigma_t}{\varepsilon^2}\xi. \tag{2.17b}$$

This can be written as

$$\frac{1}{v}\partial_t \phi = -\sigma_a \phi + \frac{\sigma_t}{\varepsilon^2}\xi + q, \tag{2.18a}$$

$$\frac{1}{v}\partial_t \xi = \frac{1}{3\sigma_t}\nabla_x^2 \left(\phi + \frac{4}{5}\xi\right) - \frac{\sigma_t}{\varepsilon^2}\xi. \tag{2.18b}$$

Remark 2. The eigenvalues of the diffusion matrix

$$\frac{1}{3\sigma_t}\begin{bmatrix} 0 & 0 \\ 1 & 4/5 \end{bmatrix}$$

are $\frac{4}{15\sigma_t}$ and 0. Thus the necessary condition for boundedness of the solution is satisfied.

Remark 3. In steady-state, these equations reduce to the steady-state SP_2 equations, cf. [9].

2.3. SP_3 approximation

The transformation of the asymptotic expansion into the SP_2 system, i.e. the definition of ξ, is unique up to a multiplicative factor. However, for the expansion up to terms of order $\mathcal{O}(\varepsilon^6)$, it is not clear how the substitutions have to be performed. We will use the guidelines outlined at the beginning of this section. Noting that Eq. (2.11) has the form of the balance equation (2.2), we write (2.11) as

$$q - \sigma_a \phi = \sigma_t T\phi - \frac{\sigma_t}{3} X^2 \left\{ \phi + \left[1 + \frac{11}{21}\varepsilon^2 X^2 - 3\alpha\varepsilon^2 T\right] \frac{4}{15}\varepsilon^2 X^2 \phi - \left[1 - \varepsilon^2 T + \frac{4}{5}(1-\alpha)\varepsilon^2 X^2\right]\varepsilon^2 T\phi \right\} + \mathcal{O}(\varepsilon^6). \tag{2.19}$$

As before, we have isolated terms that contain time-dependent diffusion operators (first-order time and second-order space derivative). Also, we have introduced a parameter $\alpha \in [0, 1]$ to split the mixed term TX^2 into two parts. We chose the parameter between zero and one in order to get diffusion equations with the correct signs.

Using Neumann's series, we write (2.19) as

$$q - \sigma_a \phi = \sigma_t T\phi - \frac{\sigma_t}{3} X^2 \left\{ \phi + \left[1 - \frac{11}{21}\varepsilon^2 X^2 + 3\alpha\varepsilon^2 T\right]^{-1} \frac{4}{15}\varepsilon^2 X^2 \phi - \left[1 + \varepsilon^2 T - \frac{4}{5}(1-\alpha)\varepsilon^2 X^2\right]^{-1}\varepsilon^2 T\phi \right\} + \mathcal{O}(\varepsilon^6). \tag{2.20}$$

Now we define

$$\phi_2 = \frac{1}{2}\left[1 - \frac{11}{21}\varepsilon^2 X^2 + 3\alpha\varepsilon^2 T\right]^{-1} \left(\frac{4}{15}\varepsilon^2 X^2 \phi\right), \tag{2.21a}$$

$$\zeta = \left[1 + \varepsilon^2 T - \frac{4}{5}(1-\alpha)\varepsilon^2 X^2\right]^{-1} (\varepsilon^2 T \phi), \tag{2.21b}$$

to obtain the system

$$\sigma_t T\phi = \frac{\sigma_t}{3} X^2[\phi + 2\phi_2 - \zeta] - \sigma_a \phi + q, \tag{2.22a}$$

$$3\alpha\sigma_t T\phi_2 = \frac{\sigma_t}{3} X^2\left[\frac{2}{5}\phi + \frac{11}{7}\phi_2\right] - \frac{\sigma_t}{\varepsilon^2}\phi_2, \tag{2.22b}$$

$$\sigma_t T\zeta - \sigma_t T\phi = \frac{\sigma_t}{3} X^2\left[\frac{12}{5}(1-\alpha)\zeta\right] - \frac{\sigma_t}{\varepsilon^2}\zeta. \tag{2.22c}$$

Diagonalizing the left hand side of (2.22), we obtain

$$\frac{1}{v}\partial_t \phi = \frac{1}{3\sigma_t}\nabla_x^2[\phi + 2\phi_2 - \zeta] - \sigma_a\phi + q, \tag{2.23a}$$

$$\frac{1}{v}\partial_t \phi_2 = \frac{1}{3\sigma_t}\nabla_x^2\left[\frac{2}{15\alpha}\phi + \frac{11}{21\alpha}\phi_2\right] - \frac{1}{3\alpha}\frac{\sigma_t}{\varepsilon^2}\phi_2, \tag{2.23b}$$

$$\frac{1}{v}\partial_t \zeta = \frac{1}{3\sigma_t}\nabla_x^2\left[\phi + 2\phi_2 + \left(\frac{12}{5}(1-\alpha) - 1\right)\zeta\right] - \sigma_a\phi + q - \frac{\sigma_t}{\varepsilon^2}\zeta. \tag{2.23c}$$

Remark 4. Note that the parameter α does not capture all possible ambiguities in the derivation of an $\mathcal{O}(\varepsilon^6)$ approximate system. For example, one could operate on the left hand side of (2.20) with certain operators and still keep the approximation order.

Remark 5. Without time-dependence, the variable ζ is zero and the above equations reduce to the steady-state SP_3 approximation.

Remark 6. The diffusion matrix of (2.23) reads

$$\frac{1}{3\sigma_t}\begin{bmatrix} 1 & 2 & -1 \\ \frac{2}{15\alpha} & \frac{11}{21\alpha} & 0 \\ 1 & 2 & \frac{12}{5}(1-\alpha) - 1 \end{bmatrix}. \tag{2.24}$$

For approximately $\alpha > 0.9$, one eigenvalue of this matrix has a negative real part. For $0 < \alpha < 0.9$ we have one positive real eigenvalue and two complex eigenvalues with positive real part. Therefore we cannot expect that the solution to the SP_3 equations satisfies the correct physical bounds, i.e., the energy ϕ is not guaranteed to be positive. Also, to obtain a system that is not ill-posed, we must take $0 < \alpha < 0.9$.

2.4. Simplification of the SP_3 system

The positivity of the radiative energy ϕ can be crucial in many applications. But our numerical results in Section 5 show that the SP_3 equations can produce negative (unphysical) solutions ϕ. We argued that this is due to the fact that the diffusion matrix has complex eigenvalues. In this section, we present an approximation of the SP_3 system that has a positive diffusion matrix (i.e. its eigenvalues are real and positive).

In Section 3, we derive the SP_3 equations with $\alpha = 2/3$ from the P_3 moment equations. We show that the variable ϕ_2 can be identified with the second-order Legendre moment of the radiative intensity. The variable ζ, on the other hand, is an auxiliary variable without a straight-forward physical interpretation. Furthermore, $\zeta = 0$ in steady-state. To simplify the SP_3 equations, we therefore make a quasi-steady approximation and neglect ζ. We obtain

$$\frac{1}{v}\partial_t\phi = \frac{1}{3\sigma_t}\nabla_x^2[\phi + 2\phi_2] - \sigma_a\phi + q, \tag{2.25a}$$

$$\frac{1}{v}\partial_t\phi_2 = \frac{1}{3\sigma_t}\nabla_x^2\left[\frac{2}{15\alpha}\phi + \frac{11}{21\alpha}\phi_2\right] - \frac{1}{3\alpha}\frac{\sigma_t}{\varepsilon^2}\phi_2. \tag{2.25b}$$

We call these the SSP_3 (simplified-simplified P_3) equations.

Remark 7. From Eq. (2.23), we see that ζ is of order $\mathcal{O}(\varepsilon^2)$. Hence, Eqs. (2.25) are asymptotically correct up to $\mathcal{O}(\varepsilon^2)$. This means that the SSP_3 equations are of the same order as SP_1 asymptotically.

Remark 8. The diffusion matrix of (2.25) reads

$$\frac{1}{3\sigma_t}\begin{bmatrix} 1 & 2 \\ \frac{2}{15\alpha} & \frac{11}{21\alpha} \end{bmatrix}. \tag{2.26}$$

For $0 < \alpha < 1$, its eigenvalues are real and positive.

3. SP_3 via P_3

The one-dimensional time-dependent P_3 equations are written in scaled form as

$$\varepsilon^2\frac{1}{v}\partial_t\psi_0 + \varepsilon\partial_z\psi_1 = \sigma_t(4\pi S - \psi_0), \tag{3.1a}$$

$$\varepsilon^2\frac{1}{v}\partial_t\psi_1 + \varepsilon\partial_z\left(\frac{1}{3}\psi_0 + \frac{2}{3}\psi_2\right) = -\sigma_t\psi_1, \tag{3.1b}$$

$$\varepsilon^2\frac{1}{v}\partial_t\psi_2 + \varepsilon\partial_z\left(\frac{2}{5}\psi_1 + \frac{3}{5}\psi_3\right) = -\sigma_t\psi_2, \tag{3.1c}$$

$$\varepsilon^2\frac{1}{v}\partial_t\psi_3 + \varepsilon\partial_z\frac{3}{7}\psi_2 = -\sigma_t\psi_3. \tag{3.1d}$$

Next we derive equations for ψ_0 and ψ_2 within an error of $\mathcal{O}(\varepsilon^8)$. From Eqs. (3.1b) and (3.1d), we get that $\psi_1, \psi_3 \sim \mathcal{O}(\varepsilon)$. Eq. (3.1c) then implies that $\psi_2 \sim \mathcal{O}(\varepsilon^2)$

$$\begin{aligned}\psi_1 &= -\left(1 + \frac{\varepsilon^2}{v\sigma_t}\partial_t\right)^{-1}\frac{\varepsilon}{3\sigma_t}\partial_z(\psi_0 + 2\psi_2),\\ &= -\left(1 - \frac{\varepsilon^2}{v\sigma_t}\partial_t + \frac{\varepsilon^4}{v^2\sigma_t^2}\partial_t^2\right)\frac{\varepsilon}{3\sigma_t}\partial_z(\psi_0 + 2\psi_2) + \mathcal{O}(\varepsilon^7)\end{aligned} \tag{3.2}$$

and

$$\begin{aligned}\psi_3 &= -\left(1 + \frac{\varepsilon^2}{v\sigma_t}\partial_t\right)^{-1}\frac{3\varepsilon}{7\sigma_t}\partial_z\psi_2,\\ &= -\left(1 - \frac{\varepsilon^2}{v\sigma_t}\partial_t\right)\frac{3\varepsilon}{7\sigma_t}\partial_z\psi_2 + \mathcal{O}(\varepsilon^7).\end{aligned} \tag{3.3}$$

Substituting (3.2) and (3.3) into (3.1c), we obtain

$$\frac{\varepsilon^2}{v}\partial_t\psi_2 - \frac{2\varepsilon^2}{15\sigma_t}\partial_z^2\psi_0 - \frac{11\varepsilon^2}{21\sigma_t}\partial_z^2\psi_2 + \frac{\varepsilon^2}{v}\partial_t\left(\frac{2\varepsilon^2}{15\sigma_t^2}\partial_z^2\psi_0 + \frac{11\varepsilon^2}{21\sigma_t^2}\partial_z^2\psi_2 - \frac{2\varepsilon^4}{15v\sigma_t^3}\partial_t\partial_z^2\psi_0\right) = -\sigma_t\psi_2 + \mathcal{O}(\varepsilon^8). \tag{3.4}$$

This implies

$$\psi_2 = \frac{2\varepsilon^2}{15\sigma_t^2}\partial_z^2\psi_0 + \mathcal{O}(\varepsilon^4). \tag{3.5}$$

Using (3.5) in the sixth term of the left hand side of (3.4), we obtain

$$\left(1-\frac{\varepsilon^2}{v\sigma_t}\partial_t\right)\left(\frac{\varepsilon^2}{v\sigma_t}\partial_t\psi_2-\frac{2\varepsilon^2}{15\sigma_t^2}\partial_z^2\psi_0-\frac{11\varepsilon^2}{21\sigma_t^2}\partial_z^2\psi_2\right)=-\psi_2+\mathcal{O}(\varepsilon^8). \tag{3.6}$$

This gives

$$\begin{aligned}\frac{\varepsilon^2}{v\sigma_t}\partial_t\psi_2-\frac{2\varepsilon^2}{15\sigma_t^2}\partial_z^2\psi_0-\frac{11\varepsilon^2}{21\sigma_t^2}\partial_z^2\psi_2&=-\left(1-\frac{\varepsilon^2}{v\sigma_t}\partial_t\right)^{-1}\psi_2+\mathcal{O}(\varepsilon^8),\\&=-\left(1+\frac{\varepsilon^2}{v\sigma_t}\partial_t+\frac{\varepsilon^4}{v^2\sigma_t^2}\partial_t^2\right)\psi_2+\mathcal{O}(\varepsilon^8).\end{aligned} \tag{3.7}$$

We arrive at

$$2\frac{\varepsilon^2}{v\sigma_t}\partial_t\psi_2-\frac{2\varepsilon^2}{15\sigma_t^2}\partial_z^2\psi_0-\frac{11\varepsilon^2}{21\sigma_t^2}\partial_z^2\psi_2=-\psi_2-\frac{\varepsilon^4}{v^2\sigma_t^2}\partial_t^2\psi_2+\mathcal{O}(\varepsilon^8). \tag{3.8}$$

Next, substituting (3.2) into (3.1a), we get:

$$\varepsilon^2\frac{1}{v}\partial_t\psi_0-\frac{\varepsilon^2}{3\sigma_t}\partial_z^2\left(1-\frac{\varepsilon^2}{v\sigma_t}\partial_t+\frac{\varepsilon^4}{v^2\sigma_t^2}\partial_t^2\right)(\psi_0+2\psi_2)=\sigma_t(4\pi S-\psi_0)+\mathcal{O}(\varepsilon^8). \tag{3.9}$$

The second term of the left hand side of (3.9) can be transformed in the following way:

$$\begin{aligned}&\frac{\varepsilon^2}{3\sigma_t}\partial_z^2\left(\psi_0+2\psi_2-\frac{\varepsilon^2}{v\sigma_t}\partial_t\psi_0-2\frac{\varepsilon^2}{v\sigma_t}\partial_t\psi_2+\frac{\varepsilon^4}{v^2\sigma_t^2}\partial_t^2\psi_0\right)+\mathcal{O}(\varepsilon^8)\\&\quad=\frac{\varepsilon^2}{3\sigma_t}\partial_z^2\left(\psi_0+2\psi_2-\frac{\varepsilon^2}{v\sigma_t}\partial_t\psi_0-\frac{4\varepsilon^2}{15v\sigma_t^3}\partial_t\partial_z^2\psi_0+\frac{\varepsilon^4}{v^2\sigma_t^2}\partial_t^2\psi_0\right)+\mathcal{O}(\varepsilon^8)\\&\quad=\frac{\varepsilon^2}{3\sigma_t}\partial_z^2\left(\psi_0+2\psi_2-\left[1-\frac{4\varepsilon^2}{15\sigma_t^2}\partial_z^2+\frac{\varepsilon^2}{v\sigma_t}\partial_t\right]^{-1}\frac{\varepsilon^2}{v\sigma_t}\partial_t\psi_0\right)+\mathcal{O}(\varepsilon^8)\\&\quad=\frac{\varepsilon^2}{3\sigma_t}\partial_z^2(\psi_0+2\psi_2-\hat{\zeta})+\mathcal{O}(\varepsilon^8).\end{aligned} \tag{3.10}$$

The unknown $\hat{\zeta}$ is defined by Eq. (2.16) with ψ_0 replacing ϕ. Here we used (3.5) again. As a result, the 1-D P_3 equations can be written, with an error of $\mathcal{O}(\varepsilon^8)$, as follows:

$$\varepsilon^2\frac{1}{v}\partial_t\psi_0-\frac{\varepsilon^2}{3\sigma_t}\partial_z^2(\psi_0+2\psi_2-\hat{\zeta})=\sigma_t(4\pi S-\psi_0), \tag{3.11a}$$

$$\varepsilon^2\frac{1}{v}\partial_t\psi_2-\frac{\varepsilon^2}{15\sigma_t}\partial_z^2\psi_0-\frac{11\varepsilon^2}{42\sigma_t}\partial_z^2\psi_2=-\frac{\sigma_t}{2}\psi_2-\frac{\varepsilon^4}{2v^2\sigma_t}\partial_t^2\psi_2, \tag{3.11b}$$

$$\varepsilon^2\frac{1}{v}\partial_t(\hat{\zeta}-\psi_0)-\frac{4\varepsilon^2}{15\sigma_t}\partial_z^2\hat{\zeta}=-\sigma_t\hat{\zeta}. \tag{3.11c}$$

The three-dimensional SP_3 equations are obtained by replacing ∂_z^2 with ∇_x^2,

$$\frac{1}{v}\partial_t\psi_0=\frac{1}{3\sigma_t}\nabla_x^2(\psi_0+2\psi_2-\hat{\zeta})-\sigma_a\phi+q, \tag{3.12a}$$

$$\frac{1}{v}\partial_t\psi_2=\frac{1}{3\sigma_t}\nabla_x^2\left(\frac{1}{5}\psi_0+\frac{11}{14}\psi_2\right)-\frac{\sigma_t}{2\varepsilon^2}\psi_2-\frac{\varepsilon^2}{2v^2\sigma_t}\partial_t^2\psi_2, \tag{3.12b}$$

$$\frac{1}{v}\partial_t(\hat{\zeta}-\psi_0)=\frac{4}{15\sigma_t}\nabla_x^2\hat{\zeta}-\frac{\sigma_t}{\varepsilon^2}\hat{\zeta}. \tag{3.12c}$$

Remark 9. Comparing the result (3.12) with the SP_3 equations (2.22) derived by asymptotic analysis, if we set $\alpha=2/3$, we obtain almost the same equations. The only difference is the term $\frac{\varepsilon^2}{2v^2\sigma_t}\partial_t^2\psi_2$ in (3.12b).

4. Boundary conditions and initial values

In this section, we derive boundary conditions for the SP_3 (2.23) and SSP_3 equations. The results for SP_1 and SP_2 can be derived accordingly and are just stated.

4.1. Boundary conditions for SP_3

We use Marshak's method [10], i.e. we ignore the tangential derivative near the boundary and equate ingoing half fluxes

$$\int_{n\cdot\Omega<0}(n\cdot\Omega)\psi\,\mathrm{d}\Omega=\int_{n\cdot\Omega<0}(n\cdot\Omega)\psi_b\,\mathrm{d}\Omega, \tag{4.1}$$

$$\int_{n\cdot\Omega<0}P_3(n\cdot\Omega)\psi\,\mathrm{d}\Omega=\int_{n\cdot\Omega<0}P_3(n\cdot\Omega)\psi_b\,\mathrm{d}\Omega. \tag{4.2}$$

We assume that ψ_b is independent of time. Using (2.6), the left sides of (4.1) and (4.2) can be written as

$$\int_{n\cdot\Omega<0}(n\cdot\Omega)\psi\,\mathrm{d}\Omega=\left\{-1-\frac{2}{3}\varepsilon(n\cdot X)+\varepsilon^2\left[-\frac{1}{2}(n\cdot X)^2+T\right]+\varepsilon^3\left[\frac{4}{3}(n\cdot X)T-\frac{2}{5}(n\cdot X)^3\right]\right\}\pi S+\mathcal{O}(\varepsilon^4), \tag{4.3}$$

$$\int_{n\cdot\Omega<0}P_3(n\cdot\Omega)\psi\,\mathrm{d}\Omega=\left\{\frac{1}{4}+\varepsilon^2\left[-\frac{1}{12}(n\cdot X)^2-\frac{1}{4}T\right]-\frac{4}{35}\varepsilon^3(n\cdot X)^3\right\}\pi S+\mathcal{O}(\varepsilon^4). \tag{4.4}$$

From (2.9), it can be seen that

$$\pi S=\frac{1}{4}\left(\phi+\varepsilon^2T\phi-\frac{1}{3}\varepsilon^2X^2\phi\right)+\mathcal{O}(\varepsilon^4), \tag{4.5}$$

and from (2.21) we get

$$\phi_2=\frac{2}{15}\varepsilon^2X^2\phi+\mathcal{O}(\varepsilon^4), \tag{4.6a}$$

$$\zeta=\varepsilon^2T\phi+\mathcal{O}(\varepsilon^4). \tag{4.6b}$$

Additionally, we assume that ϕ does not vary on the boundary, i.e. we set $\zeta=0$. Substituting (4.5) into (4.3) and (4.4), and using (4.6a) and (4.6b), then (4.1) and (4.2), up to $\mathcal{O}(\varepsilon^4)$, become

$$\phi+\frac{5}{4}\phi_2+\frac{2}{3}\varepsilon(n\cdot X)(\phi+2\phi_2-\zeta)=l_1, \tag{4.7}$$

$$\phi-5\phi_2-\frac{24}{7}\varepsilon(n\cdot X)\phi_2=l_2, \tag{4.8}$$

where

$$l_1=-4\int_{n\cdot\Omega<0}(n\cdot\Omega)\psi_b\,\mathrm{d}\Omega,\quad l_2=16\int_{n\cdot\Omega<0}P_3(n\cdot\Omega)\psi_b\,\mathrm{d}\Omega.$$

We obtain the boundary conditions

$$\varepsilon(n\cdot X)\phi=-\frac{25}{12}\phi+\frac{25}{24}\phi_2+\frac{3}{2}l_1+\frac{7}{12}l_2 \tag{4.9a}$$

$$\varepsilon(n\cdot X)\phi_2=\frac{7}{24}\phi-\frac{35}{24}\phi_2-\frac{7}{24}l_2 \tag{4.9b}$$

$$\zeta=0. \tag{4.9c}$$

Remark 10. We have derived these using Marshak's method [10]. There exist alternative ideas to come up with consistent boundary conditions, e.g. Mark's method or a boundary layer analysis, which may give better boundary values.

4.2. Boundary conditions for SP_1 and SP_2

Analogously, boundary conditions for SP_1 and SP_2 can be derived. For the SP_1 equations, we have

$$n \cdot \nabla_x \phi = \frac{\sigma_t}{\varepsilon}\left(\frac{3}{2} l_1 - \frac{3}{2}\phi\right), \tag{4.10}$$

and the SP_2 boundary conditions read

$$n \cdot \nabla_x (\phi + \frac{4}{5}\xi) = \frac{\sigma_t}{\varepsilon}\left(\frac{3}{2}(l_1 - \phi - \frac{\varepsilon^2}{\sigma_t} q + \varepsilon^2 \frac{\sigma_a}{\sigma_t}\phi) - \frac{9}{4}\xi\right). \tag{4.11}$$

Remark 11. Without time-dependence, all the above boundary conditions reduce to previously-proposed boundary conditions for the steady-state SP_N equations [14,2,9].

4.3. Initial values

Given an initial particle distribution, it is straight-forward to calculate an initial value for ϕ. From the asymptotic analysis, the physical meaning of the auxiliary variables (ξ, ϕ_2, ζ) is not obvious. Therefore it is not clear what the appropriate initial conditions for these variables are. In many cases, the initial setting is a steady state. In addition, the time-dependent SP_N equations reduce to the steady-state SP_N equations. Thus, for the SP_2 equations, we propose to compute ϕ from the initial distribution and then solve the steady-state version of (2.16), which is an elliptic equation, for ξ. For the SP_3 equations, we would have to solve (2.21) for ϕ_2 and ζ. Of course, this gives $\zeta = 0$. Alternativley, ϕ_2 could be identified as the second-order Legendre moment and thus be computed from the initial value for ψ.

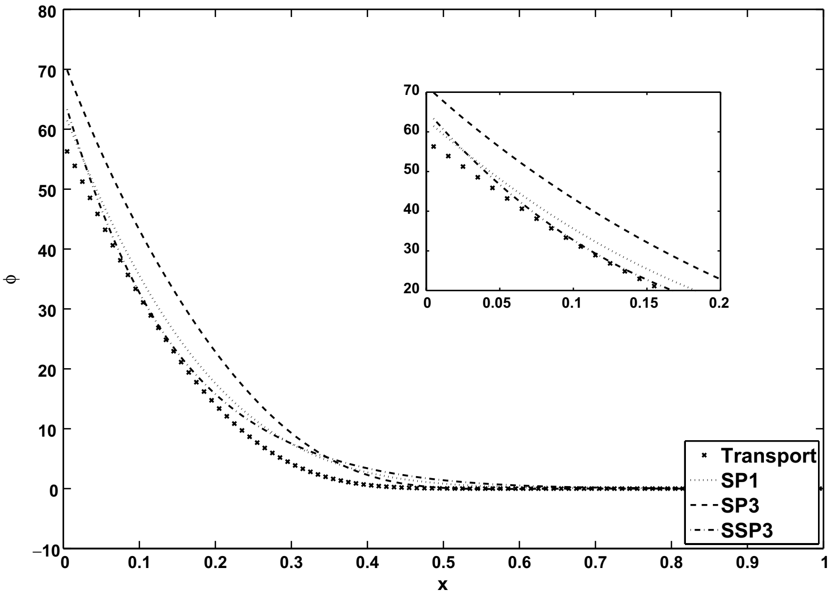
5. Numerical results

In this section, we compare the solutions to the time-dependent SP_N equations to the solution of the Boltzmann transport equation in several test cases. To solve the SP_N equations we use a standard finite difference discretization. The transport solution is computed by a high order (120 directions) discrete-ordinates method.

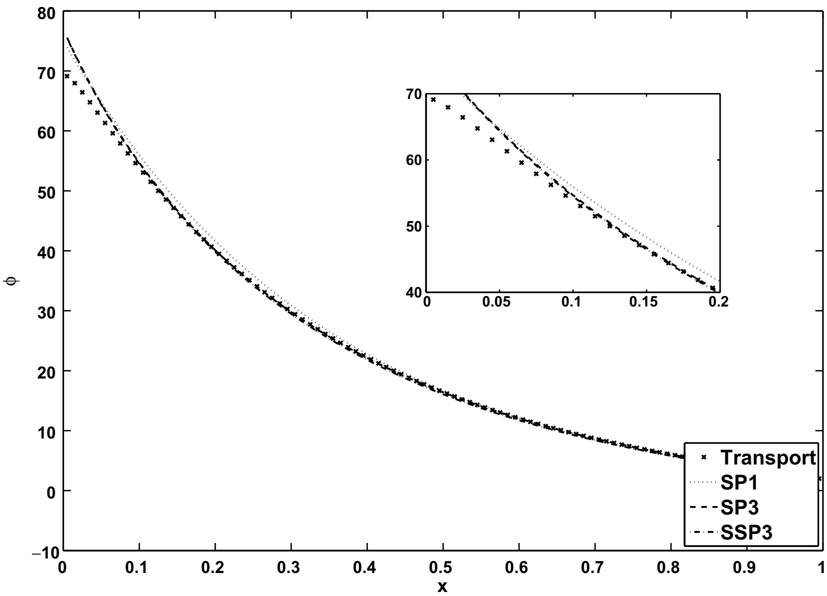
5.1. Marshak wave

Our first example is shown in Fig. 1. We consider a Marshak wave problem on the interval $[0, 1]$. There is no source inside the medium, $q = 0$. On the right side, there is no ingoing radiation, i.e. $\psi_b = 0$. On the left side, we prescribe an isotropic ingoing radiation, $\psi_b = 100$. As initial values we prescribe zero for all variables. Thus the radiation will propagate through the medium from left to right. We prescribe scattering and absorption coefficients that are consistent with the asymptotic scaling. To that end we choose $\sigma_s = 5.0$ larger than $\sigma_a = 0.5$. The particle mean free path is roughly $1/\sigma_t = 0.2$. Therefore initially a boundary layer for $x < 0.2$ can be seen. To compare the models more precisely, we computed the total particle number and the average depth $\int_0^1 z\phi(t,z)\mathrm{d}z \Big/ \int_0^1 \phi(t,z)\mathrm{d}z$. The results are shown in Table 1. As time increases and thus the system approaches a steady-state, time and space derivatives become small. This is the regime where ε is small and we therefore expect the SP_N solutions to be close to the transport solution. This can in fact be observed. We can also see that the higher-order approximations are more accurate than SP_1. Based on the average depths, one could say that in terms of diffusivity, SSP_3 is most diffusive, followed by SP_1 and SP_3.

The following test case is designed to show the non-positivity of the higher-order approximations. Instead of being isotropic, the incident radiation of the left side $(x_1 = 0)$ is chosen to be a mono-directional normally incident beam $\psi_b(\mu) = 100\delta(1 - \mu)$. Numerically, the δ-function is approximated by a Gaussian with small width. We choose $\sigma_a = 0.5$ and $\sigma_s = 0$. Thus the medium does not satisfy the assumptions necessary for the asymptotic analysis to be valid. This means that in this case ε is not small, and we cannot expect the SP_N equations to be good approximations to the transport equation. But the results in Fig. 2 show that the odd-order



(a) $t = 0.1$.



(b) $t = 1.0$.

Fig. 1. Marshak wave problem. Medium with $\sigma_s = 5.0$, $\sigma_a = 0.5$, no source $q = 0$. Boundary values $\psi_b = 100$ on the left side, $\psi_b = 0$ on the right side. Initial values zero. Comparison between SP_1, SP_3 ($\alpha = 2/3$), SSP_3 and exact transport solution.

SP_N approximations still give reasonable results. As is well known [9], the SP_2 approximation can give less accurate results than the lower order SP_1 approximation. The biggest differences between the models can be seen for small times. The boundary layer on the left side of the system cannot be captured accurately by any method. The average depths are 0.055 for the transport solution, 0.147 for SP_3, 0.150 for SP_1, and 0.161 for SSP_3. However, in this case the SP_3 solution has an unphysical negative energy and furthermore it contains roughly three times the number of particles as the transport solution, whereas SP_1 and SSP_3 contain less than twice the number. This might be due to the boundary conditions we used, since this test case is

Table 1
Particle number and average depth for Marshak wave problem (panel A, $t = 0.1$; panel B, $t = 1.0$)

Model	Transport	SP_1	SP_3	SSP_3
Panel A				
No. of particles (%)	100	120	143	117
Average depth	0.107	0.127	0.123	0.134
Panel B				
No. of particles (%)	100	103	101	100
Average depth	0.279	0.275	0.276	0.274

Medium with $\sigma_s = 5.0$, $\sigma_a = 0.5$, no source $q = 0$. Boundary values $\psi_b = 100$ on the left side, $\psi_b = 0$ on the right side. Initial values zero. Comparison between SP_1, SP_3 ($\alpha = 2/3$), SSP_3 and exact transport solution.

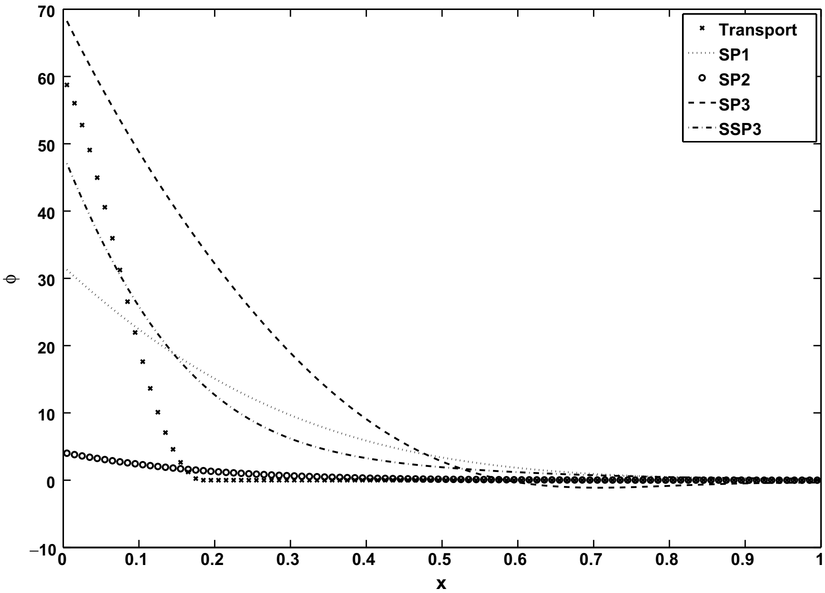


Fig. 2. Marshak wave problem. Medium with $\sigma_s = 0.0$, $\sigma_a = 0.5$, no source $q = 0$. Mono-directional normally incident beam $\psi_b(\mu) = 100\delta(1-\mu)$ on the left side, $\psi_b = 0$ on the right side. Initial values zero. Comparison between SP_N for $N = 1, 2, 3$ ($\alpha = 2/3$), SSP_3 and exact transport solution at $t = 0.1$.

dominated by the inflow through the boundary. It remains to investigate whether other sets of boundary conditions give better results.

We use the same physical setting in Fig. 3. Here, we vary the parameter α in the SP_3 approximation. Again, the purpose of this example is to investigate the positivity property. We choose $\alpha = 0.1, 0.4, 0.7, 0.8$ (we can neither choose $\alpha = 0$ nor $\alpha = 1$, and for α roughly greater than 0.9, the system becomes ill-posed). For $0 < \alpha \leqslant 0.6$ the solution is only weakly dependent on α. The solutions for $\alpha = 0.1$ and $\alpha = 0.4$ in the figure almost coincide. But if we increase α, the solution changes. In this example, for small times, the solution increases, whereas it decreases for large times. If we increase α further ($\alpha > 0.8$), then the solution oscillates and has a negative energy. This behavior foreshadows the ill-posedness for $\alpha > 0.9$. The positive real part of the eigenvalues, which damps oscillations, is already very small. On the other hand, the real parts of the eigenvalues are larger for α small. This means that oscillations are damped more strongly and negative energies are less likely to be observed in numerical results. But the eigenvalue structure is similar to the case of larger α's; thus we expect that negative solutions can also be observed for small α. As a guideline, we can conclude that α should not be chosen too large, i.e. $\alpha < 0.7$. However, it is not clear which value to take. In the other examples, we chose $\alpha = 2/3$, since this is the choice that arises from the P_3 equations.

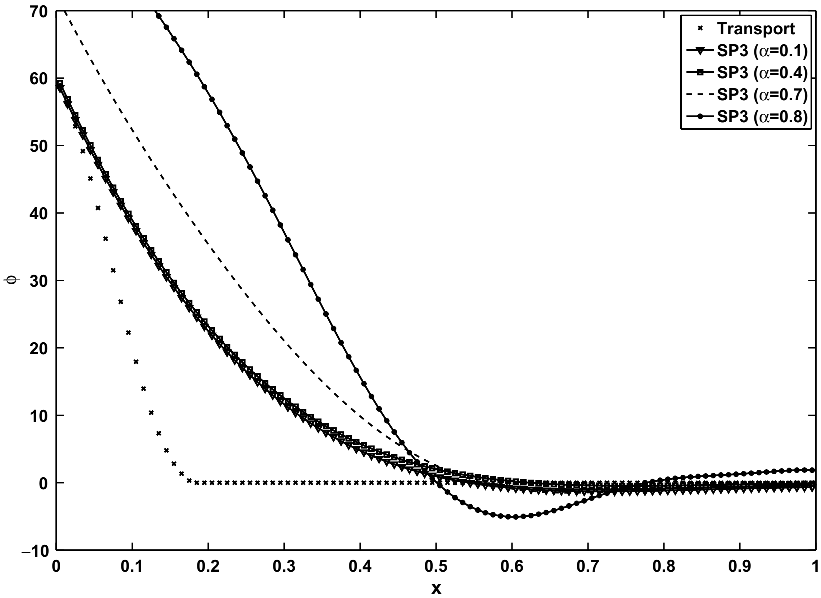


Fig. 3. Marshak wave problem. Medium with $\sigma_s = 0.0$, $\sigma_a = 0.5$, no source $q = 0$. Mono-directional normally incident beam $\psi_b(\mu) = 100\delta(1-\mu)$ on the left side, $\psi_b = 0$ on the right side. Initial values zero. Comparison between exact transport solution and SP_3 for different parameters α at $t = 0.1$.

5.2. Benchmark for non-equilibrium radiative transfer

The methodology in this paper can also be applied to radiative transfer problems. Here we compare the time-dependent SP_N solutions to an analytical benchmark solution generated by Su and Olson for non-equilibrium radiative transfer [13]. The radiative transfer equation is coupled to a material balance equation. In 1-D, the equations are

$$\frac{1}{v}\partial_t I(t,x,\mu) + \mu\partial_x I(t,x,\mu)$$
$$= \sigma_a\left(\frac{a}{2}T^4(t,x) - I(t,x,\mu)\right) + \sigma_s\left(\frac{1}{2}\int_{-1}^{1} I(t,x,\mu')\mathrm{d}\mu' - I(t,x,\mu)\right) + Q(t,x) \tag{5.1a}$$

$$\frac{1}{v}c_v(T(t,x))\partial_t T(t,x) = \sigma_a\left(\int_{-1}^{1} I(t,x,\mu')\mathrm{d}\mu' - aT^4(t,x)\right). \tag{5.1b}$$

Eq. (5.1a) has the form of the transport Eq. (1.1) with a special source $q = \sigma_a aT^4 + 2Q$. Therefore, the SP_N asymptotic method can be applied to (5.1a). In the benchmark, c_v is set to $c_v = 4aT^3$; thus the problem is linear in I and aT^4. The medium is infinite ($x \in \mathbb{R}$) and initially cold ($I = 0$ and $aT^4 = 0$ for $t = 0$). Furthermore, $v = 1$. The source is isotropically distributed in angle, and uniformly distributed in a finite space, but only switched-on for a finite amount of time

$$Q = \begin{cases} \frac{1}{4x_0} & \text{for } 0 \leqslant t \leqslant t_0,\ -x_0 \leqslant x \leqslant x_0, \\ 0 & \text{otherwise.} \end{cases} \tag{5.2}$$

Here, $x_0 = 0.5$ and $t_0 = 10$. A medium with $\sigma_a = 0.5$ and $\sigma_s = 0$ is considered. The comparison to the benchmark solution is shown in Fig. 4. Compared to the benchmark, the SP_N error is less than half that of diffusion. Smaller values of the parameter α do not significantly change the result. For comparison, we have also computed the solution to the time-dependent P_3 equations. The P_1, P_3 and P_7 solutions have been compared in [11]. The P_3 solution is more accurate than the SP_3 solution, especially for short times. This can be expected since we made some additional simplifications. The SSP_3 solution (not shown here) is slightly less accurate (error 10% larger) than the SP_3 solution. In the case $\sigma_a = 0.25$, $\sigma_s = 0.25$, similar assertions can be made.

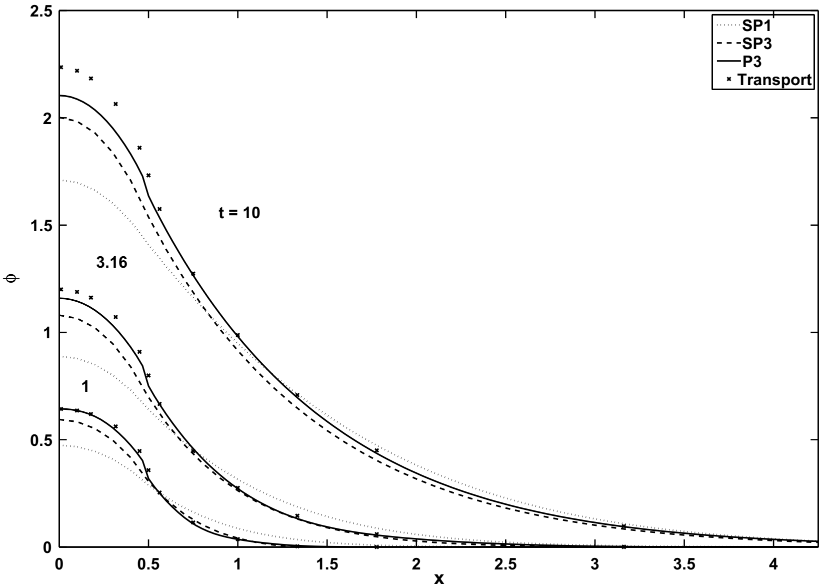


Fig. 4. Comparison between SP_3 ($\alpha = 2/3$), P_3, diffusion, and benchmark transport solution for times $t = 1, 3.16, 10$.

6. Conclusions and future work

We have derived the Simplified P_N equations for time-dependent transport problems by an asymptotic analysis. The equations have first-order time and second-order space derivatives. If we start with the one-dimensional P_N equations, it is not possible to derive equations of this form using the classical formal procedure of Gelbard.

Concerning the validity of the time-dependent SP_N equations, assertions similar to the steady case can be made. Physically, the parabolic scaling and ε small mean that we require the Knudsen number (the inverse of the factor multiplying the scattering operator, ratio of mean free path and characteristic length scale) and the kinetic Strouhal number (multiplying the time derivative, characteristic length divided by the product of characteristic time and velocity) to be small of order ε. We also note that the Neumann series is applied to the unbounded directional derivative operator $\Omega \cdot \nabla_x$, and therefore this series must be understood as an asymptotic approximation to the original transfer equation.

The numerical results show that the SP_N approximations improve diffusion theory in the sense that not too far away from the diffusive limit a better approximation is obtained. In the case of the benchmark of Su and Olson, the difference between the SP_3 solution and the transport solution is less than half the difference between diffusion and transport. Especially for short times and near sources, the higher order SP_N solutions are more accurate. However, as shown in the second Marshak wave example, this range of applicability does not extend to very forward-peaked beams and thin media. As in the steady case, one should take only odd values for N. Computation times roughly scale with the number of equations. The SSP_3 system consists of only two equations but is more accurate than SP_1. The P_3 model consists of four equations.

The time-dependent SP_1 equations satisfy a maximum principle. The radiative energy or particle number is always positive. We have found that the time-dependent SP_3 equations do not guarantee a positive energy. A positive diffusion matrix is a necessary condition for a positive energy. This condition is satisfied by the SSP_3 equations, and in simulations these always showed a positive energy. If in a particular application, the positivity of the energy is crucial, we would use the SSP_3 equations and otherwise the SP_3 equations. In the derivation of the SP_3 equations, several terms can be defined in different ways. We have studied these ambiguities by introducing a parameter α. Numerical results show that α should not be chosen too large, since then oscillations occur. In our examples, we fixed $\alpha = 2/3$ since this is the choice which can be derived from the P_3 equations, and in simulations it usually gives good results. From the simulations, it also appears that the smaller α

is chosen the less likely ϕ becomes negative. We note that in the limit $\alpha = 0$, the time derivative in (2.22b) vanishes. The SP_3 equations become a set of partial differential-algebraic equations. The properties of these equations should be investigated further.

Further work includes simulations in two and three space dimensions. Also, the use of the SP_N approximations as pre-conditioners for transport calculations will be investigated. We expect that the time-dependent SP_N equations can be generalized to anisotropic scattering in a similar manner as in the steady-state case [7]. In the derivation of the equations, we assumed a homogeneous medium. In steady-state, a variational analysis yielded the SP_N equations for non-homogeneous media as well as interface and boundary conditions [2,14]. The only difference for space-dependent coefficients is that the spatial derivatives have to be modified like

$$\frac{1}{\sigma_t}\nabla_x^2 \to \nabla_x \frac{1}{\sigma_t(x)}\nabla_x.$$

For steady-state problems, this modification of the spatial derivatives is asymptotically correct in planar geometry and we expect that it is asymptotically correct for time-dependent planar geometry problems. The interface conditions for media with non-continuous scattering coefficients (especially those containing void-like regions) should also be of a similar form. But this will have to be analyzed in more detail. Finally, there may be other ways to obtain different and better boundary conditions.

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Appendix A. Solutions with positive energy

There exist no general maximum principles for systems of equations of parabolic type [1]. Therefore we cannot expect the solutions to the SP_N equations for $N > 1$ to be positive. However, the following simple example indicates that the positivity property of the diffusion matrix is necessary for the positivity of the solution.

Example 12. Consider the Schrödinger-like Cauchy problem

$$\begin{bmatrix} u \\ v \end{bmatrix}_t = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}_{xx} \quad \text{on } \mathbb{R} \tag{A.1}$$

with initial value $[u_0, v_0]^{\mathrm{T}}$. The diffusion matrix, i.e. the matrix in front of the Laplacian, has the eigenvalues $\pm i$. The solution can be written explicitly as a convolution

$$u(t,x) = \frac{1}{\sqrt{2\pi t}} \int_{\mathbb{R}} \left[v_0(y) \cos\left(\frac{(x-y)^2}{4t}\right) + u_0(y) \sin\left(\frac{(x-y)^2}{4t}\right) \right] \mathrm{d}y \tag{A.2}$$

$$v(t,x) = \frac{1}{\sqrt{2\pi t}} \int_{\mathbb{R}} \left[v_0(y) \sin\left(\frac{(x-y)^2}{4t}\right) - u_0(y) \cos\left(\frac{(x-y)^2}{4t}\right) \right] \mathrm{d}y \tag{A.3}$$

The kernels with which the initial data is convoluted are not positive. Therefore it is easy to construct negative solutions to the Cauchy problem.

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