Two-Streams Revisited: General Equations, Exact Coefficients, and Optimized Closures

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Key Points:

- A general form of the Two-Stream Equations better lends itself to physical interpretation than the standard form.
- Numerically-optimized coupling coefficients reproduce reflectance and transmittance accurate to within 10^{-4}.
- These optimized coefficients explain the accuracy regimes of existing two-stream closures.

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Abstract

Two-Stream Equations are the most parsimonious general models for radiative flux transfer with one equation to model each of upward and downward fluxes; these are coupled due to the transfer of fluxes between hemispheres. Standard two-stream approximation of the Radiative Transfer Equation assumes that the ratios of flux transferred (coupling coefficients) are both invariant with optical depth and symmetric with respect to upwelling and downwelling radiation. Two-stream closures are derived by making additional assumptions about the angular distribution of the intensity field, but none currently works well for all parts of the optical parameter space. We determine the exact values of the two-stream coupling coefficients from multi-stream numerical solutions to the Radiative Transfer Equation. The resulting unique coefficients accurately reconstruct entire flux profiles but depend on optical depth. More importantly, they generally take on unphysical values when symmetry is assumed. We derive a general form of the Two-Stream Equations for which the four coupling coefficients are guaranteed to be physically explicable. While non-constant coupling coefficients are required to reconstruct entire flux profiles, numerically-optimized constant coupling coefficients (which admit analytic solutions) reproduced reflectance and transmittance with relative errors no greater than 4×10^{-5} over a large range of optical parameters. The optimized coefficients show a dependence on the solar zenith angle and total optical depth that diminishes as the latter increases. This explains why existing coupling coefficients, which often omit the former and mostly neglect the latter, tend to work well for only thin or only thick atmospheres.

Plain Language Summary

Two-Stream Equations are the most parsimonious general models for the propagation of fluxes through a medium and are almost universally used to compute reflectance and transmittance – the ratio of radiation reflected or transmitted by a medium – in climate models. Their accuracy depends on how their coefficients are specified, i.e. the closure, and no existing closure works well in all situations. We diagnose what these coefficients ought to be from high resolution radiative transfer models and in the process formulated a general form of the Two-Stream Equations that better lends itself to physical interpretation. Although coefficients that vary with the vertical coordinate are required to reconstruct entire flux profiles, numerically-optimized constant coefficients reproduced reflectance and transmittance to very high accuracy. The optimized coefficients provide important insights into closure parameterizations and explain why existing two-stream closures tend to work well for only thin or only thick atmospheres.

1 A Century of Two-Stream Theory

The flow of electromagnetic radiation of a given frequency through space – the intensity field u – depends in general on position and direction. The flow of radiation through a surface – the irradiance or flux F – can be described with two scalars, one for each side of the surface, at each position. Two-stream equations describing the dependence of flux on position were developed in the early 20th century (Schuster, 1905; Eddington, 1916) to understand the behavior of stars. This formulation, a pair of coupled ordinary differential equations for fluxes emerging from either side of a surface normal to a one-dimensional positional coordinate, predates by decades the substantially more complicated governing equation for intensity developed by Chandrasekhar (1960). Efforts to adapt two-stream methods to the problem of sunlight in planetary atmospheres, where the source of radiation is a collimated beam of starlight rather than internal emission, were surveyed by Meador and Weaver (1980). They found that the choice of coefficients to couple the evolution of fluxes in the two directions can be traced to assumptions about the angular distribution of the intensity (and, by implication, the angular detail of the scattering phase function). They used such assumptions as the starting point for closure derivations. Some assumptions have limited validity: the Eddington (1916) assumption, that intensity is linear in the cosine of the zenith angle in a plane-parallel atmosphere, yields negative coupling coefficients and negative albedo when the medium is strongly forward-scattering and strongly absorbing; this problem is not alleviated by delta-Eddington scaling (Joseph et al., 1976). While many two-stream closures work well in asymptotic regimes, no assumption discovered to date works well for all parts of the parameter space (Meador & Weaver, 1980; King & Harshvardhan, 1986; Harshvardhan & King, 1993; Lu et al., 2009; Barker et al., 2015) despite ongoing efforts to develop new closures (Matagne, 2011; Yin & Song, 2022; Temgoua et al., 2024).

Two-stream methods are of practical importance because they are computationally inexpensive and so remain the solution method underlying calculations in almost every numerical model of the atmosphere (Edwards & Slingo, 1996; Schmidt et al., 2006; Iacono et al., 2008; Hogan & Bozzo, 2018; Pincus et al., 2019). They also provide the foundation for approaches to problems beyond the plane-parallel homogeneous paradigm (Shonk & Hogan, 2008; Jakub & Mayer, 2015; Hogan et al., 2016). The methods are conceptually important because they are parsimonious, matching the complexity of the governing equations with the level of detail required of the solution.

Here we revisit the two-stream equations to develop both deeper conceptual understanding and near-perfect accuracy within the framework of a plane-parallel homogeneous atmosphere. High-resolution radiative transfer calculations across a wide range of optical parameters show that the widely-used form of the two-stream equations contains two key assumptions about the coupling coefficients – constancy and symmetry – which are frequently violated. We derive a more general set of two-stream equations in which the coupling coefficients and resulting solutions are guaranteed to be non-negative and bounded. We demonstrate that, while non-constant coupling coefficients are required to reconstruct entire flux profiles, constant coefficients (for which analytic solutions are provided) are able to reproduce bulk layer reflectance and transmittance. We use numerical optimization to produces sets of coupling coefficients for the symmetric and general two-stream solution forms. Both sets of equations can produce near-perfect calculations of reflectance and transmittance but the symmetric equation form may require coefficients with negative values. The coefficients for the general form, in contrast, vary smoothly and explicably between optically-thin and optically-thick regimes.

2 On the Form of the Two-Stream Equations

2.1 Governing Equations

Consider a plane-parallel, horizontally homogeneous atmosphere with vertical coordinate τ (optical depth) increasing from top to bottom, and directional coordinates ϕ for the azimuthal angle and $\mu = \cos\theta$ for the polar direction, with $\mu > 0$ pointing up following the convention of Meador and Weaver (1980). The medium is illuminated by a direct collimated beam of starlight with intensity I_0 entering the atmosphere at incident angle (μ_0, ϕ_0). Under these conditions the diffuse intensity $u(\tau, \mu, \phi)$ propagating in direction (μ, ϕ) is described by the radiative transfer equation (Chandrasekhar, 1960):

$$\begin{aligned} \mu \frac{\partial u(\tau,\mu,\phi)}{\partial \tau} = u(\tau,\mu,\phi) &- \frac{\omega}{4\pi}\int_{-1}^{1}\int_{0}^{2\pi} p\left(\mu,\phi;\mu',\phi'\right) u\left(\tau,\mu',\phi'\right) \mathrm{d}\phi' \mathrm{d}\mu' \\ &- \frac{I_0\omega}{4\pi} p\left(\mu,\phi;-\mu_0,\phi_0\right) \exp\left(-\mu_0^{-1}\tau\right) \end{aligned} \tag{1}$$

Here, ω is the single-scattering albedo and p the scattering phase function. We neglect sources of radiation internal to the atmosphere and assume no other sources are present (homogeneous Dirichlet boundary conditions). Fluxes can be computed from the solution to (1) by integrating over the upward and downward hemispheres:

$$F^{\pm} = \int_0^1 \int_0^{2\pi} \mu u(\tau, \pm\mu, \phi) d\phi d\mu \tag{2}$$

The form of the analogous two-stream equations differentiates only between up- and downwelling flux (Shettle & Weinman, 1970; Meador & Weaver, 1980):

$$\begin{aligned} \frac{d}{d\tau}F^{+}(\tau) &= \gamma_1 F^{+}(\tau) - \gamma_2 F^{-}(\tau) - I_0\omega\gamma_3 \exp\left(-\mu_0^{-1}\tau\right) \\ \frac{d}{d\tau}F^{-}(\tau) &= \gamma_2 F^{+}(\tau) - \gamma_1 F^{-}(\tau) + I_0\omega\gamma_4 \exp\left(-\mu_0^{-1}\tau\right) \end{aligned} \tag{3}$$

and the corresponding (homogeneous Dirichlet) boundary conditions are $F^{+}(0) = 0 = F^{-}(\tau_0)$. The coupling coefficients γ_1, γ_2 describe respectively the sinks and sources of diffuse fluxes while γ_3, γ_4 describe contributions of the direct beam to the diffuse fluxes. Specific two-stream models differ in their specification of these coefficients (Meador & Weaver, 1980), i.e. their closures.

In principle, the problem described by the two-stream equations (3) is the same as that posed by the radiative transfer equation (1) and its angular integral (2). Applying (2) to both sides of (1) eventually yields

$$\begin{aligned} \frac{1}{2\pi}\frac{d}{d\tau}F^{+}(\tau) &= \int_0^1 \bar{u}(\tau,\mu)\mathrm{d}\mu - \int_{-1}^1 \hat{p}\left(\mu\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu - \frac{I_0\omega}{2\pi}\beta_0 \exp\left(-\mu_0^{-1}\tau\right) \\ \frac{1}{2\pi}\frac{d}{d\tau}F^{-}(\tau) &= -\int_0^1 \bar{u}(\tau,-\mu)\mathrm{d}\mu + \int_{-1}^1 \hat{p}\left(-\mu\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu + \frac{I_0\omega}{2\pi}(1-\beta_0) \exp\left(-\mu_0^{-1}\tau\right) \end{aligned} \tag{4}$$

which are equations (10) and (11) of Meador and Weaver (1980). Our normalization differs slightly such that $\bar{p}$, $2\pi\bar{u}$ and $\pi^{-1}I_0$ equal p I and F in Meador and Weaver (1980) respectively. Here overbars indicate azimuthal averages and hats hemipheric averages. Equations (4) contain the terms

$$\begin{aligned} \beta_0 &= \frac{1}{\omega}\hat{p}(\mu_0) \\ \hat{p}(\mu) &= \frac{1}{2}\int_0^1 \bar{p}\left(-\mu', \mu\right)\mathrm{d}\mu' \end{aligned}$$

where $\hat{p}$ is the *backscattering ratio* function (Stamnes et al., 2017, 7.5.2 *The Backscattering Ratios*), and β_0 is the backscattering ratio specifically for radiation with incident cosine polar angle μ_0 (radiation from the direct beam in particular) and is normalized to exclude absorption.

One way to proceed from (4) is to assume the form of $\bar{u}$ and $\hat{p}$ which leads to equations that, in many circumstances, can be directly matched to (3) (Meador & Weaver, 1980). Here we take a more general approach. The scattering integrals of (4) can be split between upwelling and downwelling hemispheres with the extinction term of each equation (for each flux) combined with the appropriate hemispheric integral to produce

$$\begin{aligned} \frac{1}{2\pi}\frac{d}{d\tau}F^{+}(\tau) &= \int_0^1 \left(1-\hat{p}\left(\mu\right)\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu - \int_0^1 \hat{p}\left(-\mu\right)\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu - \frac{I_0\omega}{2\pi}\beta_0 \exp\left(-\mu_0^{-1}\tau\right) \\ \frac{1}{2\pi}\frac{d}{d\tau}F^{-}(\tau) &= \int_0^1 \hat{p}\left(-\mu\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu - \int_0^1 \left(1-\hat{p}\left(\mu\right)\right)\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu + \frac{I_0\omega}{2\pi}(1-\beta_0) \exp\left(-\mu_0^{-1}\tau\right) \end{aligned}$$

Defining

$$\begin{aligned} D_1^{+}(\tau) &= 2\pi\int_0^1 \left(1-\hat{p}\left(\mu\right)\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu & D_2^{-}(\tau) &= 2\pi\int_0^1 \hat{p}\left(-\mu\right)\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu \\ D_2^{+}(\tau) &= 2\pi\int_0^1 \hat{p}\left(-\mu\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu & D_1^{-}(\tau) &= 2\pi\int_0^1 \left(1-\hat{p}\left(\mu\right)\right)\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu \end{aligned} \tag{5}$$

allows the integrated equations to be written as

$$\begin{aligned}\frac{d}{d\tau}F^{+}(\tau) &= D_1^{+} - D_2^{-} - I_0\omega\beta_0 \exp\left(-\mu_0^{-1}\tau\right)\\ \frac{d}{d\tau}F^{-}(\tau) &= D_2^{+} - D_1^{-} + I_0\omega(1-\beta_0) \exp\left(-\mu_0^{-1}\tau\right)\end{aligned} \tag{6}$$

These equations are hemispherically-integrated radiative transfer equations that are coupled due to the transfer of fluxes between hemispheres and they are *exact* in the sense that $F^{\pm}$ on the left-hand side are identically the $F^{\pm}$ computed from (1) and (2).

As with the γ terms in (3), the $D_1^{\pm}$ terms represent sinks and the $D_2^{\pm}$ terms sources of diffuse radiation. More precisely, the sink term D_1^{+} for the upward flux describes a loss of flux due to extinction offset by (post-absorption) scattering back into the upper hemisphere – this interpretation is inherited from the radiative transfer equation. The source term D_2^{-} for the upward flux describes a gain in flux due to scattering from the lower hemisphere into the upper hemisphere. The sink term D_1^{-} and source term D_2^{+} for the downward flux have analogous interpretations.

Equations (6) suggest a general form of the two-stream equations (Stamnes et al., 2017, 7.5.5 *Generalized Two-Stream Equations*):

$$\begin{aligned}\frac{d}{d\tau}F^{+}(\tau) &= \gamma_1^{+}F^{+}(\tau) - \gamma_2^{-}F^{-}(\tau) - I_0\omega\gamma_3 \exp\left(-\mu_0^{-1}\tau\right)\\ \frac{d}{d\tau}F^{-}(\tau) &= \gamma_2^{+}F^{+}(\tau) - \gamma_1^{-}F^{-}(\tau) + I_0\omega\gamma_4 \exp\left(-\mu_0^{-1}\tau\right)\end{aligned} \tag{7}$$

Comparison of (7) to (6) shows that $\gamma_3 = \beta_0$ and $\gamma_4 = 1 - \beta_0$. The four coupling coefficients are given exactly by

$$\begin{aligned}\gamma_1^{+}(\tau) &= \frac{D_1^{+}(\tau)}{F^{+}(\tau)} \qquad \gamma_2^{-}(\tau) = \frac{D_2^{-}(\tau)}{F^{-}(\tau)}\\ \gamma_2^{+}(\tau) &= \frac{D_2^{+}(\tau)}{F^{+}(\tau)} \qquad \gamma_1^{-}(\tau) = \frac{D_1^{-}(\tau)}{F^{-}(\tau)}\end{aligned} \tag{8}$$

These formulas are only valid on $(0, \tau_0)$ given homogeneous Dirichlet boundary conditions but can be analytically continued to $[0, \tau_0]$. To the extent that the general coupling coefficients can be determined, solutions to the general two-stream equations (7) perfectly reconstruct entire flux profiles.

The general two-stream equations (7) differ from the widely-used symmetric form (3) in two key ways. First, the coupling coefficients generally vary with optical depth, τ, because the angular distribution of the intensity field varies with τ even if the phase function is τ-independent. Second and more fundamentally, the source and sink terms can differ between the two hemispheres because there is no *a priori* constraint on the angular symmetry of the integrals in (5).

2.2 The Condition for Symmetry

The exact values of the four general coupling coefficients (8) can be diagnosed from the azimuthally-averaged intensity field $\bar{u}$. The two coupling coefficients required by the symmetric form can also be diagnosed, even if symmetry does not hold, by equating the right-hand sides of (3) and (6):

$$\begin{aligned}\gamma_1 F^{+} - \gamma_2 F^{-} &= D_1^{+} - D_2^{-}\\ \gamma_2 F^{+} - \gamma_1 F^{-} &= D_2^{+} - D_1^{-}\end{aligned}$$

This pair of equations can be re-expressed as the linear system

$$\begin{bmatrix} F^{+} & -F^{-} \\ -F^{-} & F^{+} \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} D_1^{+} - D_2^{-} \\ D_2^{+} - D_1^{-} \end{bmatrix}$$

with the unique solution

$$\begin{aligned}\gamma_1(\tau) &= \left\{\frac{\left(D_1^+ - D_2^-\right)F^+ + \left(D_2^+ - D_1^-\right)F^-}{\left(F^+ - F^-\right)\left(F^+ + F^-\right)}\right\}(\tau)\\ \gamma_2(\tau) &= \left\{\frac{\left(D_1^+ - D_2^-\right)F^- + \left(D_2^+ - D_1^-\right)F^+}{\left(F^+ - F^-\right)\left(F^+ + F^-\right)}\right\}(\tau)\end{aligned} \tag{9}$$

The exact coupling coefficients for the general and symmetric forms, diagnosed here from high resolution (multi-stream) calculations of $\bar{u}$ with a home-built Python implementation of the discrete ordinates method (`PythonicDISORT`, see Ho (2023)), are shown for an example problem in Figure 1. Solutions to the general and symmetric two-stream equations with their corresponding exact coupling coefficients perfectly reconstruct the flux profile but the behavior of the two sets of coefficients differ markedly.

Exact general coupling coefficients (8) are non-negative and bounded since every term in (8) is positive for all $\tau \in (0, \tau_0)$. Sink coefficient of each hemisphere are equivalent to the source coefficient of the opposite hemisphere when $\omega = 1$ due to conservation of energy, otherwise the former are greater than the latter for all τ.

The exact symmetric coupling coefficients (9), in contrast, appear unphysical in the conditions shown here. There is a singularity at the value of τ for which net flux $F^{\text{net}}(\tau) := F^+(\tau) - F^-(\tau) = 0$ (the linear system that produces (9) is generally inconsistent at that point and has no solution). The negative values and sign changes of these coefficients are incompatible with an interpretation of the terms of the symmetric two-stream equations (3) as sinks or sources. In other words, for some optical parameters the symmetric form of the two-stream equations can produce perfect flux profiles only with unphysical coupling coefficients.

Under what conditions can the symmetric coupling coefficients be expected to be non-negative and bounded? The condition for symmetry, that $\gamma_1^+ \equiv \gamma_1^-$ and $\gamma_2^+ \equiv \gamma_2^-$, can be determined from definitions (5) and (8) to be

$$\begin{aligned}\frac{\int_0^1 \left(1 - \hat{p}\left(\mu\right)\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu}{\int_0^1 \mu\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu} &= \frac{\int_0^1 \left(1 - \hat{p}\left(\mu\right)\right)\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu}{\int_0^1 \mu\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu}\\ \frac{\int_0^1 \hat{p}\left(-\mu\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu}{\int_0^1 \mu\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu} &= \frac{\int_0^1 \hat{p}\left(-\mu\right)\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu}{\int_0^1 \mu\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu}\end{aligned} \tag{10}$$

This can be distilled into the slightly stricter condition

$$\bar{u}(\tau,\mu) = r(\tau)\bar{u}(\tau,-\mu), \quad \mu > 0$$

for some ratio function $r(\tau)$, with $r(\tau) = 1$ whenever the intensity field at τ is continuous at $\mu = 0$. In other words, multiplicative symmetry between the intensity fields in the upper and lower hemispheres is required if the flux transfer in one direction is to be described using the same coupling coefficients that describe the flux transfer in the opposite direction.

Condition (10) is satisfied by the Schuster (1905) assumption that the intensity field is hemispherically isotropic, and the symmetric form of the two-stream equations was originally proposed around this assumption. Symmetry conditions are not discussed in Meador and Weaver (1980), however, and the defining assumption for the Eddington model $\bar{u}(\tau,\mu) = U_0(\tau)+\mu U_1(\tau)$ (Meador & Weaver, 1980, p. 633) does not satisfy (10). This is the reason the Eddington source coefficient γ_2 can take on unphysical (negative) values.

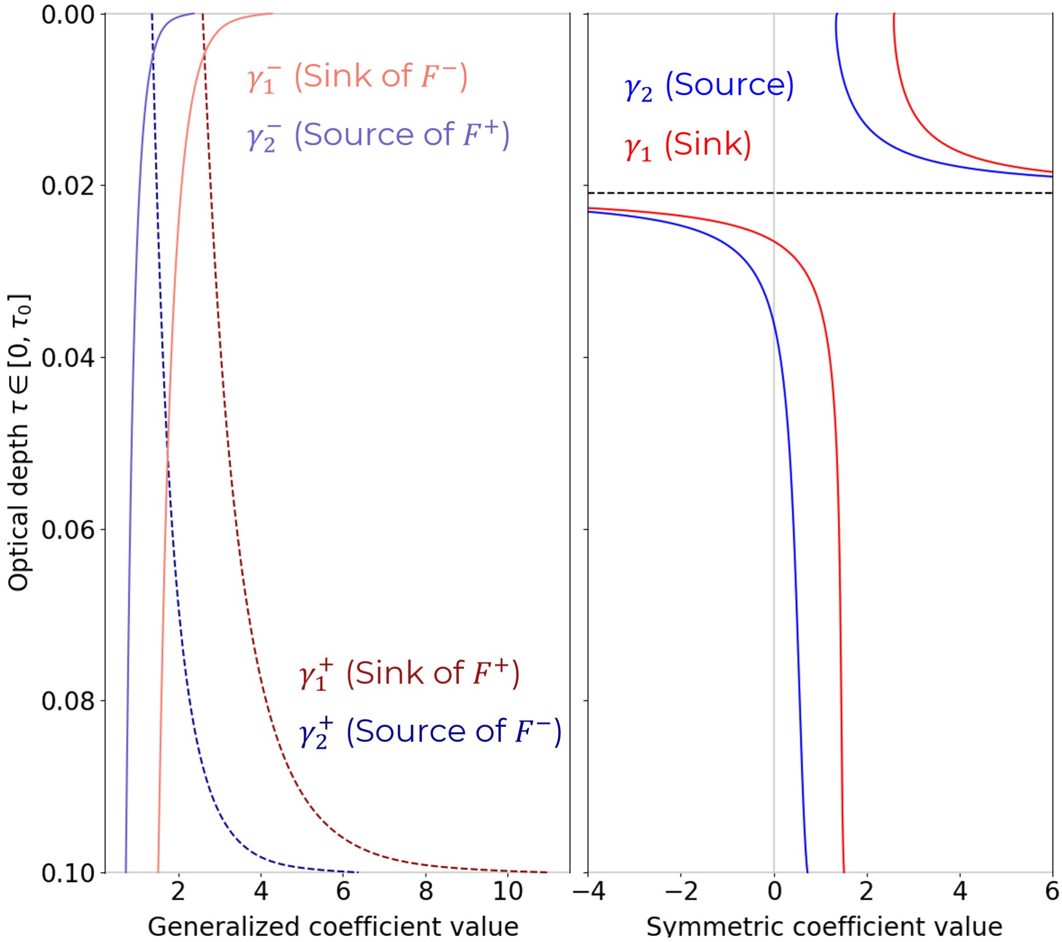

Figure 1. Exact coupling coefficients for the general (left) and symmetric (right) two-stream equations given $g = 0.65$, $\omega = 0.75$, $\mu_0 = 0.45$, $\tau_0 = 0.1$ (Henyey-Greenstein phase function) based on high-resolution computations using the discrete ordinates method. All coupling coefficients depend on optical depth τ. The general coupling coefficients (left) are non-negative and bounded. When absorption is present, the sink coefficient of each hemisphere will be larger than the source coefficient of the opposite hemisphere for all τ. The symmetric coupling coefficients (right) are, in contrast, unphysical due to the singularity and negative values.

The two symmetric coefficents can be determined from the four general coefficients by using (8) to substitute the D terms in (9) to arrive at

$$\begin{aligned}\gamma_1(\tau) &= \left\{\gamma_1^{\pm} + F^{\mp}\left(\frac{F^{\mp}(\gamma_1^{+}-\gamma_1^{-}) + F^{\pm}(\gamma_2^{+}-\gamma_2^{-})}{(F^{+}-F^{-})\,(F^{+}+F^{-})}\right)\right\}(\tau)\\ \gamma_2(\tau) &= \left\{\gamma_2^{\pm} + F^{\mp}\left(\frac{F^{\mp}(\gamma_2^{+}-\gamma_2^{-}) + F^{\pm}(\gamma_1^{+}-\gamma_1^{-})}{(F^{+}-F^{-})\,(F^{+}+F^{-})}\right)\right\}(\tau)\end{aligned} \tag{11}$$

In the general case, (11) shows that γ_1 may be attained by perturbing either γ_1^+ or γ_1^- (and similarly for γ_2). In other words, if the intensity field is not in fact symmetric then the source and sink values have to be artificially redistributed to fit the symmetric form of (3). This artificial redistribution compromises the explicability of the model and the perturbation of the two-stream coefficients is what causes them to take on unphysical values (e.g. Fig. 1). Consequently, (10) can be interpreted as the condition for true two-stream symmetry. No perturbation can be defined where net flux is 0 (as in the right panel of Fig. 1).

Equation (11) suggests that the symmetric two-stream equations are likely to admit non-negative coefficients throughout the medium if $\left(\gamma_1^+ - \gamma_1^-\right)$ and $\left(\gamma_2^+ - \gamma_2^-\right)$ are small relative to the directional and net fluxes, i.e. the intensity field is almost symmetric. One of the largest factors affecting the symmetry of the intensity field, especially in optically thin media, is the source of diffuse radiation from the direct beam. Two-stream methods were originally developed for stellar atmospheres with isotropic blackbody emission sources (Schuster, 1905). For collimated sources, however, the intensity field near the top of the atmosphere is dominated by the scattering phase function which can be strongly anisotropic e.g. for clouds.

2.3 Reduced Constraints and Closed-Form Solutions

As noted at the end of Section 2.1, the general two-stream equations (7) differ from the widely-used form (3) in not assuming symmetry and, as explored in the previous section, in requiring coupling coefficients that depend in general on optical depth. The latter presents a particular challenge since coupling coefficients with arbitrary dependence on optical depth do not admit closed-form solutions.

The search for optimal coupling coefficients can be formulated as an optimization problem. For the problem to be well-posed it is necessary for the degrees of freedom to match the number of constraints. If the goal is to reconstruct the flux profiles in their entirety, then the optimization problem has two functional constraints, i.e. the F^+ and F^- flux profiles, and two functional degrees of freedom will be required. The symmetric τ-dependent two-stream equation falls under this paradigm. Requiring non-negative coupling coefficients imposes two more functional constraints, which is consistent with Fig. 1 and the fact that the symmetric form of the two-stream equations has two coupling coefficients but the general form has four.

This also implies that the τ-dependence of the constraints is tied to the τ-dependence of the coupling coefficients. Two-stream models are often used to compute only the reflectance $R = F^+(0)/F^-(0)$ and transmittance $T = F^-(\tau_0)/F^-(0)$. Scalar constraints (e.g. on R and T) can be satisfied with scalar coupling coefficients. This is consistent with the Meador and Weaver (1980) paradigm of only using τ-independent coupling coefficients to target accurate R and T rather than entire flux profiles.

The solution to the general two-stream equations (7) with τ-independent coefficients is given by

$$\begin{aligned} F^+(\tau) &= F_{\text{inc}}\omega\Big\{\alpha_1\left(e^{\lambda^+\tau+\lambda^-\tau_0}-e^{\lambda^+\tau_0+\lambda^-\tau}\right)-\alpha_5\Big[\alpha_3\left(e^{\lambda^+\tau-\frac{\tau_0}{\mu_0}}-e^{\lambda^+\tau_0-\frac{\tau}{\mu_0}}\right) \\ &\quad -\alpha_4\left(e^{\lambda^-\tau-\frac{\tau_0}{\mu_0}}-e^{\lambda^-\tau_0-\frac{\tau}{\mu_0}}\right)\Big]\Big\}\left\{\alpha_7\left(\alpha_3e^{\lambda^+\tau_0}-\alpha_4e^{\lambda^-\tau_0}\right)\right\}^{-1} \\ F^-(\tau) &= F_{\text{inc}}\omega\Big\{\alpha_2\left(e^{\lambda^-\tau-\frac{\tau_0}{\mu_0}}-e^{\lambda^+\tau-\frac{\tau_0}{\mu_0}}\right)+\alpha_6\Big[\alpha_3\left(e^{\lambda^+\tau_0-\frac{\tau}{\mu_0}}-e^{\lambda^+\tau_0+\lambda^-\tau}\right) \\ &\quad -\alpha_4\left(e^{\lambda^-\tau_0-\frac{\tau}{\mu_0}}-e^{\lambda^+\tau+\lambda^-\tau_0}\right)\Big]\Big\}\left\{\alpha_7\left(\alpha_3e^{\lambda^+\tau_0}-\alpha_4e^{\lambda^-\tau_0}\right)\right\}^{-1} \end{aligned} \tag{12}$$

where $F_{\text{inc}} = I_0\mu_0$ is the incident flux and

$$\begin{aligned} k &= \sqrt{\left(\gamma_1^+\right)^2+2\gamma_1^+\gamma_1^-+\left(\gamma_1^-\right)^2-4\gamma_2^+\gamma_2^-} \\ \lambda^\pm &= \frac{1}{2}\left(\gamma_1^+-\gamma_1^-\pm k\right) \\ \alpha_1 &= 2\gamma_2^-\left(\left(\gamma_1^+\gamma_4+\gamma_2^+\gamma_3\right)\mu_0+\gamma_4\right) \\ \alpha_2 &= 2\gamma_2^+\left(\left(\gamma_1^-\gamma_3+\gamma_2^-\gamma_4\right)\mu_0-\gamma_3\right) \\ \alpha_3 &= \gamma_1^++\gamma_1^-+k \\ \alpha_4 &= \gamma_1^++\gamma_1^--k \\ \alpha_5 &= \left(\gamma_1^-\gamma_3+\gamma_2^-\gamma_4\right)\mu_0-\gamma_3 \\ \alpha_6 &= \left(\gamma_1^+\gamma_4+\gamma_2^+\gamma_3\right)\mu_0+\gamma_4 \\ \alpha_7 &= \left(\gamma_1^+\gamma_1^--\gamma_2^+\gamma_2^-\right)\mu_0^2+\left(\gamma_1^--\gamma_1^+\right)\mu_0-1 \end{aligned}$$

Although the eigenvalues $\lambda^\pm$ can be complex the boundary conditions ensure that $F^\pm$ are always real. The diffuse (excluding direct beam) reflectance and transmittance are given by

$$\begin{aligned} R &= \frac{\omega\left(\alpha_1\left(e^{\lambda^-\tau_0}-e^{\lambda^+\tau_0}\right)+\alpha_5\left(\alpha_3\left(e^{\lambda^+\tau_0}-e^{-\frac{\tau_0}{\mu_0}}\right)+\alpha_4\left(e^{-\frac{\tau_0}{\mu_0}}-e^{\lambda^-\tau_0}\right)\right)\right)}{\alpha_7\left(\alpha_3e^{\lambda^+\tau_0}-\alpha_4e^{\lambda^-\tau_0}\right)} \\ T &= \omega\Big\{\alpha_2\left(e^{\tau_0\left(\lambda^--\mu_0^{-1}\right)}-e^{\tau_0\left(\lambda^+-\mu_0^{-1}\right)}\right)+\alpha_6\Big[\alpha_3\left(e^{\tau_0\left(\lambda^+-\mu_0^{-1}\right)}-e^{\tau_0\left(\lambda^++\lambda^-\right)}\right) \\ &\quad +\alpha_4\left(e^{\tau_0\left(\lambda^++\lambda^-\right)}-e^{\tau_0\left(\lambda^--\mu_0^{-1}\right)}\right)\Big]\Big\}\left\{\alpha_7\left(\alpha_3e^{\lambda^+\tau_0}-\alpha_4e^{\lambda^-\tau_0}\right)\right\}^{-1} \end{aligned} \tag{13}$$

The derivations are in Appendix A. Equations (25) and (26) in Meador and Weaver (1980) can be recovered from our (13) by having $\gamma_1^+ = \gamma_1^-$, $\gamma_2^+ = \gamma_2^-$ and by adding the direct beam transmittance: $\exp(-\tau_0/\mu_0)$ to our formula for T.

3 Optimized Coupling Coefficients

Practical application of the general two-stream expression for reflectance and transmittance (13) requires specifying the coupling coefficients $\gamma_1^+, \gamma_1^-, \gamma_2^+, \gamma_2^-$ as a function of the problem parameters g, ω, τ_0 and μ_0, with g typically used to represent the phase function (Meador & Weaver, 1980). We approach the search for these dependencies as a problem in numerical optimization over the problem space shown in Figure 2. Parameter choices are appropriate for condensed materials (clouds and aerosols) in the Earth's atmosphere.

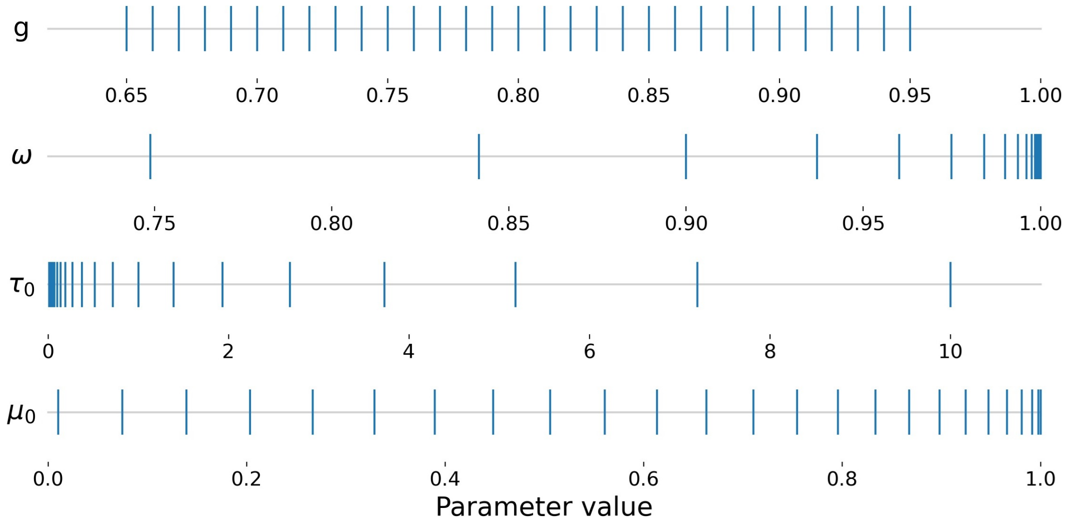

Figure 2. The distribution of each problem parameter. The values of the asymmetry parameter $g \in [0.65, 0.95]$ (Henyey-Greenstein phase function) represent the highly forward-peaked scattering of clouds and explore the delta-function limit. The values of the single-scattering albedo $\omega \in [0.75, 1)$ ensure significant multiple scattering so that the coupling coefficients will be significant. The values of the total optical depth $\tau_0 \in [0.01, 10]$ represent both thick and thin atmospheres. Finally, the values of the cosine of the solar zenith angle $\mu_0 \in [0.01, 1]$ spans the full range with equispaced $\arccos \mu_0$. Due to limitations in the algorithms on which both `PythonicDISORT` and its Fortran antecedent are based, $\omega = 1$ is not a valid input and so $\omega = 1 - 10^{-6}$ is used in its place.

3.1 Objective Functions and Optimization Details

We search for optimal coupling coefficients for each set of parameter values independently. We numerically optimize for coupling coefficients such that the sources and sinks of the two-stream equations match, the true vertically-integrated, angularly resolved sources and sinks, i.e. the D terms in (5).

The general two-stream equations have four degrees of freedom (coupling coefficients) which allow it to satisfy four constraints, and these are chosen to be the vertically-integrated (total) true sources and sinks. This gives the objective function

$$\begin{aligned} O_1(\vec{\gamma}) = &\\ &\left(\frac{\gamma_1^+ \int_0^{\tau_0} F^+(\tau;\vec{\gamma})\,\mathrm{d}\tau - \int_0^{\tau_0} D_1^+(\tau)\mathrm{d}\tau}{\int_0^{\tau_0} D_1^+(\tau)\mathrm{d}\tau}\right)^2 + \left(\frac{\gamma_1^- \int_0^{\tau_0} F^-(\tau;\vec{\gamma})\,\mathrm{d}\tau - \int_0^{\tau_0} D_1^-(\tau)\mathrm{d}\tau}{\int_0^{\tau_0} D_1^-(\tau)\mathrm{d}\tau}\right)^2 \\ &+ \left(\frac{\gamma_2^+ \int_0^{\tau_0} F^+(\tau;\vec{\gamma})\,\mathrm{d}\tau - \int_0^{\tau_0} D_2^+(\tau)\mathrm{d}\tau}{\int_0^{\tau_0} D_2^+(\tau)\mathrm{d}\tau}\right)^2 + \left(\frac{\gamma_2^- \int_0^{\tau_0} F^-(\tau;\vec{\gamma})\,\mathrm{d}\tau - \int_0^{\tau_0} D_2^-(\tau)\mathrm{d}\tau}{\int_0^{\tau_0} D_2^-(\tau)\mathrm{d}\tau}\right)^2 \end{aligned} \tag{14}$$

where $\vec{\gamma} := \left(\gamma_1^+, \gamma_1^-, \gamma_2^+, \gamma_2^-\right)$. That is, we specify the objective function as the squared 2-norm of the relative error of the total sources and sinks. This choice generalizes well to the optimization for the two coupling coefficients of the symmetric form and provides more accurate results than other objective functions we have tried, partly because the source and sink terms are of comparable scale.

The D terms in the objective functions and the reference values of reflectance R and transmittance T are computed with `PythonicDISORT v0.8.0` (Ho, 2023). Every integral in (14) can be analytically solved: the fluxes from the general two-stream equations can be integrated with respect to optical depth given the formulas (12), while solutions to the radiative transfer equation (6) can be integrated analytically because, in the discrete ordinates method, the azimuthally-averaged intensity $\bar{u}$ is the analytical solution to a system of ordinary differential equations with variable τ (Stamnes et al., 1988). Since the objective function can be evaluated analytically it is amenable to auto-differentiation allowing the gradient to be evaluated quickly and to machine precision, speeding optimization efforts.

The objective function for the symmetric coupling coefficients should have only two constraints to match the two degrees of freedom of (3). The number of constraints can be reduced from four to two by combining the source and sink terms in each equation of (6), and in (3), to obtain the net sources. The objective function is the normalized sum of the squared vertically-integrated difference between these two source terms:

$$
\begin{aligned}
O_2(\vec{\gamma}) = &\left(\frac{\int_0^{\tau_0}\left[\gamma_1 F^+(\tau;\vec{\gamma}) - \gamma_2 F^-(\tau;\vec{\gamma})\right]\mathrm{d}\tau - \int_0^{\tau_0}\left[D_1^+(\tau) - D_2^-(\tau)\right]\mathrm{d}\tau}{\int_0^{\tau_0}\left[D_1^+(\tau) - D_2^-(\tau)\right]\mathrm{d}\tau}\right)^2 \\
&+ \left(\frac{\int_0^{\tau_0}\left[\gamma_2 F^+(\tau;\vec{\gamma}) - \gamma_1 F^-(\tau;\vec{\gamma})\right]\mathrm{d}\tau - \int_0^{\tau_0}\left[D_2^+(\tau) - D_1^-(\tau)\right]\mathrm{d}\tau}{\int_0^{\tau_0}\left[D_2^+(\tau) - D_1^-(\tau)\right]\mathrm{d}\tau}\right)^2
\end{aligned}
\tag{15}
$$

i.e. the squared 2-norm of the relative error of the total net sources.

Both objective functions (14) and (15) are non-convex. We use monotonic basin-hopping (`scipy.optimize.basinhopping` with `T=0`) with the Broyden–Fletcher–Goldfarb–Shanno algorithm (Nocedal & Wright, 2006) as the local optimizer. Basin-hopping is the only global optimizer in `scipy.optimize` that uses an initial value. Every other global optimizer requires bounds but the coupling coefficients are in principle unbounded above. Monotonic basin-hopping is a stochastic algorithm but our results are quite consistent across realizations.

Initial values for the optimization at the first point in the parameter grid (Fig. 2) are chosen through trial-and-error. The first set of optimized coupling coefficients are used as the initial values for the optimization at an adjacent point making it more likely that the optimized coefficients will vary smoothly with the parameters. An acceptance test is imposed on the global, but not local, step-taking procedure (through the argument `accept_test`) to reject steps that result in negative coefficients or fluxes. The acceptance test acts as a soft constraint against spurious minima but still allows negative optimized coefficients for the symmetric two-stream equations (see Sec. 2.2).

3.2 Accuracy and Trade-Offs

Numerical optimization produces coupling coefficients that reproduce R and T with relative errors less than 4×10^{-5} across the entire parameter range (Fig. 2). For comparison, Figure 3 shows the worst-case R, T errors of three baseline two-stream methods: Coakley and Chylek (1975, *Two-stream model 1*) and Eddington (Eddington, 1916; Meador & Weaver, 1980) which were formulated to be accurate for thin and thick atmospheres respectively, as well as the Zdunkowski et al. (1980) method adopted by the widely-used `RRMTG` comprehensive radiation package (Iacono et al., 2008) and still in widespread use (Hogan & Bozzo, 2018; Pincus et al., 2019). Zdunkowski and Eddington, which are identical when $\omega = 1$, use delta-scaling (Joseph et al., 1976) which requires $\gamma_3 = (2-3g\mu_0)/4$ as the coefficient of the source of diffuse radiation from the direct beam, whereas $\gamma_3 = \beta_0$ for the optimized and Coakley-Chylek models which do not use delta-scaling. Unlike the optimized methods which are accurate everywhere, the baseline methods are only

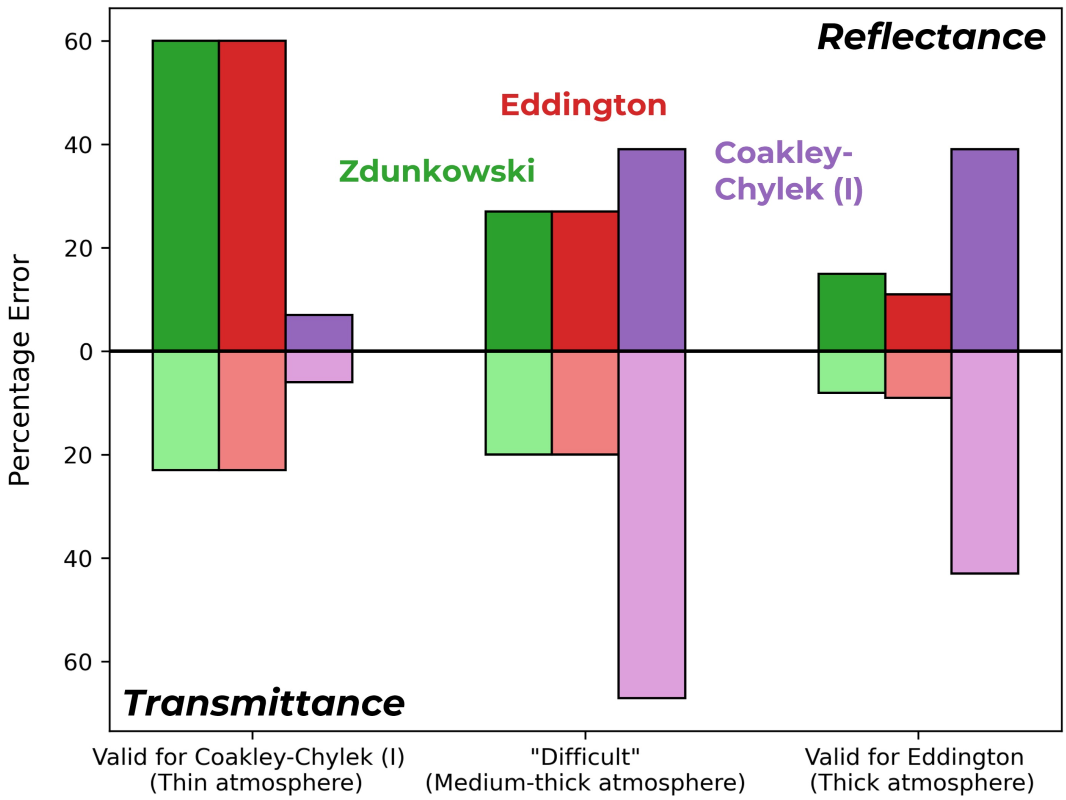

Figure 3. Worst-case percentage errors for two-stream methods using numerically-optimized coupling coefficients and for baseline methods Coakley-Chylek (I), Eddington, and Zdunkowski in different parameter ranges. The (adjusted) "ranges of validity" and "difficult range of variables" (King & Harshvardhan, 1986, p. 785) are from left to right: $\mu_0 \geq 0.1$, $\tau_0 \leq 0.1$ (thin atmosphere); $\mu_0 \in [0.1, 0.5]$, $g \in [0.8, 0.9]$, $\omega = 1$, $\tau_0 \in [1, 5]$ (medium-thick atmosphere); and $\mu_0 \geq 0.5$, $g \in [0.8, 0.9]$, $\omega \geq 0.96$, $\tau_0 \in [3, 10]$ (thick atmosphere). Parameter ranges not mentioned default to those shown in Fig. 2. The overall worst-case (R, T)% errors for the Coakley-Chylek (I), Eddington, and Zdunkowski methods are $(85, 107)$, $(85, 107)$, $(66, 467)$ respectively. In comparison, the optimized methods have a worst-case error of 10^{-3}% to 10^{-5}% in each parameter range and overall, in fact, they are more accurate for every set of problem parameters.

accurate in limited "ranges of validity" (King & Harshvardhan, 1986). The optimized methods are more accurate than any other closure for every set of problem parameters.

While the optimized models produce more accurate R and T (endpoint values), the flux profiles they construct may be less accurate than those constructed by other two-stream models (see Figure 4). In addition, some flux profiles constructed by the optimized general model are, for most τ-points, less accurate than those constructed by the optimized symmetric model. Thus, no formulation of the two-stream coupling coefficients is ideal. Rather, the choice involves a trade-off between four desirable properties: accuracy in R and T; accuracy across the flux profile; tractability and simplicity – i.e. the number and τ-(in)dependence of coupling coefficients; and non-negative, bounded and thus physically explicable coupling coefficients. The optimized symmetric model provides simple and accurate R and T but its mechanisms may be artificial. The optimized general model determines R and T in a physically explicable way but requires the specification of two more coupling coefficients and more complicated analytic solutions. Both optimized models may construct flux profiles that are, apart from the endpoints, less accurate than other two-stream models, and this is consistent with the fact that τ-dependent coupling coefficients are necessary for a two-stream model to accurately construct entire flux profiles (see Sec. 2.3).

3.3 Parameter Dependence

The numerically-optimized coupling coefficients vary smoothly with optical parameters (Figures 5 and 6) suggesting that the optimization produced values at or near the true global optimum despite the lack of proof for the well-posedness of the optimization problems set up in Section 3.1. Smooth variations allow for interpretation of the parameter dependence of the optimized coefficients which then informs the parameterization of two-stream closures. The limited range of validity of all existing closures is due to their lack of τ_0-dependence.

Two-stream methods differ in how the sink, γ_1, and source, γ_2, coefficients depend on single-scattering parameters g, ω (Meador & Weaver, 1980, Table 1). The dependence of the optimized coupling coefficients on these parameters (Fig. 5) is smooth but rich and changes qualitatively with macroscopic parameters τ_0, μ_0. In some parts of the phase space the dependence of the source and sink coefficients on g, ω shows mild curvature, suggesting that linear closures such as Eddington and Zdunkowski may be too simple. The optimized source coefficient for the symmetric form of the two-stream equations, γ_2, is negative in optically thin atmospheres when ω is small and g is close to 1 – i.e. regions in which the intensity field is dominated by the direct beam and thus highly anisotropic.

The source and sink coefficients in some but not all existing two-stream closures depend on μ_0 (see, for example, Table 1 of Meador and Weaver (1980)). The optimized coupling coefficients do depend on μ_0 (Fig. 6), and, unlike all existing closures, also depend on τ_0. Both dependencies diminish as τ_0 increases. These behaviors can be understood by recalling that the exact coupling coefficients depend on both optical depth and the solar zenith angle (Sec. 2.1). Each optimal (τ-independent) coupling coefficient is therefore a weighted average of the corresponding exact (τ-dependent) coefficient and inherits its underlying dependence on τ_0 and μ_0. Both dependencies diminish with τ_0 because multiple scattering, which increases in relative significance with optical depth, homogenizes the radiation field. The interior of thick media (large τ_0) falls within the *diffusion domain*: "the range of optical depths far enough from the boundaries (or from internal source layers) to let the radiation be transported by simple diffusion as if the medium were unbounded" (Van de Hulst, 1968, p. 79), and within which the direct beam is negligible relative to the diffuse intensity field (King, 1981, p. 2032). In the interior of thick atmospheres the exact coupling coefficients are quite close to the μ_0- and τ-independent *diffusion approximations* (Figure 7) which are derived in Appendix B. The proportion of the atmosphere in the diffusion domain increases with τ_0 and this pulls the value of each optimized coupling coefficient toward the value of its diffusion approximation.

These results have two implications. First, there exists a soft upper bound to the τ_0 values above which further increases should not substantially vary the optimal source and sink coefficients. This bound is higher the closer g is to 1 (see Figure 6; note that μ_0 and ω are also relevant) since the existence of the diffusion domain requires a thicker atmosphere (King, 1981) under conditions of stronger single-scattering anisotropy. That such a bound exists simplifies optimization since the parameter space $(g, \omega, \tau_0, \mu_0)$ with the Henyey-Greenstein phase function becomes effectively bounded. Second, the "range of validity" (King & Harshvardhan, 1986) of each two-stream method is limited by the parameters on which it depends, and specifically whether the source and sink strengths depend on μ_0. The Coakley-Chylek closure is invalid for thick atmospheres since it is dependent on μ_0, whereas the Eddington closure is invalid for thin atmospheres since it is independent of μ_0, and this is consistent with the errors shown in Fig. 3. Coupling

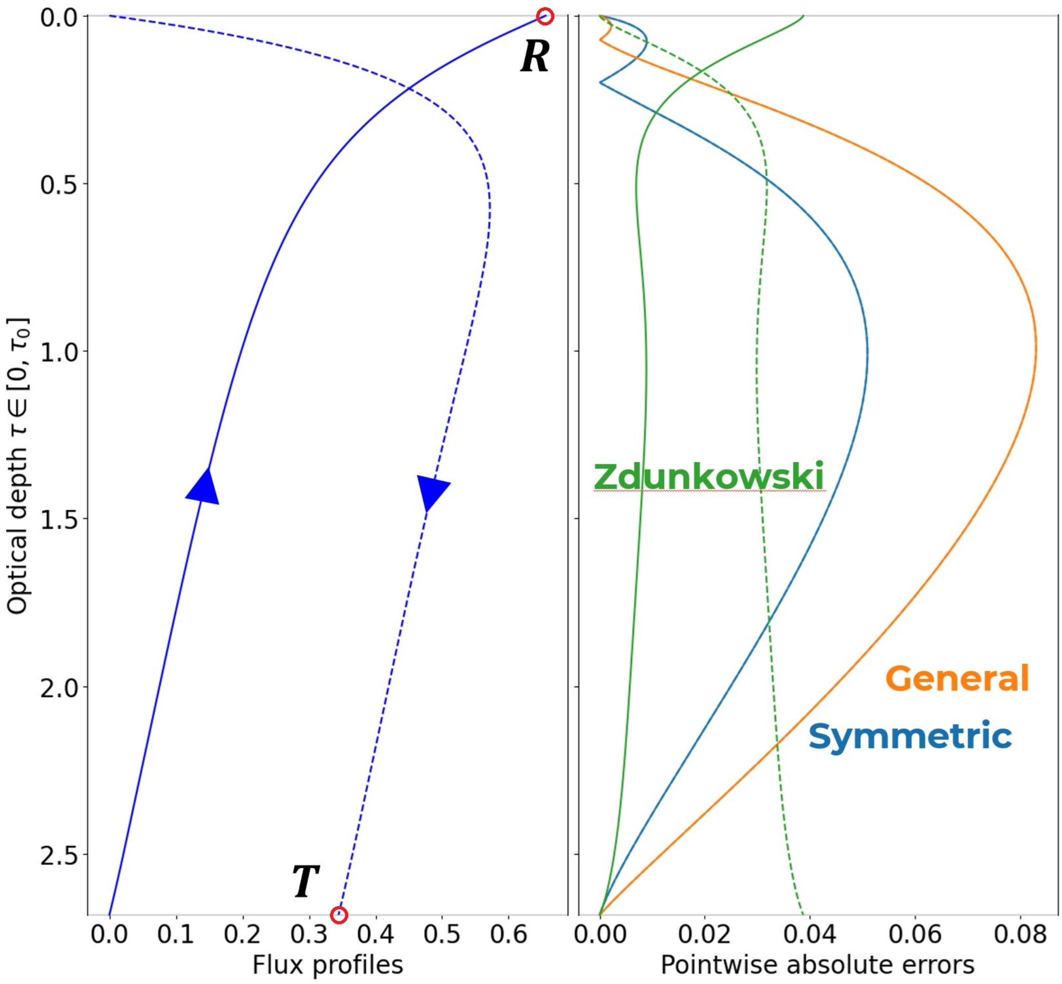

Figure 4. The left panel shows the true upward (solid line) and downward (dotted line) flux profiles given $g = 0.65$, $\omega = 1$, $\mu_0 = 0.2$, $\tau_0 = 2.7$ with the Henyey-Greenstein phase function. The right panel shows the pointwise absolute error for each flux profile constructed by the optimized and Zdunkowski (commonly used to model thick atmospheres) two-stream models. Note that for the optimized models, the errors for the upward and downward fluxes are very similar and so the lines overlap. The optimized methods produce more accurate R and T (endpoint fluxes), but for most other τ-points they produce less accurate fluxes than the Zdunkowski method. In addition, the flux profiles constructed by the optimized general model are, for most τ-points, less accurate than those constructed by the optimized symmetric model, though the former is guaranteed to have non-negative coupling coefficients.

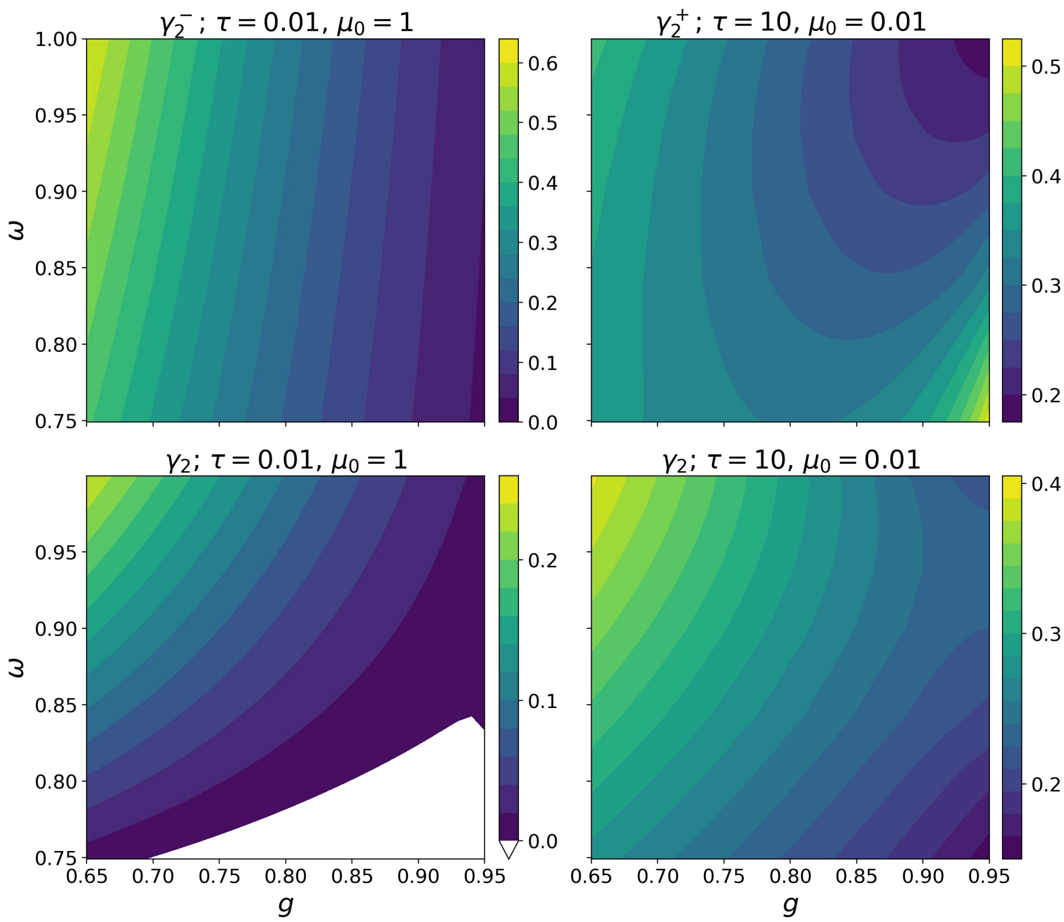

Figure 5. Dependence of optimized coupling coefficients on single-scattering parameters g, ω for fixed τ_0, μ_0. The patterns of variation with g and ω differ between panels and are nonlinear in some cases, with more patterns in the data that are not shown. The lower left panel shows that the optimized γ_2 takes on negative values when ω is small and g is close to 1 (similar to the Eddington γ_2), though this is only true for thin atmospheres and when μ_0 is close to 1.

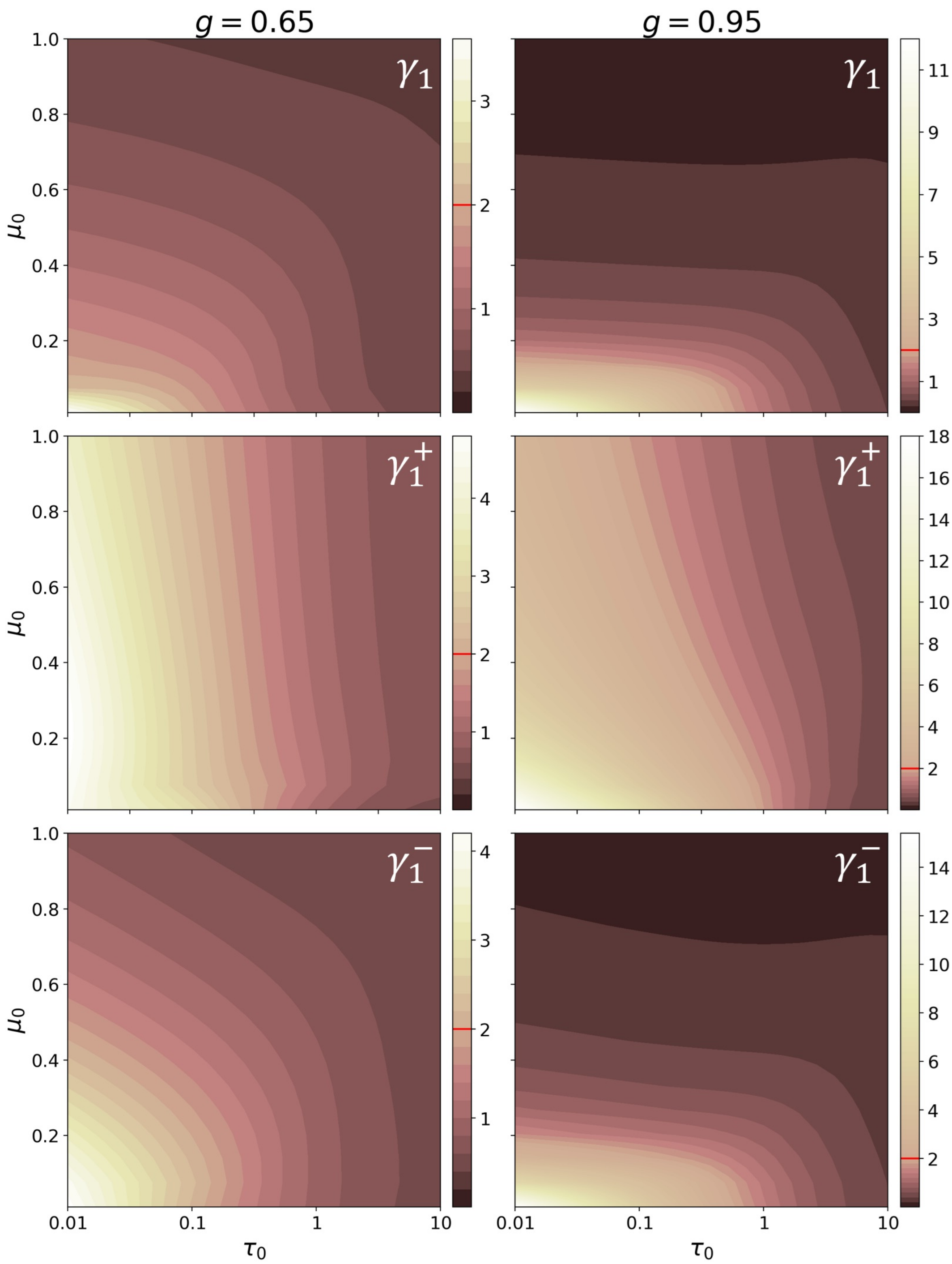

Figure 6. Dependence of optimized coupling coefficients on macroscopic parameters τ_0, μ_0 for fixed $g = 0.65$ (left column) or 0.95 (right column) and $\omega = 0.9$. Each color range is normalized between 0 and 2 (with a fixed number of contour lines in this range) and separately normalized between 2 and the maximum coefficient value for that panel. Three pairs of optimized sink and source coefficients: (γ_1, γ_2), (γ_1^+, γ_2^+), (γ_1^-, γ_2^-) are qualitatively similar and so only the sink coefficients are plotted. The dependence of the optimized coefficients on τ_0 and μ_0 diminishes as τ_0 increases. This decay is slower when the degree of forward scattering is greater as evidenced by the larger gradients in the panels on the right (for which g is greater).

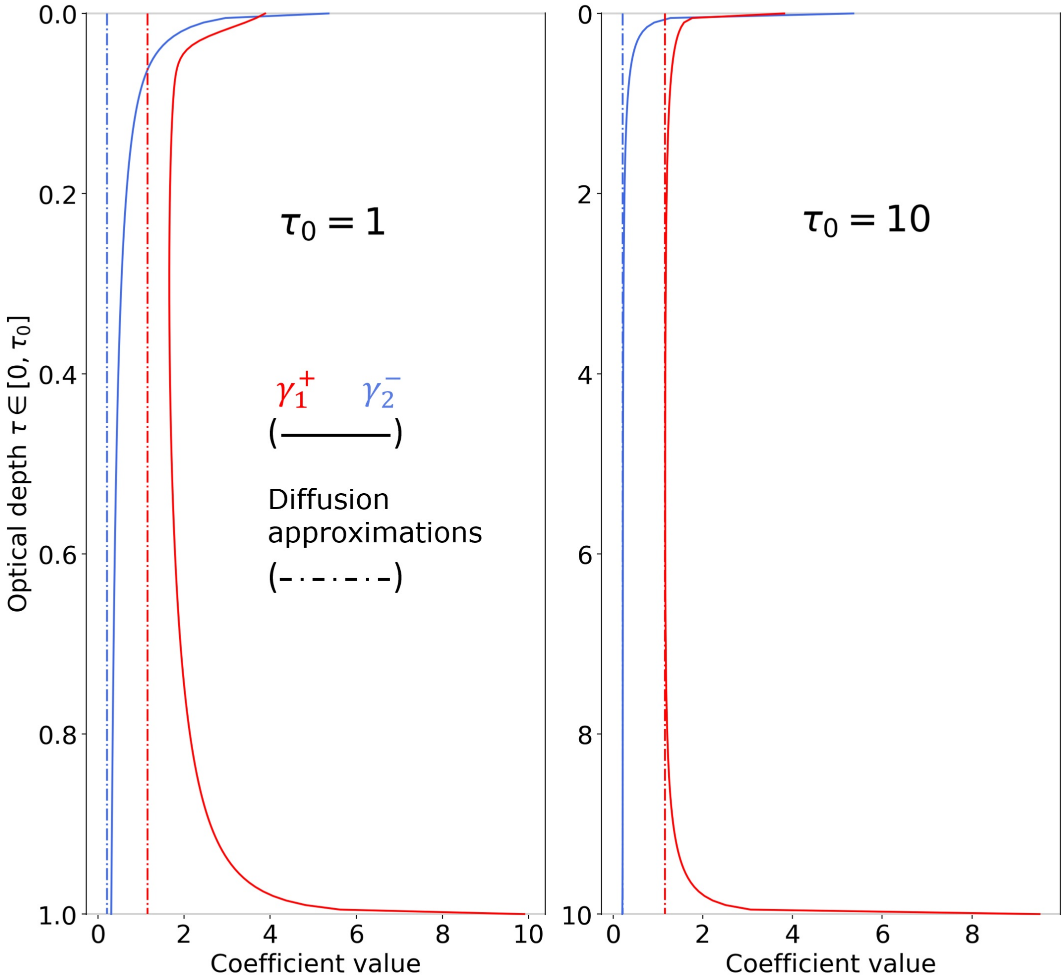

Figure 7. Exact (τ-dependent) source, γ_1^+, and sink, γ_2^-, coefficients of the general two-stream equations (solid lines) and their τ-independent diffusion approximations (dot-dashed lines) at $\tau_0 = 1$ (left) and $\tau_0 = 10$ (right) for fixed $g = 0.65$, $\omega = 0.75$, $\mu_0 = 0.01$. The other two exact general coupling coefficients are qualitatively similar; they, and the exact symmetric coupling coefficients, also converge to corresponding diffusion approximations in the diffusion domain. The proportion of the atmosphere in the diffusion domain increases with τ_0.

coefficients for a thin-atmosphere model should also be strongly dependent on τ_0 but this is obscured by the fact that the τ_0 values of thin atmospheres necessarily span a small range. A two-stream closure that works well for all parts of the parameter space must have τ_0-dependence so that it can shift between the μ_0-independent thick-atmosphere and μ_0-dependent thin-atmosphere regimes.

4 Insights, Implications and Limitations

Two-stream concepts and methods have been a cornerstone of radiative transfer for more than a century, providing conceptual clarity and computational efficiency to the calculation of fluxes in strongly scattering media. As we have shown, however, two fundamental assumptions – that the source and sink coefficients for upwelling and downwelling radiation are symmetric and independent of optical depth – do not hold in general in the case of a beam source (i.e. sunlight in earth's atmosphere). The two assumptions have practical implications: the assumption of symmetry requires coefficients to take on unphysical values in some parameter regimes, while the assumption of τ-independence means that two-stream models cannot reconstruct entire flux profiles. Numerically-optimized values of τ-independent coupling coefficients can reproduce reflectance and transmittance to very high accuracy but these coefficients have nonlinear dependence on g, ω, τ_0, μ_0. The dependence on τ_0 and μ_0 diminishes as τ_0 increases and more of the medium is occupied by diffusion-like radiative transfer. These results explain why existing closures work well exclusively in optically-thick or optically-thin limits (King & Harshvardhan, 1986) and suggests that any closure that does not depend on τ_0 will be less accurate in some limits than in others.

As two-stream methods are used in many radiation codes coupled to dynamical models, our results have both practical implications and important limitations. Two-stream methods are sometimes identified as a key limit to the accuracy of radiative transfer calculations (see Li and Ramaswamy (1996); Li et al. (2015) or Wild et al. (2000); Hsu et al. (2017) on actinic flux to which our findings should generalize). We have shown that the methods are inherently limited only by the choice of closure. The use of tabulated closures such as those we have generated would be unwieldy, however, and practical implementations would benefit from compact analytic representation of the closures. The results would also need extension from the Henyey-Greenstein phase function to more realistic cloud phase functions since neglecting higher-order Legendre coefficients of "phase functions for typical cloud particle size distributions" results in systematic errors (Barker et al., 2015, pp. 4069–4070), as well as to more isotropic Rayleigh scattering phase functions for use in clear skies. The dependence on τ_0 will also need extension to atmospheres in which vertical inhomogeneity is explicitly resolved. Finally, although our results suggest that errors in angular integration introduced by two-stream methods can be reduced by orders of magnitude, these errors are in many circumstances a small part of the overall error budget (Barker et al., 2015), which can be dominated at larger scales by unresolved variability in clouds and at smaller scales by the neglect of horizontal transport.

Appendix A Closed-Form Solutions to the General Two-Stream Equations

We seek closed-form solutions to the general two-stream equations (7) with τ-independent coupling coefficients:

$$\partial_\tau \begin{bmatrix} F^+ \\ F^- \end{bmatrix} = \begin{bmatrix} \gamma_1^+ & -\gamma_2^- \\ \gamma_2^+ & -\gamma_1^- \end{bmatrix} \begin{bmatrix} F^+ \\ F^- \end{bmatrix} + \begin{bmatrix} -I_0\omega\gamma_3 \\ I_0\omega\gamma_4 \end{bmatrix} \exp\left(-\mu_0^{-1}\tau\right)$$

given homogeneous Dirichlet boundary conditions: $F^+(0) = 0 = F^-(\tau_0)$. The two-stream equations can be re-expressed as

$$\partial_\tau F = AF + X\exp\left(-\mu_0^{-1}\tau\right) \tag{A1}$$

Assume matrix A has two distinct and non-zero eigenvalues $\lambda^{\pm}$, then A can be diagonalized as

$$A = GDG^{-1}, \quad D = \begin{bmatrix} \lambda^+ & 0 \\ 0 & \lambda^- \end{bmatrix}$$

where matrices G and D can be analytically determined as they are 2×2. The homogeneous solution can be determined through

$$\begin{aligned} &\partial_\tau F = GDG^{-1}F \\ &\implies \partial_\tau \left(G^{-1}F\right) = D\left(G^{-1}F\right) \\ &\implies \left(G^{-1}F\right) = \exp\left(D\tau\right)C \\ &\implies F = G\exp\left(D\tau\right)C \end{aligned}$$

The next step is to determine a particular solution. The ansatz to use is

$$B\exp\left(-\mu_0^{-1}\tau\right)$$

Substitution of the ansatz into (A1) gives

$$\begin{aligned} &-\mu_0^{-1}B\exp\left(-\mu_0^{-1}\tau\right) = AB\exp\left(-\mu_0^{-1}\tau\right) + X\exp\left(-\mu_0^{-1}\tau\right) \\ &\implies -\mu_0^{-1}B = AB + X \\ &\implies -\left(\mu_0^{-1}I + A\right)B = X \end{aligned}$$

which can be solved for B. The full solution in vector form is

$$F = G\exp\left(D\tau\right)C + B\exp\left(-\mu_0^{-1}\tau\right) \tag{A2}$$

The boundary conditions give

$$\begin{bmatrix} G^+\exp\left(D\tau_0\right) \\ G^- \end{bmatrix} C = -\begin{bmatrix} B^+\exp\left(-\mu_0^{-1}\tau_0\right) \\ B^- \end{bmatrix}$$

from which C can be determined. Substitute matrices G and D as well as vectors C and B into (A2), then perform the matrix multiplications. Substantial simplification is required to get (12) but after that it should be trivial to derive (13).

Precautions against overflow should be taken when implementing formulas (12) and (13). One approach is to multiply each numerator and denominator by $\exp\left(-\lambda^+\tau_0\right)$ if $\mathrm{Re}(\lambda^+) > 0$, and again by $\exp\left(-\lambda^-\tau_0\right)$ if $\mathrm{Re}(\lambda^-) > 0$ to ensure the real part of every exponent is always non-positive.

Appendix B Diffusion Approximations of the Exact Coupling Coefficients

We seek to study the behavior of the exact coupling coefficients in the diffusion domain. The formulas for the exact general coupling coefficients (8) with the substitution of the D terms (5) give

$$\begin{aligned} \gamma_1^+(\tau) &= \frac{\int_0^1 \left(1 - p\left(\mu\right)\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu}{\int_0^1 \mu\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu} & \gamma_2^-(\tau) &= \frac{\int_0^1 p\left(-\mu\right)\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu}{\int_0^1 \mu\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu} \\ \gamma_2^+(\tau) &= \frac{\int_0^1 p\left(-\mu\right)\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu}{\int_0^1 \mu\bar{u}\left(\tau,\mu\right)\mathrm{d}\mu} & \gamma_1^-(\tau) &= \frac{\int_0^1 \left(1 - p\left(\mu\right)\right)\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu}{\int_0^1 \mu\bar{u}\left(\tau,-\mu\right)\mathrm{d}\mu} \end{aligned} \tag{B1}$$

One way to proceed from (B1) is to use the discrete ordinates method to approximate $\bar{u}$ (see Stamnes et al. (1988) and Ho (2023, Comprehensive Documentation)). First, discretize the variable $\mu \in [-1,1]$ as the vector $\boldsymbol{\mu}$. For positive eigenvalues λ_n,

$$\bar{u}(\tau,\boldsymbol{\mu}) \approx \sum_n \left(\boldsymbol{a}_n e^{-\lambda_n\tau} + \boldsymbol{b}_n e^{-\lambda_n(\tau_0-\tau)}\right) + \boldsymbol{c}\exp\left(-\mu_0^{-1}\tau\right) \tag{B2}$$

There exists a unique pair of smallest eigenvalues $\pm\lambda_s$ such that $\lambda_s < \lambda_n$ for all $n \neq s$. This implies that away from the boundaries, i.e. when τ and $\tau_0 - \tau$ are large, (B2) can be further approximated as

$$\bar{u}(\tau, \boldsymbol{\mu}) \approx \boldsymbol{a}_s e^{-\lambda_s \tau} + \boldsymbol{b}_s e^{-\lambda_s(\tau_0 - \tau)} \tag{B3}$$

This corresponds to equation (5) of Van de Hulst (1968) and equation (1) of King (1981) except that their $\tau = 0$ is defined to be the center of the atmosphere (our $\tau = 0$ is the top of the atmosphere), and so their τ and $-\tau$ (their positive is downward) are our τ and $\tau_0 - \tau$ respectively. From King (1981, p. 2032), $\boldsymbol{a}_s$ and $\boldsymbol{b}_s$ are "the strengths of the diffusion streams in the positive [downward] and negative [upward] τ directions, respectively". Since our phase functions are strongly forward-scattering (see Fig. 2), $\boldsymbol{a}_s \gg \boldsymbol{b}_s$, and so (B3) can be further approximated once more as

$$\bar{u}(\tau, \boldsymbol{\mu}) \approx \boldsymbol{a}_s e^{-\lambda_s \tau} \tag{B4}$$

Bisect the vector $\boldsymbol{\mu}$, and by extension $\boldsymbol{a}_s$, into the vector of upward, $\boldsymbol{\mu}^+$, and downward, $\boldsymbol{\mu}^-$, directions and substitute (B4) into (B1) to cancel out the τ-dependence and get

$$\gamma_1^+ \approx \frac{\int_0^1 (1 - p(\mu))\, a_s^+(\mu) \mathrm{d}\mu}{\int_0^1 \mu a_s^+(\mu) \mathrm{d}\mu} \qquad \gamma_2^- \approx \frac{\int_0^1 p(-\mu)\, a_s^-(-\mu) \mathrm{d}\mu}{\int_0^1 \mu a_s^-(-\mu) \mathrm{d}\mu}$$

$$\gamma_2^+ \approx \frac{\int_0^1 p(-\mu)\, a_s^+(\mu) \mathrm{d}\mu}{\int_0^1 \mu a_s^+(\mu) \mathrm{d}\mu} \qquad \gamma_1^- \approx \frac{\int_0^1 (1 - p(\mu))\, a_s^-(-\mu) \mathrm{d}\mu}{\int_0^1 \mu a_s^-(-\mu) \mathrm{d}\mu}$$

where functions a_s^+ and a_s^- can be interpolations of their corresponding vectors or the integrals around them can be evaluated using quadrature since it is common to choose $\boldsymbol{\mu}^+$ and $\boldsymbol{\mu}^-$ to be quadrature points (Sykes, 1951; Stamnes et al., 2000; Ho, 2023). These τ-independent approximations of the exact coupling coefficients in the diffusion domain are the *diffusion approximations* – in this case, of the exact general coupling coefficients. The approximation (B4) can also be substituted into (9) to derive the diffusion approximations of the exact symmetric coupling coefficients.

The diffusion approximations only depend on the single-scattering albedo ω and phase function p (or asymmetry factor g). They are independent of macro parameters τ_0 and μ_0. As $\tau_0 \to \infty$, each optimized coupling coefficient will converge to the corresponding diffusion approximation with some perturbation to account for the transfer of fluxes near the boundaries. That the optimized coefficients converge at all as $\tau_0 \to \infty$ explains their diminishing dependence on τ_0.

Data Availability Statement

The dataset of optimized coupling coefficients and Jupyter Notebook for creating figures shown in this paper are publicly available at Ho (2024). The Jupyter Notebook also includes 3D interactive versions of Fig. 5 and 6. `PythonicDISORT` is publicly available at Ho (2023) and the required version is `0.8.0` or above.

Acknowledgments

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