Design and Verification of a New Monochromatic Thermal Emission Component for the I3RC Community Monte Carlo Model

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ABSTRACT

The Intercomparison of 3D Radiation Codes (I3RC) community Monte Carlo model has been extended to include a source of photon emission from the surface and atmosphere, thereby making it capable of simulating scalar radiative transfer in a 3D scattering, absorbing, and emitting domain with both internal and external sources. The theoretical basis, computational implementation, verification of the internal emission, and computational performance of the resulting model, the “IMC+emission,” is presented. Thorough verification includes fundamental tests of reciprocity and energy conservation, comparison to analytical solutions, and comparison with another 3D model, the Spherical Harmonics Discrete Ordinate Method (SHDOM). All comparisons to fundamental tests and analytical solutions are accurate to within the precision of the simulations—typically better than 0.05%. Comparison cases to SHDOM were typically within a few percent, except for flux divergence near cloud edges, where the effects of grid definition between the two models manifest themselves. Finally, the model is applied to the established I3RC case 4 cumulus cloud field to provide a benchmark result, and computational performance and strong and weak scaling metrics are presented. The outcome is a thoroughly vetted, publicly available, open-source benchmark tool to study 3D radiative transfer from either internal or external sources of radiation at wavelengths for which scattering, emission, and absorption are important.

1. Introduction

Radiative transfer models are needed to compute the net radiation absorbed by Earth’s atmosphere and surface and the radiation reaching our remote sensors. The plane-parallel approximation, which assumes the atmosphere and its radiative boundary conditions are horizontally homogeneous, is used ubiquitously in computing radiative heating and photolysis rates in environmental prediction models. This approximation simplifies the radiative transfer calculation to one

dimension (1D), namely, the vertical, which results in tremendous savings in computational cost. The 1D approximation is also used by remote sensing algorithms, since it allows for tangible solutions to the inverse problem. Nature, of course, manifests itself in three spatial dimensions (3D) and is heterogeneous over a wide range of scales in vertical and horizontal directions. This is evident just about everywhere we look (e.g., clouds and land surfaces), and the bias resulting from the 1D approximation provokes a continued push to understand and account for 3D radiative transfer in Earth science applications (e.g., Davies 1984; Guan et al. 1997; Davis et al. 1997; Várnai 2000; Benassi et al. 2004; O’Hirok et al. 2005; Widlowski et al. 2006; Marshak et al. 2006; Wen et al. 2007; Yang and Di Girolamo 2008; Várnai and Marshak 2009; Di Girolamo et al. 2010; Davis and Marshak 2010; Fauchez et al. 2014; Klinger and Mayer 2014).

In the late 1990s, a community-led effort began that brought together a group of atmospheric scientists from around the world with an interest in 3D radiative transfer in cloudy atmospheres. This effort led to the Intercomparison of 3D Radiation Codes (I3RC;

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Cahalan et al. 2005) and is ongoing with updates posted on the I3RC website (<https://i3rc.gsfc.nasa.gov>). The goals of the I3RC are to 1) compare existing codes for calculating 3D radiative transfer in cloudy atmospheres, 2) provide benchmark results for debugging 3D radiative transfer codes, 3) publish an open-source, community 3D Monte Carlo radiative transfer model, and 4) promote education in 3D radiative transfer to students and practitioners in the atmospheric sciences. Results of the first two goals were reported in Cahalan et al. (2005). The third goal was achieved by the development of the I3RC Monte Carlo community model (Pincus and Evans 2009). The fourth goal is largely achieved through the maintenance of the I3RC website, which provides a large number of resources for students, scientists, and code developers, including an updated publication list on Earth science research involving 3D radiative transfer.

Much of the I3RC efforts have focused on shortwave monochromatic radiative transfer with a solar source and a reflective surface. The I3RC Monte Carlo community model, herein referred to as the “IMC-original” model, is also solar source only. However, one of the hoped-for community contributions to the model is a source of internal emission from the surface and the atmosphere (Cahalan et al. 2005). Incorporating internal sources of radiation in 3D Monte Carlo models is not new (e.g., Chen and Liou 2006; Fomin 2006; Eriksson et al. 2011; Fauchez et al. 2014; Klinger and Mayer 2014). The addition of this feature into the IMC-original model is based upon the knowledge gained from many sources. However, very few such models are publicly available for download, and none fully address what is accomplished here: a publicly available, thoroughly vetted 3D Monte Carlo model applicable to a wide range of the electromagnetic spectrum; capable of simulating scattering, absorption, and thermal emission; computing spectral radiance, irradiance, and heating rates from solar and internal sources; and optimized for parallel computing, with an object-oriented, open-source design that the community can build upon. The theoretical basis for the internal emission component of this model and the thorough benchmarking of its accuracy and performance is the subject of this paper.

Section 2 describes the base model and the theoretical basis for and implementation of internal emission. This is followed by section 3, which thoroughly verifies the accuracy of the model’s results with a number of test cases based on fundamental standards, analytical solutions, and comparisons with another model, namely, the spherical harmonics discrete ordinate method (SHDOM; Evans 1998). In section 4, the newly verified model is applied to a complex cloud field to provide a benchmark

result for a case similar to that defined by the I3RC. Performance and scaling metrics of the model on the Blue Waters supercomputer are provided in section 5. Finally, the results are summarized in section 6.

2. Model description

a. Review of the IMC-original base model

The IMC-original model is used as a starting point. It is coded in an “object oriented” style in Fortran 95 so that pieces of code may be easily swapped in or out for other implementations. This lends itself well to the open-source community approach to development sought after by the I3RC. Further details of the code base structure are described by Pincus and Evans (2009) and Jones (2016). It can be acquired under the GNU general public license, along with its detailed documentation, online (https://i3rc.gsfc.nasa.gov/I3RC_community_model_new.htm).

The samples drawn for a Monte Carlo radiative transfer simulation are often referred to as photons (which differs from the modern usage of the word in quantum electrodynamics; Pujol 2015) and are often conceptualized as bundles of radiative energy that can be traced along a path and partially depleted through absorption and redirected upon scattering. The IMC-original model employs a forward photon tracing technique, meaning that photons are traced forward from their source until they are extinguished or leave the top of the domain. It simulates scattering and absorption but not emission events. The horizontal boundaries are periodic, and the lower boundary is represented by a scattering surface with a specified albedo. Photons are each assigned a weight of 1.0 upon initiation, which is depleted through successive absorption events at the point of scattering as opposed to either depletion along the path or complete absorption at an interaction point.

In addition to the documentation provided with the IMC-original source code, further details of the model algorithm are described by Jones (2016). The user must supply per constituent optical properties, volume extinction coefficient, single-scattering albedo, and phase function at their desired accuracy and select their algorithmic options via a name list. This includes selecting the type of domain illumination, since only one may be selected per run. The available outputs are horizontal distributions of upward irradiance at the top of the domain, downward irradiance at the bottom of the domain, and irradiance absorbed in the atmosphere; the 3D distribution of flux divergence; and the horizontal distribution of outgoing radiance at the top of the domain in a user-specified set of directions. Since it is unlikely that a statistically significant number of photons will

scatter into the particular direction of a simulated sensor, a technique called the local estimator (e.g., [Evans and Marshak 2005](#)) is used to sample the radiance contribution of every photon into each specified direction. A variety of techniques to reduce the variance in the radiance are available but were not utilized in this study; descriptions of those techniques and how they impact the time to achieve a particular standard error can be found in [Pincus and Evans \(2009\)](#). Dividing the total number of photons simulated into a number of batches, the increment of work assigned to each processor, allows for independent batch estimates of the radiative quantities, which in turn allows the standard errors of estimated quantities to be calculated and reported. See Eq. (A1) in [appendix A](#) for the formulation of standard error in the IMC-original.

b. Addition of internal emission: The IMC+emission model

The IMC-original model with the added internal emission features described in this section will be referred to as the “IMC+emission” model. This model does not restrict thermal emission to any spectral range, and like the original model, calculations are monochromatic. The forward photon tracing technique was maintained to take advantage of the existing infrastructure within the IMC-original model. A forward tracing technique can be more computationally efficient than a backward technique when the number of output quantities is large relative to the number of emitting elements, such as simultaneous calculation of radiance into many directions. When radiance into a single direction is desired, a backward approach may be more efficient. For a discussion of trade-offs between backward and forward techniques see [Ellingson and Takara \(2005\)](#) and [Evans and Marshak \(2005\)](#).

Since the mechanisms of radiative transfer are the same regardless of the initial source of the radiation, the main algorithmic addition needed for the IMC+emission model is in the photon initialization at its source, an atmospheric constituent (gases, clouds, aerosols, etc.), or the surface. The thermally emitted photons need to be accurately distributed between the atmospheric voxels and the surface pixels, taking into account the likelihood of emission from each. Several, sometimes inconsistent, approaches to internal emission can be found in the literature ([Ellingson and Takara 2005](#); [Chen and Liou 2006](#); [Kablick et al. 2011](#); [Fauchez et al. 2014](#)). The method ultimately employed in the IMC+emission model is summarized below. Additional detail and background can be found in [Jones \(2016\)](#).

The likelihood of photon emission from a voxel within the IMC+emission model domain is governed by the

fraction of radiative power emitted by the voxel $\Phi_{\text{atm},i}$ relative to the total power emitted by the atmosphere Φ_{atm} :

$$f_{\Phi_{\text{atm},i}} = \frac{\Phi_{\text{atm},i}}{\Phi_{\text{atm}}}, \quad (1)$$

where i represents one of the total number of voxels comprising the atmosphere, $N_{\text{atm}} = N_x N_y N_z$, N_x and N_y are the number of voxels in the horizontal directions, and N_z is the number of voxels in the vertical direction. The total power emitted by the atmosphere is

$$\Phi_{\text{atm}} = \sum_{i=1}^{N_{\text{atm}}} \Phi_{\text{atm},i}, \quad (2)$$

and similarly for the surface,

$$f_{\Phi_{\text{sfc},j}} = \frac{\Phi_{\text{sfc},j}}{\Phi_{\text{sfc}}}, \quad (3)$$

$$\Phi_{\text{sfc}} = \sum_{j=1}^{N_{\text{pix}}} \Phi_{\text{sfc},j}, \quad (4)$$

where $N_{\text{pix}} = N_x N_y$ is the total number of surface pixels. For a surface pixel j having an area equal to $\Delta x \Delta y$, the spectral power emitted is

$$\Phi_j = \pi \varepsilon_{\lambda} B_{\lambda}(T_{\text{sfc}}) \Delta x \Delta y, \quad (5)$$

where ε_{λ} and T_{sfc} are the homogeneous surface emissivity and temperature and $B_{\lambda}(T_{\text{sfc}})$ is the Planck radiance for wavelength λ .

For an atmospheric voxel i of volume $V_i = \Delta x \Delta y \Delta z$, the spectral power emitted is

$$\Phi_i = \int_{4\pi} \int_V \beta_{a,i} B_{\lambda}(T_i) dV d\omega, \quad (6)$$

where $\beta_{a,i}$ is the volume absorption coefficient of voxel i accumulated across all of its contained constituents, T_i is its temperature, and ω represents the solid angle. Since the model assumes the voxel properties are internally homogeneous, Eq. (6) can be integrated to yield

$$\Phi_i = 4\pi \beta_{a,i} B_{\lambda}(T_i) \Delta x \Delta y \Delta z. \quad (7)$$

The total power emitted by the domain is the sum of the power emitted by the surface and atmosphere:

$$\Phi_{\text{domain}} = \Phi_{\text{atm}} + \Phi_{\text{sfc}}. \quad (8)$$

The total irradiance emitted by the domain F_{total} is needed by the model to convert the tallied photon

weights to radiative quantities in physical units and is given by Eq. (9), where Δx and Δy are the horizontal dimensions of each pixel:

$$F_{\text{total}} = \frac{\Phi_{\text{domain}}}{\sum_{j=1}^{N_{\text{pix}}} \Delta x \Delta y}. \quad (9)$$

The number of photons emitted by the surface is the nearest whole number of photons determined by the following relationship:

$$N_{\text{sfc}} = f_{\Phi, \text{sfc}} N_{\text{total}}, \quad (10)$$

where $f_{\Phi, \text{sfc}}$ is given by the following equation:

$$f_{\Phi, \text{sfc}} = \frac{\Phi_{\text{sfc}}}{\Phi_{\text{domain}}}. \quad (11)$$

The number of photons emitted by the atmosphere is the remainder:

$$N_{\text{atm}} = N_{\text{total}} - N_{\text{sfc}}. \quad (12)$$

When initializing a photon emitted by the atmosphere, sometimes called energy partitioning, the emitting voxel is selected by comparing a random number to the cumulative distribution of likelihood of emission for the atmosphere, which is determined by cumulatively summing the likelihood of emission determined by Eq. (1). Precise emission location within a voxel or from the surface is determined randomly from an implied uniform distribution, since the entire surface and individual pixels are considered homogeneous. Initial travel direction is assigned randomly according to the relationships described by Ellingson and Takara (2005).

The only other fundamental processes added to accurately simulate internal emission were to decrement the absorbed irradiance of the emitting column and the flux divergence of the emitting voxel and increment the radiance at the corresponding location at the top of the domain upon photon emission. Initial emission of a photon from the atmosphere decrements the flux divergence of that voxel and the absorbed irradiance of the containing column by 1.0, which is the value of the full photon weight. When calculating the contribution of a photon to the radiance emerging from a pixel at the top of the domain in a particular direction specified by the user, the phase function is used to weight the likelihood of travel in that direction. For initial emission from a voxel, the normalized isotropic phase function is $\wp(\theta) = 1/(4\pi|\mu|)$, and for initial emission from the surface, the normalized isotropic phase function of $\wp(\theta) = 1/\pi$ is used.

3. Verification

Verification of the accuracy, or benchmarking, of a 3D radiative transfer model is difficult because of the lack of an analytical solution for a heterogeneous domain. The benchmarking philosophy of the I3RC was one of intercomparison of results between various models for specific input cases. Cahalan et al. (2005) reports on simple (phase 1) and complex (phase 2) intercomparisons, which included 23 and 13 participating models, respectively. In phase 1, comparisons were made to a single reference model, while in phase 2, the consensus mean outputs from participating models were taken as the benchmark. The IMC-original was developed after phase 1 and 2 efforts. Pincus and Evans (2009) focused on comparing the IMC-original model with SHDOM, to weigh the trade-offs between cost and accuracy for both models' computation of a variety of radiative quantities.

In Cahalan et al. (2005) and in Pincus and Evans (2009), the focus was only on the solar source of radiation. For the IMC+emission model, we compare results from simulations of both solar and internal sources of radiation to analytical solutions for nonscattering atmospheres that are designed to specifically test new and altered components of the model. We also test for energy conservation and reciprocity, where appropriate, which were not considered by Cahalan et al. (2005) or Pincus and Evans (2009). Finally, we compare to SHDOM when analytical solutions are unavailable.

SHDOM is perhaps the most popular publicly available 3D radiative transfer code that includes scattering, absorption, and emission that is applicable to a wide spectral range. Its accuracy and efficiency were compared with the IMC-original model for a couple of cloud distributions by Pincus and Evans (2009). There are situation-dependent pros and cons to selecting either type of model, and interested readers should refer to Pincus and Evans (2009). Additionally, SHDOM was well within the spread of results from models participating in the I3RC (Cahalan et al. 2005). For these reasons, it is used here as a basis of comparison where analytical solutions are not available. SHDOM (Evans 1998) combines a discrete, gridded representation of the atmosphere with spherical harmonics, which speed up the calculation of the scattering integral. The model solves for source functions rather than the radiation field, since the latter can be derived from the former, and stores the source functions as spherical harmonic series at each grid point. It requires an input field of optical properties, as does the IMC+emission model, but in contrast to the IMC+emission model, it assumes those properties vary linearly between the specified values, which are the voxel vertices rather than the voxel

centers. The internal representation of the medium is interpolated trilinearly from the input optical properties, making it difficult to represent sharp boundaries on an equally spaced grid. Adaptive cell splitting is available as a feature of SHDOM but was not utilized for the present study to keep interpretation of the differences between methods simple for model inputs that are as similar as possible. The IMC+emission model's accuracy depends on the number of photons simulated, whereas SHDOM's accuracy depends on the number of streams resolved in angular space and the resolution of the grid.

Each of the major radiative quantities output by the IMC+emission model—radiance, irradiance, and per voxel flux divergence—were tested to ensure the model's accuracy for remote sensing and radiative heating applications. Tests are presented in the following subsections in order of simplest to most complex, starting with homogeneous, absorption-only cases, followed progressively by the addition of heterogeneity and scattering.

a. Isothermal, nonscattering, homogeneously absorbing atmosphere with a Lambertian surface

This simplest case of homogeneously absorbing but nonscattering atmosphere with a Lambertian surface is used to demonstrate that radiance at both nadir and off-nadir angles is calculated correctly, that the uncertainty in the solution decreases as expected with the total number of photons, and that energy is conserved within the model. To pass these tests, photon tracing and tallying must be done in an accurate way, and for an internal source of radiation, the emission must be properly divided between the surface and atmosphere.

The panel of simulations feature a $3 \times 3 \times 20$ voxel domain that extends 3 km in each horizontal direction and 2 km vertically. For the simulations with atmospheric absorption, the volume extinction coefficient was set to 0.1 km^{-1} , and the single-scattering albedo was set to 0.0 to preclude scattering. For the solar source simulations, the incoming solar irradiance was set to $1 \text{ W m}^{-2} \mu\text{m}^{-1}$ with overhead sun. The infrared emission simulations were conducted at $\lambda = 11.0 \mu\text{m}$, the atmospheric temperature was 303.1 K, and the surface temperature was also

303.1 K. In all simulations, the surface was considered Lambertian, with an albedo of 0.0, 0.3, or 1.0. Each batch contained 50 000 photons, and there were 20 000 batches for a total of 10^9 photons per simulation.

Energy conservation in the IMC+emission model can be demonstrated with a couple of these simple setups. For a solar source of photons and a surface albedo of 1.0, the average irradiance absorbed by the domain [$F_{\text{abs}} = 0.423\,697\,(11) \text{ W m}^{-2} \mu\text{m}^{-1}$] and the average irradiance exiting the domain [$F^\uparrow = 0.576\,303\,(13) \text{ W m}^{-2} \mu\text{m}^{-1}$] sum to [$F^\uparrow = 1.000\,000\,(17) \text{ W m}^{-2} \mu\text{m}^{-1}$] the irradiance entering the domain. Here and throughout, the two digits in parentheses represent the computed standard error in the last two reported digits of the radiative quantity with the same units as that quantity [e.g., $0.423\,697\,(11) \text{ W m}^{-2} \mu\text{m}^{-1}$ is equivalent to $0.423\,697 \pm 0.000\,011 \text{ W m}^{-2} \mu\text{m}^{-1}$]. For an internal emission source of photons with no atmosphere and surface albedo of 0.0 (emissivity of 1.0), the total irradiance emitted by the surface ($F_{\text{emitted}} = 31.4650 \text{ W m}^{-2} \mu\text{m}^{-1}$) does equal the average irradiance exiting the top of the domain [$F^\uparrow = 31.4650\,(20) \text{ W m}^{-2} \mu\text{m}^{-1}$]. For the same setup but an emitting surface with an albedo of 0.3 (emissivity of 0.7), total irradiance emitted by the surface ($F_{\text{emitted}} = 22.0255 \text{ W m}^{-2} \mu\text{m}^{-1}$) also equals the average irradiance exiting the top of the domain [$F^\uparrow = 22.0255\,(14) \text{ W m}^{-2} \mu\text{m}^{-1}$]. Thus, energy conservation is obeyed by the model within the precision of the simulations, 0.0017%–0.0064% in the above cases.

For an absorbing but nonscattering atmosphere with a Lambertian surface, an analytical solution for the top-of-domain upward radiance from an internal emission source is given by the following equation (see [appendix B](#), section a, for a detailed derivation), where $I^\uparrow(\infty, \mu)$ is the upwelling radiance at the top of the atmosphere, τ^* and t^* are the total vertical optical depth and transmittance of the atmosphere, μ is the cosine of the simulated detector's zenith angle, Ei represents the exponential integral, ε_λ is the surface emissivity (1.0 minus albedo), T_a is the atmospheric temperature, and T_s is the surface temperature:

$$I^\uparrow(\infty, \mu) = \{\varepsilon_\lambda B(T_s) + (1 - \varepsilon_\lambda) B_\lambda(T_a) [-t^*(1 - \tau^*) + (-\tau^*)^2 \text{Ei}(-\tau^*) + 1]\} t^{*1/\mu} + B_\lambda(T_a) (1 - t^{*1/\mu}). \quad (13)$$

For an absorbing but nonscattering atmosphere and a Lambertian surface, the analytical solution to the top-of-atmosphere outgoing radiance for a solar source is given by Eq. (14), where μ_0 is the cosine of the solar

zenith angle and S_0 is the incoming monochromatic solar irradiance at the top of the domain:

$$I^\uparrow(\infty, \mu) = \frac{S_0}{\pi} (t^{*1/\mu+1/\mu_0}) (1 - \varepsilon_\lambda). \quad (14)$$

TABLE 1. IMC+emission-modeled 11- μm nadir radiance for isothermal, homogeneously absorbing atmospheres with Lambertian lower boundaries compared to the expected radiance from analytically derived solutions [e.g., Eqs. (13) and (14)]. A total of 10^9 photons were simulated from 20 000 batches of 50 000 photons each. The last two digits in parentheses represent the uncertainty in the last two digits of the radiance.

Source	Atmosphere	Albedo	Expected radiance ($\text{W m}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$)	Simulated radiance ($\text{W m}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$)
Solar	None	0	0	0
Solar	None	0.3	0.095 493 0	0.095 491 0 (86)
Solar	None	1	0.318 310	0.318 326 (29)
Solar	Absorbing	1	0.213 369	0.213 372 (21)
Solar	Absorbing	0.3	0.064 010 8	0.064 011 6 (64)
Solar	Absorbing	0	0	0
Emission	Absorbing	0	10.0156	10.0157 (10)
Emission	Absorbing	0.3	8.284 04	8.284 24 (80)
Emission	Absorbing	1	4.243 66	4.243 84 (42)
Emission	None	1	0	0
Emission	None	0.3	7.010 94	7.011 30 (63)
Emission	None	0	10.015 64	10.016 14 (90)

The results for a nadir view angle are summarized in Table 1. Note that all simulated results are within their standard errors to the expected result and the differences between the analytical solutions and simulated results are within 0.005%. These results confirm that, for the simple case of overhead sun or internal emission and a nonscattering atmosphere in a homogeneous isothermal domain, the simulated nadir radiance is consistent with expectations derived from an analytical solution. This indicates that, for these simple setups, the division of emitted photons between the surface and the atmosphere and the contribution of each photon's emission to the radiance are handled correctly.

The accuracy of radiance values at off-nadir angles for the above simulations was also tested. Where applicable, the solar geometry was $\mu_0 = 1.0$ and $\phi_0 = 60^\circ$. The results are summarized in Table 2 for the following

simulated detector angles θ : 30° , 60° , and 88° . Results are well within the standard error from the expected radiance. The difference between the simulated radiance and the expected value is within 0.005% for the 10^9 simulated photons. This indicates that the contribution from emitted photons to the radiance is handled properly even at off-nadir angles.

Finally, we ran simulations as a function of the total number of photons simulated N_{total} to see if we get the expected $1/\sqrt{N_{\text{total}}}$ drop in standard error in the radiance and to detect any model biases due to numerical implementation and the discrete nature of computing. For each total number of photons, four simulations were carried out for the internal emission case with a surface albedo of 0.3 with atmospheric emission. The number and size of the batches used to compute each simulation are available in the online supplementary material.

TABLE 2. IMC+emission-modeled 11- μm radiance for isothermal, homogeneously absorbing atmospheres with Lambertian lower boundaries compared to analytically derived solutions for $\theta = 30^\circ$, 60° , and 88° . A total of 10^9 photons were simulated from 20 000 batches of 50 000 photons each. The last two digits in parentheses represent the uncertainty in the last two digits of the radiance.

Source	Atmosphere	Albedo	Radiance ($\text{W m}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$)					
			30°		60°		88°	
			Expected	Simulated	Expected	Simulated	Expected	Simulated
Solar	None	0	0	0	0	0	0	0
Solar	None	0.3	0.095 493 0	0.095 491 0 (85)	0.095 493 0	0.095 491 0 (85)	0.095 493 0	0.095 491 0 (85)
Solar	None	1	0.318 310	0.318 326 (28)	0.318 310	0.318 326 (28)	0.318 310	0.318 326 (28)
Solar	Absorbing	1	0.206 869	0.206 869 (21)	0.174 692	0.174 694 (17)	$8.455\,94 \times 10^{-4}$	$8.455\,92\,(44) \times 10^{-4}$
Solar	Absorbing	0.3	0.062 060 7	0.062 061 5 (62)	0.052 407 7	0.052 408 0 (52)	$2.536\,78 \times 10^{-4}$	$2.536\,65\,(25) \times 10^{-4}$
Solar	Absorbing	0	0	0	0	0	0	0
Emission	Absorbing	0	10.015 64	10.015 61 (99)	10.015 64	10.015 85 (92)	10.015 64	10.0152 (24)
Emission	Absorbing	0.3	8.336 80	8.336 93 (42)	8.597 93	8.598 18 (75)	10.008 82	10.0073 (22)
Emission	Absorbing	1	4.419 51	4.419 65 (42)	5.289 94	5.290 10 (44)	9.9928	9.9922 (16)
Emission	None	1	0	0	0	0	0	0
Emission	None	0.3	7.010 94	7.011 30 (63)	7.010 94	7.011 30 (63)	7.010 94	7.011 30 (63)
Emission	None	0	10.015 64	10.016 14 (90)	10.015 64	10.016 14 (90)	10.015 64	10.016 14 (90)

FIG. 1. For internal emission at $11\mu\text{m}$ in an isothermal, homogeneously absorbing atmosphere with a surface albedo of 0.3, (a) markers represent sample standard error from IMC+emission normalized by the sample radiance and the line is the expected $1/\sqrt{N_{\text{total}}}$ relationship and (b) IMC+emission modeled radiance as a function of total number of photons, including the analytical solution (thick black line) and standard error for each realization (thin lines).

Figure 1a shows the $1/\sqrt{N_{\text{total}}}$ drop in standard error of the radiance with increasing total number of photons. Figure 1b shows the simulated radiance and its standard error, as well as the analytical solution. While it is difficult to see, we note at 10^{10} simulated photons, all four simulations are larger than the analytical solution by about 0.002%, suggesting a slight bias given that the four simulations have a precision of 0.001%. This may arise from the accumulation of tiny errors over the numerous discrete computations involved.

b. Isothermal, nonscattering, homogeneously absorbing atmosphere with nonreflecting surface

This case demonstrates that upward irradiances at the top of the domain and downward irradiances at the surface are calculated correctly by comparing to analytical solutions. Comparisons to SHDOM are also provided to establish a baseline for comparison before moving on to cases for which there is no analytical solution. A variety of relationships between surface and atmospheric temperature with a small total optical depth are tested in addition to a more optically thick case. To pass this test, the isotropic phase function used to assign a photon's initial direction of travel must be correctly implemented as well as the accurate partitioning of emitted photons between the surface and the atmosphere given differing temperatures.

The panel of simulations feature a $3 \times 3 \times 20$ voxel domain that extended 3 km in each horizontal direction and 2 km vertically. The infrared wavelength simulated is $11.0\mu\text{m}$. The total vertical optical depth of the domain, surface temperature, and atmospheric temperature is listed next to the results in Tables 3 and 4. The IMC+emission simulations consisted of 3.2×10^9 photons, while the SHDOM results were achieved with 32 streams in zenith and 32 streams in azimuth.

Analytical solutions for the upward irradiance at the top of the domain $F^\uparrow(z = \infty)$ and downward irradiance at the surface $F^\downarrow(z = 0)$ for the simple case of a homogeneous, isothermal, and nonscattering atmosphere with no surface reflection or external sources of radiation are given by the following equations (see appendix B, section b, for full derivations):

$$F^\uparrow(z = \infty) = \pi(B(T_a) + [B(T_s) - B(T_a)]\{t^{*1/\mu}[\ln(t^*) + 1] + \ln^2(t^*)\text{Ei}[\ln(t^*)]\})), \quad (15)$$

$$F^\downarrow(z = 0) = \pi B(T_a)\{1 - t^*[\ln(t^*) + 1] + \ln^2(t^*)\text{Ei}[\ln(t^*)]\}. \quad (16)$$

As shown in Tables 3 and 4, IMC+emission has no detectable bias down to the precision of the simulations ($<0.01\%$). The SHDOM results show a positive bias of up to 0.27% relative to the analytical solutions. For the case with emission from the atmosphere but not the surface ($T_s = 0.0\text{K}$), the upward irradiance at the top of the domain and downward irradiance at the surface are within their standard errors of each other. This demonstrates that the isotropic phase function used to select an atmospherically emitted photon's initial direction of travel was implemented correctly—equal amounts of irradiance are directed upward and downward. This set of simulations with varying relationships between

TABLE 3. Upward $11\text{-}\mu\text{m}$ irradiance $F^\uparrow(z = \infty)$ at the top of the domain for isothermal, homogeneously absorbing atmospheres with blackbody surfaces and no external sources of radiation. The last two digits in parentheses represent the uncertainty in the last two digits of the irradiance. A total of 3.2×10^9 photons were simulated.

Surface temperature (K)	Atmospheric temperature (K)	Total optical depth	Simulated irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)	Expected irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)	SHDOM irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)
0	303.1	0.2	9.317 46 (79)	9.317 10	9.342 60
303.1	303.1	0.2	31.4650 (22)	31.4651	31.4890
313.1	303.1	0.2	34.7889 (24)	34.7890	34.8130
293.1	303.1	0.2	28.3977 (20)	28.3975	28.4210
275	266	1.12	17.6959 (22)	17.6944	17.7070

surface temperature and atmospheric temperature again indicate that the partitioning of emitted photons between the surface and atmosphere is handled correctly. This holds for relatively warm and cold temperatures and for optically thin and optically thick atmospheres.

c. Nonisothermal, homogeneously nonscattering, absorbing atmosphere with nonreflecting surface

Domains with homogeneous absorption but vertically varying temperature profiles were also used to test an emission of $11.0\text{-}\mu\text{m}$ nadir radiance. This set of simulations demonstrates that partitioning of photon emission from layers with varying temperature is done properly.

The domain for these simulations was $3 \times 3 \times 20$ voxels or $3.0\text{ km} \times 3.0\text{ km} \times 2.0\text{ km}$. The surface was nonreflecting and had a temperature of 303.1 K. The volume extinction coefficient was set to 0.1 km^{-1} and the single-scattering albedo set to 0.0. The simulations consisted of 3.2×10^9 photons. For the isothermal atmosphere control simulation, the atmospheric temperature was set to 303.1 K. For the decreasing temperature profile, the atmospheric temperature decreased linearly with height from 303.1 K at the surface to 273.1 K at the top of the domain. For the increasing temperature profile, the atmospheric temperature increased linearly with height from 273.1 K at the surface to 303.1 K at the top of the domain.

The nadir radiance leaving a plane-parallel atmosphere with internal sources of radiation only, no

scattering, and in stacked isothermal layers, each having the same transmittance t but differing temperatures T_i is given by the following equation:

$$I^\uparrow(\infty, \mu = 1) = B(T_s)t^n + \sum_{i=1}^n B(T_i)(1-t)t^{n-i}. \quad (17)$$

The first term on the right-hand side is the product of the radiance emitted by the surface and the transmittances of the layers above it. The second term is the product of the Planck radiance emitted by a layer of the atmosphere, the emissivity of the layer, and the transmittances of the layers above it, summed over all n layers. The expected radiance for the cases described above is determined by setting $n = 20$ in Eq. (17). The nadir radiance results are displayed in Table 5, showing that the simulated radiances all match the analytical solutions to better than 0.05%, which is well within the precision of the simulations.

d. Two-layer horizontally homogeneous, nonscattering, absorbing atmosphere with Lambertian surface

This test examines the flux divergence field when both temperature and absorptive properties vary between model levels without the complication of scattering. To pass this test, the partitioning of photon emission between atmospheric layers with different temperatures and emission coefficients must be done correctly. Results are compared with another 3D model, SHDOM.

TABLE 4. Downward irradiance $F^\downarrow(z = 0)$ at the surface for homogeneous, isothermal, nonscattering atmospheres with blackbody surfaces and no external sources of radiation. The last two digits in parentheses represent the uncertainty in the last two digits of the irradiance.

Surface temperature (K)	Atmospheric temperature (K)	Total optical depth	Simulated irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)	Expected irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)	SHDOM irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)
0	303.1	0.2	9.316 82 (80)	9.317 10	9.342 60
303.1	303.1	0.2	9.3170 (12)	9.3171	9.342 60
313.1	303.1	0.2	9.3168 (12)	9.3171	9.342 60
293.1	303.1	0.2	9.3169 (12)	9.3171	9.342 60
275	266	1.12	13.9321 (19)	13.9327	13.9460

TABLE 5. Nadir $11\text{-}\mu\text{m}$ radiance exiting nonisothermal atmospheres with homogeneous absorption and blackbody surfaces for different temperature profiles. The last two digits in parentheses represent the uncertainty in the last two digits of the radiance. A total of 3.2×10^9 photons were simulated.

Temperature profile	Simulated radiance ($\text{W m}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$)	Expected radiance ($\text{W m}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$)
Decreasing	9.743 (75)	9.742
Increasing	9.754 (75)	9.755
Isothermal	10.010 (80)	10.016

The infrared wavelength used for these simulations was $4.0\text{ }\mu\text{m}$ so that there would be a significant contribution from both solar and internal emission sources. The panel of simulations feature a $3 \times 3 \times 20$ voxel domain that extended 3 km in each horizontal direction and 2 km vertically. The lowest 10 atmospheric layers had a volume extinction coefficient of 0.5 km^{-1} and a temperature of 293.1 K. The upper 10 atmospheric layers had a volume extinction coefficient of 0.1 km^{-1} and a temperature of 303.1 K. The single-scattering albedo was set to 0.0 throughout the atmosphere. The surface albedo was 0.3, and the surface temperature was 303.1 K. For the solar simulation, the incoming solar irradiance was set to $8.6\text{ W m}^{-2} \mu\text{m}^{-1}$, $\mu_0 = 0.866$, and $\phi_0 = 60^\circ$. For the IMC+emission simulations, 50 000 photons per batch and 20 000 batches were used for a total of 10^9 photons. For the SHDOM simulations, 32 streams in zenith and 32 streams in azimuth were used.

Figure 2 shows domain-mean profiles of flux divergence as simulated by the IMC+emission model and SHDOM for both solar and internal emission sources. The slight discrepancy between the IMC+emission model and SHDOM at the layer interface is because the properties are defined at slightly offset locations. SHDOM properties are defined at voxel vertices, and IMC+emission model properties are defined at voxel centers. So the height of the boundary between the two layers is slightly different between the IMC+emission and SHDOM. Overall, the domain-mean flux divergence profiles agree very well. This demonstrates that partitioning of photon emission between atmospheric layers with different temperatures and emission coefficients is done correctly as well as the calculation of flux divergence.

e. Nonscattering and absorbing cubic cloud set in a nonscattering and absorbing atmosphere with nonreflecting surface

In a horizontally heterogeneous but nonscattering atmosphere, the emitted radiance exiting each pixel at the top of the domain at nadir should be equal to the nadir radiance exiting a plane-parallel domain with the

FIG. 2. Domain-average profiles of flux divergence from both internal (solid) and solar (dashed) sources at $4.0\text{ }\mu\text{m}$ for a two-layer nonscattering atmosphere with surface albedo of 0.3 from SHDOM (blue) and the IMC+emission model (red). IMC+emission standard error is about $1.0 \times 10^{-4} \text{ W m}^{-3} \mu\text{m}^{-1}$. A total of 10^9 photons were simulated.

same vertical distribution of properties as the column below that pixel if partitioning of the photons horizontally and vertically, the photon emission and tracing, and calculation of the contribution to radiance are being done correctly. Figure 3 represents a vertical cross section through the centers of the domains used for this test. Figures 3a and 3b show plane-parallel, two-layer atmospheres with upper-layer properties corresponding to either the cubic cloud or the surrounding atmosphere shown in Fig. 3c. The thickness of both layers is 1 km. All simulations were done at an infrared wavelength of $11.0\text{ }\mu\text{m}$. The spatial distribution of temperatures and volume absorption coefficients are as shown in Fig. 3. The panel of simulations feature a $3 \times 3 \times 20$ voxel domain that extended 3 km in each horizontal direction and 2 km vertically. The IMC+emission model simulated 20 000 batches of 50 000 photons each for a total of 10^9 photons.

Table 6 shows the nadir radiances for the setup in Fig. 3. As expected, to within the precision of the simulations, the average nadir radiance leaving the domain shown in Fig. 3a, I_a , is equivalent to the nadir radiance leaving the perimeter of the domain in Fig. 3c, I_{c1} , and the nadir radiance leaving the domain shown in Fig. 3b, I_b , is equivalent to the nadir radiance exiting the center of the domain in Fig. 3c, I_{c2} . Thus, partitioning, tracing, and radiance contribution are verified in this first 3D case.

FIG. 3. Schematic representation of domain setup for experiment. (a),(b) Nadir radiance simulated by plane-parallel two-layer domains was compared to (c) radiance values from like components of the cubic cloud domain. Single-scattering albedo is 0.0 everywhere.

TABLE 6. Nadir $11\text{-}\mu\text{m}$ radiance simulated by plane-parallel two-layer domains (Figs. 3a,b) was compared to radiance values from like components of the cubic cloud domain (Fig. 3c). The last two digits in parentheses represent the uncertainty in the last two digits of the radiance. A total of 10^9 photons were simulated.

	Cubic domain simulated radiance ($\text{W m}^{-2} \text{ sr}^{-1} \mu\text{m}^{-1}$)	Plane-parallel simulated radiance ($\text{W m}^{-2} \text{ sr}^{-1} \mu\text{m}^{-1}$)
Setup in Fig. 3a	$I_{c1} = 7.431\,26\,(80)$	$I_a = 7.431\,35\,(76)$
Setup in Fig. 3b	$I_{c2} = 7.269\,92\,(55)$	$I_b = 7.268\,76\,(71)$

f. Isothermal, homogeneously scattering and absorbing cubic cloud in a homogeneously scattering and absorbing atmosphere with a nonreflecting surface

As a final benchmark of irradiance and flux divergence, a domain incorporating spatial heterogeneity and cloudlike optical properties, including scattering, was designed. Its high-spatial-resolution grid allows for diagnosis of the spatial pattern of irradiance and flux divergence rather than just domain means or profiles. Incorporating scattering into a cubic cloud set in a scattering atmosphere precludes an analytically derived solution. So radiative quantities from the IMC+emission model are compared with those from SHDOM, bearing in mind the small SHDOM bias revealed in section 3b and the effect of grid interpolation revealed in section 3d.

The infrared wavelength used for these simulations was $4.0\,\mu\text{m}$ so that there would be a significant contribution from both solar and thermal emission sources. The domain was $100 \times 100 \times 36$ voxels, corresponding to $6.67 \text{ km} \times 6.67 \text{ km} \times 1.44 \text{ km}$. The atmosphere can be described as follows and is visualized by Fig. 4. The atmospheric temperature, volume extinction coefficient, and single-scattering albedo were homogeneous and equal to 293.1 K , 0.1 km^{-1} , and 0.5 , respectively. The Rayleigh phase function was used to represent molecular scattering. The cloud was placed in the center of the domain, extended from 0.48 to 0.96 km vertically, and was about 1.334 km in each horizontal direction. The scattering phase function within the cloud was calculated from Mie theory and was representative of a gamma distribution of water droplets with $\alpha = 7$ and effective radius of approximately $8.6\,\mu\text{m}$ with a single-scattering albedo of 0.5 . The volume extinction of the cloud was set to 21.0 km^{-1} . The surface albedo was 0.0 , and the surface temperature was 298.1 K . For the solar simulation, the incoming solar irradiance was set to $8.6 \text{ W m}^{-2} \mu\text{m}^{-1}$, $\mu_0 = 0.866$, and $\phi_0 = 60^\circ$. For the IMC+emission simulations, $50\,000$ photons per batch and $200\,000$ batches were used for a total of about 10^{10}

FIG. 4. Schematic representation of domain setup for isothermal, absorbing, and scattering cubic cloud in an absorbing and scattering atmosphere over a nonreflective surface.

photons. This is an increase from previous tests, designed to reduce Monte Carlo noise, since results will be compared to SHDOM on a per pixel basis in a higher-resolution domain. For the SHDOM simulations, 32 streams in zenith and 32 streams in azimuth were used.

The upward irradiance at the top of the domain and downward irradiance at the surface from an internal emission source for both SHDOM and the IMC+emission model are shown in Figs. 5 and 6, respectively. Some geometrically shaped artifacts are apparent in the SHDOM solution, and some Monte Carlo noise is apparent in the IMC+emission solution. Maximum pixel-level differences between models are about 1% for upward irradiance and about 4% for downward irradiance. Results of domain-average upward irradiance at the top of the domain and downward irradiance at the surface are listed in Table 7. SHDOM and IMC+emission domain-average irradiance are within 0.046%–2.6% of one another.

Profiles of domain mean flux divergence for both the solar and internal emission simulations were also constructed (Fig. 7). Two sets of SHDOM simulations are plotted to show the effect of the difference between input specifications for each model. One SHDOM simulation is of a cloud whose outer vertices are at the location of the outer edge of the cloudy voxels of the IMC+emission domain's cloud. For the other SHDOM simulation, the outer vertices specified cloudy are at the inner edge of the cloudy voxels of the IMC+emission domain's cloud. Elsewhere in this section, only results from the smaller-footprint cloud are shown. The peaks in the IMC+emission flux divergence profile (red lines) lie between the two SHDOM profiles vertically, because of the physical height difference in the cloud boundary. For the internal thermal emission simulations (solid lines),

FIG. 5. Upward $4\text{-}\mu\text{m}$ irradiance at the top of the domain $F^\uparrow(z = \infty)$ of internally emitted radiation for a cubic cloud embedded in an isothermal atmosphere from (a) the IMC+emission model and (b) SHDOM. Pixel-level standard error in the IMC+emission irradiance is about $0.0027 \text{ W m}^{-2} \mu\text{m}^{-1}$. A total of 10^9 photons were simulated.

the IMC+emission has the largest magnitude of flux divergence at cloud top. This is likely due to the sharper difference in optical properties in the IMC+emission compared to the interpolated relaxation of the properties between cloudy and clear vertices in SHDOM. In the solar simulations (dashed lines), the difference in cloud footprint is the dominant effect rather than the gradient in optical properties. Above and below the cloud, there is a cooling from atmospheric emitted radiation being absorbed by the surface or exiting the domain top. The cooling within the cloud layer is also influenced by radiation emitted out the sides of the clouds to the surrounding atmosphere. The profile of flux divergence of solar radiation is also stronger at cloud top than at cloud base; as radiation is attenuated in the cloud, less is available for absorption deeper in the cloud.

FIG. 6. Downward $4\text{-}\mu\text{m}$ irradiance at the surface $F^\downarrow(z=0)$ of internally emitted radiation for a cubic cloud embedded in an isothermal atmosphere from (a) the IMC+emission model and (b) SHDOM. Pixel-level standard error in the IMC+emission irradiance is about $0.0011 \text{ W m}^{-2} \mu\text{m}^{-1}$. A total of 10^{10} photons were simulated.

Figures 8 and 9 show horizontal cross sections of flux divergence through the center of the cloud (zoomed in to the immediate cloud area to show detail) from SHDOM (Figs. 8a,b and 9a,b) and the IMC+emission model (Figs. 8c and 9c) and separated by photon source: atmosphere and surface emission (Fig. 8) and solar (Fig. 9). There are two SHDOM cross sections

presented for every IMC+emission model cross section because the SHDOM reporting levels are staggered to the IMC+emission model levels. The first apparent feature is the Monte Carlo noise in the IMC+emission solution (Fig. 8c). Looking past the noise, Fig. 8c shows strong cloud-edge cooling ($\sim 6 \text{ W m}^{-3} \mu\text{m}^{-1}$) due to the differences in optical properties between cloud and atmosphere, especially at the cloud corners, where the cooling is maximum ($\sim 10 \text{ W m}^{-3} \mu\text{m}^{-1}$). That magnitude of cooling is not seen from SHDOM, which has cloud-edge cooling of about $5 \text{ W m}^{-3} \mu\text{m}^{-1}$ and cloud-corner cooling of about $8 \text{ W m}^{-3} \mu\text{m}^{-1}$. With $\phi_0 = 60^\circ$ and $\mu_0 = 0.866$ for the solar source in mind, Fig. 9c shows stronger absorption on the cloud sides facing the solar source ($\sim 29\text{--}44 \text{ W m}^{-3} \mu\text{m}^{-1}$). That magnitude of heating is not apparent at either level of the SHDOM simulation ($\sim 13\text{--}32 \text{ W m}^{-3} \mu\text{m}^{-1}$), although the same spatial pattern of heating occurs. This is again likely due to the interpolation of values between grid points done by SHDOM. For grid resolutions and property specifications that are as identical as possible, SHDOM is not naturally able to represent the sharp gradients in properties, which translates to lower-magnitude flux divergence.

In summary, internal emission as a source of photons has been added to the IMC-original model to produce the IMC+emission model. The resulting radiance, irradiance, and flux divergence calculations have been tested and their accuracy verified by analytical solutions and energy conservation. Comparisons were also made to SHDOM, showing good general agreement, with differences largely attributable to the grid setup—homogeneous voxels versus interpolation between vertices.

4. A benchmark for realistic distributions of clouds

As part of phase 2 of I3RC (Cahalan et al. 2005), there were optional experiments at $11.0 \mu\text{m}$ for which 3D distributions of cloud LWC and effective radius from LES, a profile of molecular absorption, aerosol optical properties, and a domain constant profile of atmospheric temperature were provided. They can be retrieved at the I3RC website (<http://i3rc.gsfc.nasa.gov/input/heatingrate.html>).

TABLE 7. Domain-average upward $4\text{-}\mu\text{m}$ irradiance at the top of the domain and downward $4\text{-}\mu\text{m}$ irradiance at the surface from solar and internal emission sources for both SHDOM and IMC+emission model simulations of a cubic cloud in an isothermal atmosphere. The last two digits in parentheses represent the uncertainty in the last two digits of the irradiance. A total of 10^{10} photons were simulated.

Photon source	Simulated upward irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)	SHDOM upward irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)	Simulated downward irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)	SHDOM downward irradiance ($\text{W m}^{-2} \mu\text{m}^{-1}$)
Solar	0.248 764 2 (93)	0.250 055 5	6.242 692 (67)	6.206 882
Internal	1.927 911 (27)	1.927 149	0.406 329 (11)	0.417 156

FIG. 7. Domain-average profiles of IMC+emission (red) and SHDOM (blue and green) flux divergence from both internal emission (solid) and solar (dashed) sources at $4.0\text{ }\mu\text{m}$ for a cubic cloud in an isothermal absorbing and scattering atmosphere with a black surface. Two SHDOM simulations show that slightly larger (blue) and smaller (green) clouds bound the results from IMC+emission. IMC+emission standard error is about $2.0 \times 10^{-5}\text{ W m}^{-3}\text{ }\mu\text{m}^{-1}$. A total of 10^{10} photons were simulated.

The domain consists of $100 \times 100 \times 36$ voxels, corresponding to $6.67\text{ km} \times 6.67\text{ km} \times 1.44\text{ km}$. Figure 10 shows the temperature profile (Fig. 10a), cloud-top heights (Fig. 10b), and the planar view of the cloud optical depth (Fig. 10c) for the cumulus fields of case 4. However, none of the participant models submitted results for the thermal emission tests, likely because most participant models did not support internal emission. Since the IMC+emission model's veracity has been verified in section 3, the simulations presented below can act as a benchmark result for model intercomparisons, for example, a new round of I3RC activities, at least until another model's veracity has been similarly demonstrated.

a. No scattering or surface reflection

To create an absorption-only version of case 4, the volume extinction coefficient of the cloud water in each voxel was set to the volume absorption coefficient; hence, the single-scattering albedo was set to 0.0. The profile of molecular absorption was retained. The molecular (Rayleigh) scattering component was turned off, the aerosol optical properties were ignored, and the surface is a blackbody. The surface temperature was prescribed at 303.1 K. The simulation consisted of 10^{10} photons. Figure 11 shows the nadir radiance (Fig. 11a)

FIG. 8. Horizontal cross sections of $4\text{-}\mu\text{m}$ flux divergence through the two levels closest to center of the cloud at (a) 0.76 and (b) 0.72 km from an SHDOM simulation of internal emission and (c) through the center of the cloud (0.74 km) from an IMC+emission simulation of internal emission. Voxel-level standard error in the IMC+emission flux divergence is about $0.0098\text{ W m}^{-3}\text{ }\mu\text{m}^{-1}$. A total of 10^{10} photons were simulated.

FIG. 9. Horizontal cross sections of $4\text{-}\mu\text{m}$ flux divergence through the two levels closest to center of the cloud at (a) 0.76 and (b) 0.72 km from an SHDOM simulation of a solar source and (c) through the center of the cloud (0.74 km) from an IMC+emission simulation of a solar source. Voxel-level standard error in the IMC+emission flux divergence is about $0.0009 \text{ W m}^{-3} \mu\text{m}^{-1}$. A total of 10^{10} photons were simulated.

FIG. 10. Several parameters of the I3RC case 4 cumulus domain: (a) temperature profile, (b) cloud-top height, and (c) planar view of total optical depth.

and standard error expressed as a percentage of the pixel radiance (Fig. 11b) as well as the brightness temperature (Fig. 11c) for the case 4 simulation. Most of the non-cloud-covered pixels show a brightness temperature between 301 and 302 K as expected given the molecular absorption and the atmospheric temperature profile. In optically thick regions, cloud-top brightness temperatures are at their coldest, between 288 and 290 K, for the highest cloud tops, which is again consistent with Fig. 10.

FIG. 11. IMC+emission model results for the I3RC case 4 cumulus domain at $11.0\ \mu\text{m}$ considering absorption and emission only: (a) nadir radiance, (b) nadir radiance standard error as a percentage of the radiance, and (c) brightness temperature. A total of 10^{10} photons were simulated.

In the most optically thin cloud-covered regions, surface contributions to warmer brightness temperatures are evident.

b. Scattering and absorbing clouds and atmosphere with Lambertian surface

Figure 12 represents the case 4 simulation with cloud and molecular absorption and cloud scattering taken into account as well as surface reflection but not aerosol optical properties. The surface albedo was set to 0.1, and the surface temperature was set to 303.1 K. The simulation consisted of 10^{10} photons. The differences in the radiance compared to the previous case, which had no scattering in the atmosphere or off the surface, are as expected. For example, there is a net reduction of radiance in the clear pixels relative to those in Fig. 11a, owing to the lower surface emissivity. However, a lower surface emissivity gives rise to a larger surface albedo. As a result, the contribution to the clear-sky radiance from radiation originating in the cloud and scattering off the surface and molecular atmosphere is evident, with the largest contributions occurring closest to the cloud. The influence of scattering on cloudy pixel radiance for this simulation is minor as expected given the low single-scattering albedo for cloud drops in this simulation.

c. Demonstration of directional reciprocity

Like energy conservation, reciprocity is a fundamental benchmark that should be obeyed by the model under appropriate boundary conditions and proper model setup, even in a heterogeneous environment. Here, we use the same distribution of cloud as above in case 4 but with cloud and molecular optical properties at $\lambda = 2.13\ \mu\text{m}$, including molecular scattering, a surface albedo of 0.0, and a solar source only. While the pixel-level bidirectional reflectance distribution functions (BRDFs) at the top of the domain are not expected to obey directional reciprocity (Di Girolamo et al. 1998; Di Girolamo 1999), the domain-averaged BRDF should exactly obey directional reciprocity (Di Girolamo 2002); that is, the domain-averaged BRDF is invariant when solar and viewing angles are interchanged. We run two simulations of 200 000 batches of 50 000 photons for total of 10^{10} photons per simulation. The first simulation has $\theta = 30^\circ$ and $\phi = 10^\circ$, while $\theta_0 = 60^\circ$ and $\phi_0 = 240^\circ$. In the second simulation, $\theta = 60^\circ$ with $\phi = 240^\circ$, while $\theta_0 = 30^\circ$ and $\phi_0 = 10^\circ$. The domain-averaged BRDF is calculated by normalizing the domain-averaged radiance by the solar zenith angle, giving us a domain-averaged BRDF of 0.019 862 3 (26) for the first simulation and 0.019 857 3 (35) for the second simulation. Thus, the two values are indistinguishable from each other within the precision of the simulations (0.02%), implying that domain-averaged directional reciprocity is obeyed by our model.

We note that phases 1 and 2 of I3RC also provided several sun-view geometry reciprocal experiments, but

FIG. 12. IMC+emission model results for the I3RC case 4 cumulus domain at $11.0\ \mu\text{m}$ considering absorption, emission, and scattering: (a) nadir radiance, (b) nadir radiance standard error as a percentage of the radiance, and (c) brightness temperature. The color bar is the same as Fig. 11 for easier comparison. A total of 10^{10} photons were simulated.

only the phase 1 “step cloud” case is expected to obey domain-averaged directional reciprocity, since all other cases involved a nonreciprocal surface boundary condition. Of the 21 participating Monte Carlo models, only 9 ran both reciprocal sets for the step-cloud case and reported standard errors for their simulations. We examined their values for the setup with single-scattering albedo of 1.0, as archived at the I3RC website, and found that only one model (from the Institute of Atmospheric Optics, Russia) obeyed reciprocity to within the precision of its simulations (0.06%). Deviations from reciprocity were smaller than 1.0% for four of the models and between 1% and 3% for the remaining four models. SHDOM deviated from reciprocity for this case by 0.2% and 0.5%, respectively, for the low-resolution and high-resolution model setups that were used. Our simulations for the step-cloud case obeyed reciprocity to within the precision of our simulations (0.02%).

5. Computational performance

One of the best features of a Monte Carlo model, from a computational standpoint, is the independent nature of the samples, in this case, batch estimates of radiative quantities. This means that work can be easily parallelized. The MPI paradigm is used for parallelization in this model. The total number of batches are divided evenly among processes, and each batch is independent and indistinguishable from any other batch, so processes need no knowledge of the results from other processes. Therefore, communication, which can reduce the code’s scalability if done often, is limited to one collective call at the end of the simulation to sum results across all processes. There are some limiting factors on the configuration of batch size and number of batches. For example, standard error can only be estimated for more than one batch, and memory constraints put an upper limit on the number of photons per batch. For various configurations of batch size and number of batches that equal the same total number of photons, we can assume the compute time used in the actual photon tracing is the same. So the only factors impacting the total compute time are the per-batch and per-process overhead: the fewer batches and processes, the less overhead. However, in terms of wall-clock time, more batches allow for more parallelization over more processes to arrive at the answer sooner.

All simulations presented here were completed on the Blue Waters supercomputer. The Blue Waters system (Bode et al. 2013) employs the Cray Gemini interconnect between nodes, which implements a 3D torus topology. Blue Waters is composed of 22 640 Cray XE6 nodes and 4228 Cray XK7 nodes that include NVIDIA

FIG. 13. Performance of the IMC+emission model run in both internal emission mode and solar source mode for (a),(b) strong scaling experiments and (c),(d) weak scaling experiments. (a),(c) Throughput, defined as the number of photons simulated per minute of wall-clock time, and (b),(d) throughput efficiency (%) are shown as a function of number of processes. Note that logarithmic spacing is used on the horizontal axis in all panels and on the vertical axis for (a) and (c).

graphics processor acceleration. The IMC+emission model does not currently take advantage of graphics processing unit (GPU) acceleration. Each XE node contains 32 integer cores and has access to 64 GB of memory. The node is composed of Advanced Micro Devices (AMD) 6276 “Interlagos” processors, which have a nominal clock speed of 2.3 GHz. When compared to a typical laptop, the XE node has 16 times the memory and processors. The IMC+emission model was compiled with the Cray computing environment Fortran compiler.

Scalability of a code refers to how efficiently it completes the job as the number of processes increases, relative to a baseline cost to complete the job on the

fewest processes possible. Strong scaling tests demonstrate how a code’s time to solution or throughput varies with the number of processes, while keeping the total problem size fixed, which in this case was 200 000 batches of 50 000 photons each. Weak scaling tests demonstrate how a code’s time to solution or throughput varies with the number of processes, while keeping the problem size per process fixed, which in this case was 20 batches of 50 000 photons each, thus increasing the total problem size as the number of processes increases.

a. Strong scaling

Figure 13a shows the throughput, defined as photons simulated per minute of wall-clock time, and Fig. 13b

shows the throughput efficiency E for strong scaling, defined below, where T is the throughput, N is the number of processes used, and the subscript “base” refers to the simulation on the fewest processes, 16 in this case:

$$E = \frac{T_N/T_{\text{base}}}{N/N_{\text{base}}} \times 100\%. \quad (18)$$

For perfect strong scaling, the throughput would increase from the base throughput by a factor of N/N_{base} . Ideally, the base simulation would be completed on a single process. However, a reasonable number of photons for the complex domain described in the previous section could not be completed on a single process within the wall-clock limits of Blue Waters. Throughput increases as the work is divided among more processes until somewhere between 50 000 and 200 000 processes (Fig. 13a). At 200 000 processes, each process is only computing a single batch, so the overhead associated with each process outweighs the gain from increased parallelization. In terms of efficiency, the drop-off happens at fewer processes (Fig. 13b), which gives an indication of how many batches per process balance the overhead for this batch size and domain. The drop-off in efficiency between 1000 and 10 000 processes is more dramatic for the solar source than internal emission; however, the overall throughput is higher for a solar source.

b. Weak scaling

Figures 13c and 13d show the throughput and the throughput efficiency, respectively, for weak scaling. For perfect weak scaling, the throughput should increase by a factor of N as the number of processes increases. Unlike strong scaling throughput, the weak scaling throughput does continue to increase through 200 000 processes (Fig. 13c). Similar to the strong scaling, the solar source throughput is higher than internal emission, and the efficiency drops off more quickly for a solar source than for an internal source of photons. Although simulations on a single process are possible for the weak scaling experiment, the base used to calculate the weak scaling efficiency is 16 processes to make the plot more comparable to strong scaling efficiency (thus $E > 100\%$ for one process). The efficiency is above 80% through 10 000 processes for both solar and internal sources and then declines to 60% at worst by 100 000 processes (Fig. 13d).

The IMC+emission model shows better weak scaling than strong scaling through the full range of processes tested on this case. However, the strong scaling efficiency is about 70% or better through 10 000 processes. For the strong scaling experiment, at 10 000 process, each process is simulating 20 batches of 50 000 photons

each. This is the same workload per process as the weak scaling experiment. This demonstrates the importance of considering workload per process when setting up the IMC+emission model to run in parallel. For best conservation of allocation resources, each process should be assigned at least 20 batches to run this domain. However, if the time to a solution is the greatest concern, throughput continues to increase with increasing processes if at least four batches per process are assigned. Some fluctuation in these rules of thumb can be expected for input atmospheres of different complexity. So one should conduct throughput and efficiency tests to determine the optimal computational load before submitting large production simulations.

6. Summary

I3RC created a working group to provide a community-developed 3D Monte Carlo model. In its publicly released form, the “I3RC-original” model simulates only external sources of monochromatic radiation. It adopted an open-source paradigm with the intent of community input for further development. The goal of the present work has been to present the theoretical basis for and implementation, verification, performance, and application of the model with the addition of an internal source of radiation emitted from the surface and atmospheric constituents, the “IMC+emission” model. The benefit of such a model is a publicly available, thoroughly vetted, open-source, benchmark tool to study 3D radiative transfer from both external and internal sources at wavelengths for which both absorption and scattering may be important. It is publicly available on GitHub under the repository name IMC-emission along with select benchmark results (Jones 2017). The project web page, which hosts documentation, the latest code version, and licensing information, can be found online (<https://alexandraljones.github.io/IMC-emission/>).

The IMC+emission model’s algorithm determines emission location based on the construction of a cumulative distribution function of the probability of emission from the surface or the atmosphere. The probability of emission varies according to the emissive power, which is a function of temperature, emissivity, and the extent of the surface’s area or voxel’s volume. The initial direction of travel is chosen according to an isotropic phase function. The rest of the changes from the IMC-original incorporate the photon’s initial contribution to absorption, flux divergence, and radiance and implementation considerations for accurate construction of cumulative distribution functions and standard error. Jones (2016) discusses this in more detail.

Traditional metrics for radiative transfer models such as directional reciprocity and energy conservation were shown to hold to within the simulation precision (0.02% and better than 0.0064%, respectively). Additionally, the standard error of radiance was shown to decrease with increasing samples according to the expected $1/\sqrt{N_{\text{total}}}$ relationship. Several tests compared irradiance and radiance to those expected from analytical solutions demonstrating the successful implementation of the new components of the model associated with internal sources of radiation, such as accurate partitioning of photons between the surface and atmospheric layers with varying emissive properties, calculating the contribution of photon emission to radiance and the isotropic distribution of emitted radiation. In all cases, accuracy with respect to the analytical solution was found to hold to within simulation precision (typically better than 0.05%). With the above metrics for accuracy verified, the IMC+emission model was applied to an LES-produced cumulus cloud field, case 4 from the I3RC. Those solutions are available in the GitHub repository. They can act as benchmark results for model intercomparisons, at least until a model with similar or better veracity comes about. With the benchmarks provided here and the large increase in 3D radiative transfer models that include emission, we strongly recommend a new round of I3RC activities to test emission capabilities of those models. However, care should be taken when constructing a multimodel-mean benchmark result in future activities. Only models that are capable of passing analytical and energy conservation tests should be included in that mean.

The performance of the code was documented for this case in terms of throughput, or number of photons simulated per minute, and throughput efficiency for both weak and strong scaling experiments. For both weak and strong scaling experiments, the solar source of photons exhibits a faster drop-off in efficiency but has an overall higher throughput than the internal source of photons. The model shows better weak scaling efficiency than strong scaling efficiency for both sources of photons over the range of processes tested. However, the most important factor to consider when setting up a simulation

for maximum efficiency is the number of batches of photons per process. Before large or production simulations of new cases, throughput and efficiency tests should be conducted to determine a satisfactory workload that satisfies allocation constraints and desired throughput.

Finally, we also recommend and welcome continued development of this community model. For example, the addition of a backward photon tracing technique would be welcomed for applications for which it is more efficient. Other additions could be in the surface representation to allow for spatially inhomogeneous temperatures and albedos or including calculation of irradiance and radiance within the domain, not just at the boundaries.

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APPENDIX A

Minor Code Modifications

The standard error as computed within the “IMC-original” is given by the following equation:

$$SE = \sqrt{\frac{\max\left\{0.0, \left[F_{\lambda} \sum_{NR} \sum_{NBpR} (X)^2 / NB\right] - \left[F_{\lambda} \sum_{NR} \sum_{NBpR} (X) / NB\right]^2\right\}}{NB - 1}}, \quad (A1)$$

where NR is the number of computational ranks, NBpR is the number of independent batches of photons per rank, NB is the total number of batches,

F_{λ} is the incoming solar irradiance, and X is the tallied photon weight corresponding to a radiative quantity.

A small adjustment needed to be made to the calculation of standard error for internal emission. Equation (A1) is biased for any F_λ not equal to $1.0 \text{ W m}^{-2} \mu\text{m}^{-1}$,

which is almost always the case for internal emission. Equation (A1) was rearranged to the formulation below to make it applicable to either illumination source:

$$\text{SE} = \sqrt{\frac{\max\left\{0.0, \left[\sum_{\text{NR}} \sum_{\text{NBpR}} (F_\lambda X)^2 / \text{NB}\right] - \left[\sum_{\text{NR}} \sum_{\text{NBpR}} (F_\lambda X) / \text{NB}\right]^2\right\}}{\text{NB} - 1}}. \quad (\text{A2})$$

APPENDIX B

Derivations of Analytical Solutions

a. Radiance

The general solution of Schwarzschild's equation for the top-of-atmosphere radiance $I^\uparrow(\infty, \mu)$ over a Lambertian reflecting surface and for a plane-parallel atmosphere is given by Petty (2006):

$$I^\uparrow(\infty, \mu) = \left[\varepsilon B(T_s) + (1 - \varepsilon) \int_0^\infty B(z) W_F^\downarrow(z) dz \right] t^{*1/\mu} + \int_0^\infty B(z) W^\uparrow(z, \mu) dz, \quad (\text{B1})$$

where ∞ represents the altitude z at the top of the atmosphere, μ is the cosine of the viewing zenith angle, ε is the surface emissivity, T_s is the surface temperature, t^* is the total vertical transmittance of the atmosphere, and $B(z)$ is the Planck spectral radiance evaluated for the temperature at altitude z . The weighting function $W^\uparrow(z, \mu)$ may be written as

$$W^\uparrow(z, \mu) = \frac{\beta_a(z)}{\mu} t(z, \infty)^{1/\mu}, \quad (\text{B2})$$

where $t(z, \infty)$ is the transmittance between altitude z and the top of the atmosphere. The flux weighting function $W_F^\downarrow(z)$ is given by Petty (2006):

$$W_F^\downarrow(z) = 2 \int_0^1 \frac{\beta_a(z)}{\mu} t(0, z)^{1/\mu} \mu d\mu. \quad (\text{B3})$$

For an isothermal atmosphere, the rightmost term in Eq. (B1) is simply

$$\int_0^\infty B(z) W^\uparrow(z, \mu) dz = B(T_a)(1 - t^{*1/\mu}). \quad (\text{B4})$$

For a vertically homogeneous atmosphere [i.e., $\beta_a(z)$ is constant with altitude], the middle term of Eq. (B1) becomes

$$\int_0^\infty B(z) W_F^\downarrow(z) dz = \int_0^\infty B(z) 2\beta_a \int_0^1 t(0, z)^{1/\mu} d\mu dz, \quad (\text{B5})$$

which, for an isothermal atmosphere of temperature T_a , becomes

$$\int_0^\infty B(z) W_F^\downarrow(z) dz = 2B(T_a) \int_0^1 \mu(1 - t^{*1/\mu}) d\mu. \quad (\text{B6})$$

The following integral identity is used in evaluating Eq. (B6):

$$\int x(1 - a^{1/x}) dx = \frac{1}{2} \left\{ -a^{1/x} [x \ln(a) + x^2] + \ln^2(a) \text{Ei} \left[\frac{\ln(a)}{x} \right] + x^2 \right\}, \quad (\text{B7})$$

where Ei is the exponential integral defined as $\text{Ei}(x) = -\int_{-x}^\infty \exp(-u)/u du$. Applying this integral identity to the limits of integration in Eq. (B6) leads to

$$2B(T_a) \int_0^1 \mu(1 - t^{*1/\mu}) d\mu = B(T_a) [-t^*(1 - \tau^*) + (-\tau^*)^2 \text{Ei}(-\tau^*) + 1]. \quad (\text{B8})$$

Finally, substituting these component solutions back into Eq. (B1) leads to

$$I^\uparrow(\infty, \mu) = \{ \varepsilon B(T_s) + (1 - \varepsilon) B(T_a) [-t^*(1 - \tau^*) + (-\tau^*)^2 \text{Ei}(-\tau^*) + 1] \} t^{*1/\mu} + B(T_a)(1 - t^{*1/\mu}), \quad (\text{B9})$$

which is equivalent to Eq. (13) in section 3a. Note that the first term on the rhs of Eq. (13) is the contribution from surface emission, the second term on the rhs is the contribution from surface reflection, and the third term on the rhs is the contribution from atmospheric emission.

b. Irradiance

Starting from the relationship between downwelling radiance and irradiance,

$$F^\downarrow(z=0) = \int_0^{2\pi} \int_0^1 I^\downarrow(z=0, \mu, \phi) \mu d\mu d\phi. \quad (\text{B10})$$

In our case of a plane-parallel, absorbing, and emitting atmosphere, there is no dependence on ϕ . So

$$F^\downarrow(z=0) = 2\pi \int_0^1 I^\downarrow(z=0, \mu) \mu d\mu. \quad (\text{B11})$$

For an isothermal, plane-parallel atmosphere with no external sources of radiation, where T_a is the atmospheric temperature and t^* is the total vertical transmittance of the atmosphere,

$$I^\downarrow(z=0, \mu) = B(T_a)(1 - t^{*/\mu}), \quad (\text{B12})$$

$$F^\downarrow(z=0) = 2\pi B(T_a) \int_0^1 (1 - t^{*/\mu}) \mu d\mu. \quad (\text{B13})$$

The integral identity given by Eq. (B7) is again used, which after carrying out the integration of Eq. (B13) over its limits, leads to

$$F^\downarrow(z=0) = \pi B(T_a) \{1 - t^*[\ln(t^*) + 1] + \ln^2(t^*) \text{Ei}[\ln(t^*)]\}. \quad (\text{B14})$$

The upward irradiance at the top of the domain with a nonreflecting surface can be derived similarly:

$$F^\uparrow(z=\infty) = 2\pi \int_0^1 I^\uparrow(z=\infty, \mu) \mu d\mu. \quad (\text{B15})$$

For an isothermal, plane-parallel atmosphere over a black surface of temperature T_s ,

$$I^\uparrow(z=\infty, \mu) = B(T_s)t^{*/\mu} + B(T_a)(1 - t^{*/\mu}), \quad (\text{B16})$$

$$F^\uparrow(z=\infty) = 2\pi \int_0^1 [B(T_s)t^{*/\mu} + B(T_a)(1 - t^{*/\mu})] \mu d\mu. \quad (\text{B17})$$

Substituting the integral identity Eq. (B7) and carrying out the integration leads to

$$F^\uparrow(z=\infty) = \pi [B(T_a) + [B(T_s) - B(T_a)]\{t^{*/\mu}[\ln(t^*) + 1] + \ln^2(t^*) \text{Ei}[\ln(t^*)]\}]. \quad (\text{B18})$$

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