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# Non-Equlibrium Radiative Transfer Solutions using a Two-Group Diffusion Model

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# We need benchmarks for code verification, but most benchmarks are gray (1-group).

- The pursuit and discovery of benchmark solutions for code verification has a long history in the high-energy density radiative transfer community.
- The formulation of a material model that linearizes the equations by **Pomraning:1979fj** led to a series of solutions to gray (i.e., one-group) radiative transfer problems over the ensuing decades using various transport models.
  - Diffusion (**Ganapol:1983go**; **Su:1996wr**)
  - $P_1$ (**Mcclarren:2008dl**)
  - Transport (**Su:1997ux**)
- There have also been solutions that include the additional physics from a 3 temperature model using diffusion (**Mcclarren:2011km**) and transport (**mcclarren2011benchmarks**).
- The utility of these verification solutions is evident in their widespread use in the academic and laboratory communities in code verification.

- We present semi-analytic solutions to this model using non-equilibrium diffusion.
- These benchmark problems can be solved by radiative transfer codes that implement the multigroup model and allow different opacity and emissivity constants, as well as temperature-dependent heat capacities.
- Temperature independent heat capacities are required to solve the existing Su-Olson benchmarks.
- Opacities and emissivities that are not equivalent are required for non-LTE physics, so it does exist in many codes.
    - This gives the additional benefit of verifying some parts of the non-LTE capability.

# The existing non-gray benchmarks are not multigroup.



- A non-gray solution to the radiative transfer equations using transport and diffusion has been presented by Su and Olson (**Su:1999tk**) and extended by (**wollaeger2013radiation**).
- These solutions use the "picket fence" photon energy model that assumes there are two different values for the opacity that exist in adjacent, **differentially-sized** ranges of energy that repeat.
- While fences "make good neighbours", Pulitzer prize-winning plays, 1990's television dramas, and middlemen for stolen property, their value in describing the properties of radiative transfer is considerably less useful.
    - Most physics codes do not adopt the picket fence model except for running this benchmark.
- The picket fence model is very different than the common multigroup model used in most radiation transport codes.

Consider the non-equilibrium radiation diffusion system in slab geometry for the spectral radiation energy density, $E_\nu(x, \nu, t)$, and the material temperature, $T(x, t)$:

$$\frac{\partial E_\nu}{\partial t} - \frac{\partial}{\partial x}\frac{c}{3\kappa(x,\nu,T)}\frac{\partial}{\partial x}E_\nu + c\kappa(x,\nu,T)E_\nu = 4\pi\chi(x,\nu,T)B(\nu,T) + Q_\nu(x,t), \tag{1}$$

$$C_\mathrm{v}\frac{\partial T}{\partial t} = \int_0^\infty \left(c\kappa(x,\nu,T)E_\nu - 4\pi\chi(x,\nu,T)B(\nu,T)\right)\, d\nu. \tag{2}$$

In these equations $\kappa(x, \nu, T)$ is the spectral opacity, $\chi(x, \nu, T)$ is the emissivity of the material, and the Planck function is given by

$$B_\nu(\nu, T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{kT}} - 1}, \tag{3}$$

with $k$ and $h$ being the Boltzmann and Planck constants respectively.

A two-group model is defined by a cutoff frequency $\nu_0$ and integrating the Planck function to define two integral emission sources:

$$B_1(T) = \int_0^{\nu_0} B(\nu, T)\, d\nu, \qquad B_2(T) = \int_{\nu_0}^{\infty} B(\nu, T)\, d\nu. \tag{4}$$

The sum of these is equal to the integral of the Planck function over all frequency:

$$B_1(T) + B_2(T) = \int_0^{\infty} B(\nu, T)\, d\nu = \frac{acT^4}{4\pi}, \tag{5}$$

where

$$a = \frac{8\pi^5 k^4}{15h^3c^3} = \frac{4\sigma_{\text{SB}}}{c} = 0.01372\ \frac{\text{GJ}}{\text{cm}^3\text{-keV}}, \tag{6}$$

with $\sigma_{\text{SB}}$ the Stefan-Boltzmann constant. We define

$$B_1(T) = f(T)\frac{ac}{4\pi}T^4, \qquad B_2(T) = (1 - f(T))\frac{ac}{4\pi}T^4. \tag{7}$$

- Note that $0 \leq f(T) \leq 1$ is the fraction of emission in group 1.
- The $B_i(T)$ are each a positive fraction of the total emission.
- A quickly converging form for $f(T)$ with $r = h\nu_0/kT$ is

$$f(T) = 1 - \frac{15}{\pi^4} \sum_{n=1}^{\infty} \left( \frac{r^3}{n} + \frac{3r^2}{n^2} + \frac{6r}{n^3} + \frac{6}{n^4} \right) e^{-nr}, \tag{8}$$

- $$\lim_{\nu_0 \to 0} f(T) = 0, \qquad \lim_{\nu_0 \to \infty} f(T) = 1. \tag{9}$$

- These limits indicate that as the group cutoff goes to zero there is no emission in group 1, and as the cutoff goes to infinity, all of the emission is in group 1.
- The sum converges to a maximum absolute error of less than $2 \times 10^{-3}$ with only five terms in the sum and less than $10^{-6}$ with 70 terms.

We also define averaged radiation energy densities

$$E_1(x,t) = \int_0^{\nu_0} E_\nu(x,\nu,t)\,d\nu, \qquad E_2(x,t) = \int_{\nu_0}^{\infty} E_\nu(x,\nu,t)\,d\nu, \quad (10)$$

and similarly we define $Q_1(x,t)$ and $Q_2(x,t)$. Then using appropriately averaged values for the opacities and emissivities, (i.e., Planck or Rosseland means) we get the equations

$$\frac{\partial E_1}{\partial t} - \frac{\partial}{\partial x}\frac{c}{3\kappa_1(x,T)}\frac{\partial}{\partial x}E_1 + c\kappa_1(x,T)E_1 = acT^4\chi_1(x,T)f(T) + Q_1(x,t), \quad (11)$$

$$\frac{\partial E_2}{\partial t} - \frac{\partial}{\partial x}\frac{c}{3\kappa_2(x,T)}\frac{\partial}{\partial x}E_2 + c\kappa_2(x,T)E_2 = acT^4\chi_2(x,T)f(T) + Q_2(x,t), \quad (12)$$

$$C_\mathrm{v}\frac{\partial T}{\partial t} = c\left(\kappa_1(x,T)E_1 + \kappa_2(x,T)E_2\right) - acT^4\left[\chi_1(x,T)f(T) + \chi_2(x,T)(1-f(T))\right] \quad (13)$$

- We consider problems where $\kappa_1$ and $\kappa_2$ are independent of time, space, and temperature.
- The emissivity in group 1 is constant, $\bar{\chi}_1$.
- The emissivity in group 2 is prescribed to be

$$\chi_2 = \bar{\chi}_2 \frac{f(T)}{1 - f(T)}. \tag{14}$$

- This is done so that the resulting equations have emission that has the same temperature dependence in both groups.
- When the temperature dependence is the same for each group, we will be able to linearize.

Upon making these substitutions we get

$$\frac{\partial E_1}{\partial t} - \frac{c}{3\kappa_1}\frac{\partial^2}{\partial x^2}E_1 + c\kappa_1 E_1 = \bar{\chi}_1 acf(T)T^4 + Q_1(x,t), \tag{15}$$

$$\frac{\partial E_2}{\partial t} - \frac{c}{3\kappa_2}\frac{\partial^2}{\partial x^2}E_2 + c\kappa_2 E_2 = \bar{\chi}_2 acf(T)T^4 + Q_2(x,t), \tag{16}$$

$$C_v\frac{\partial T}{\partial t} = c\left(\kappa_1 E_1 + \kappa_2 E_2\right) - acf(T)T^4\left(\bar{\chi}_1 + \bar{\chi}_2\right). \tag{17}$$

- We specify the heat capacity of the problem to be

$$C_{\mathrm{v}} = \frac{\partial}{\partial T} f(T) a T^4. \tag{18}$$

- This makes

$$\frac{\partial}{\partial t} f(T) a T^4 = \left[ \frac{\partial}{\partial T} f(T) a T^4 \right] \frac{\partial T}{\partial t} = C_{\mathrm{v}} \frac{\partial T}{\partial t}. \tag{19}$$

- In the limit $\nu_0 \longrightarrow \infty$, i.e., a one group problem, we recover the familiar form of $C_{\mathrm{v}} \propto T^3$ because $f(T) = 1$ in this limit.
- We define a new variable $U(x,t)$ as

$$U(x,t) = f(T) a T^4. \tag{20}$$

- Therefore, to go from $U$ to $T$ we have to solve a nonlinear equation.

We introduce a scaling where $\tau = c\kappa_1 t$, $z = \kappa_1 x$, and

$$\tilde{E}_i = \frac{E_i}{aT_{\mathrm{H}}^4}, \quad \tilde{U} = \frac{U}{aT_{\mathrm{H}}^4}, \quad \tilde{Q}_i = \frac{Q_i}{\kappa_1 caT_{\mathrm{H}}^4}, \tag{21}$$

where $i = 1, 2$ and $T_H$ is a reference temperature. With these definitions we get a set of non-dimensional equations:

$$\frac{\partial \tilde{E}_1}{\partial \tau} - \frac{1}{3}\frac{\partial^2}{\partial z^2}\tilde{E}_1 + \tilde{E}_1 = \tilde{\chi}_1 \tilde{U} + \tilde{Q}_1(z, \tau), \tag{22}$$

$$\frac{\partial \tilde{E}_2}{\partial \tau} - \frac{1}{3\tilde{\kappa}_2}\frac{\partial^2}{\partial z^2}\tilde{E}_2 + \tilde{\kappa}_2 \tilde{E}_2 = \tilde{\chi}_2 \tilde{U} + \tilde{Q}_2(z, \tau), \tag{23}$$

$$\frac{\partial \tilde{U}}{\partial \tau} = \left(\tilde{E}_1 + \tilde{\kappa}_2 \tilde{E}_2\right) - \tilde{U}\left(\tilde{\chi}_1 + \tilde{\chi}_2\right). \tag{24}$$

$$\tilde{\kappa}_2 = \frac{\kappa_2}{\kappa_1} \quad \tilde{\chi}_i = \frac{\bar{\chi}_i}{\kappa_1}.$$

- We consider a source in group 1 of the form

$$\tilde{Q}_1(z,\tau) = \begin{cases} \delta(z) & 0 \le \tau \le \tau_0 \\ 0 & \text{otherwise} \end{cases}, \qquad \tilde{Q}_2 = 0 \tag{25}$$

- This source is on from time $\tau = 0$ until $\tau = \tau_0$.
- The initial conditions are $\tilde{E}_1(z,0) = \tilde{E}_2(z,0) = \tilde{U}(z,0) = 0$.
- The boundary conditions are that the solutions go to zero as $|z| \to \infty$, i.e., we are in an infinite medium.
- Taking a Fourier transform in space and a Laplace transform in time Eqs. (22) - (24) become

$$\left(\tilde{s} + \frac{k^2}{3} + 1\right)\tilde{E}_1(k,s) = \tilde{\chi}_1\tilde{U}(k,s) + \frac{\frac{1}{s} - \frac{e^{-as}}{s}}{\sqrt{2\pi}}, \tag{26}$$

$$\left(\tilde{s} + \frac{k^2}{3\tilde{\kappa}_2} + \tilde{\kappa}_2\right)\tilde{E}_2(k,s) = \tilde{\chi}_2\tilde{U}(k,s), \tag{27}$$

$$s\tilde{U}(k,s) = \tilde{E}_1(k,s) + \tilde{\kappa}_2\tilde{E}_2(k,s) - (\tilde{\chi}_1 + \tilde{\chi}_2)U(k,s). \tag{28}$$

- The inverse Laplace transform can be performed analytically using computer algebra software; we use `Mathematica`.
- The resulting functions are too long to detail here, as they would take several pages to write out due to the fact that the roots of a cubic polynomial with symbolic coefficients appear repeatedly.
- Instead we write the inverse Laplace transformed solutions as $\tilde{E}_1(k,\tau)$, $\tilde{E}_2(k,\tau)$, $\tilde{U}(k,\tau)$ respectively.
- To get the solution as a function of $z$ and $\tau$ we must perform the inverse Fourier transform numerically.
- In particular we must compute

$$\tilde{E}_1(z,\tau) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{E}_1(k,\tau) e^{-ikz}\, dk, \tag{29}$$

and similar evaluations are required for $\tilde{E}_2(z,\tau)$ and $\tilde{U}(z,\tau)$.

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- In particular we must compute

$$\tilde{E}_1(z,\tau) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{E}_1(k,\tau) e^{-ikz}\, dk, \tag{30}$$

and similar evaluations are required for $\tilde{E}_2(z,\tau)$ and $\tilde{U}(z,\tau)$.

- We use the Green's function to solve a problem of a finite source of strength over the range $z \in [-z_0/2, z_0/2]$ such that

$$\tilde{Q}_1(z,\tau) = \begin{cases} 1 & z \in [-z_0/2, z_0/2] \text{ and } \tau \leq 10 \\ 0 & \text{otherwise} \end{cases},$$

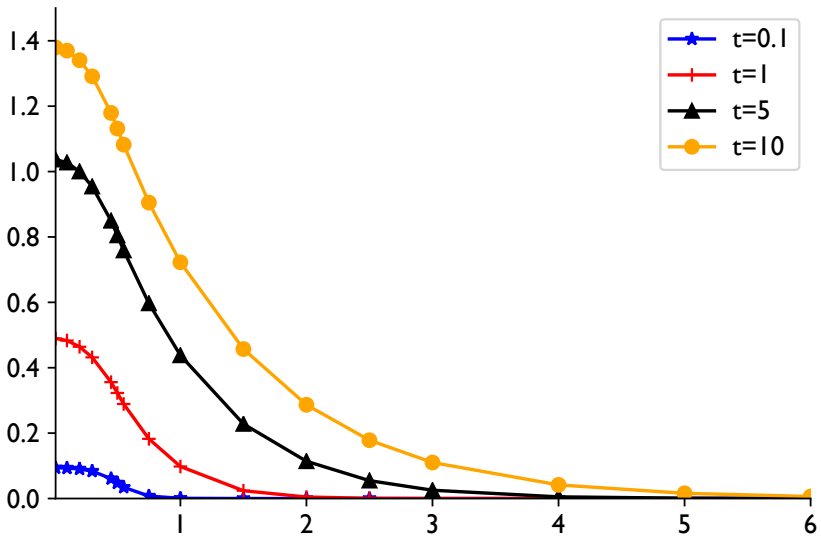
by replacing $z$ in Eq. (30) with $|z - z'|$ and integrating over $z'$ from $-z_0/2$ to $z_0/2$. This leads to the solution for $\tilde{E}_1$

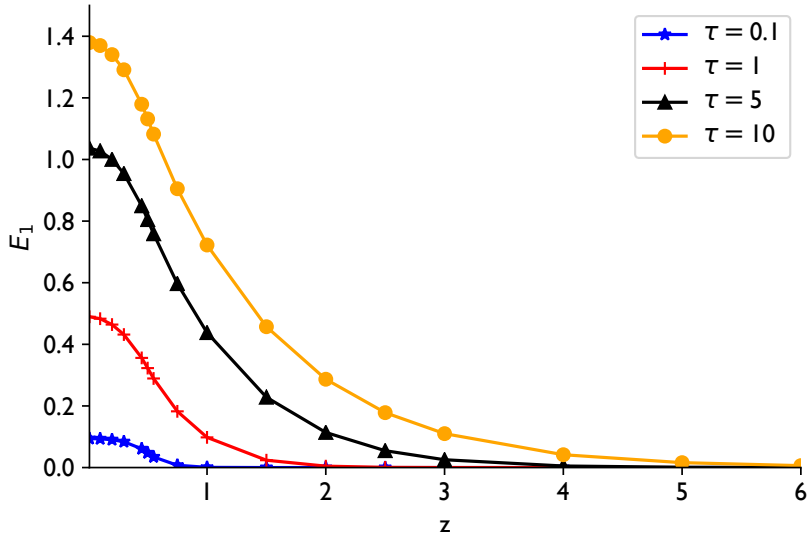
$$\tilde{E}_1(z,\tau) = \frac{1}{\sqrt{2\pi}} \int_{-z_0/2}^{z_0/2} dz' \int_{-\infty}^{\infty} dk\, \tilde{E}_1(k,\tau) e^{-ik|z-z'|} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{E}_1(k,\tau) S(z,k)\, dk, \tag{31}$$

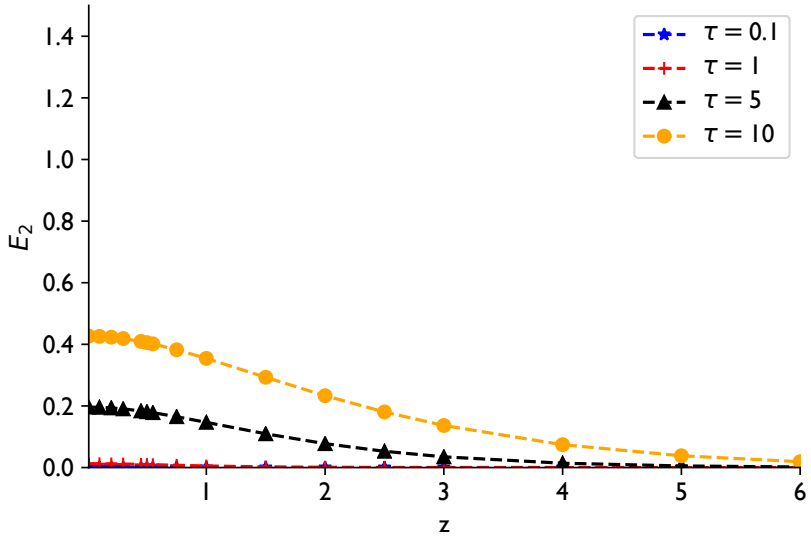
$$S(z,k) = \int_{-z_0/2}^{z_0/2} dz'\, e^{-ik|z-z'|} = \begin{cases} \frac{1}{k}\left(2ie^{-\frac{1}{2}ikz_0}\cos(kz) - 2i\right) & -\frac{z_0}{2} \leq z \leq \frac{z_0}{2} \\ \frac{1}{k}\left(2e^{-ikz}\sin\left(\frac{kz_0}{2}\right)\right) & \text{otherwise} \end{cases}. \tag{32}$$

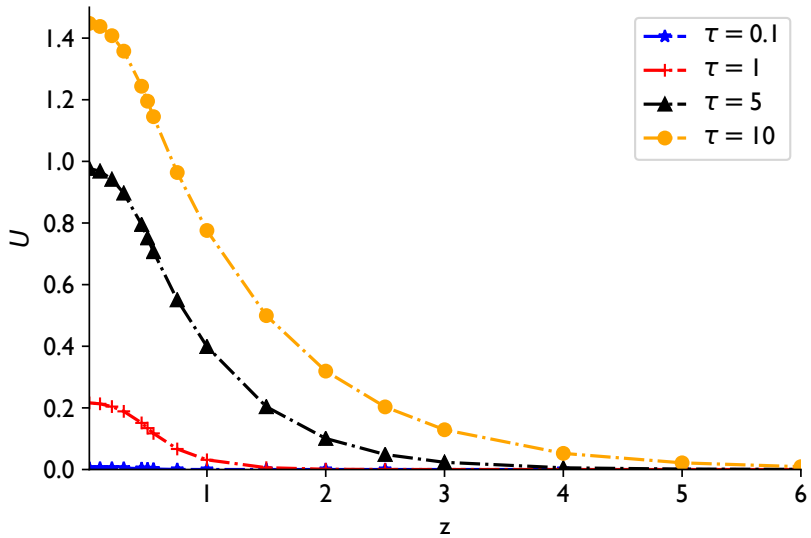
- We need only compute a single numerical integral to get the solution.
- The other functions are found in a similar manner.
- In performing the integrals, we can make further simplifications.
  1. The solutions $\tilde{E}_1(z,\tau)$, $\tilde{E}_2(z,\tau)$, $\tilde{U}(z,\tau)$ are all real, so the imaginary part can be ignored.
  2. The solution will be symmetric about the origin so the Fourier transform of the solution will also be even. Therefore, we only need to integrate over the range $k \in [0,\infty)$ and multiply the result by 2 to compute the inverse transform.

- The source is in group 1, making $\tilde{E}_1 > \tilde{E}_2$.
- $U$ is larger than $E_1$ at $\tau = 10$ because a significant amount of energy has been absorbed and radiated by the material into both groups.
- The values shown are computed using `Mathematica`'s `NIntegrate` function using the multi-periodic integration strategy (**krommer1998computational**) with a working precision of 40 digits and converge to 7 digits of accuracy, though we only report 6 digits in our tables.






late_times.pdf

# Here are the solutions in real units with $T_{\mathrm{H}} = 1$ keV and $\kappa_1 = 1\,\mathrm{cm}^{-1}$



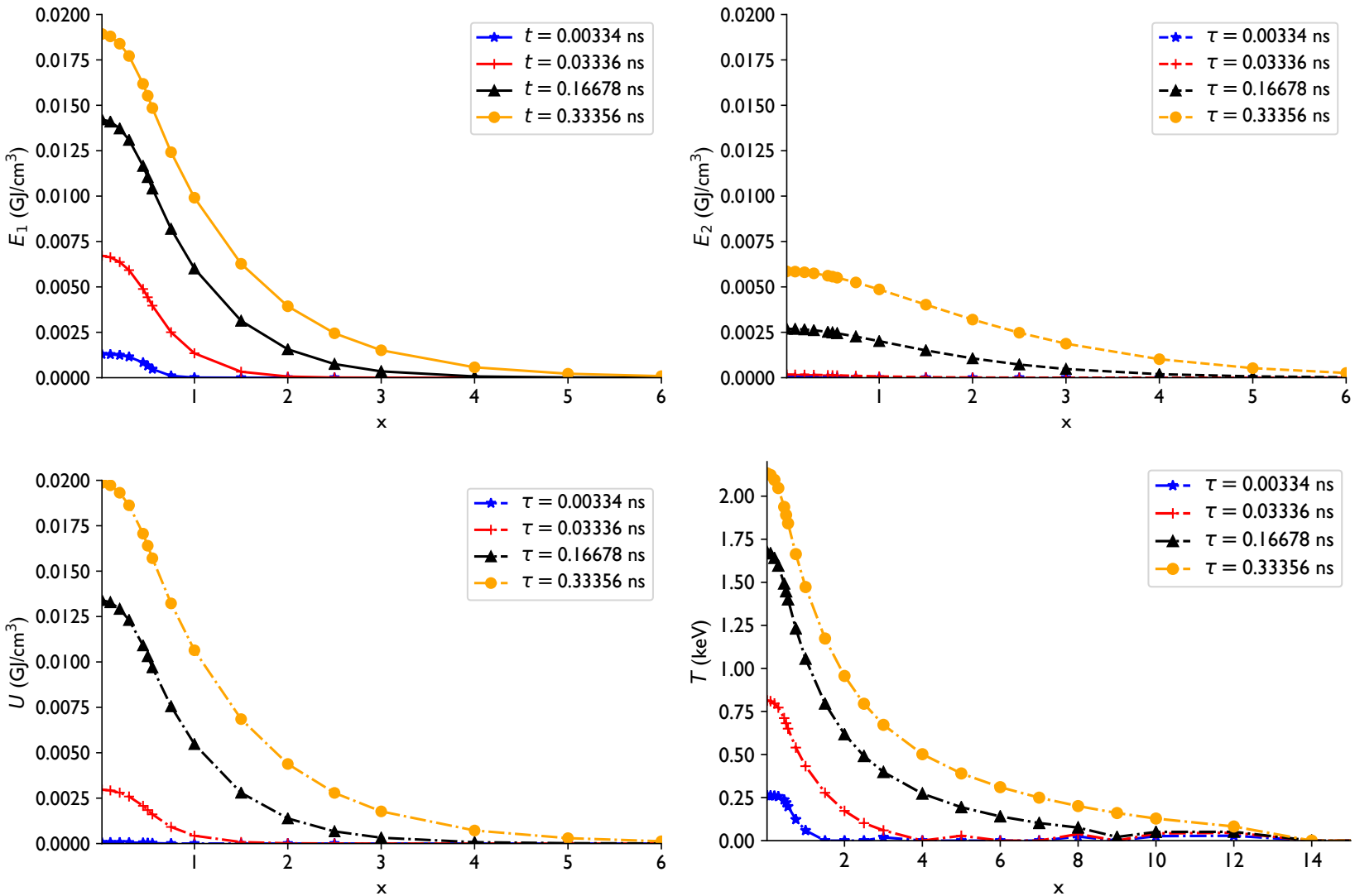


Table: $\tilde{E}_1(z,\tau)$ for a problem with $\tilde{\kappa}_2 = 1/3$, $\tilde{\chi}_1 = 3/4$, $\tilde{\chi}_2 = 1/4$, $\tau_0 = 10$, and $z_0 = 1$.

| $z/\tau$ | 0.1 | 0.316228 | 1 | 3.162278 | 10 | 31.622777 | 100 |
|---|---|---|---|---|---|---|---|
| 0.01 | 0.093989 | 0.242639 | 0.489454 | 0.846950 | 1.379522 | 0.291839 | 0.141724 |
| 0.1 | 0.093217 | 0.239110 | 0.483215 | 0.838600 | 1.369842 | 0.291741 | 0.141714 |
| 0.17783 | 0.091239 | 0.231200 | 0.469482 | 0.820304 | 1.348658 | 0.291527 | 0.141692 |
| 0.31623 | 0.082265 | 0.204393 | 0.425117 | 0.761931 | 1.281306 | 0.290849 | 0.141621 |
| 0.45 | 0.060833 | 0.159212 | 0.355952 | 0.672960 | 1.179299 | 0.289838 | 0.141516 |
| 0.5 | 0.047639 | 0.136293 | 0.322820 | 0.631130 | 1.131599 | 0.289371 | 0.141467 |
| 0.56234 | 0.031693 | 0.108128 | 0.281324 | 0.578011 | 1.070468 | 0.288721 | 0.141399 |
| 0.75 | 0.007546 | 0.050649 | 0.182492 | 0.440691 | 0.905040 | 0.286319 | 0.141146 |
| 1 | 0.000641 | 0.015768 | 0.097978 | 0.302342 | 0.722392 | 0.282111 | 0.140699 |
| 1.33352 | | 0.002435 | 0.039205 | 0.177924 | 0.532940 | 0.274809 | 0.139906 |
| 1.77828 | | 0.000109 | 0.009789 | 0.083539 | 0.352972 | 0.262376 | 0.138508 |
| 3.16228 | | | | 0.005595 | 0.094088 | 0.209985 | 0.131814 |
| 5.62341 | | | | | 0.008832 | 0.109659 | 0.112791 |
| 10 | | | | | 0.000151 | 0.019773 | 0.069430 |
| 17.78279 | | | | | | 0.000334 | 0.015993 |

Table: $\tilde{E}_2(z,\tau)$ for a problem with $\tilde{\kappa}_2 = 1/3$, $\tilde{\chi}_1 = 3/4$, $\tilde{\chi}_2 = 1/4$, $\tau_0 = 10$, and $z_0 = 1$.

| $z/\tau$ | 0.1 | 0.316228 | 1 | 3.162278 | 10 | 31.622777 | 100 |
|---|---|---|---|---|---|---|---|
| 0.01 | 0.000037 | 0.000827 | 0.012442 | 0.103160 | 0.426661 | 0.263759 | 0.138118 |
| 0.1 | 0.000036 | 0.000815 | 0.012326 | 0.102704 | 0.425781 | 0.263688 | 0.138109 |
| 0.17783 | 0.000035 | 0.000787 | 0.012077 | 0.101717 | 0.423872 | 0.263533 | 0.138088 |
| 0.31623 | 0.000031 | 0.000701 | 0.011316 | 0.098680 | 0.417946 | 0.263044 | 0.138023 |
| 0.45 | 0.000023 | 0.000581 | 0.010259 | 0.094364 | 0.409382 | 0.262312 | 0.137926 |
| 0.5 | 0.000020 | 0.000530 | 0.009805 | 0.092462 | 0.405545 | 0.261974 | 0.137881 |
| 0.56234 | 0.000015 | 0.000465 | 0.009211 | 0.089916 | 0.400334 | 0.261503 | 0.137818 |
| 0.75 | 0.000006 | 0.000290 | 0.007382 | 0.081440 | 0.382280 | 0.259761 | 0.137585 |
| 1 | 0.000001 | 0.000135 | 0.005172 | 0.069360 | 0.354348 | 0.256700 | 0.137171 |
| 1.33352 | | 0.000041 | 0.002970 | 0.053833 | 0.313693 | 0.251358 | 0.136439 |
| 1.77828 | | 0.000007 | 0.001276 | 0.036438 | 0.259107 | 0.242180 | 0.135147 |
| 3.16228 | | | | 0.008417 | 0.124200 | 0.202213 | 0.128948 |
| 5.62341 | | | | | 0.024836 | 0.118042 | 0.111229 |
| 10 | | | | | 0.000803 | 0.026662 | 0.070148 |
| 17.78279 | | | | | | 0.000636 | 0.017277 |

Table: $\tilde{U}(z,\tau)$ for a problem with $\tilde{\kappa}_2 = 1/3$, $\tilde{\chi}_1 = 3/4$, $\tilde{\chi}_2 = 1/4$, $\tau_0 = 10$, and $z_0 = 1$.

| $z/\tau$ | 0.1 | 0.316228 | 1 | 3.162278 | 10 | 31.622777 | 100 |
|---|---|---|---|---|---|---|---|
| 0.01 | 0.004657 | 0.038104 | 0.216108 | 0.706021 | 1.447721 | 0.388874 | 0.188821 |
| 0.1 | 0.004637 | 0.037628 | 0.213206 | 0.698641 | 1.437848 | 0.388742 | 0.188807 |
| 0.17783 | 0.004577 | 0.036528 | 0.206771 | 0.682453 | 1.416247 | 0.388454 | 0.188778 |
| 0.31623 | 0.004238 | 0.032486 | 0.185556 | 0.630645 | 1.347603 | 0.387544 | 0.188684 |
| 0.45 | 0.003151 | 0.024726 | 0.151256 | 0.551223 | 1.243751 | 0.386186 | 0.188544 |
| 0.5 | 0.002341 | 0.020397 | 0.134328 | 0.513701 | 1.195232 | 0.385559 | 0.188479 |
| 0.56234 | 0.001374 | 0.015126 | 0.113312 | 0.466215 | 1.132999 | 0.384686 | 0.188388 |
| 0.75 | 0.000227 | 0.005791 | 0.066626 | 0.345870 | 0.963841 | 0.381462 | 0.188052 |
| 1 | 0.000012 | 0.001386 | 0.031387 | 0.228898 | 0.775692 | 0.375816 | 0.187456 |
| 1.33352 | | 0.000153 | 0.010575 | 0.128652 | 0.578770 | 0.366022 | 0.186402 |
| 1.77828 | | 0.000005 | 0.002124 | 0.057239 | 0.389652 | 0.349363 | 0.184541 |
| 3.16228 | | | | 0.003761 | 0.111381 | 0.279376 | 0.175633 |
| 5.62341 | | | | | 0.012613 | 0.146096 | 0.150316 |
| 10 | | | | | 0.000266 | 0.026726 | 0.092592 |
| 17.78279 | | | | | | 0.000470 | 0.021382 |

# We have developed the first two-group, thermal radiation diffusion benchmarks.

- We have developed a novel model for producing truly multigroup radiative transfer benchmark solutions.
- These solutions can be used as benchmark solutions for radiation diffusion codes by specifying the problem with a temperature dependent heat capacity given by Eq. (18) utilizing the summation formula for $f(T)$ given in Eq. (8).
- The value for the emissivity in group 2 must be temperature dependent and given by Eq. (14).
- To convert the values in the solution tables for $\tilde{U}$ to temperatures, one must first multiply $\tilde{U}$ by $aT_H^4$ and then solve the nonlinear equation:

$$\tilde{U}(z,\tau)aT_H^4 = f(T)aT^4(z,\tau),$$

for $T(z,\tau)$. This solution can be computed once and tabulated for a given unit system.

# Bibliography I