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Simulations of high yield air bursts using gray and multigroup diffusion; Comparison of Raptor and Lasnex*

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Abstract

We describe a realistic test problem which simulates a strong explosion in air at STP. We consider two yields, $Y = 11$ kT and $Y = 1$ MT. We compare results obtained using gray with those using multigroup diffusion. For low Y, the two models give nearly identical results. In the early-time, radiation-dominated regime, the low Y simulation resembles a classical spherically expanding thermal wave with strongly coupled ($T = T_r$) temperatures. For large Y, the gray and multigroup runs differ considerably. The large yield, gray diffusion simulation, after proper scaling, is nearly identical to the low yield result. However, for large Y, the multigroup temperatures are equal only for T larger than 5–10 keV. Beyond, T_r decouples from T and an energetic pulse of radiation, populated by 100 keV photons, streams out from the fireball. Our large Y result contradicts established theory. However, two LNL codes, Raptor and Lasnex, show excellent agreement for large Y.

This work stems from a Validation & Verification (V&V) exercise for the radiation multigroup diffusion (MGD) module recently developed by Shestakov and Offner [5]. The module has been incorporated into LLNL's radiation-hydrodynamic code Raptor, which is massively parallel, multidimensional, Eulerian, with adaptive mesh refinement (AMR). Although MGD has been tested on a variety of test problems, e.g., Shestakov et al [6], it is important to check its accuracy while running in a mode that utilizes all physics and computational modules. To wit: using multiple, real materials, coupling hydrodynamics, heat conduction and radiation diffusion, running with multiple AMR levels, and verifying that when relevant, the code's 3D Cartesian executable produces the same result as its 1D spherical analogue.

Thus, we formulate the following "hot ball" problem. An Aluminum (Al) sphere of radius $r_A = 15.5$ cm is suspended in air. The initial densities are $\rho = 2.68118198$ and 0.00129 g/cc for Al and air, respectively. Both materials are initially at $T = 375.936$ deg.[1] There is initially no radiation energy $T_r|_{t=0} = 0$. At $t = 0$, we source energy into

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[1] Inputs are tailored so that our EOS returns equal pressures for both materials, approximately 1 bar.

the radiation field, but only into the domain covered by Al and only for the first 0.1 ns, at which time we have loaded a yield Y into the domain.[2] For runs using multigroup diffusion, energy is sourced with a Planckian spectrum. The Raptor AMR runs use two levels of refinement; $h = 8$, 4, and 2 cm.

We compare Raptor simulations, in which radiation is modeled by gray diffusion, to runs using MGD. We present results for $Y \approx 11$ kT and $Y \approx 1$ MT.[3] Since our high yield MGD Raptor result conflicts with established theory, we compare Raptor's $Y = 1$ MT profiles with those from a Lasnex run and find that the codes produce nearly identical results *only if* the codes use the same opacity models.

The results lead us to conclude that for high yield air bursts at STP, the established theory, e.g., Brode [1], which was based on gray diffusion, gives incorrect results in the early-time, radiation-dominated regime.

We stress that our results are totally dependent on the equation-of-state (EOS) and opacity tables. For the former, we use LEOS, material numbers 130 (Al) and 2260 (Air). The EOS tables have the min and max table ranges for the input variables: $10^{-10} \leq \rho \leq 10^3$ (g/cc) and $1.2 \leq T \leq 1.16 \cdot 10^9$ deg. The gray LEOS opacity tables have the narrower range: $10^{-4} \leq \rho \leq 10^3$ and $1.2 \cdot 10^4 \leq T \leq 1.16 \cdot 10^9$. For multigroup we use tables supplied by J. Castor [2]. Castor's tables compute the scattering opacity using the nuclear charge instead of the more commonly used free electron density (Lasnex's default.) Forcing Lasnex to likewise use the nuclear charge was crucial to arriving at the excellent agreement we present below.

The above-mentioned table ranges lead to a certain uncertainty, viz., what to do for table look-ups if the inputs are outside of the table ranges. For example, what opacity to use if $T < 1.2 \cdot 10^4$ deg. In the simulations, we opt for the simplest approach. Table lookups use the closest table input values, i.e., inputs are min-maxed with the extremal table ranges. Our approach is guided by the motivation of this paper: a test of Raptor's multigroup *scheme* and *not* a V&V exercise of opacity data.

The hot ball problem simulates a strong explosion in air; with our parameters, one with a nuclear source. The effects are well known: Zel'dovich and Raizer [7] Ch. IX, Brode [1], Landshoff [3]. Initially, the dynamics is dominated by radiation: a fast thermal wave propagates through the surrounding air. When the wave slows to sonic speeds (of the hot air), the steep pressure gradient gives rise to a strong shock. Then, hydrodynamics dominates. Salient effects are well approximated by a simulation of a point explosion using hydro and nonlinear heat conduction, as described in Shestakov [4], "Non-Self-Similar-Problem" section.

To summarize our results: for the lower yield, gray and MGD simulations are very similar. However, for $Y = 1$ MT, gray and MGD simulations differ significantly.

We begin by discussing Raptor's low yield (gray and MGD) and the gray high yield results. Figures 1, 2 and 3 display densities, temperatures and velocities, respectively. Each figure contains three curves. Two are from simulations with $Y = 11$ kT, one with gray, another with multigroup diffusion. The third curve is from a simulation using gray diffusion and a yield $Y = 1$ MT. The 1 MT curves are drawn after implementing

[2]The source rate is only meant to stress the numerics, not represent a particular explosion.

[3]Using the conversion $4.18 \cdot 10^{19}$ erg/kT, the actual yields are 10.9731 kT, 0.9870682 MT, 10.9665 kT, and 0.9862604 MT for the two gray and two MGD runs, respectively.

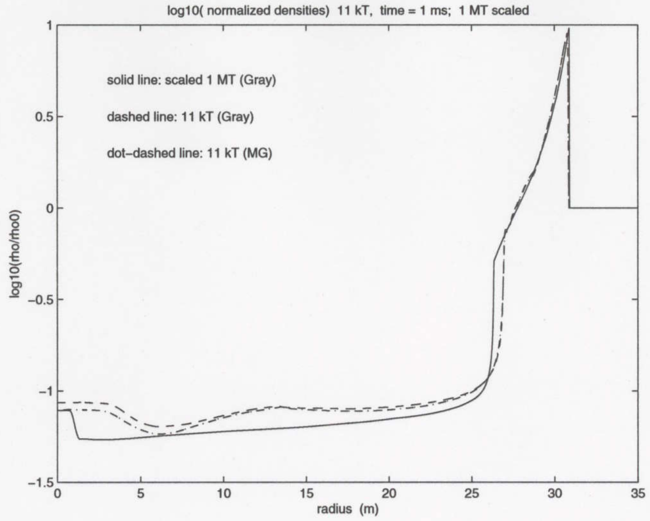

Figure 1: Log of normalized density ρ/ρ_0; $Y = 11$ kT, $t = 1$ ms, gray and multigroup diffusion; $Y = 1$ MT gray curve is scaled; see text. Raptor code.

Sachs scaling, i.e., by scaling time and radii by the cube root of the yield ratio $R_Y = (Y_1/Y_2)^{1/3}$, where $Y_1 = 11$ and $Y_2 = 1000$. Hence, while the $Y = 11$ results are taken at $t = 1$ ms, the 1 MT results are at $t = 4.48$ ms and the 1 MT radii have been divided by R_Y. Figure 1 displays $\log_{10}(\rho/\rho_0)$, where $\rho_0 = 0.00129$ is the ambient air density. Although the close agreement displayed in Figs. 1, 2 and 3 may not surprise, it is indeed remarkable how well the scaled 1 MT curves, which use gray diffusion, compare with the lower yield results. The similarity of the $Y = 11$ kT gray and MGD curves implies say that for small Y, gray diffusion is adequate.

In order to validate our gray $Y = 1$ MT simulation, we continue the run to $t = 7$ ms and when we compare with Brode [1], find good qualitative agreement. Quantitatively, at $t = 7$ ms, we get a strong shock at $r = 164$ m, whereas Brode puts it at $r \approx 190$. Both of us get a nearly tenfold density rise at the shock, while inside the fireball, $\rho \approx 5 \cdot 10^{-5}$. For the central ($r = 0$) temperatures: at $t = 7$ ms, we have $T = 2.04 \cdot 10^5$ deg vs. $\approx 2 \cdot 10^5$ for Brode; our fireball radius is 138 m (≈ 160 for Brode); and our shock temperature is $1.65 \cdot 10^4$ (≈ 1.6–$1.7 \cdot 10^4$ for Brode).

We now compare the lower yield gray and MGD results at the earlier time, $t = 1$ μs, when the solution is dominated by radiation. At this time, since the thermal wave is supersonic, it suffices to only examine the temperatures T and T_r for both gray and MGD simulations. Figure 4, which displays the temperatures, shows little difference between gray and multigroup. Both models display a fireball extending to $r = 8.1$-8.4 m and a central $T \approx 2.5 \cdot 10^6$ deg; both also display the start of a shock emanating at the Al/air interface, as evidenced by the spike at $r \approx 0.8$ m.

However, for high yield, the gray and MGD simulations differ dramatically. Fig-

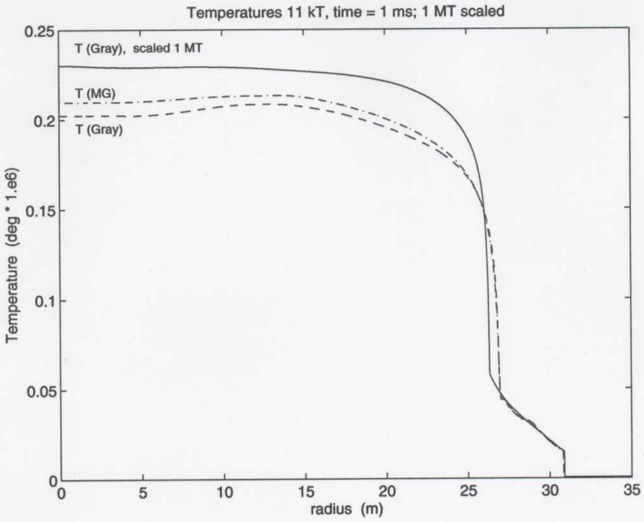

Figure 2: Temperatures T; $Y = 11$ kT, $t = 1$ ms, gray and multigroup diffusion; $Y = 1$ MT gray curve is scaled; see text. Raptor code.

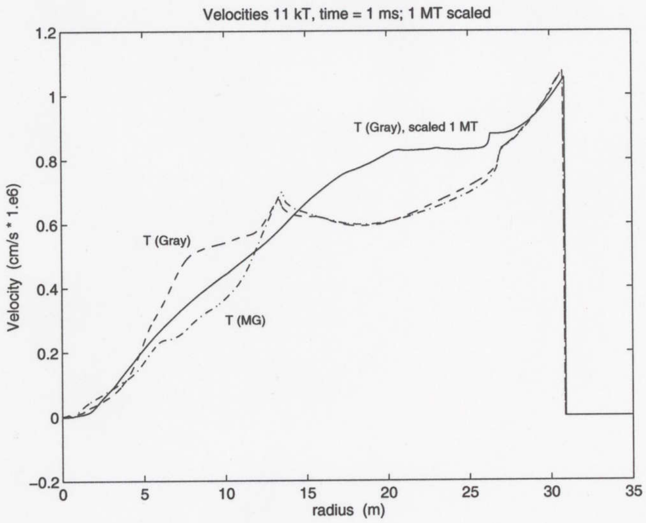

Figure 3: Velocities v; $Y = 11$ kT, $t = 1$ ms, gray and multigroup diffusion; $Y = 1$ MT gray curve is scaled; see text. Raptor code.

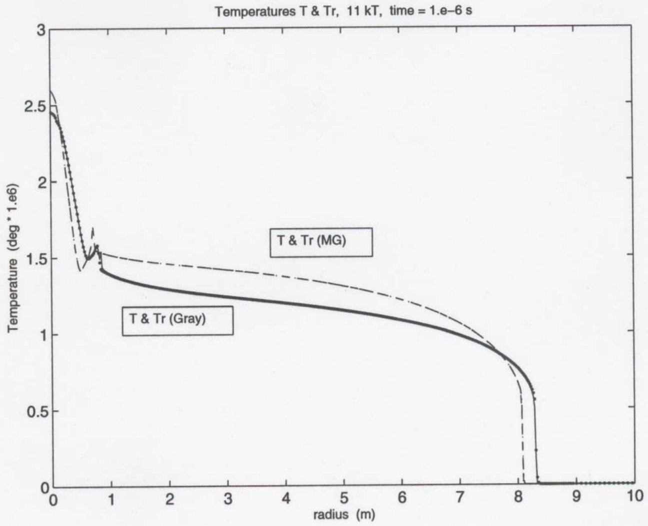

Figure 4: Gray and multigroup temperatures T and T_r, $Y = 11$ kT, $t = 1\mu$s; Raptor.

ure 5 displays T and T_r for $Y = 1$ MT at $t = 1\mu$s. We see that for gray diffusion, $T = T_r$; just as for $Y = 11$ kT. The gray diffusion thermal wave, which still moves supersonically, has a front at $r \approx 30$ m. However, the MGD result is strikingly different. Multigroup diffusion lowers the central temperatures by more than 10%. But, more surprising is that the multigroup T and T_r temperatures are tightly coupled only out to $r \approx 20$ m. Beyond that, at $T \approx 8.5 \cdot 10^5$ deg, T and T_r decouple. The radiation temperature, i.e., the fourth root of E_r, extends to $r \approx 300$ m, which is the free streaming limit. The Raptor MGD result is corroborated by Lasnex, as we now show.

To examine why the high-yield gray and MGD simulations differ, we turn off hydrodynamics and heat conduction physics, repeat the simulation, and find temperatures similar to Fig. 5. This does not surprise since the dynamics is radiation-dominated. We present a series of plots that compare Raptor and Lasnex results. The Lasnex simulation also shuts off hydrodynamics and heat conduction. Additionally, in Lasnex, we use the two temperature ($T_i = T_e$) model, turn off Compton scattering and use the TABOP opacities [2], taking care to set the full-ionization switch to ensure that scattering opacities are based on the nuclear charge. Figures 6 and 7 display the Raptor and Lasnex temperatures, respectively; now in keV units. We set the figures' maximum ordinate to 0.2 keV. However, inside the Al sphere the temperatures are much hotter. A close inspection shows that in both codes $T = T_r = 0.87$ keV at $r = 0$. Excellent agreement is also evident in the transitional region at $r \approx 22$ m. There, the two temperatures separate at T just below 0.07 keV. Beyond, the matter temperature continues its steep drop to $T \approx 0.04$ kev, then changes slope and drops to ambient values at $r \approx 100$ m. On the other hand, T_r stays hot out to the streaming limit $r = 300$ m.

To gain more insight, we examine spectra. Figures 8 (Raptor), and 9 (Lasnex)

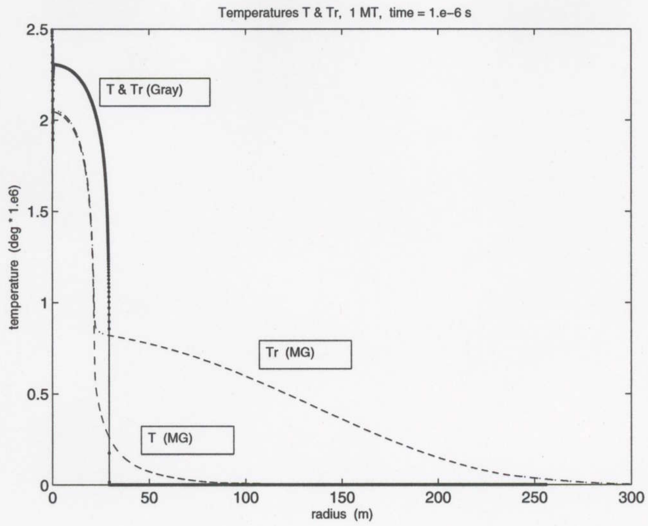

Figure 5: Gray and multigroup temperatures T and T_r, $Y = 1$ MT, $t = 1\mu$s; Raptor.

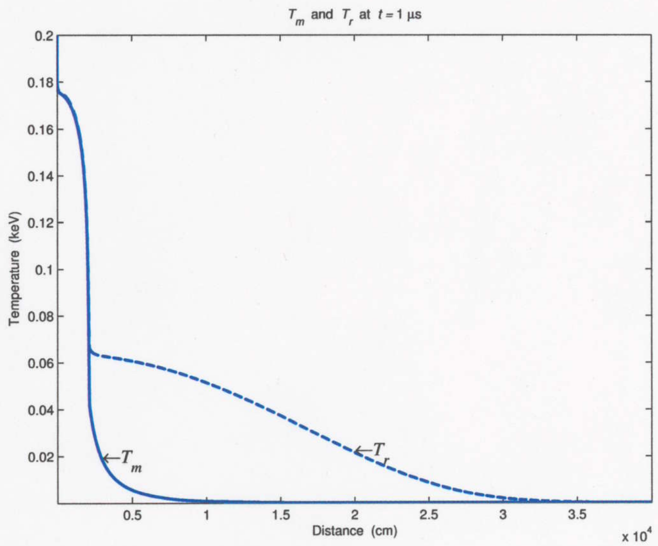

Figure 6: Multigroup temperatures T and T_r, $Y = 1$ MT, $t = 1\mu$s; Raptor.

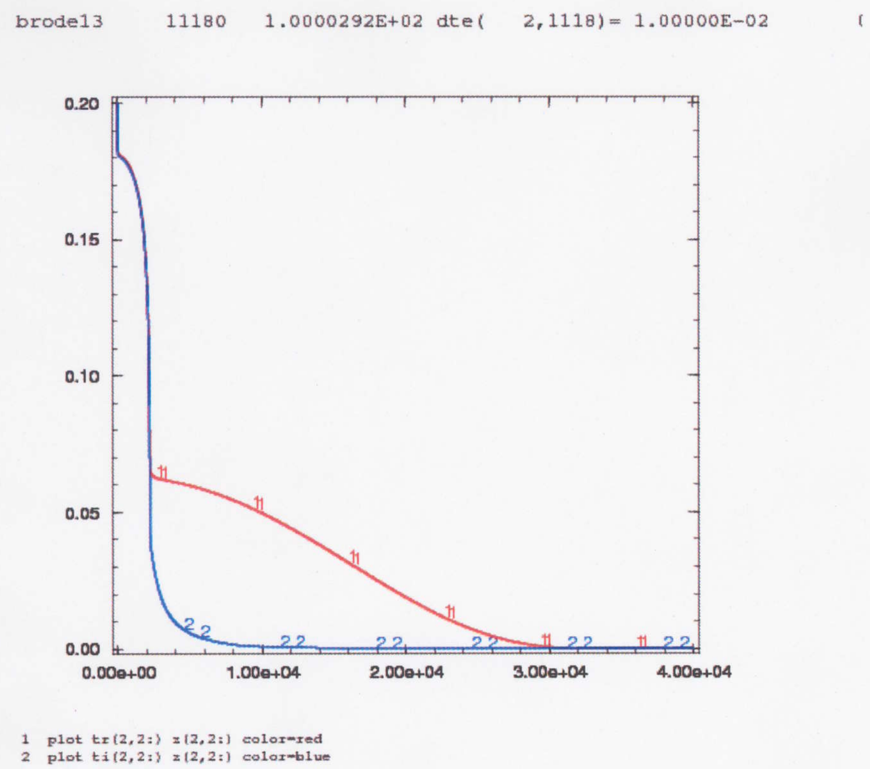

Figure 7: Multigroup temperatures T and T_r, $Y = 1$ MT, $t = 1\mu$s; Lasnex code.

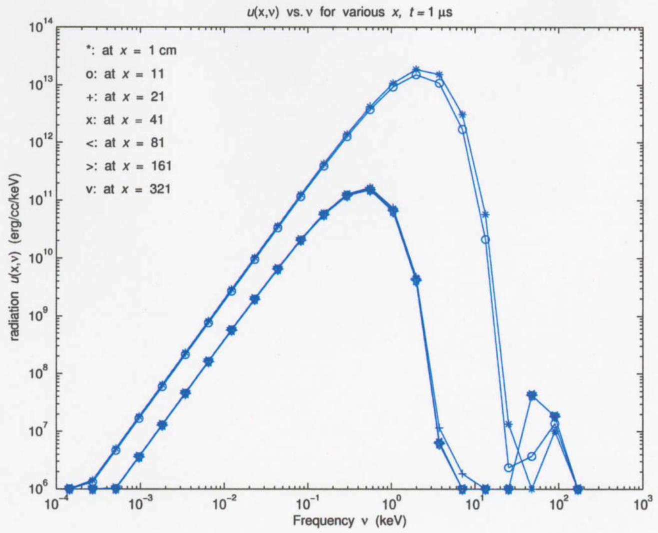

Figure 8: Spectral radiation energy vs. frequency at various radii; multigroup physics only; $Y = 1$ MT, $t = 1\mu$s; Raptor.

display the spectral radiation energy vs. frequency at close-in radii: $r = 0.01$–3.21 m. Similarly, Figs. 10 (Raptor), and 11 (Lasnex) display the far-field radiation energy, $r =$ 25–300 m.

The spectral plots help understand why the two temperatures decouple at $r \approx 22$ m. Evidently, the frequency dependent air opacity is responsible. Near-in, the radiation spectrum develops a hole at 10 keV. As r increases, the hole progresses to lower frequencies so that at 100-200 m, the spectrum consists of two peaks, one at the high frequencies (30–200 keV), another near the visible range. These photons travel largely unimpeded. Hence, do not couple and do not heat the air. The high frequency photons, since they contain more energy, are responsible for the radiation "tongue," displayed in Fig. 5, that extends to $r = 300$ m.

We feel that the $Y = 11$ kT multigroup simulation does not display a decoupling of temperatures for the following reason. The two yields differ by a factor of 100. Since energy is sourced with a Planckian spectrum, the initial maximum temperatures differ by roughly the fourth root, or approximately 3. Since the initial temperatures are of order 3–5 keV, the high frequencies have a nearly Wien distribution, $\nu^3\, e^{-\nu/T}$. Hence, we expect the $Y = 11$ kT spectrum to be $e^{\nu/3T}/e^{\nu/T}$ or $e^{-2\nu/3T}$ times smaller than the high yield case. Substituting $T = 3$ and $\nu = 100$ keV gives a very small number. The conclusion is that the $Y = 11$ kT case has an insignificant number of those energetic photons that are not absorbed by air and are the source of the "tongue."

We conclude the Raptor V&V by comparing results obtained with the 1D spherical and 3D Cartesian versions. We return to running with hydro, heat conduction, and with two AMR levels. For the Cartesian simulation, the Al "ball" consists of a cube 31 cm

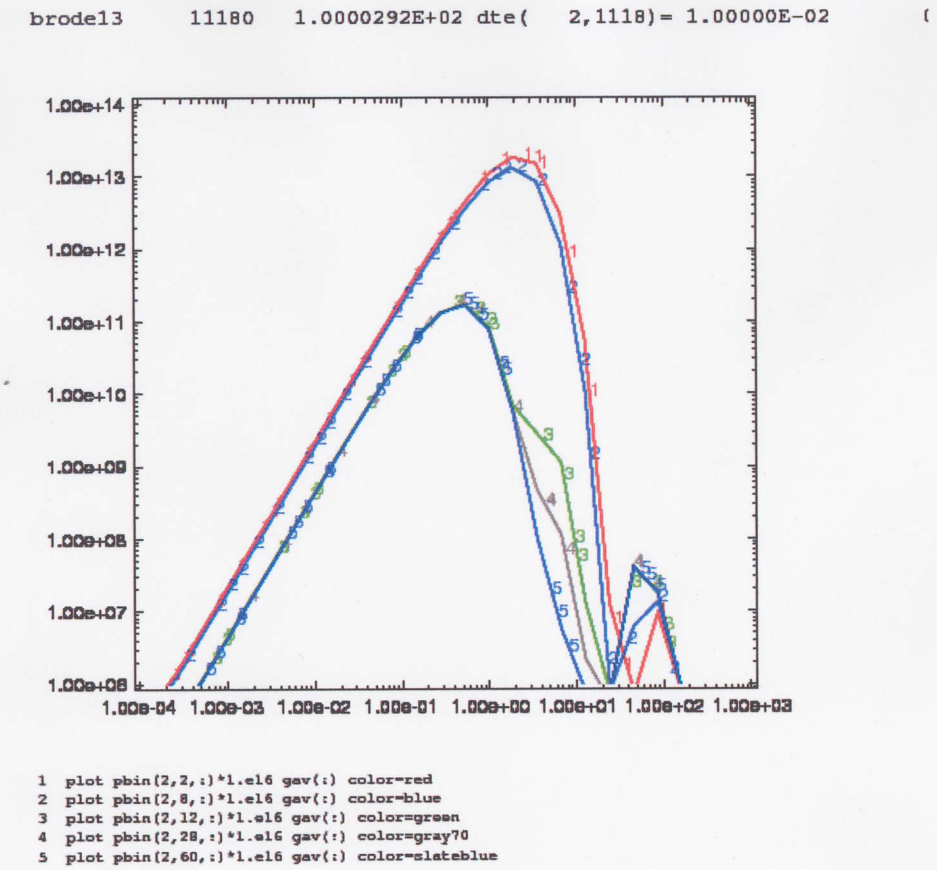

Figure 9: Spectral radiation energy vs. frequency at various radii; multigroup physics only; $Y = 1$ MT, $t = 1\mu$s; Lasnex.

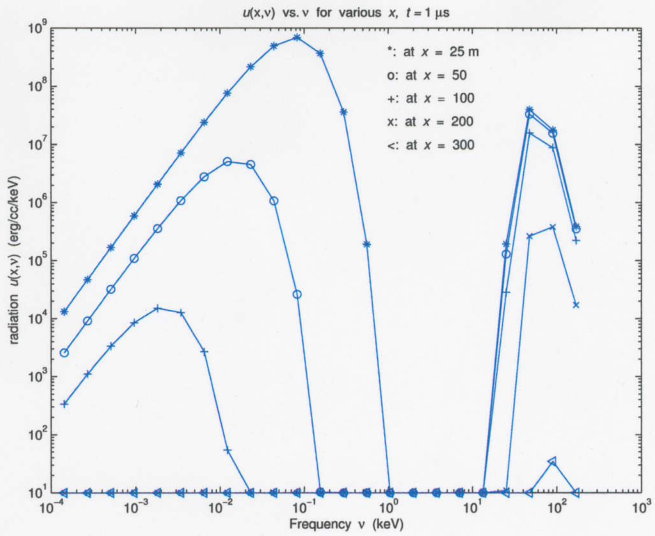

Figure 10: Spectral radiation energy vs. frequency at various radii; multigroup physics only; $Y = 1$ MT, $t = 1\mu s$; Raptor.

per side (in contrast to the 1D spherical ball of 31 cm diameter.) The difference in the Al volumes implies that the initial central, Cartesian temperatures are necessarily smaller in order to have the same yield. Results are presented in Fig. 12 where we display the radial 1D results and a x-axis lineout of the Cartesian run. The agreement of the profiles is self-evident.

To summarize, we have described a non-trivial test problem and compared results obtained with the Raptor and Lasnex codes. The test consists of simulating two air bursts with yields $Y = 11$ kT and 1 MT. Our results show that for low Y, gray and MGD give similar results. However, for large Y, they differ; at least for early times when the dynamics is dominated by radiation.

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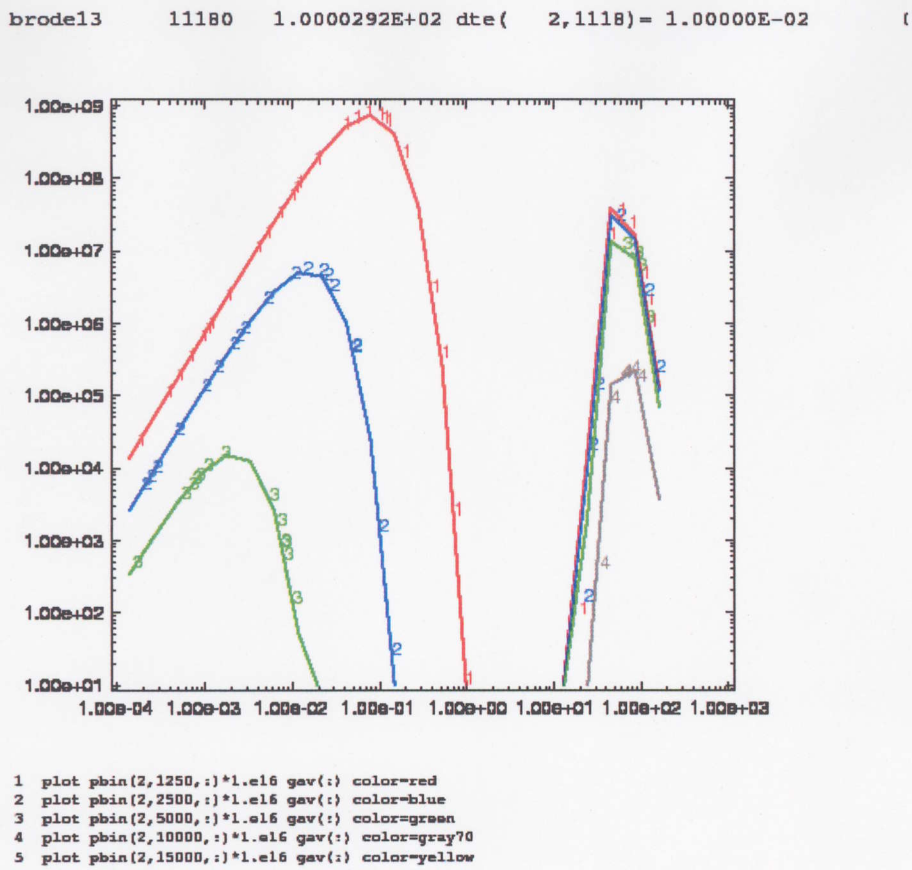

Figure 11: Spectral radiation energy vs. frequency at various radii; multigroup physics only; $Y = 1$ MT, $t = 1\mu s$; Lasnex.

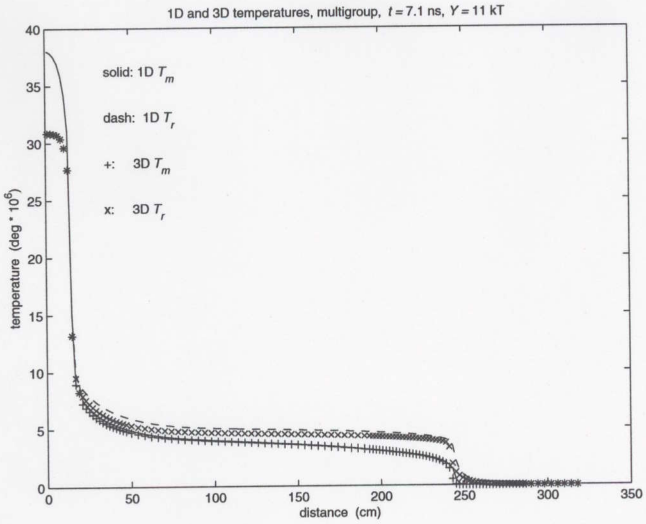

Figure 12: Comparison of T and T_r for 3D Cartesian and 1D spherical multigroup runs; $Y = 11$ kT, $t = 7.1$ ns; Raptor.

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