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ABSTRACT

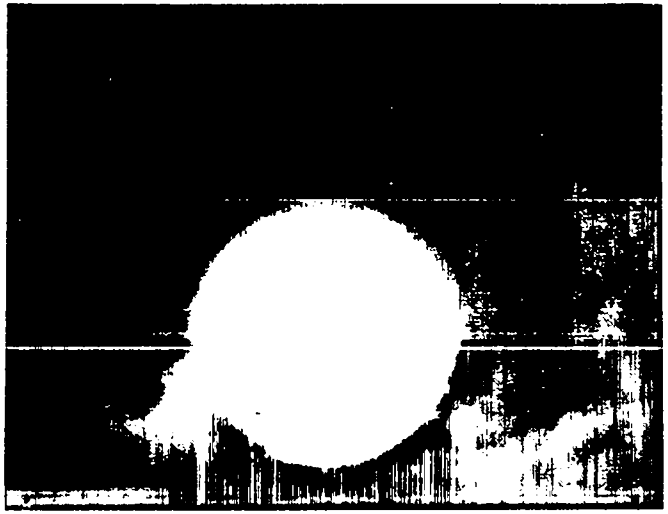
In a study of 2D radiative transfer methods, equilibrium diffusion, nonequilibrium diffusion and S_n, as applied to the interaction of the reflected shock with a fireball near the surface, the following results were obtained. The equilibrium diffusion method requires modifications to transfer energy through optically thin zones. The present S_n method, as included in YAQUI-SN, i.e., the TWOTRAN code, has troubles in the treatment of a thick/thin interface. Improvements are possible using methods developed by I. Grant or D. Barfield. The nonequilibrium diffusion or Moments method appears to be the most useful since it will limit properly in the optically thick and thin regions, but methods to determine the variable Eddington factors have not been successfully developed as yet.

I. INTRODUCTION

In modeling effects in two dimensions, we may have to trade off the importance of including detailed "physics" for reduced computer time usage. A complete Monte Carlo-type solution could be obtained for almost any geometry but the cost in computer time would be prohibitive. We propose to look for radiative transfer methods that may be used specifically to solve the particular problem at hand. The problem that we are considering is the interaction of an initially spherical fireball with a flat surface which occurs during the time of second maximum. Second maximum is the time during which the fireball rebrightens and radiates some 30% of its initial energy. This problem therefore requires the coupling between a 2D hydrodynamic code and methods of 2D radiative transfer. Photographs of a typical fireball interacting with a surface during this time are shown in Fig. 1. A strong shock develops from the hot bubble which then reflects back into the fireball, distorting its shape and therefore its optical signature, as observed at different viewing angles. The fireball is also rising during this time. The proposed study is to see how the variation in explosion height, yield and viewing angle affects the optical signature during second maximum light. The complete results will be discussed in another document. The actual fireballs modeled and the results are classified. In most of this study, we have utilized the YAQUI hydrodynamics code developed in T-3.[1] This code has the ability to do Lagrangian or Eulerian hydrodynamics and Arbitrary Lagrangian Eulerian (ALE) hydrodynamics by the use of an algorithm. For the most part, our studies have relied only on the Eulerian version of the code.

What we plan to discuss in this report is the adaptation of the three methods, equilibrium diffusion, nonequilibrium diffusion, and the S_n method, coupled into the YAQUI code, to the fireball interaction problem. In Sec. II, we discuss the use of the equilibrium diffusion method as adapted from RADOIL, a 2D code from Wallace Johnson.[2] The nonequilibrium diffusion method was obtained from the 2D VERA code[3] which was developed at Systems, Science and Software (S^3) and is discussed in Sec. III.

In Sec. IV, we discuss the application of the YAQUI-SN code developed in J-10 with the help of T-1.[4] This code has a variety of versions and we have utilized the grey-S_n version, the multigroup S_n, and a multi-S_n rezone version in our studies. Possible modifications of these codes will be discussed in Sec. V. As a test of the various methods, we have utilized a typical fireball structure, developed by the 1D code SPECFB, as starting conditions for the 2D calculations. The discussions of these calculations and the comparisons will be given in Sec. VI. Finally, in Sec. VII we discuss the results of this study indicating that a diffusion-like method is needed for the calculation of the "cooling wave" effect,[5] occurring during second maximum time. The most reasonable code for carrying out this aspect of fireball history, including the 2D effects of shock interaction, appears to be the nonequilibrium diffusion or Moments code (2DVERA or HIGHBALL II). A modification to the SN code, as described in Sec. V, could make it more acceptable for this phase of the 2D fireball interaction problem.



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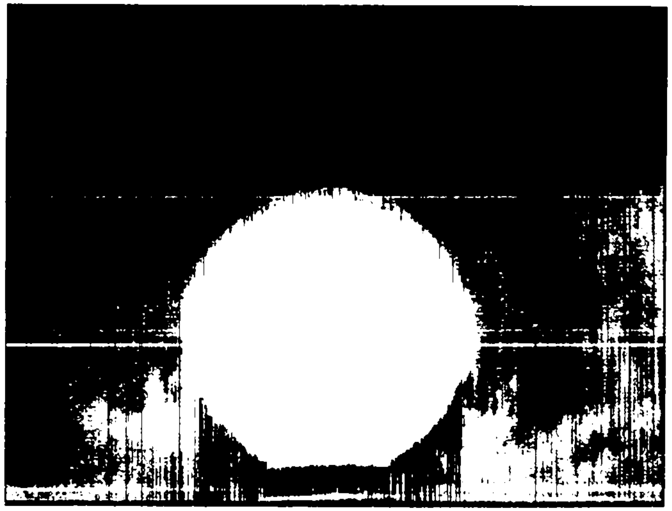

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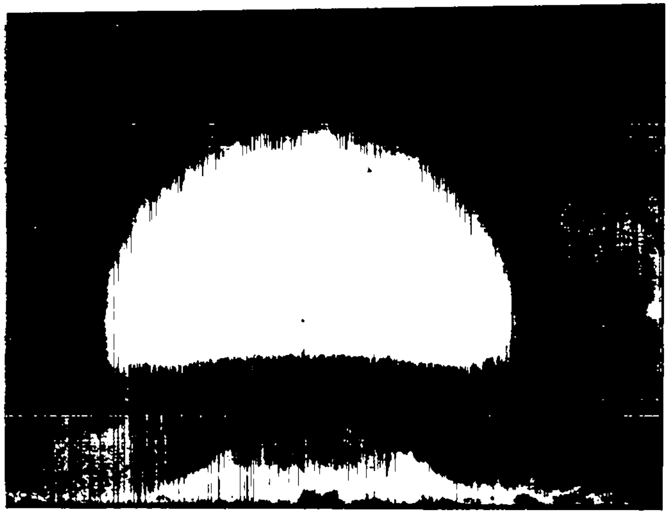

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Fig. 1.
Event GRABLE, Film No. 17981; sequence of frames showing effect of shock wave on fireball.

II. EQUILIBRIUM DIFFUSION

The most used approximation for solving the radiative transfer equation, in one or two dimensions, has been that of equilibrium diffusion. Starting from the basic transport equation

$$\frac{1}{c}\frac{\partial I}{\partial t} + \bar{\Omega}\cdot\nabla I = \sigma(B-I) \tag{1}$$

we can obtain the 1D diffusion equation making the following approximations:

1. The time dependence of the equations is not important. (Distances are small compared to ct.)
2. The radiation field is nearly isotropic ($I = I_0 + I_1\,\mu$).
3. The radiation field is in equilibrium with the material field (aT^4).
4. The frequency dependence of the transfer is not important (grey).

First, we can integrate Eq. (1) along a characteristic ray at a fixed μ where the time dependence has been incorporated as a retarded term and the following equation is obtained for the intensity.

$$I_i = I_{i-1}\, e^{-(\tau_i-\tau_{i-1})/\mu} + \int_{\tau_{i-1}}^{\tau_i} Be^{-(\tau_i-\tau)/\mu}\, d\tau/\mu \tag{2}$$

where τ is the optical depth ($=\int\sigma dr$) and B is the Planck Source function. An integration by parts of Eq. (1) results in the "SPUTTER"[6] equation, i.e.,

$$I_i = (B-\partial B/\partial\tau)_i + \left[I_{i-1} - (B-\partial B/\partial\tau)_{i-1}\right] e^{-\Delta\tau} + \text{higher order terms} \tag{3}$$

where for large optical depth ($\Delta\tau$) we obtain the diffusion limit, that is,

$$I = B - \partial B/\partial\tau \;\; ; \;\; \tau \text{ is now defined as } \;\; 1/\mu \int_0^x \sigma dx. \tag{4}$$

The resulting flux from the equation $F_1 = 2\pi\int_{-1}^{+1} I\mu d\mu$ is

$$F = -\frac{c}{3}\lambda_R \frac{dB}{dx} \tag{5}$$

where $d\tau$ is now written as dx/λ_R and

$$\lambda_R = \int_0^\infty \frac{1}{(\mu_a' + \mu_s)} \frac{dB_\nu}{dT} d\nu \bigg/ \int_0^\infty \frac{dB_\nu}{dT} d\nu \tag{6}$$

is by definition the Rosseland mean free path.

In two dimensions the equilibrium diffusion equation, in cylindrical coordinates, is

$$\frac{\partial E}{\partial t} = \frac{\partial \phi}{\partial t}\left(1 + \rho \frac{C_V}{4a\theta^3}\right) = \frac{c}{3}\left[\frac{1}{r}\frac{\partial r\lambda}{\partial r}\left(\frac{\partial \phi}{\partial r}\right) + \frac{\partial}{\partial z}\lambda\left(\frac{\partial \phi}{\partial z}\right)\right] \quad ; \quad \phi = T^4 . \tag{7}$$

$$\frac{\lambda'}{\Delta z} = \frac{\frac{\lambda}{\Delta z}}{\left\{1 + K\frac{\lambda}{\Delta z}\left|\frac{\nabla E}{E}\right|\left[1 + 3\exp\left(-\frac{\lambda}{2}\left|\frac{\nabla E}{E}\right|\right)\right]\right\}} .$$

λ' is a modification to the mean free path (λ) in the diffusion equation (7) in order to limit the flux to cE across a thick-thin interface. The particular limiter described here was devised by LLL[7] and used extensively by them in various codes. We used this equation in our 2D equilibrium diffusion version (YAQUI-RADOILR).

In the solution of these equations, we use the method proposed by Johnson, though there is some question as to directional effects. The method relies on the "splitting" technique where passes are made in the radial and axial directions separately in a semi-implicit fashion. Even though the direction of these passes are alternated on successive cycles, there is still some question as to the directional nature of the solution. However, from our experience with the code, the method seems to work well and preserves the sphericity of the fireball during the early phase. The same type of solution is applied to the nonequilibrium diffusion equations which will be discussed next. Refer to Ref. 2 for a more complete discussion of the method.

III. NONEQUILIBRIUM DIFFUSION

The nonequilibrium diffusion equations result from an expansion of the transport equation, Eq. (1), in terms of the moments of the angular distribution of the intensity. The first three 1D moments, which have some physical significance, are

$$E = \int_{-1}^{+1} I \, d\mu \quad ; \quad F = \int_{-1}^{+1} I\mu \, d\mu \quad ; \quad P_{rr} = \int_{-1}^{+1} I\mu^2 d\mu \; . \tag{8}$$

These are then the energy density (E), the radiative flux (F) and radial component of the radiation pressure tensor (P_{rr}). The actual 1^{st} and 0^{th} moments of the transport equation in cylindrical geometry are

$$\left.\begin{aligned} \frac{1}{c}\frac{\partial F_r}{\partial t} + c\,\frac{1}{r}\frac{\partial(rfE)}{\partial r} + \frac{\partial(hE)}{\partial z} &= -\frac{F_r}{\lambda_r} \\ \frac{1}{c}\frac{\partial F_z}{\partial t} + c\,\frac{\partial(gE)}{\partial z} + \frac{1}{r}\frac{\partial(rhE)}{\partial r} &= -\frac{F_z}{\lambda_z} \end{aligned}\right\} \quad 1^{st} \tag{9}$$

$$\frac{\partial E}{\partial t} + \frac{\partial F_z}{\partial z} + \frac{1}{r}\frac{\partial rF_r}{\partial r} = c\mu\left(\frac{4\pi B}{c} - E\right) \qquad 0^{th}$$

where f, g and h are the variable Eddington factors.

As a closure of the expansion, P_{rr} was set equal to fE, P_{zz} to gE and P_{rz} to hE. The reason these equations are called diffusion equations is that the expansion is only to P_1 or $(1 + \cos\theta)$. Higher order terms could be included, as in S_n, but this removes the simplicity of the solution of the fully retarded transport equation. In 1D geometries, either an analytic solution[8] or a transport snapshot may be used to determine f. This latter approach is used in the 1D SPEC codes (SPECFB). The main improvement over the equilibrium diffusion equation is now evident: (1) the radiation field will now limit correctly in optically thin regions, and obviously in the optically thick regions, to the diffusion, i.e., the radiation field is not necessarily in equilibrium with the material field; (2) the correct angular distribution can be included in f, g and h. That these equations limit to the wave equation can be demonstrated by using the plane geometry set of nonequilibrium diffusion Moments equations, i.e., ,

$$\begin{aligned} \frac{\partial E}{\partial t} + \frac{\partial F}{\partial x} &= c\mu_p \left(\frac{4\pi B}{c} - E\right) \\ \frac{1}{c}\frac{\partial F}{\partial t} + cf\,\frac{\partial E}{\partial x} &= \mu_R F \ . \end{aligned} \tag{10}$$

When the material has zero absorption and scattering, i.e., ($\mu_s = \mu_a' = 0$), then

$$\frac{\partial^2 E}{\partial t^2} + c^2 f\ \frac{\partial^2 E}{\partial x^2} = 0 \tag{11}$$

where the velocity of the radiation front is $\bar{c} = c\sqrt{f}$. In the present application of the Moments method, we have decided to use the Eddington approximation in 2D, i.e., f = g = 1/3 and h = 0; and therefore the wave front velocity is $c/\sqrt{3}$. A cylindrical transformation of the spherical Eddington factors is available in 2DVERA or HIGHBALL II (TD-3) but difficulty in running problems with these factors has been experienced. It is possible to approximate the correct effects of retardation by not including the $1/c\ \partial F/\partial t$ term in the 1st Moment equation but to include a flux limiter, the use of the term ($1/c\ \partial F/\partial t$) can cause instabilities. For stability, we have used the flux limiter described in Sec. II with K = 0.10 and have dropped the time derivative term ($1/c\ \partial F/dt$).

If we wished to carry the variable Eddington factors, using the splitting technique, then the cross derivative terms must be done explicitly in the following fashion.

$$F_z^{n+\frac{1}{2}} = F_z^{n} - c\ \frac{\partial (hE)^{n+\frac{1}{2}}}{\partial z}\ c\Delta t\ . \tag{12}$$

This aspect of using variable Eddington factors will also result in instabilities, which has also contributed to our decision to set f = g = 1/3 and

$h = 0$. With these approximations we can solve the nonequilibrium diffusion equations by the splitting method as discussed in Sec. II.

Another method that has been tried for solving the traditional diffusion equation is the ADI or Alternating Direction Implicit Method of Douglas and Gunn.[9] This method effectively uses three passes through the mesh, treating the cross derivative terms directly. Difficulties were found in this method as applied by Wei et al (TD-3) in the HIGHBALL II code to our fireball problem (see Sec. VI).

Finally, there is the full matrix inversion method, a fully implicit method, used by S^3. In order to implement this method, S^3 has gone to a minimatrix inversion technique that depends on including the surrounding cells that are only a photon flight path away. The number of mesh cells included in the inversion also depends on the subsequent time for convergence, i.e., the number of iterations needed to converge. The method, when applied properly, seems to require about as much time as the splitting method to complete the problem. When using a fully implicit method though, it appears difficult to easily modify terms in the equations if new physics needs to be added. For the study made here, the splitting method is the only method of solution used.

IV. S_n TRANSPORT

S_n is recognized by now as the standard numerical scheme for use in the solution of neutron transfer problems. Recently, Lathrop and Brinkly have released a transportable version of the 2D S_n code TWOTRAN,[10] and this is the code adapted by Reed (T-1) for use in the J-10 YAQUI code. S_n effectively replaces the exponentials in the transport equations by numerical differences. The equation for the intensities at the interfaces ($N_{i,j,m}$), as transcribed from the S_n report (formula 23), is

$$\begin{aligned}&\mu\ (A_{i+\frac{1}{2}}N_{i+\frac{1}{2}} - A_{i-\frac{1}{2}}N_{i-\frac{1}{2}})\\&+ (A_{i+\frac{1}{2}} - A_{i-\frac{1}{2}})\ (\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}})/w\\&+ \eta B\ (N_{j+\frac{1}{2}} - N_{j-\frac{1}{2}}) + \sigma_t VN = VS\ .\end{aligned} \tag{13}$$

Where the recursion relation $\alpha_{m+\frac{1}{2}} = \alpha_{m-\frac{1}{2}} - m_m \mu_m$, is used to determine α then σ_t is the total cross section, S the source, μ, n are direction cosines to r and z respectively, A is the surface area and V the volume of the cell. For a complete discussion of these equations, see Ref. 10. For photon transport, the step differencing scheme is used instead of the diamond difference scheme normally used in TWOTRAN. From discussions with Lathrop and others, it is evident that step differencing is less accurate but stable. Diamond differencing is known to give negative intensities in 1D if $\sigma\Delta x/2\mu > 1$ is not satisfied.

Differences in r and μ enter the equations and these differences require interpolations. The centered difference equations therefore retain second order accuracy for optically thin zones but introduce possibly very large errors for optically thick zones. Another problem with S_n in 1D is that the same number of sampling angles applies to regions near the center of the cylinder as to regions near the boundary. The usual requirement of isotropy at the center indicates that compared to this selection scheme a preferable scheme would be to place light rays nearer the surface. Some attempt at codes of this nature, i.e., direct integration methods, have been tried (Campbell).[11]

V. MODIFICATIONS

The equilibrium diffusion scheme can be modified in an ad hoc manner to account for transfer of flux through the optically thin air. One can integrate in from the boundaries of the mesh to $\tau = 2/3$ and then remove energy from the edge of the fireball as $\kappa_p \sigma T^4_{2/3}$ where T is the temperature at $\tau = 2/3$. One turns off the $\nabla \cdot F$ term by a large increase of opacity at the fireball surface.

The nonequilibrium diffusion equations lack proper methods for calculating the variable Eddington factors. With reasonable factors, limiting to f = 1/3 in diffusion regions and f = 1 in streaming regions, a complete transfer solution could be obtained.

Various modifications have been made to the standard neutron S_n equations for use in photon transport. In 1D spherical geometry, I. Grant[12] and B. Wendroff[13] have made use of the integral equation, Eq. (2), for the source term with an indicated improvement in the results. In the TWOTRAN code, Barfield[14] has used a transformation of variables, i.e., $\overline{I} = I/B$ which results in some improvement of the results. In two dimensions it is more difficult to determine the correct dB/dT from the spatial distributions. None of these improvements, apparently, have been attempted in the present YAQUI-SN code.

Two important aspects of radiative transfer that have not been considered in this report are the question of frequency dependence and the proper energy equation. From our 1D studies, we have determined that grey opacities are sufficient for calculating the temperature time history of the fireball during second maximum. The spectral characteristics of the fireball structure are then determined by utilizing a multigroup snapshot code. For the energy equation all the methods discussed, even the S_n transport method, utilize the left-hand side of the 0^{th} moment equation, Eq. (9), without the retardation term ($\partial E/\partial t$). This term is more easily formed for use in the diffusion region of the fireball structure. In the semitransparent region where precursors may form, which is outside of the diffusion fireball edge, it would be more appropriate to use the right-hand side of the 0^{th} moment in Eq. (9). From our studies so far, precursors do not form during the time of second maximum for sea level fireballs.

VI. INTERCOMPARISONS

As mentioned in the Introduction, the various 2D radiative transfer schemes described were coupled into the YAQUI hydrodynamics code, using the Eulerian option except for the HIGHBALL II calculation. The equation-of-state and opacity data used in this study were developed in Group J-15 with the help of Group T-4.

The fireball problems were started with a 1D SPECFB calculation at the time when the shock strikes the surface (0.09 s). In all cases the initial zoning was the same using equal Δr, Δz steps of 0.02 km. As a test of the various schemes the calculations of the so-called cooling wave of Zeldovich and Bethe, in terms of temperature profiles versus time, are intercompared. The temperature profiles from the 1D calculation, clearly showing the cooling wave, are shown in Fig. 2. It is necessary that the 2D transfer schemes give nearly the same profiles in the horizontal direction in order to obtain agreement with observations, i.e., to times near second maximum. In Fig. 3, we show the horizontal profiles in temperature for a nonequilibrium diffusion (HIGHBALL II) and the grey and multigroup S_n calculations at 0.1 s to be compared to the 1D results (Fig. 2). As seen, the HIGHBALL II profile indicates a higher energy density than SPECFB while the S_n profiles show that too much energy loss has ocurred by this time. The HIGHBALL II calculation then blew up at 0.2 s. The reasons are not clear but may be related to the method of solution used.

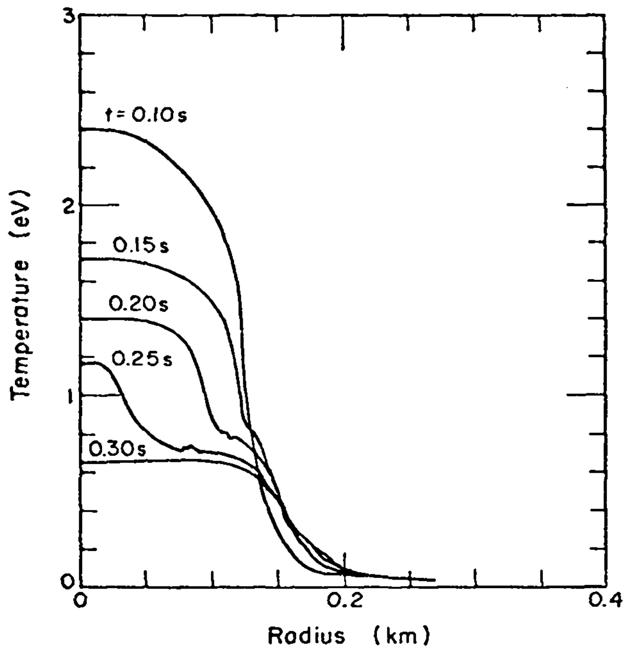


Fig. 2.
1D fireball temperatures vs radius at selected times. Observe "cooling wave" effect.

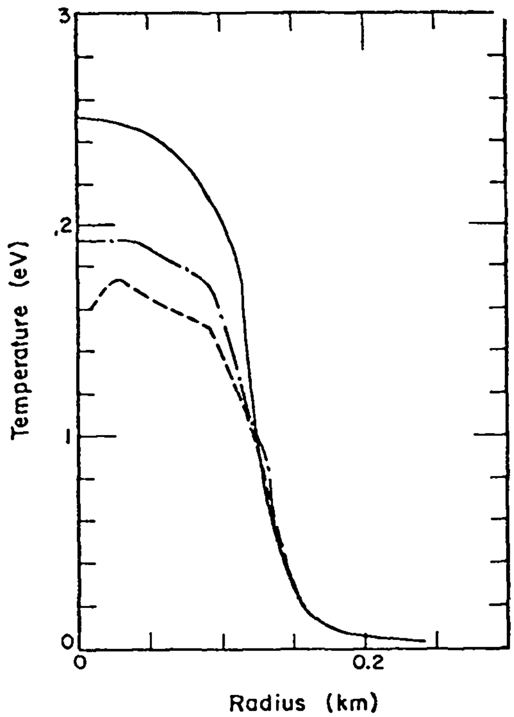
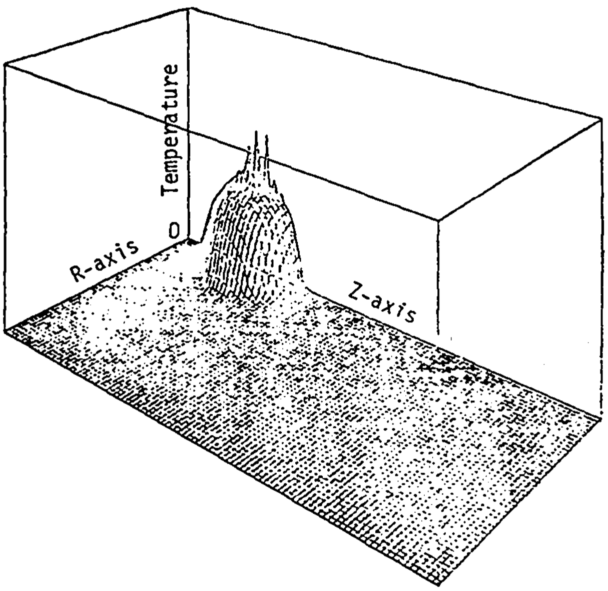


Fig. 3.
2D horizontal fireball temperatures vs radius at 0.10 s for nonequilibrium diffusion (solid line), multigroup S_n (dash-dot), and grey S_n (dash).

In Fig. 4, we show a 2D plot of the temperature from the S_n calculation at 0.1 s showing an instability near the center of the fireball. This instability apparently is related to the coupling with YAQUI. From these comparisons and others, we decided to continue only the nonequilibrium diffusion (YAQUI-MOMENT) calculation to late times. The reasons will be discussed next.

In Fig. 5, we show the time-temperature profiles using the nonequilibrium equations introduced into the YAQUI-MOMENTS code with f = g = 1.3, h = 0 and splitting. In general, these results look better than in the above-mentioned comparisons except for the peak in temperature near the middle at 0.1 s and the late breakthrough of the cooling wave as compared to the 1D results.

In order to obtain an optical signature from these two-dimensional fireball results, we use a ray calculation developed for the YAQUI code by J. Kodis.[15]



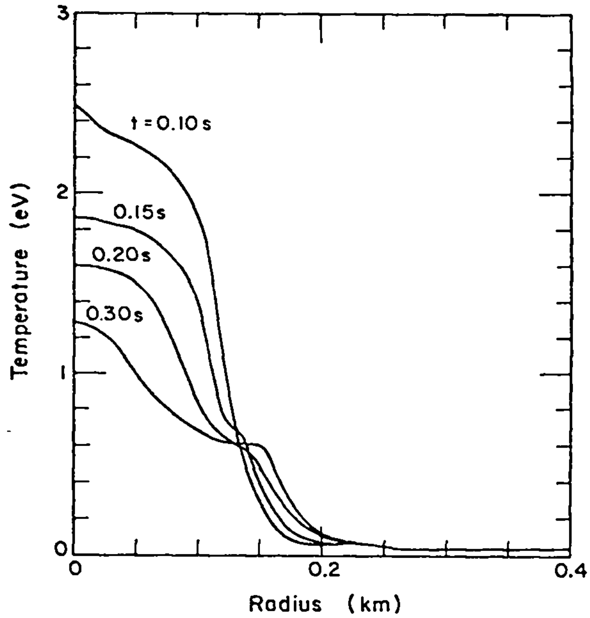


Fig. 4.
2D display of temperature for the grey S_n at 0.1 s showing some instability near center of fireball.

Fig. 5.
2D horizontal fireball temperatures vs radius at selected times from the Moments calculation.

Using these rays in our coupled 1D snapshot program SNAP DRAGON, we are able to develop space-integrated luminosities during the time of the interaction until past second maximum. By second maximum time, the actual luminosities are affected by bomb debris emissions and these are not included in these calculations. These snapshot rays can be used to produce isophotes in a manner devised by Kodis. The results for a horizontal view angle and one at 45° are shown in Fig. 6. The actual integrated light output from these view angles is shown in Fig. 7. The differences indicated appear real, but the overall effect is minimal.

VII. RESULTS

As indicated in Sec. VI, our initial study, using the existing 2D radiative transfer codes HIGHBALL II and YAQUI-SN, gave disappointing results. The adaptation of the Moment equations to YAQUI, using the splitting technique for solution, on the other hand, gave encouraging results. A time shift occurs in second maximum, compared to the 1D results, but the "cooling wave" is evident in the 2D temperature profiles. Some evidence of real two-dimensional effects appear in the luminosities as viewed from 0° and 45°. The computer time spent on this calculation was approximately 3-1/2 hours of CDC 7600 time.

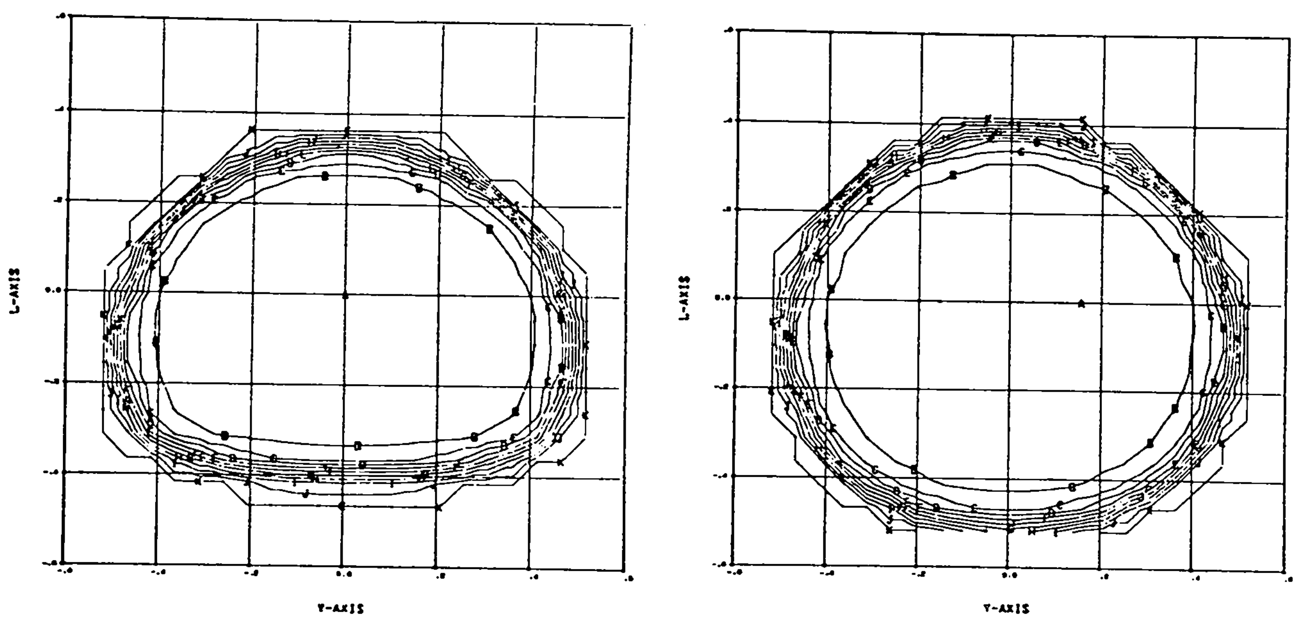


Fig. 6.
Isophotes from 2D fireball structure at 0.7 s at viewing angles of 0°(left) and 45° (right).

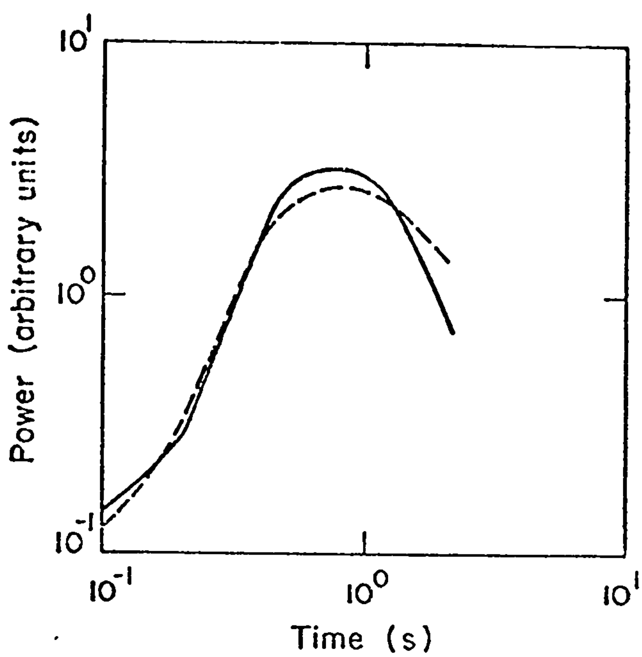


Fig. 7.
Integrated fireball luminosities vs time from the 2D structure developed by the Moments method. Code viewed at 0° (dashed) and 45° (solid).

Finally, it appears that modifications along the lines of Grant or Barfield could be made to YAQUI-SN to make it more acceptable for the fireball calculation during second maximum.

ACKNOWLEDGMENTS

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