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Theoretical Simulations of the Gas Explosive Simulation Technique (GEST) Experiments

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ABSTRACT

To calibrate our ability to predict the dynamic behavior of nuclear fireballs we have simulated the balloon detonations conducted under DNA sponsership in November of 1973. These well-instrumented shots provide excellent data to test the reliability of hydrodynamic models for the rise and expansion of very low yield explosions. We present the results of our calculations and draw conclusions concerning the applicability of such techniques to nuclear fireball simulations.

I. INTRODUCTION

Considerable success has been achieved in the past in predicting the gross geometric properties of nuclear fireballs as a function of time. However, the amount of physics that is desirable in such calculations is more than that usually contained in hydrodynamic computer codes so that when a discrepancy between the numerical simulations and the experimental data does occur, it is often attributed to phenomena missing from the codes, e.g., radiation, moisture, dust, equations of state of the many constituents of a nuclear burst, etc. This leaves little opportunity for a good evaluation of the importance of these effects on predictions of large-scale dynamic behavior. Furthermore, one cannot discount the possibility that the mismatch between theory and experiment resides in the assumption that fireball behavior can be approximated by a hydrodynamic model even with a simplified version of turbulence.

To reduce the number of unknown variables often associated with nuclear effects, several large balloons filled with a mixture of methane and oxygen were detonated. These experiments were well instrumented and, thus, serve as good benchmark test cases involving primarily hydrodynamic phenomena. We shall compare our calculations with two of the large detonations that produced similar gross geometric properties as a function of time. These shots consisted of centrally detonated Mylar balloons, originally 9.7 m in diameter, for which the yields were predicted to be 4×10^9 J. The detonation point was 43 m above ground and the calculations were picked up at 8.3 ms at which time the radius of the fireball was calculated to be 7.8 m.

The configuration at 8.3 ms was predicted by a one-dimensional combustion code, the results of which were obtained from the Air Force Weapons Laboratory. The code yielded density, velocity, and specific internal energy as a function of radius. The pressure was then obtained from the Doan-Nickel equation of state for heated air and an equation of state for the methane/oxygen combustion products. The form of these equations of state assumes the pressure dependence may be written as

$$p = [\gamma(\text{material}, \rho, I) - 1]\, \rho I ,$$

where ρ is the material density, I is the specific internal energy, and γ is a function of ρ and I dependent on the particular material involved. Thus, an input of ρ and I into the appropriate routine

yields γ and, hence, the pressure. From the initial configuration of velocities, densities, and internal energy as a function of radius, the calculations were carried forward in time by the two-dimensional hydrodynamics code, YAQUI,[1] which was designed and constructed expressly for the purpose of predicting fireball behavior. It was written employing a capability for continuously rezoning the mesh. We have found, empirically, that this feature considerably enhances our ability to make reliable predictions for fireball dynamics. The effect of pressure on the mass and momentum equations is handled implicitly though this is only important for fireballs at late times when the flow is quite subsonic. YAQUI also has the capability to simulate turbulence through a transport equation for the turbulence energy density and an empirical formulation of the characteristic turbulence scale.

The boundaries of the computational mesh are rigid, free-slip boundaries. The effect of this on the calculation will also be discussed in more detail later.

As far as the continuous mesh rezone is concerned, we used our standard rezone treatment which moves mesh vertices with a two-part grid velocity: a component equal to the fluid velocity (Lagrangian component) and a part to prevent excessive distortion. The latter part relaxes the mesh such that each vertex moves toward the average position of its nearest neighbors. This may be expressed in terms of a grid velocity as

$$\vec{u}_{g,i} = \vec{u}_{f,i} + \frac{f}{\delta t}\left(\langle\vec{x}\rangle - \vec{x}_i\right) , \qquad (1)$$

where f is a parameter, of the order of 0.05. $\vec{u}_{f,i}$ is the Lagrangian fluid velocity of the ith cell. This algorithm would relax the mesh in approximately 20 cycles if the fluid velocity were zero, and has the advantage that if distortion decreases the time step, requiring more cycles per unit time, the relaxation procedure is carried out more frequently, keeping pace with the greater tendency to distort.

We will not discuss the details of the numerical technique here, since it is well documented in Ref. 1. Rather we report in some detail the calculations made employing this technique for the methane balloon experiments. Some important conclusions can be drawn from this series of simulations.

Several calculations were made in order to be able to do more than simply compare theory with experiment. With the relatively clear data provided by the balloon detonations it is feasible to learn, at least in part, what approximations in the numerical simulations most affect the agreement with experiment. In particular, for certain comparisons with nuclear bursts, it has been difficult to fit both the fireball rise rate and its radial expansion rate out to late times. By performing several different calculations and by comparing with data available from the balloon detonations, we are able to reach some important conclusions.

II. DISCUSSION OF RESULTS

The standard mesh for our series of simulations was 30 cells wide by 45 cells high with cylindrical symmetry about the vertical line, I = 1. Initially there was a square central portion of cells 2 m on a side with the cells exterior to this region increasing in size geometrically, about 10% per cell, to the mesh boundaries. The right-hand boundary was initially found at 193 m, the top boundary at 236 m, and the ground at its proper location, since the reflected ground shock is an important aspect of the calculation. Using marker particles to locate the position of the fireball, we moved the right and top boundaries to maintain at least six fireball radii between the hot region and these boundaries throughout the calculation. At 30 s after burst when the calculations were terminated, the right boundary was at about 200 m, having moved hardly at all, while the top boundary had reached nearly 450 m above the ground. It is clearly an approximation to confine the calculational region between rigid boundaries. Signals that originate at the fireball are trapped in the mesh and may reflect back across the burst region. These reflections will eventually smooth themselves out and lead to a uniform overpressure everywhere in the mesh. What we would like, and indeed try to do, is to move the mesh boundaries out at such a rate as to remove, or at least minimize, the influence of reflected signals from the region of interest.

To test the effectiveness of our efforts, we made two calculations particularly to address this question: one in which the boundaries were forced to be at least eight radii from the burst region and one in which a simplified version of an outflow boundary was employed. In neither case were the geometric properties materially affected. From these tests we concluded that rigid boundaries at six radii have only a slight influence on the results.

In this report we shall compare three calculations made with the basic configuration outlined above. In each we will show the effect of a particular physical phenomenon. A comparison of the results leads us to certain conclusions concerning the sensitivity of the calculations to various parameters and indicates how such a code should be used to obtain information concerning fireball behavior.

The geometric configuration of the fireball was obtained from the numerical simulations by examining the Lagrangian marker particles. The radius was read from the right-most particle, while the altitude was calculated from the average of the highest and lowest marker particles. Initially these particles were distributed evenly over the fireball.

Figures 1(a)-1(c) compare the experimental results and theoretical predictions for the rise rate and radial expansion of two balloon shots. We include the data from both shots to give some feeling for the reproducibility of the experiments and hence an idea of the experimental error one might associate with these data.[2]

Consider first the calculation shown in Figure 1(a). An equation of state of the form $P = (\gamma-1)\rho I$, with $\gamma = 1.4$, was used everywhere, both in the hot fireball interior and in the exterior ambient region. The agreement between experiment and data is excellent; in fact this calculation agrees better than do the simulations that purport to be better realizations of the actual physical situation.

Calculations that use exclusively either the Doan-Nickel equation of state for air or the equation of state for "methane" throughout the mesh exhibit fits equally as good as the $\gamma = 1.4$ result. It appears that, within some range of γ's, constant γ calculations give excellent representations of the data.

Nevertheless, calculations were performed that made a distinction between the interior region, containing combustion products, and the exterior region in which air is the dominant constituent. This was done by carrying along an equation for the concentration of combustion products (of methane and oxygen). For brevity we shall often refer to the combustion products as "methane." We assumed the "methane" was not mixed with air but convected only, that is,

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = 0 \ .$$

The "methane" concentration was initially set to unity inside a sphere of radius 7.8 m, where the specific internal energy exceeded 10^{10} ergs/g. The concentration was zero elsewhere. The γ used in the equation of state for any cell was then determined from a linear combination of γ's for air and "methane" from the relation

$$\gamma = c\,\gamma_{\text{methane}} + (1 - c)\gamma_{\text{air}} \ .$$

The individual γ's were obtained from routines that provided γ as a function of ρ and I for the combustion products and heated air, respectively.

The results of this calculation are shown in Fig. 1(b). We note a rise rate that is a bit excessive at late times and a radius versus time that underestimates the experimental data. A comparison of this calculation with the $\gamma = 1.4$ simulation demonstrates what is perhaps the most important result that emerges from our study: namely that the equation of state crucially affects the radial expansion of the fireball. Considerable investigation of this point leads us to conclude that the early time pressure balance between interior and exterior regions affects for all time the geometric development of the fireball. A constant $\gamma = 1.4$ calculation appears from the results to model the physical situation most closely. Our attempt to improve the physics seems to have led us to introduce a pressure field that hinders the free expansion of the fireball.

It is hard to determine exactly how this happens. We do know that the γ for the combustion products is less than that for heated air for all

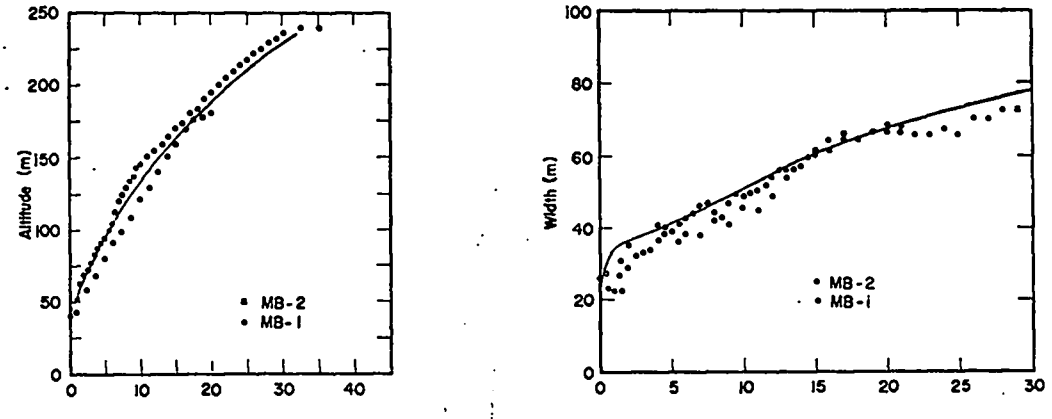

Figure 1 (a)

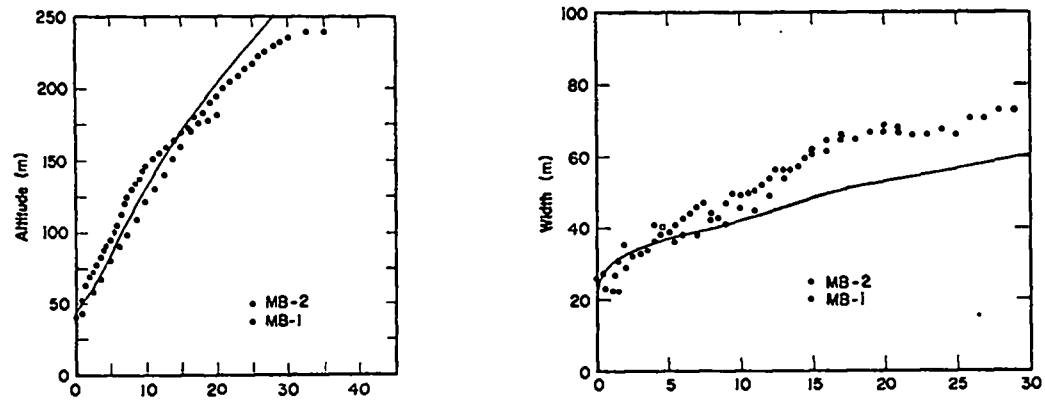

Figure 1 (b)

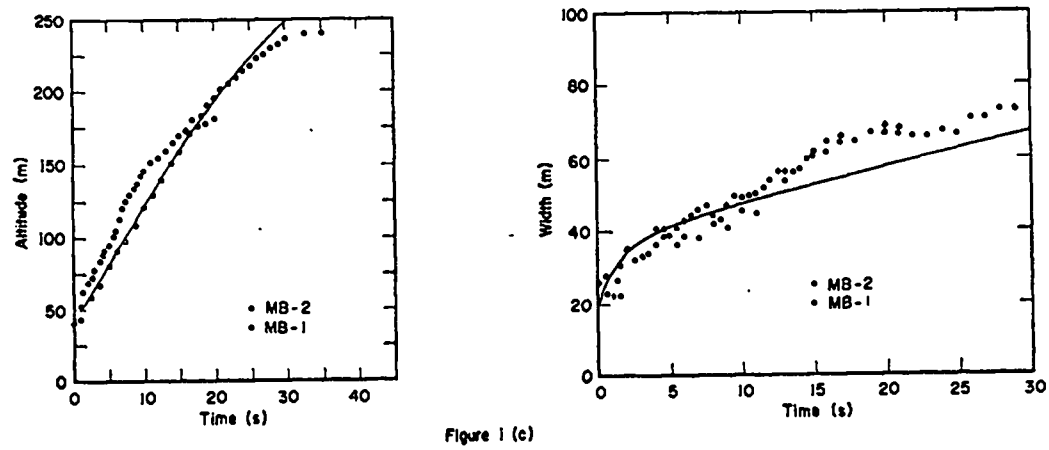

Figure 1 (c)

Fig. 1. Altitude and radius as a function of time for methane/oxygen filled balloon detonations. The calculations of Fig. 1(a) were performed with a simple γ-law equation of state, γ=1.4. For Fig. 1(b) γ was obtained as a linear combination of the γ's for the combustion products and γ's for heated air. Fig. 1(c) included a turbulence model and a γ as for Fig. 1(b). The linear combination is, of course, altered by the inclusion of turbulence.

temperatures and densities of interest. Hence, for a given density and temperature, if the proportion of "methane" to air in a cell is too large, the pressure would be too low leading to an inward pressure gradient inhibiting radial expansion.

Past calculations on nuclear fireballs have shown that the radius versus time curve is the more difficult feature to predict. In those earlier calculations only the most primitive equations of state were included, generally just for heated air. One is led to hypothesize that to do accurate simulations of nuclear events, considerable thought should be given to including better models for the equation of state.

Since the ratio of "methane" to air affected the results, it seemed natural to turn on the turbulence model[3] that already existed in the code. This would allow the "methane" to mix with air through turbulent diffusion. The equation for the concentration was modified to include this term and was written as

$$\frac{\partial c}{\partial t} + \vec{u} \cdot \nabla c = \nabla \cdot \sigma \nabla c \ .$$

For details on the remaining equations, see Ref. 3.

Because the marker particles are used to mark the position of the fireball and give the radius and altitude, it was necessary to superimpose a diffusion[4] onto their basic Lagrangian movement. The results of the calculation that includes the turbulence model are depicted in Fig. 1(c). Clearly the inclusion of turbulence improved the fit to the data. The addition of the turbulent diffusion had the effect of slowing down the rise and increasing the radius, though the fit is still not as impressive as the simple model with $\gamma = 1.4$.

If the turbulent mixing should occur earlier and more violently than our model allows, the "methane" interior in our calculation may retain its identity for too long a time and cause insufficient radial expansion.

There are many uncertainties in our turbulence model. Past experience had indicated that these do not have large effects on the dimensional data; however, we had never worked with a model in which the equations of state are affected by the turbulence through material diffusion. For the record, the turbulence was seeded at 0.5 s as proportional to the vorticity in those regions where the vorticity was less than 10% of its maximum absolute value over the mesh; it was set to zero elsewhere. This prescription has been found empirically to give a reasonable representation of an early time turbulence that rapidly finds its equilibrium value. The scale was taken to be 10 m, which is the radius of the fireball at the earliest times. This is only an approximation to the scale, hopefully an upper bound. A much smaller value would have led to a too rapid decay of the turbulence energy and minimized the effect of the turbulent diffusion. In any case it appears that the results are much more sensitive to the equation of state than to the inclusion of turbulence.

III. CONCLUSIONS

Several important conclusions can be drawn from these results. Most important is that, at least for shots of the size calculated here, the hydrodynamics does describe the important features of the observed fireball behavior. The code gives rather accurate predictions for the position and size of these fireballs. Since care was taken to keep as many parameters of the code the same as used in nuclear fireball simulations and not to specialize in any way for these smaller shots, the balloon simulations have increased our confidence in the ability of codes to predict the hydrodynamic evolution of fireballs from the initial one-dimensional input conditions.

The discrepancy observed with some of the nuclear events, then, must be due either to a lack of accurate initial data or to some feature of the simulations that cannot be scaled up from the balloon events. In this latter category could be the stratification of the atmosphere over distances involved in nuclear events or the much more complex composition of the fireball which must be modeled with a simplified equation of state. Almost all nuclear fireball calculations have been made with a single equation of state - that for heated air. Although this must be largely correct, it is an approximation, particularly at the edge of the burst region where it can affect radial pressure gradients and significantly modify the growth of the fireball.

For nuclear fireballs simulated previously there has always been some uncertainty concerning the tradeoff between rise rate and radial expansion. One could fit them both for up to, say, 10 torus formation times but then the rise rate would drop below the experimental rate. If one did the calculation with as little numerical diffusion as possible, the result was to achieve too much rise and too little radial expansion. At early times, say 1-3 torus formation times, the fits to all geometric data tended to be good almost independently of the details of the simulation.

From the experience obtained in previous work on nuclear events and from the careful simulations of the balloon shots we are led to conclude that rather good predictions of fireball behavior are possible. The continuous rezone capability and the possibility of moving boundaries away from the burst region as the fireball expands are important attributes of a code that is to succeed in such an effort. Less crucial seems to be the inclusion of a turbulence model, at least after times comparable to one torus formation time. Less clear is the situation with regard to the turbulence at very early times. Its most important influence appears to be in the mixing of materials with different equations of state, particularly in the transition region between heated detonation products and the ambient medium.

IV. NOTE ADDED IN PROOF

To test the sensitivity of the rezoning algorithm a calculation was performed by E. M. Jones using marker particles to perform the rezone.[5] The code is run in the Lagrangian mode until a sensor detects some level of distortion. Then a remapping to equal rectangular cells is performed, using marker particles to assign masses, momenta, and energies to the new cells. The frequency of rezoning is of course problem dependent and depends on the preassigned distortion threshold. At early times rezoning is done every 1/3 of a second. At about five seconds, rezoning takes place each 1/2 second; the interval between mappings gradually increases. At late times, the rezoning is only needed each $1\frac{1}{2}$ seconds of problem time. This calculation was performed with the equation of state for heated air throughout. Moreover, the mesh was 70 x 100 cells, 0.2 m across the fireball initially. This provides much greater resolution than the calculations of Fig. 1.

However, this rezone algorithm follows the shock outward until it becomes weak enough to be ignored. This implies encompassing a much larger region of space for a considerable period of time. Hence the resolution is variable and at some point, perhaps 2-3 s, is comparable to the calculations of Fig. 1. At later times, when the shock can in fact be ignored, the grid is remapped inward and the resolution once more is dramatically improved. Despite these considerable differences, the rate of rise as shown in Fig. 2 agrees well with the data and also with the other simulations. The radial expansion also seen in Fig. 2 proceeds slightly more rapidly than our calculation of Fig. 1(a), which also was done with a single equation of state. Nonetheless, in the balance, it appears that the simulations agree well enough that concern about the form of the rezone prejudicing the results is unwarranted.

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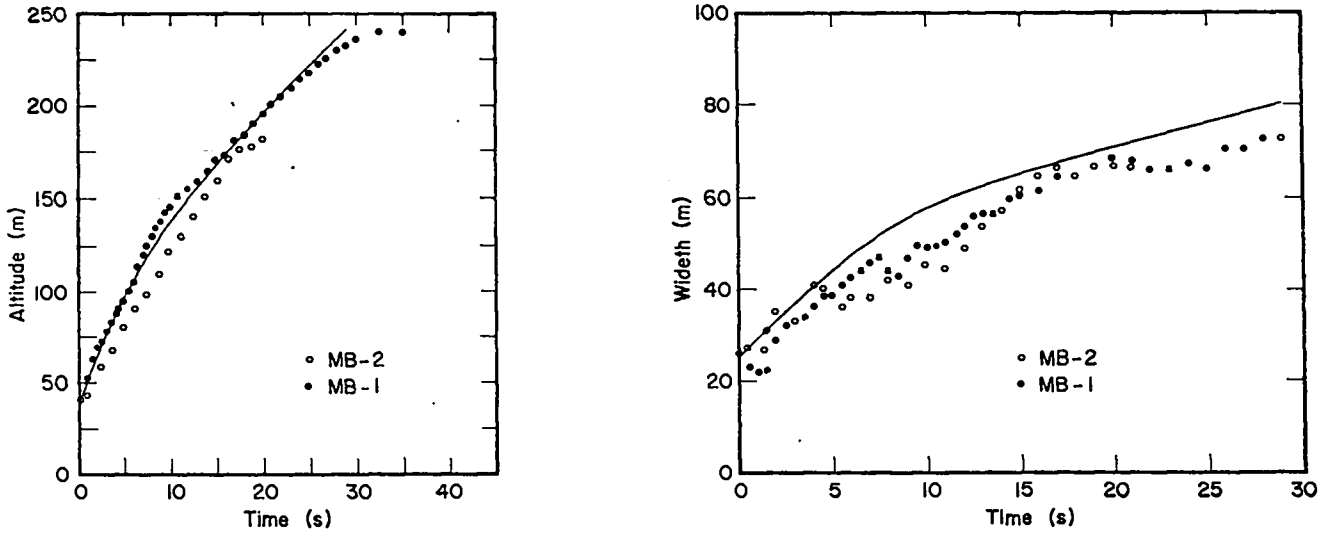

Fig. 2. Altitude and radius as a function of time calculated with a combination Lagrangian code and remapping procedure.