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**Simulation of Complex Shock Reflections from
Wedges in Inert and Reactive Gaseous Mixtures**

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The Flux-Corrected Transport (FCT) technique for solving fluid equations reduces numerical diffusion, permitting calculations with Reynolds numbers considerably in excess of the cell Reynolds number. Recent advances in FCT, including a multidimensional flux limiter and a dynamic adaptive rezone, are illustrated in the problem of transient reflections of planar shocks from wedges in inert and reactive media. Abstract (continues)			

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18. Supplementary Notes (Continued)

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20. Abstract (Continued)

Results are obtained with high resolution which are in quantitative agreement with experiments.

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1A

SIMULATION OF COMPLEX SHOCK REFLECTIONS
FROM WEDGES IN INERT AND REACTIVE GASEOUS MIXTURES

1. Advances in FCT Techniques

In this paper we describe new adaptations of the Flux-Corrected Transport (FCT) algorithms developed by Boris and Book (1973, 1976) for solving fluid equations, and discuss their application to multidimensional shock reflections in inert and reacting gaseous mixtures. In particular, we consider planar constant-velocity shocks reflecting from wedges. Under certain circumstances double Mach stems are formed. Historically these have proven to be difficult to calculate with high accuracy, although many schemes have been available to analyze compressible flow on a computationally discretized mesh: the method of characteristics, spline techniques, Glimm-type random choice schemes, and finite element, finite difference, and spectral methods. We believe that the calculational difficulties experienced on this problem were the result of excessive numerical diffusion, especially in the region of the contact surface.

In any Eulerian calculation, numerical diffusion arises because material which has just entered a computational cell, and is still near one boundary, becomes smeared over the whole cell. FCT minimizes this effect. FCT algorithms can be constructed as a weighted average of a low-order and a high-order finite-difference scheme. If the fluid equations are written in conservative form, both schemes are implemented using transportive fluxes. Each flux describes the transfer of mass (or some other extensive quantity) from one point to a neighboring point. The procedure for assigning weights involves limiting or "correcting" the fluxes at certain points. The higher-order scheme is used to the greatest possible extent, consistent with avoiding the introduction of dispersive ripples (undershoots and overshoots). The weights for the low-order scheme are chosen to be just sufficient to eliminate these ripples, thus assuring the property of "monotonicity" or "positivity." The result is an algorithm which effectively reduces to the higher-order scheme wherever the fluid properties change gradually. Near sharp discontinuities, however, enough diffusion is supplied to retain monotonicity. At shock fronts this procedure automatically produces the correct local viscous heating.

The prototype second-order finite-difference formula

$$\rho_j^{n+1} = \rho_j^n - \frac{1}{2} \epsilon_{j+1/2} (\rho_{j+1}^n + \rho_j^n) + \frac{1}{2} \epsilon_{j-1/2} (\rho_j^n + \rho_{j-1}^n) + v_{j+1/2} (\rho_{j+1}^n - \rho_j^n) - v_{j-1/2} (\rho_j^n - \rho_{j-1}^n)$$

illustrates the procedure. Here j labels grid position, n denotes time level and $\epsilon_{j+1/2} = v_{j+1/2} \Delta t / \Delta x$, and $v_{j+1/2}$ are dimensionless advection and diffusion coefficients, respectively. We write $\epsilon_{j+1/2} = \frac{1}{2} [1 + (|\epsilon| + c)]$, where c is a "clipping factor" measuring the extra diffusion added to achieve positivity. When $c = 0$, the above scheme is second-order; in the vicinity of shocks $c \sim 1$ and it effectively reduces to first order.

A numerical diffusion Reynolds number $(Re)_{np} = 2L/c\Delta x$ can be defined, where L is the characteristic size of a structure in the flow. Even the most accurate spectral simulations require setting $c = 1$ to guarantee positivity linearly. This gives rise to the usual definition of the numerical Reynolds number, $2L/\Delta x$. Algorithms such as FCT which

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guarantee monotonicity nonlinearly can have average values $\langle c \rangle \sim 10^{-1} - 10^{-2}$, introducing much less overall dissipation and permitting calculations with effective Reynolds numbers such that $Re \sim (Re)_{ND} \gg 2L/\delta x$.

Four advances in FCT techniques have enabled us to perform a series of shock and detonation calculations with high accuracy. These techniques are easy to program, and they have wide applicability to general quasi-linear hyperbolic equations (i.e., equations describing continuum conservation laws).

The first of these, a generalization of FCT due to Zalesak (1979), removes the necessity of timestep splitting in multidimensional hydrodynamics. This reduces errors associated with time splitting in regions of the flow which are nearly incompressible. The second refers to the development of FCT algorithms in which the spatial derivatives can be approximated to arbitrarily high order (fourth, sixth, eighth, etc., or pseudo-spectral). These innovations, which relate to the transport algorithm itself, have been implemented in a two-dimensional hydrocode which utilizes the leafrog-trapezoidal (L-T) algorithm and is therefore dissipationless. Both complex and double Mach stem structures are obtained (cf. Ben-Dor, 1978; Ben-Dor and Glass, 1978, 1979).

The third new technique, adaptive rezoning, is an extension to two dimensions of the dynamic rezoning employed in detailed one-dimensional reactive flow simulations by Oran, et al. (1979). This concentrates needed spatial resolution in the vicinity of moving shocks, contact discontinuities and reactive surfaces. The technique is illustrated with shock calculations using a time-split code (FAST2D). In air for $M=5$ and $\theta=45^\circ$, the results fall very close to the boundary between regular and Mach reflection. The calculated wall pressures are in detailed agreement with the results of Bertrand (1972). The fourth technique is a generalization of the induction time approximation used in earlier flame, ignition and shock work (Oran et al, 1980a, b). This provides a simple, efficient, yet reasonably accurate global chemical kinetics package to be used in connection with these comprehensive two-dimensional hydrodynamics calculations.

Section 2 describes the results of calculations in which a planar shock is reflected from a wedge in an inert gas. In Section 3 we present the results of calculations of detonations initiated by shock reflections in stoichiometric mixtures of H_2 in air at low pressure. Section 4 summarizes our conclusions.

2. Shock Reflections in Air

The utility of these advanced FCT methods has been demonstrated by applying them to transient reflections of planar shocks from wedges for various shock strengths M and wedge angles θ . For nonreacting flows at Mach numbers greater than about 2.5 and wedge angles between 20 and 50 degrees, double Mach stems can develop. Numerical schemes previously used for this problem reproduce qualitatively the wave structure and shape, but have difficulty making accurate predictions of flow details such as density contours (a conclusion drawn by Ben-Dor and Glass, 1978) even in the single Mach stem case. To our knowledge, successful calculations of the double Mach stem case have not yet been published. In this paper we discuss the series of calculations summarized in Table 1.

Open boundary conditions are used on the left, right, and top edges of the mesh, i.e., density, pressure and velocity are set equal to their pre-shock or post-shock values, depending on whether the incident shock front has passed that point. Reflecting conditions are imposed on the bottom of the mesh, which corresponds to the wedge surface. Examples of the calculated density contours and wave structure for the double and complex Mach reflection cases are shown in Fig. 1. The incident shock, I , the contact surface, CS , and the first and second Mach stems, M_1 and M_2 , are indicated in Fig. 1a. Note in particular the forward curl of the contact surface near the wall and the small region (4 by 7 mesh points) of high-density gas just to the left of the point where the contact surface impacts the wall. The latter causes a second peak in the pressure and density distribution on the wall, as shown in Fig. 1c. The accuracy of the calculations has been verified by comparison with experimental density distributions along the wall, as shown in Fig. 2, and with experimental pressure measurements (Bertrand, 1972). Note that FCT provides adequate resolution of the key surfaces (contact surface and second Mach stem) in regions as small as 5 by 5 cells.

Two additional cases were calculated with larger values of θ (Fig. 3). As the wedge angle increases, the Mach stem develops more slowly, being W separated from the wedge by a triple-point angle of only one or two degrees. [The triple-point angle α is the angle subtended by the Mach stem as viewed from the end of the wedge at which the shock was first incident (Fig. 4.) To reduce the size of the mesh needed, it is necessary to calculate in the frame of the Mach stem and to rezone. For these calculations we employed the time-split code FAST2D (with a 150×50 mesh), which incorporates an automatic continuous ("sliding zone") regridding procedure (Oran et al., 1979). For the small θ cases discussed above, where regridding is necessary, FAST2D yielded results very W similar to those obtained with the L-T code. The cases with wedge angles of 44° and 46.5° constitute a severe test of the numerical algorithm because of the small triple-point angle. Because α is approximately equal to 2.8° and 1.5° , respectively, considerable spatial resolution and a large amount of running time are usually necessary to get accurate flow fields. Figure 4 illustrates our adaptive rezone technique on a grid of 60×40 cells with varying cell dimensions, δx , δy . This method requires one-fifth the number of cells required in a uniform grid calculation. A uniform region consisting of the smallest cells covers part of the incident shock front, the Mach stems, and the reflected shock structure. Outside this finely gridded region, we have transition zones in which the cell dimensions increase smoothly to their maximum values, $10\delta x_{\min}$ and $10\delta y_{\min}$.

We have investigated the accuracy of the numerical simulation by comparing the results with experimental data (Bertrand et al, 1972). Because the cases $\theta = 44^\circ$ and 46.5° are so similar, we will discuss only the latter. The computed value of α for $\theta = 46.5^\circ$ is approximately 2.5° for a real-air equation of state and approximately 3.2° for an ideal gas with $\gamma = 1.35$. Both agree with the measurements to within the experimental errors, $\sim 2\%$. In Fig. 5, we compare the calculated (using a real-air equation of state) and experimental values of the pressure at the surface of the wedge for $\theta = 46.5^\circ$. The agreement in the shapes of the pressure curve is striking—the values of the lower pressure peak, corresponding to the Mach stem, are nearly identical. The calculated value of the second pressure peak is 11% lower than the experimental value and is thus within experimental uncertainty. Figure 6 shows the history of the pressure on the wedge calculated for an ideal gas with $\gamma = 1.35$. We note that the curves have much the same shape as for the real-air simulations; however, the first pressure peak is again 11% lower than the experimental value. Figure 7 shows that the double Mach reflection shock structure is well resolved in the simulation.

3. Detonations

We have also considered analogous shock reflections in reactive gases (stoichiometric mixtures of H_2 in air) at low pressure (0.1 atm). The induction time hypothesis (e.g., Oran et al, 1980) represents the chemistry through a composite process, in which reactants begin to combine into combustion products only after a finite time has elapsed. The rate at which the energy-releasing reactions proceed depends upon a single parameter, the induction time. This in turn is a function of the local thermodynamic variables.

Figure 8 shows the time development of a detonation initiated by a weak reflecting shock. The incident shock was chosen so that the pressure behind it is too low to cause detonation to take place within the time of the calculation. As with the calculation of Section 2, we have used open boundary conditions at the sides and top of the system. The sequence of six pressure contour plots traces the evolution of a detonation wave initiated by complex Mach reflection at the surface of the wedge. Figure 8a shows the pressure contours corresponding to an incident shock with $\theta_i = 25^\circ$ and $M = 4.0$ which has just begun to reflect. The Mach stem is initially too small to be resolved. In Fig. 8b the Mach stem becomes discernible, but as yet no apparent reaction has occurred. By frame (c) the material has begun to ignite at a position well behind the current location of the Mach stem. When the Mach stem passed that position the pressure increase heated the mixture sufficiently to cause ignition after a short induction time characteristic of the H_2 -air mixture. In frames (d) and (e), at later times, the pressure at the Mach stem continues to grow, leading to shorter characteristic induction times for material between the Mach stem and the original ignition point. Thus we see the ignited region accelerate along the wedge surface toward the Mach stem. Because more energy is being released as the burning continues, the boundary of the

ignited region also accelerates in the direction of the reflected shock front, compressing and heating the material into which the burned gases expand. In the last frame the burn front has overtaken the reflected shock and Mach stem, as we see from the decrease in the separation of the pressure contours near both locations. A stable detonation pattern has not yet emerged, however. This is evident from the bending out of the Mach stem and the lower density of contours between the Mach stem and the reflected shock/detonation front.

We anticipate that shock tube experiments will confirm this wave structure and that such reactive flow calculations will be extremely useful in quantitatively explaining the experimentally observed multicell structure of detonations (Oppenheim 1970).

4. Conclusions

Our calculations of complex and double Mach reflection are in close agreement with measurements for shocks reflecting in air from wedges. Because of the accuracy and speed of FCT algorithms and the effectiveness of adaptive rezoning, the calculations are accurate and economical even when the Mach stem develops very slowly. All of the important features (location of surfaces of discontinuity, pressure loading on the wedge surface, density contours) are correctly predicted. The results do not depend sensitively on whether the L-T or FAST2D code is used. Of the advances discussed in Section 1, multidimensional flux limiting and the adaptive regridding technique seem to be the most efficacious for reflections in nonreactive media. We conclude that FCT algorithms reduce numerical diffusion dramatically, assuring qualitative improvements in accuracy. We believe that to achieve comparable accuracy and efficiency, other hydrocodes must employ similar nonlinear algorithms and rezoning techniques.

Our calculations in reactive gas mixtures show that detonations tend to begin where a secondary pressure peak arises as the slip surface approaches the wedge. Because of the finite induction time in our kinetics model, the detonation begins somewhat behind this pressure peak. The high resolution our calculations achieve enables us to follow multiple reflections and is capable of providing quantitative predictions of detonation phenomena.

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Table 1 - Shock Reflection Simulations

CODE	MACH NO.	WEDGE ANGLE	TYPE OF SHOCK	E.O.S. $\gamma =$	REZONE	# STEPS	EXPERIMENT
L-T	6.9	20°	CMR(A)	1.35	NO	1,000	BEN-DOR
L-T	8.06	26.56°	DMR(A)	1.35	NO	800	BEN-DOR
FAST2D	8.06	26.56°	DMR(A)	1.35	NO	800	BEN-DOR
FAST2D	5.173	44°	DMR(D)	1.35	YES	600	BRL
FAST2D	5.074	44°	DMR(D)	REAL AIR	YES	1,000	BRL
FAST2D	5.148	46.5°	DMR(D)	1.35	YES	1,000	BRL
FAST2D	5.046	46.5°	DMR(D)	REAL AIR	YES	1,500	BRL

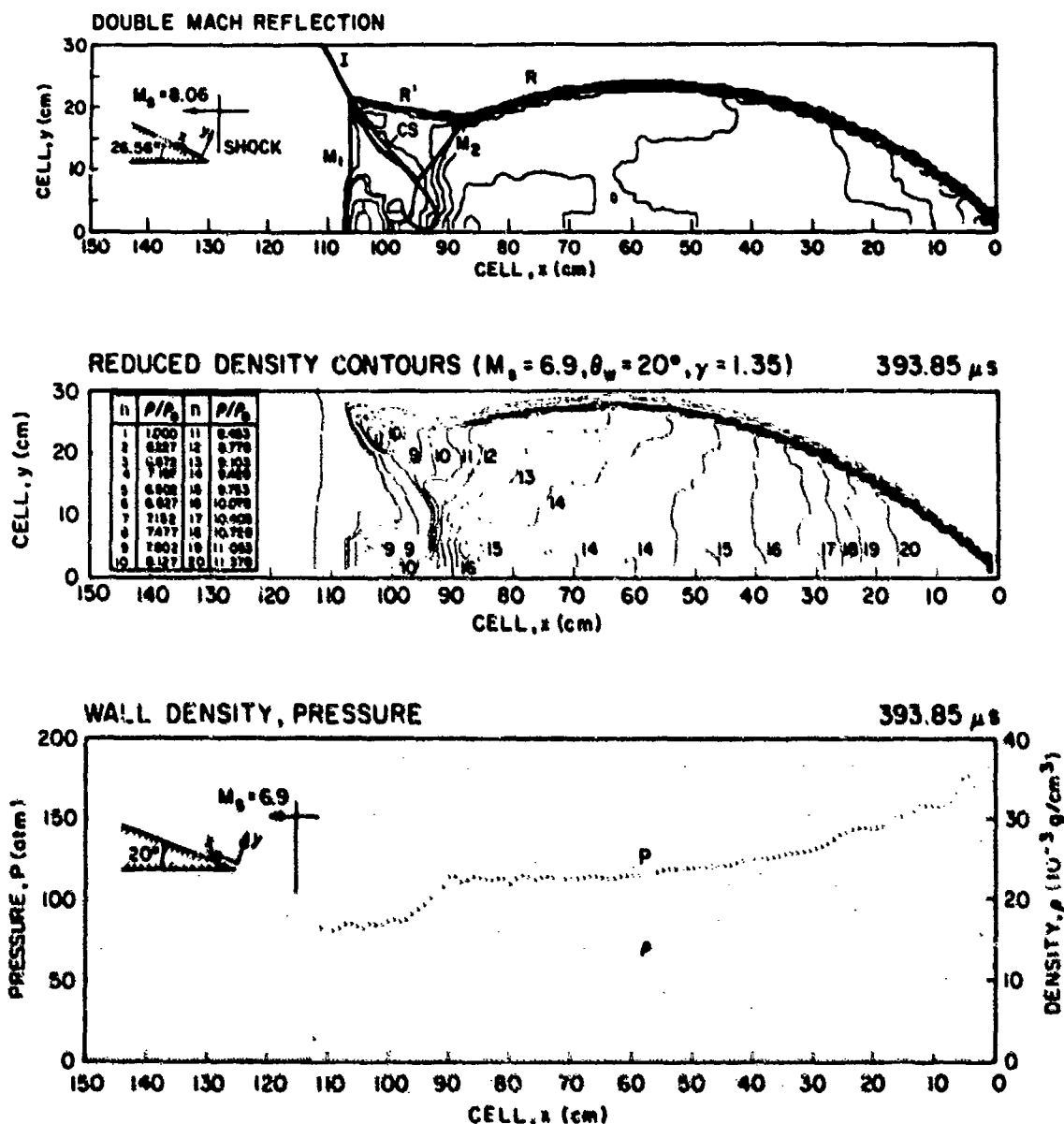


Fig. 1 - (a) Wave structure and density contours for double Mach reflection from a wedge; (b) reduced density contours (ρ/ρ_0) for complex Mach reflection with levels chosen to agree with those of Ben-Dor and Glass (1978); (c) corresponding pressure and density profiles on the wedge, plotted against cell number.

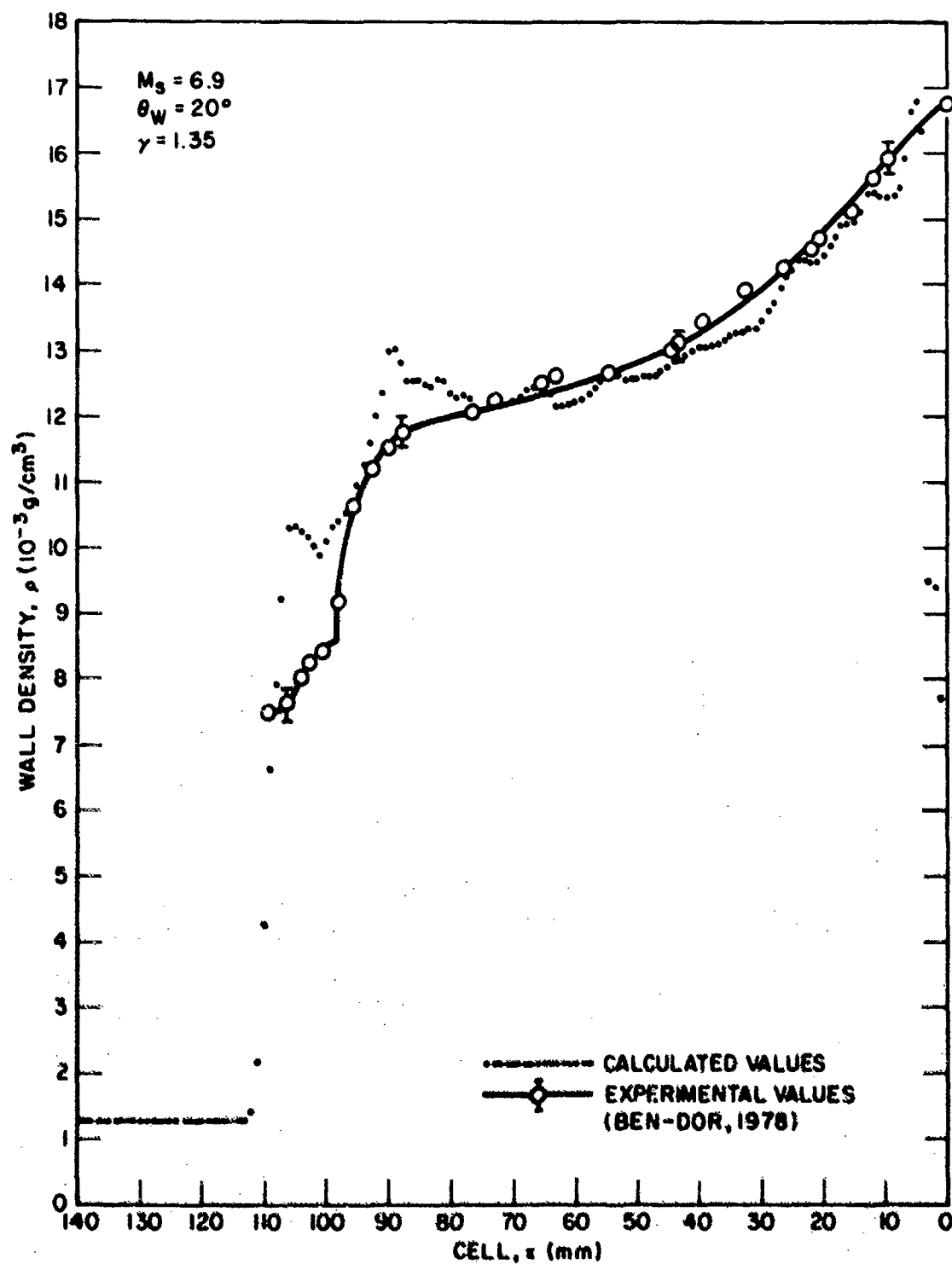


Fig. 2 - Comparison of the calculated density profile on the wedge (Fig. 1(b)) with measured values (Ben-Dor and Glass, 1978).

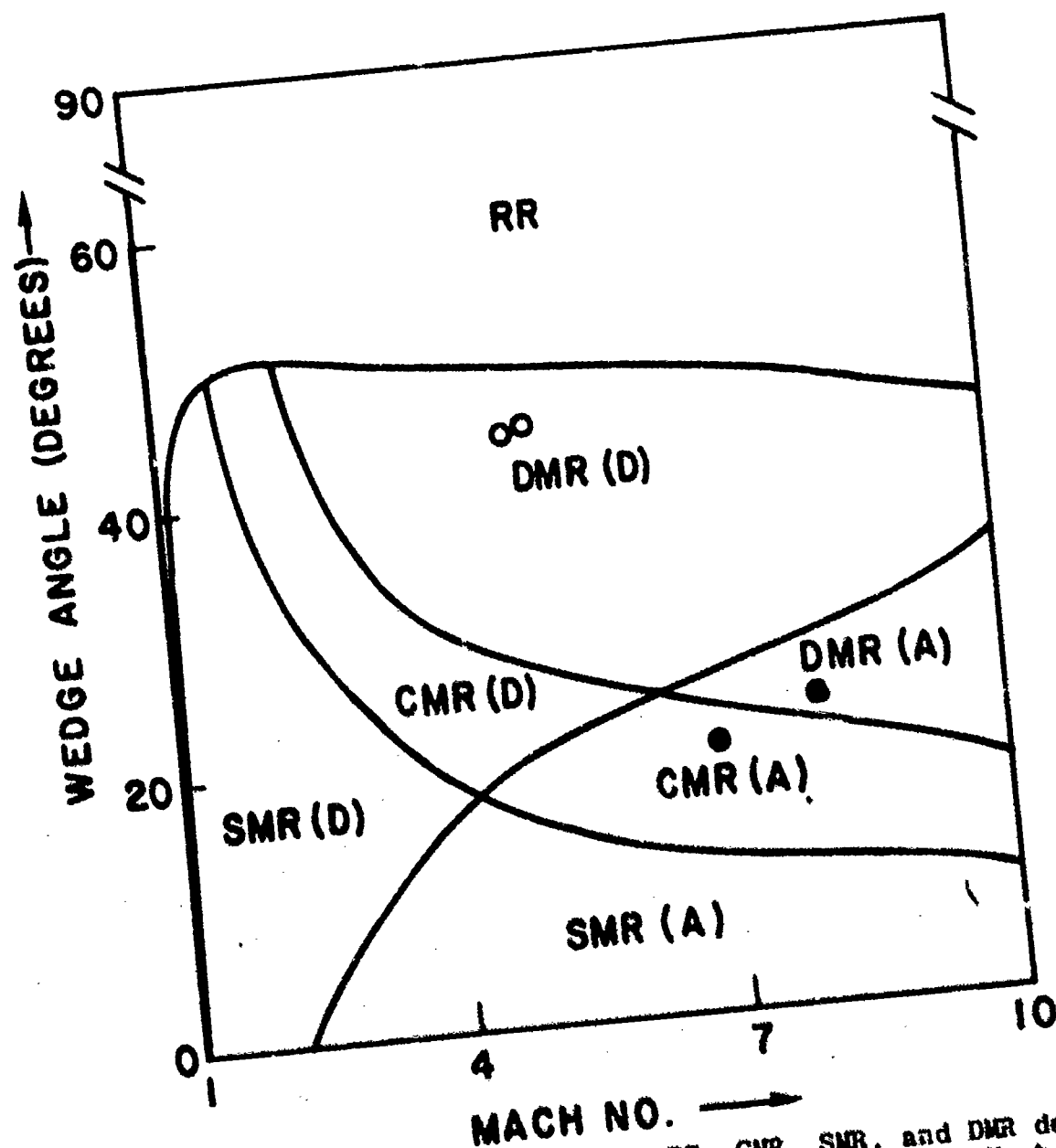


Fig. 3 - Types of shock reflections; RR, CMR, SMR, and DMR denote regular reflection and single, complex, and double Mach reflection, respectively. The D and A refer to detached and attached shocks.

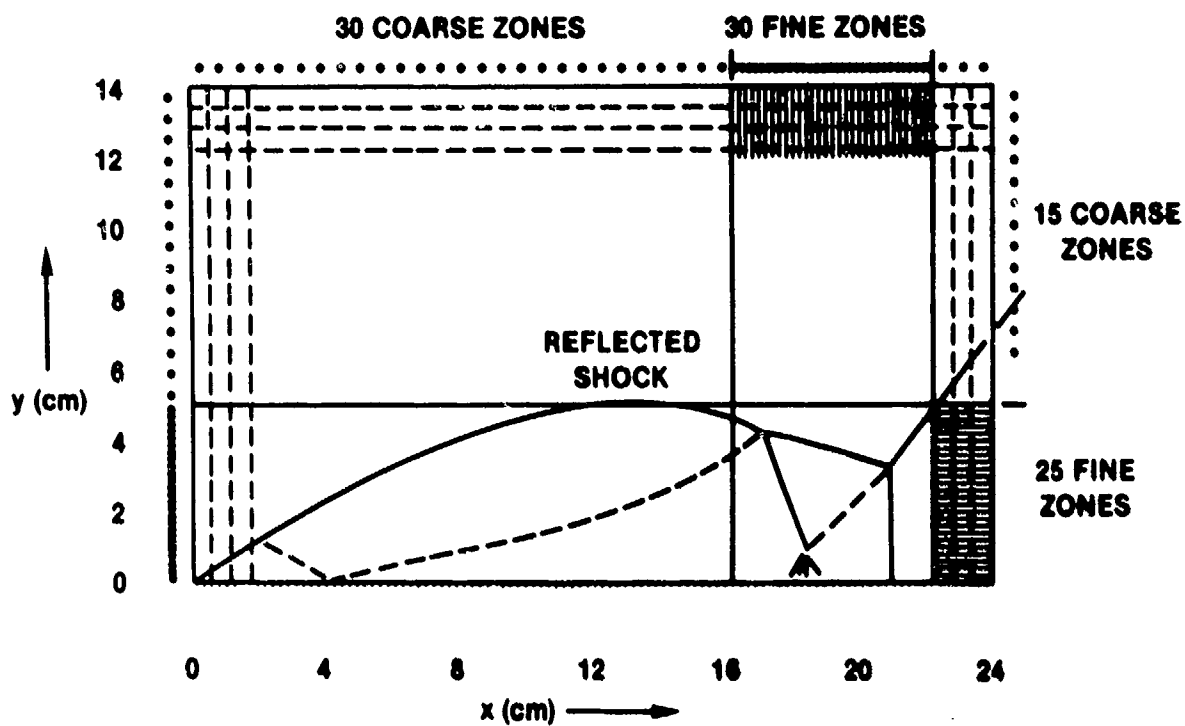


Fig. 4 - Gridding for complex shock reflection problems with FAST2D code. Shown are incident, reflected and Mach shocks (solid lines) and slip surfaces (dotted lines) for incident shock coming from the left.

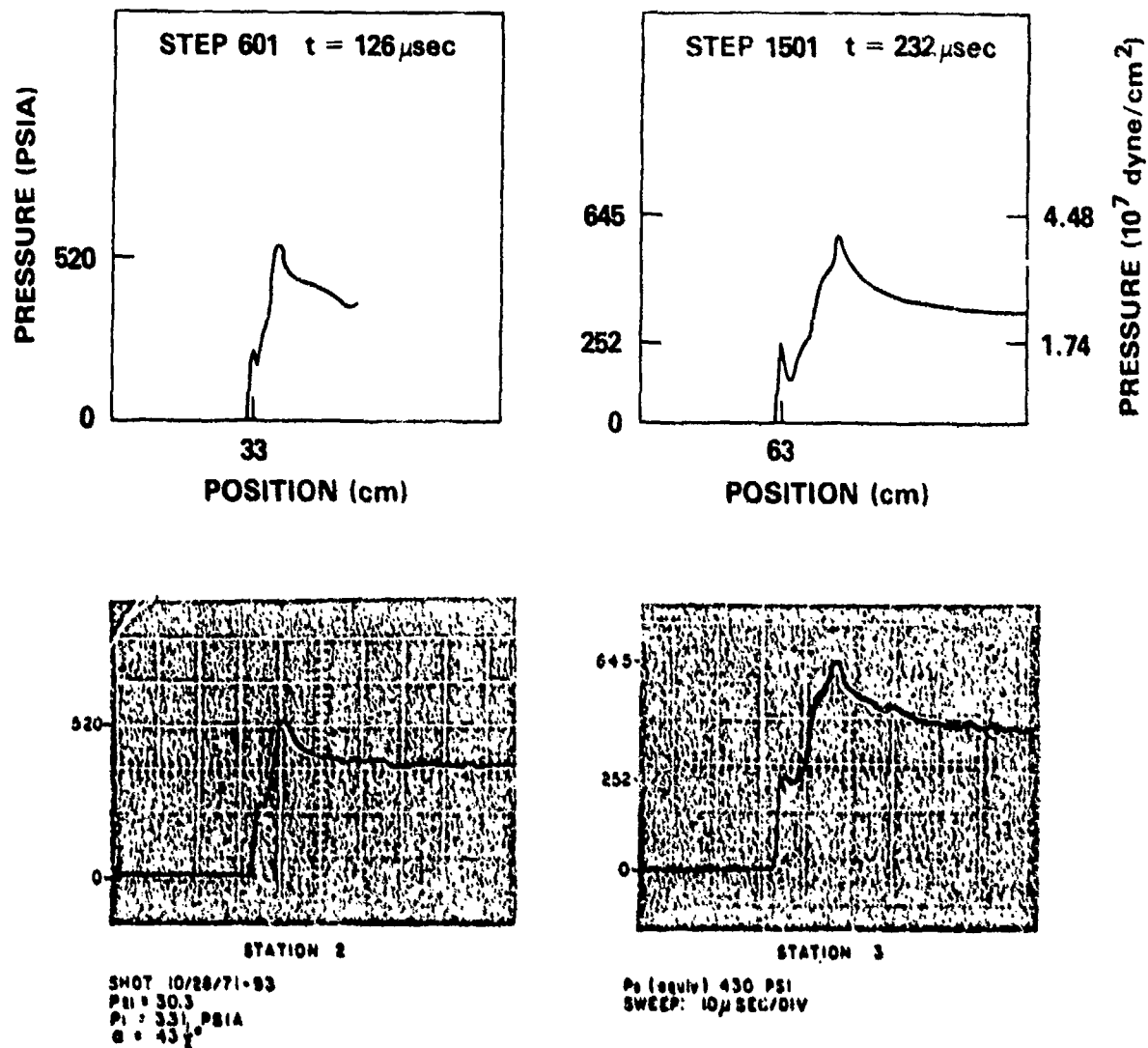


Fig. 5 - Upper and lower diagrams show pressure in PSIA on the wedge as a function of position for $\theta_w = 46.5^\circ$ (real air equation of state) at two times in the simulation and as a function of time at two stations in the experiment, respectively.

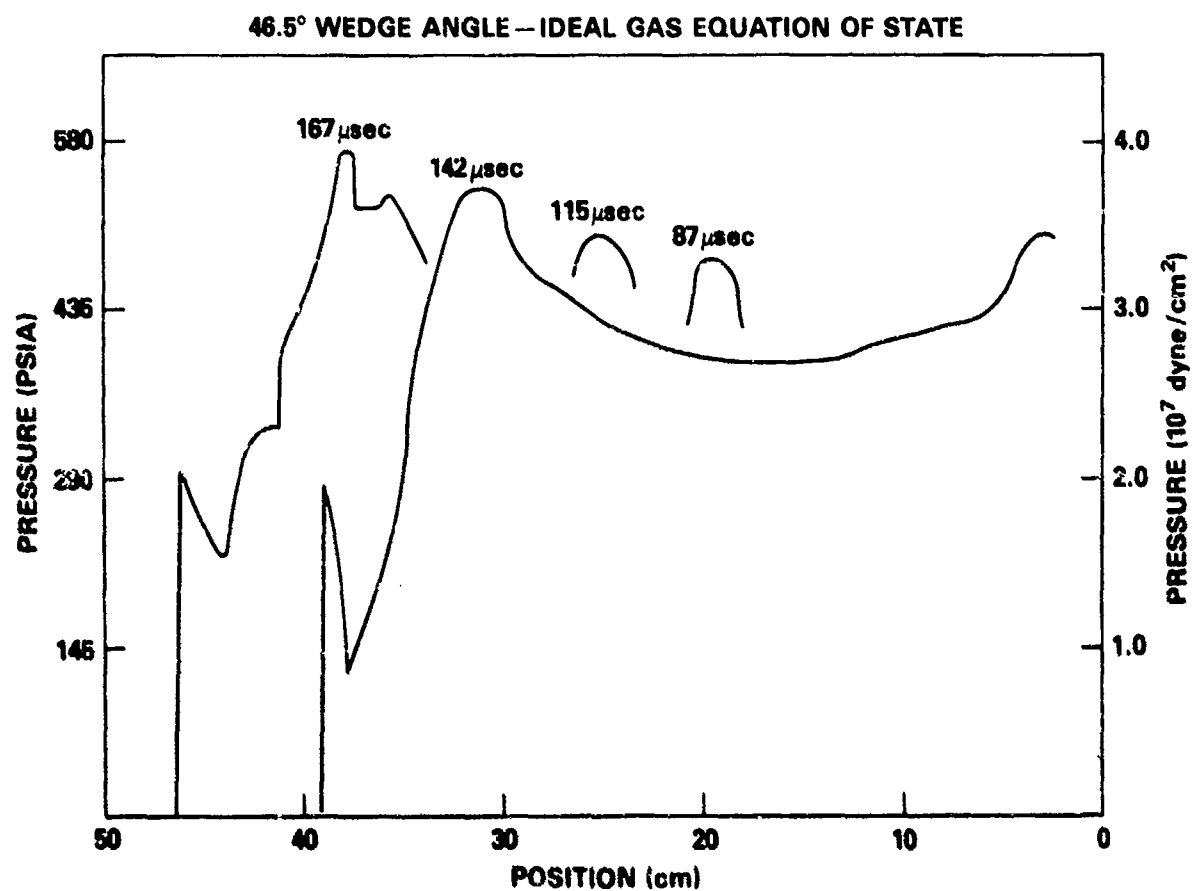


Fig. 6 - Structure of the calculated shock ($\theta_w = 46.5^\circ$, $M = 5.15$, $\gamma = 1.35$) as a function of position for several times.

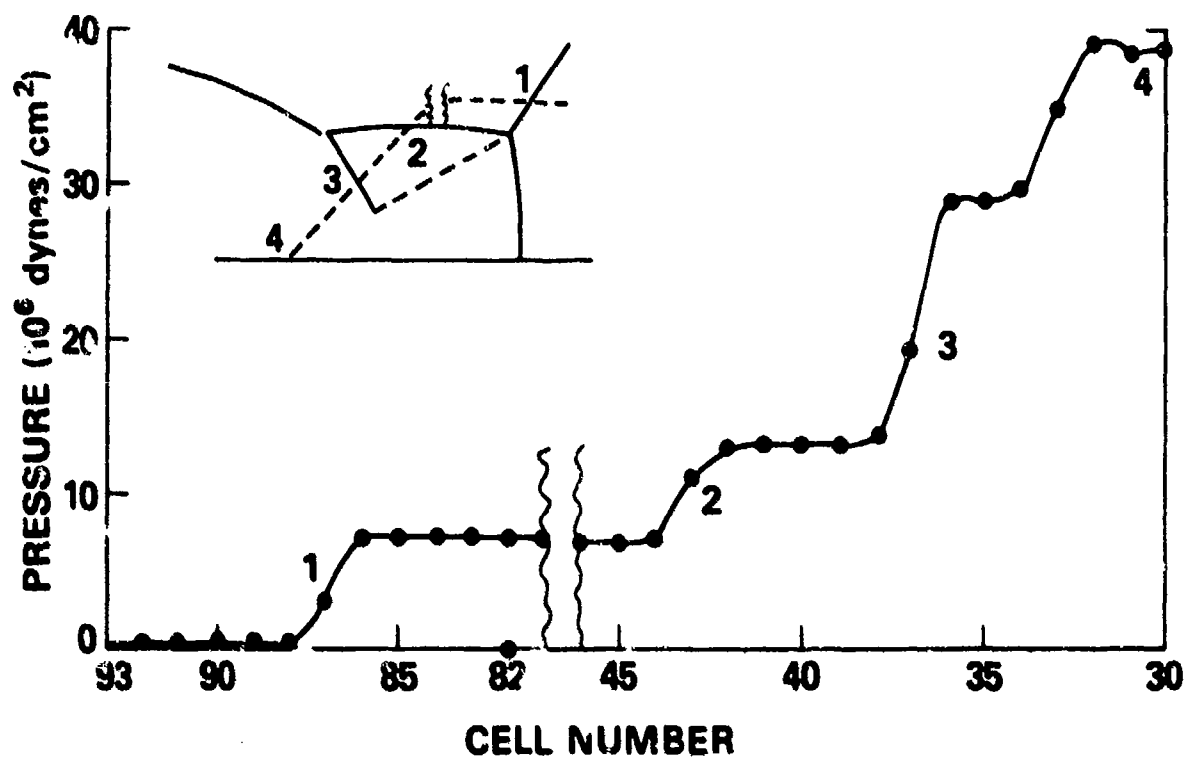


Fig. 7 - Plot of pressure vs distance along the trajectory 1-2-3-4 shown in the inset, which intersects all surfaces of discontinuity normally.

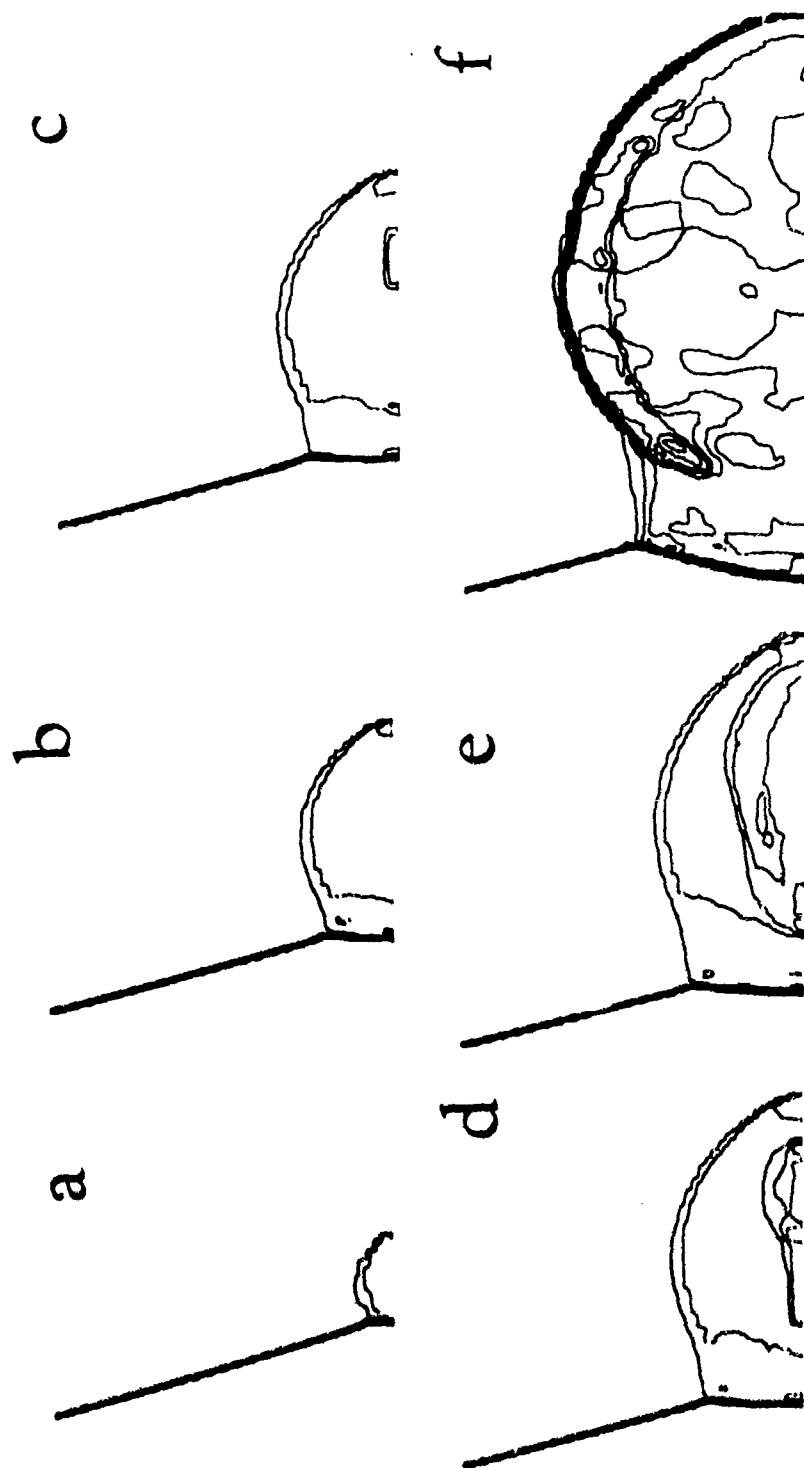


Fig. 8 - Sequence of six pressure contour plots tracing the development of detonation in a stoichiometric H_2 --air mixture at 0.1 atm due to complex Mach reflection from wedge.

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