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Flow Refraction by an Uncoupled Shock and Reaction Front

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Nomenclature

C_p = specific heat
E = activation energy
M = Mach number
p = pressure
Q = heat release
$\hat{Q}$ = $(1-\beta_2)Q$
$\bar{Q}$ = Q/RT_f
R = gas constant
T = temperature
u,v = velocity components
β = reaction progress variable
γ = specific heat ratio
δ = shock angle
θ = wedge angle
$(\ )_f$ = fresh gas
$(\ )_n$ = normal to front
$(\ )_1$ = upstream of front
$(\ )_2$ = downstream of front

Introduction

CONSIDER an oblique detonation wave supported, for example, by a wedge. Given the freestream conditions, the heat released in the wave, and the wedge (flow-deflection) angle, we can ask if a wave angle can be found so that the Rankine-Hugoniot conditions are satisfied. Gross[1] has shown that when the freestream conditions and the heat released are prescribed, this is possible provided the wedge angle is smaller than some critical value. Moreover, additional conditions, arising from consideration of the wave structure, define a *minimum* wedge angle. The permissible range of wedge angles, determined in this way, is of practical concern in any flow configuration in which oblique detonations are expected, e.g., in Ref. 2.

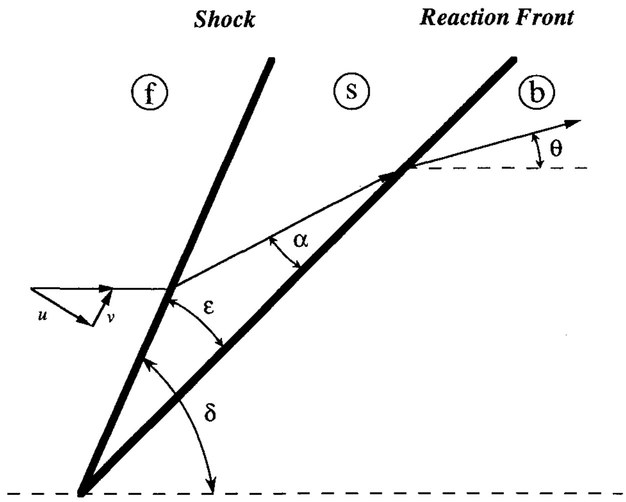

Fig. 1 Refraction by dual fronts.

Recently, Fujiwara et al.[3] have carried out numerical simulations of flow past wedges and have computed steady solutions (as the late time limit of unsteady ones) characterized by oblique detonations. The calculations employ a 2-step kinetic scheme in which the first (irreversible) step has an Arrhenius temperature dependence with a large activation energy. The associated one-dimensional steady detonation structure is characterized by a nearly isothermal induction zone behind the lead shock, terminated by a thin reaction zone or fire. In a genuine oblique detonation wave, remote from any disturbance (such as a blunted wedge nose), this fire will be parallel to the shock, and the structure will be one-dimensional. However, in some cases, Fujiwara et al. found steady solutions in which the shock and the fire are uncoupled in the sense that they drift apart as the distance from the symmetry axis increases. The refraction of the flow is then generated by a two-dimensional structure, and qualitative conclusions drawn from calculations similar to those of Gross must be modified. In the present paper, we approximate the structure by two fronts, the shock and the fire, inclined relative to each other, and we calculate the refraction that they generate. We find that such dual fronts are more effective than an oblique detonation wave in turning the flow (i.e., larger wedge angles are possible).

Flow Refraction by a Single Front

Consider a uniform flow which passes through a single front ($\epsilon = 0$ in Fig. 1). Then the Rankine-Hugoniot conditions are

$$\rho_1 u_1 = \rho_2 u_2$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \tag{1}$$

$$v_1 = v_2$$

$$C_p T_1 + \frac{1}{2}(u_1^2 + v_1^2) + Q = C_p T_2 + \frac{1}{2}(u_2^2 + v_2^2)$$

The equation of state is

$$p = \rho R T \tag{2}$$

valid on each side of the front, and geometrical conditions are

$$\tan\delta = u_1/v_1, \qquad \tan(\delta - \theta) = u_2/v_2 \tag{3}$$

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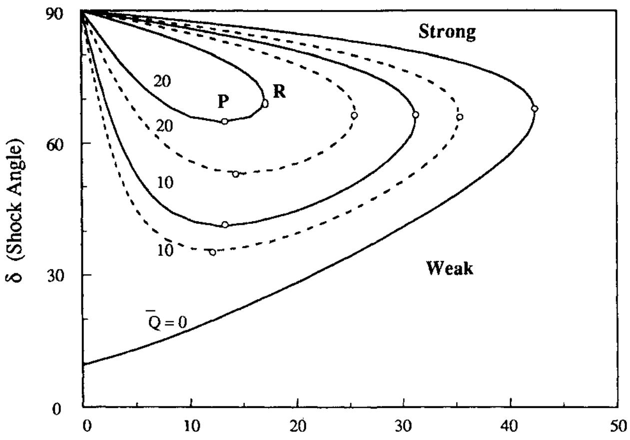

Fig. 2 Variations of shock angle and wedge angle, $M_f = 6$, $\bar{Q} = 0$, 10, 20; solid lines: $\beta_2 = 0$; dotted lines: equilibrium chemistry.

From these conditions we find

$$\frac{\rho_1}{\rho_2} = \frac{u_2}{u_1} = \frac{\tan(\delta - \theta)}{\tan\delta}$$

$$= \frac{(1 + \gamma M_{1n}^2) \pm [(M_{1n}^2 - 1)^2 - 2(1 + \gamma)M_{1n}^2 Q/C_pT_1]^{1/2}}{(1 + \gamma)M_{1n}^2} \tag{4}$$

$$\frac{T_2}{T_1} = 1 + \frac{(\gamma - 1)}{2}M_{1n}^2(1 - \rho_1^2/\rho_2^2) + \frac{Q}{C_pT_1}$$

$$M_{1n} = M_1 \sin\delta \tag{5}$$

$$\frac{p_2}{p_1} = \frac{\rho_2 T_2}{\rho_1 T_1} \tag{6}$$

These results are appropriate when the heat released (Q) is prescribed.

We are also interested in the situation where the heat released is determined by equilibrium chemistry. Fujiwara et al. (loc. cit.) use a two-step kinetic scheme in which a progress variable α is consumed adiabatically at a rate $w_\alpha = -K_1\rho \exp(-E_1/RT)$ and falls to zero, and this triggers a second reaction in which β is consumed exothermically at a rate

$$w_\beta = -K_2\rho^2 \left\{\beta^2 \exp\left(-\frac{E_2}{RT}\right) - (1 - \beta)^2 \exp\left(\frac{-E_2 + Q}{RT}\right)\right\}$$

Thus if β changes from 1 to β_2 across the wave, β_2 is determined by the equilibrium formula

$$\beta_2^2 = (1 - \beta_2^2) \exp\left(-\frac{Q}{RT_2}\right) \tag{7}$$

and the released heat is

$$\hat{Q} = (1 - \beta_2)Q \tag{8}$$

This replaces Q in Eqs. (1), (4), and (5). Since β_2 is a function of T_2, the Rankine-Hugoniot conditions must be solved iteratively in this case. Results calculated in this way are valid for the gas used by Fujiwara et al. in their numerical calculations.

The solid lines in Fig. 2 are typical of the results obtained when $\beta_2 = 0$ and Eq. (7) is discarded (assigned heat release). This is the case considered by Gross.[1] Consider first the curve $\bar{Q} = 0$, which intercepts the vertical axis (vanishing wedge angle) at two points. The upper one ($\delta = \pi/2$) corresponds to a normal shock, the lower one to a Mach wave, and so it is the lower point which is physically relevant when a wedge of vanishing thickness is placed in the flow. The curve has two branches, and the solutions on the upper branch are called strong oblique shock waves and are characterized by a subsonic postshock state. Solutions on the lower branch are called weak oblique shock waves and are characterized, for the most part, by a supersonic postshock state.[4] The weak branch is the physically relevant one, in the context of flow past an unbounded wedge, contiguous as it is with the physically relevant Mach wave at $\theta = 0$. In other situations, e.g., duct flows, the strong branch might be relevant.

When heat is added ($\bar{Q} > 0$), the curve closes with the shock angle approaching $\pi/2$ as the wedge angle vanishes (the limit Mach wave solution disappears). If we assume that for $\theta \neq 0$ the physically relevant solutions depend continuously on Q then, again, the lower or weak branch is the physically relevant one for wedge flows.

On that part of the lower curve that has a negative slope the normal Mach number behind the wave is greater than one corresponding to *underdriven* detonations. Elsewhere on the curve we have *overdriven* detonations with the normal Mach number behind the wave being less than one. Exceptional circumstances are required for the existence of a solution to the detonation wave structure in the underdriven case (what are called weak detonations in the detonation literature). The difficulty is in passing by addition of heat from $M_n < 1$ immediately behind the lead shock to $M_n > 1$ in the burnt gas. Thus, in general, the point where the slope is zero (e.g., P) and $M_{2_n} = 1$, defines a *minimum* wedge angle. The point of infinite slope (e.g., R) defines a *maximum* wedge angle. In this way, necessary (but not sufficient) conditions are defined for the existence of one-dimensional oblique detonation waves.

The dotted lines in Fig. 2 show results obtained when Eq. (7) is retained so that the heat released is determined by equilibrium chemistry. Note that the reduction in the heat released for given $\bar{Q}$ increases the maximum refraction angle. For $\bar{Q} = 20$, this angle is approximately 26 deg. And yet, for precisely these parameter values ($\bar{Q} = 20$; $M_f = 6$, equilibrium chemistry), Fujiwara et al. describe steady numerical solutions for a 30-deg wedge angle. This apparent contradiction arises because in the numerical simulations the detonation wave is never truly one dimensional. To explore the consequences of a two-dimensional structure on the refractive efficacy of a detonation wave we now consider the following.

Flow Refraction by Dual Fronts

The configuration is sketched in Fig. 1. A shock compresses and refracts the incoming flow turning it away from the shock normal. A reaction front then refracts the shocked gas turning it toward the front normal. We shall suppose that ϵ is prescribed; it must be smaller than the deflection generated by the shock. In the context of the flow considered by Fujiwara et al. (loc. cit.), this configuration is only representative at points far from the wedge nose.

The justification for representing the wave in this way is rooted in asymptotics—at large activation energy the structure will resemble the classical square-wave[5]—and in the results of Fujiwara et al. (see, in particular, Fig. 5 of their paper).

The Rankine-Hugoniot conditions are to be applied across each front but with heat release only across the second one. Suppose that δ is prescribed. Equations (4-6) with $Q = 0$, then describe the shocked gas (state 2) in terms of the fresh gas (state 1). Of the two roots in Eq. (4), only the second (with the minus sign) is relevant, and the first root yields a state 2 identical to state 1.

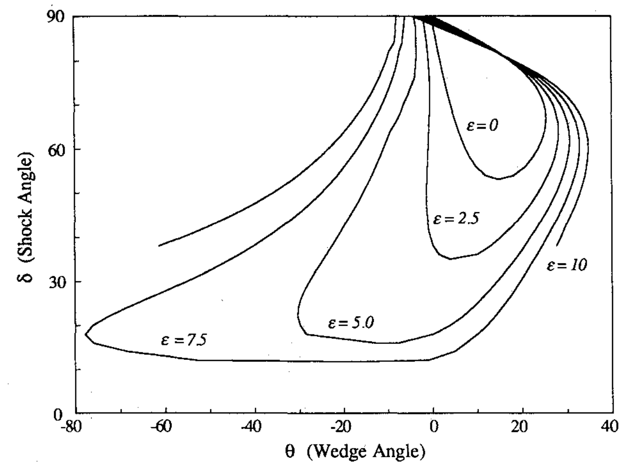

Fig. 3 Variations of shock angle and wedge angle, $M_f = 6$, $\bar{Q} = 20$, equilibrium chemistry, $\epsilon = 0, 2.5, 5, 7.5, 10$.

With the shocked state determined, the velocity can be resolved into components normal and parallel to the reaction front and formulas similar to Eqs. (4–6) applied again, now with Q nonvanishing. In this case there are two roots. When $\epsilon = 0$, this procedure recovers the results of the single-front calculation.

Figure 3 is typical of the results obtained in this way. Curves that terminate do so at points where the shocked flow is parallel to the reactive front ($\alpha = 0$). Note that negative wedge angles are formally possible but seem unlikely to have physical significance.

These results are of interest in the context of the calculations of Fujiwara et al. for they show that increases in ϵ lead to a commensurate increase in the final refraction angle. Specifically, $\epsilon = 6$ deg increases the maximum deflection by about 6 deg so that a wedge angle of 30 deg is possible. Since the numerical results for $\bar{Q} = 20$, $M_f = 6$ reveal a value of ϵ of about 10 deg (see Fig. 5 of Ref. 3), there is no contradiction between the numerical results and the necessary conditions defined by the Rankine-Hugoniot conditions.

Conclusions

Some of the numerical results for oblique detonations obtained by Fujiwara et al. are not consistent with limits defined by single-front Rankine-Hugoniot conditions. However, when two-dimensional effects are accounted for in an approximate fashion using a dual-front model, the inconsistency is eliminated.

Acknowledgment

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Accuracy of Upwind Schemes Applied to the Navier-Stokes Equations

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Introduction

UPWIND schemes for solving the compressible Euler and Navier-Stokes equations have been known for almost 30 years, but they have been applied to predictions of flows about complex geometries only relatively recently.

The Euler solvers based on the van Leer flux-vector splitting[1,3,6] are generally capable of accurate and reliable predictions of two- and three-dimensional flows. They have been extended to the Navier-Stokes equations by, among others, Thomas and Walters,[2] with mixed results. On grids with sufficiently high resolution, the results were generally good. However, on coarser grids and grids with significant stretching, the boundary layers were badly diffused. It has been shown recently by Hänel et al.[3] that some of this excessive diffusion is because of the application of flux limiters and formulations that are formally of lower order accuracy than the third-order upwind-biased MUSCL procedures.[2] Van Leer et al.[1] point out that the van Leer flux-vector splitting in its finite-volume form is actually neglecting the interaction of linear waves at cell interfaces and, therefore, solves the corresponding Riemann problem only approximately. A more accurate solution to the Riemann problem at the cell interfaces (interface between two states) as proposed by, for example, Roe,[4] will reduce the effect of artificial dissipation. This has been demonstrated conclusively in Ref. 1 for a few hypersonic cases. However, based on these few cases, it is still difficult to make a general statement.

The purpose of this Note is to present the results of a systematic comparison of the different forms of the van Leer flux-vector splitting with Roe's flux-difference splitting as applied to a simple viscous configuration. Attention is paid to the effects of spacial accuracy, grid resolution, and grid stretching on the accuracy of the resulting flowfield.

Approach

The comparison of the different schemes was carried out for a flat plate at a freestream Mach number $M_\infty = 0.5$ and reference Reynolds number $Re_o = 5 \times 10^3$. A rectangular grid with uniform spacing along the plate and various degrees of stretching in the normal direction extended two unit lengths downstream and three unit lengths (10 boundary-layer thicknesses at the outflow) in the direction normal to the plate. The main goal of the present work was the determination of the accuracy of the different schemes as a function of the various rates of stretching of the grid in the normal direction; therefore, the usual grid refinement study was performed for constant grid stretching. Since a simple geometric grid distribution was taken in the normal direction, the stretching factor f was constant throughout the grid and was defined as the ratio of two spacings in the y direction (normal to the plate), $f = (\Delta y_i / \Delta y_{j-1})$. Three rates of stretching were selected for this study:

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