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Computation of Thermally Perfect Oblique Shock Wave Properties

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Summary

A set of compressible flow relations describing flow properties across oblique shock waves, derived for a thermally perfect, calorically imperfect gas, is applied within the existing thermally perfect gas (TPG) computer code. The relations are based upon the specific heat expressed as a polynomial function of temperature. The updated code produces tables of compressible flow properties of oblique shock waves, as well as the original properties of normal shock waves and basic isentropic flow, in a format similar to the tables for normal shock waves found in NACA Rep. 1135. The code results are validated in both the calorically perfect and the calorically imperfect, thermally perfect temperature regimes through comparisons with the theoretical methods of NACA Rep. 1135. The advantages of the TPG code for oblique shock wave calculations, as well as for the properties of isentropic flow and normal shock waves, are its ease of use and its applicability to any type of gas (monatomic, diatomic, triatomic, polyatomic, or any specified mixture thereof).

Nomenclature

Symbols:

a	speed of sound
A	cross-sectional area of stream tube or channel
A_j	coefficients of polynomial curve fit for c_p/R
c_p	specific heat at constant pressure
c_v	specific heat at constant volume, $c_p - R$
M	Mach number, V/a
p	pressure
q	dynamic pressure, $\frac{\rho V^2}{2}$
R	specific gas constant
T	temperature
u	velocity component normal to the shock wave
V	flow velocity
w	velocity component tangential to the shock wave
Y	mass fraction
z	lateral coordinate to upstream flow, measured from wedge leading edge
γ	ratio of specific heats, c_p/c_v
δ	flow deflection angle; 2-D wedge half-angle
Θ	molecular vibrational energy constant[1,5]
μ	characteristic Mach angle
ρ	mass density
σ	shock wave angle relative to the upstream flow direction

Subscripts:

1	upstream flow reference point; e.g., upstream of a shock wave
2	downstream flow reference point; e.g., downstream of a shock wave
i	i^{th} component gas species of mixture
lim	limiting conditions for oblique shock waves
max	maximum value
mix	gas mixture
n	total number of gas species that comprise a gas mixture
perf	calorically perfect
therm	thermally perfect
t	total (stagnation) conditions

Abbreviations:

1-D	one-dimensional
2-D	two-dimensional
CFD	computational fluid dynamics
CPG	calorically perfect gas
cpu	(computer) central processing unit
GASP	General Aerodynamic Simulation Program

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NACA	National Advisory Committee for Aeronautics
NASP	National Aero-Space Plane
TPG	thermally perfect gas

Introduction

The traditional computation of one-dimensional (1-D) isentropic compressible flow properties, and properties across normal and oblique shock waves, has been performed with calorically perfect gas equations such as those found in NACA Rep. 1135[1]. When the gas of interest is air and all shock waves present are normal to the flow direction, the tables of compressible flow values provided in NACA Rep. 1135 are often used. For shock waves in air that are oblique to the flow direction, NACA Rep. 1135 contains charts of certain flow properties. These tables and charts were generated from the calorically perfect gas equations with a value of 1.40 for the ratio of specific heats γ. The application of these equations, tables, and charts is limited to that range of temperatures for which the calorically perfect gas assumption is valid. However, many aeronautical engineering calculations extend beyond the temperature limits of the calorically perfect gas assumption, and the application of the tables or equations of NACA Rep. 1135 can result in significant errors. These errors can be greatly reduced by the assumption of a thermally perfect, calorically imperfect gas in the development of the compressible flow relations. (For simplicity within this paper, the term *thermally perfect* will be used to denote a thermally perfect, calorically imperfect gas.) Previous papers[2,3] described a computer code, and the underlying mathematical formulation, which implements 1-D isentropic compressible flow and normal shock wave relations derived for a thermally perfect gas. The current paper, along with a related NASA contractor report[4], presents an enhanced computer code, and the corresponding mathematical derivation, for the computation of the oblique shock wave relations based upon the assumption of a thermally perfect gas.

A calorically perfect gas is by definition a gas for which the values of specific heat at constant pressure c_p and specific heat at constant volume c_v are constants. NACA Rep. 1135[1], as well as many compressible flow textbooks, derive and summarize calorically perfect compressible flow relations based upon this definition. The accuracy of these equations is only as good as the assumption of a constant c_p (and therefore a constant γ). For any non-monatomic gas, the value of c_p actually varies with temperature and can be approximated as a constant for only a relatively narrow temperature range. As the temperature increases, the c_p value begins to increase appreciably due to the excitation of the vibrational energy of the molecules. For air, this phenomenon begins around 450 to 500 K. The variation of c_p with temperature (and *only* with temperature) continues up to temperatures at which dissociation begins to occur, approximately 1500 K for air. Thus, air is thermally perfect over the range of 450 to 1500 K and application of the calorically perfect relations can result in substantial errors. A similar range can be defined for other gases over which the gas is calorically imperfect, but still thermally perfect. At yet higher temperatures c_p becomes a function of both temperature and pressure, and the gas is no longer considered thermally perfect.

NACA Rep. 1135 presents one method for computation of the 1-D compressible flow properties of a thermally perfect gas (see "Imperfect Gas Effects"[1]) in which the variation of heat capacity due to the contribution from the vibrational energy mode of the molecule is determined from quantum mechanical considerations by the assumption of a simple harmonic vibrator model of a diatomic molecule[5]. With this assumption the vibrational contribution to the heat capacity of a diatomic gas takes the form of an exponential equation in terms of static temperature and a single constant Θ. Tables of these thermally perfect gas properties are not provided because each value of total temperature T_t would yield a unique table of gas properties. Instead, NACA Rep. 1135 provides charts of the isentropic and normal shock properties for air normalized by the calorically perfect air values and plotted versus Mach number for select values of total temperature. For oblique shock waves, an even more limited set of charts is presented for shock wave angle σ, downstream Mach number M_2, and pressure coefficient as functions of deflection angle δ for four static temperatures at two total temperatures.

Because the imperfect gas method of NACA Rep. 1135 is applicable only to diatomic gases (e.g., N_2, O_2, and H_2), a different method of computing the 1-D isentropic and normal shock flow properties of a thermally perfect gas was developed and described in NASA TP-3447[2] and AIAA-96-0681[3]. The method utilizes a polynomial curve fit of c_p versus temperature to describe the variation of heat capacity for a gas. The data required to generate this curve fit for a given gas can be found in tabulated form in published sources such as the NBS "Tables of Thermal Properties of Gases"[6] and the "JANAF Thermochemical Tables"[7]. Actual coefficients for specific types of polynomial curve fits are published in NASP TM 1107[8], NASA SP-3001[9], and NASA TP-3287[10]. Use of these curve fits based upon tables of standard thermodynamic properties of gases enables the application of this method to any type of gas: monatomic, diatomic, and polyatomic (e.g., H_2O, CO_2, and CF_4) gases or mixtures thereof.

In this report, a set of thermally perfect gas equations, derived for the specific heat as a polynomial function of temperature, is applied to the calculation of flow properties across oblique shock waves. This set of equations was coded into a previously developed computer program referred to as the Thermally Perfect Gas (TPG) code. The new oblique shock wave capability was added as an optional output to the isentropic flow and normal shock wave tables of the original code. All output tables of the TPG code are structured to resemble the tables of compressible flow properties that appear in NACA Rep. 1135, but can be computed for arbitrary gases at arbitrary Mach numbers and/or static temperatures, for given total temperatures. All properties are output in tabular form, thus eliminating the need for graphical interpolation from charts. As in the original TPG code, the biggest advantage is the validity in the thermally perfect temperature regime as well as in the calorically perfect regime, and its applicability to any type of gas (monatomic, diatomic, triatomic, polyatomic, or any specified mixture thereof). The code serves the function of the tables and charts of NACA Rep. 1135 for any gas species or mixture of species, and significantly increases the range of valid temperature application due to its thermally perfect analysis.

Derivation of Oblique Shock Relations

Polynomial Curve Fit for c_p

The selection of a suitable curve fit function for c_p is the starting point for the development of thermally perfect compressible flow relations. The form chosen for the TPG code was the eight-term, fifth-order polynomial expression given below, in which the value of c_p has been nondimensionalized by the specific gas constant.

$$\frac{c_p}{R} = A_1\left(\frac{1}{T^2}\right) + A_2\left(\frac{1}{T}\right) + A_3 + A_4(T) + A_5(T^2) + A_6(T^3) + A_7(T^4) + A_8(T^5) \quad (1)$$

This functional form is valid for each of the curve fit data sets of the most useful references[8,9,10]. See previous documentation of the TPG code for more detail on this form[2,3]. Different algebraic expressions for c_p/R could be exchanged for that of equation (1) within the TPG code. The form of equation (1) was selected in the current work because of its ease of implementation, and the wealth of already available data[8,9,10]. The only requirements are that closed-form solutions to both $\int c_p dT$ and $\int (c_p/T) dT$ must be known[2].

Mixture Properties

The TPG code can be used to compute the thermally perfect gas properties for not only individual gas species but also for mixtures of individual gas species (e.g., air). The variation of the heat capacity for the specified gas mixture is

$$c_{p_{mix}} = \sum_{i=1}^{n} Y_i c_{p_i} \quad (2)$$

where Y_i is the mass fraction of the i^{th} gas species. The value of c_{p_i} is determined from equation (1) for each component species. With a known curve fit expression for c_p of the gas mixture, the value of γ for a given temperature can be directly computed, as can mixture properties of gas constant and molecular weight. Derivations of the 1-D isentropic relations and the normal shock relations from these properties are given elsewhere[2,3].

Oblique Shock Relations

Figure 1 illustrates the geometric relationships associated with a shock wave at an arbitrary shock angle σ relative to the upstream flow direction. These relationships can be expressed as

$$\tan\sigma = \frac{u_1}{w} \quad \text{and} \quad (3)$$

$$\tan(\sigma - \delta) = \frac{u_2}{w} \quad (4)$$

where u_1 and u_2 are the upstream and downstream velocity components normal to the shock, and $w = w_1 = w_2$ is the tangential velocity component which is conserved across the shock. Since only the normal component of velocity changes across the shock, the flow is turned through an angle δ. Solving equations (3) and (4) for w, a single equation can be written:

$$\frac{\tan(\sigma - \delta)}{\tan\sigma} = \frac{u_2}{u_1} \tag{5}$$

The normal velocity components can be expressed as

$$u_1 = V_1 \sin\sigma \quad \text{and} \tag{6}$$

$$u_2 = V_2 \sin(\sigma - \delta) \tag{7}$$

Thus, equation (5) can be rewritten as

$$\frac{\tan(\sigma - \delta)}{\tan\sigma} = \frac{V_2 \sin(\sigma - \delta)}{V_1 \sin\sigma} , \tag{8}$$

a function of shock angle σ, deflection angle δ, and the upstream and downstream velocities V_1 and V_2.

The continuity and momentum equations for 1-D flow across a shock wave in a shock-fixed coordinate system (a *stationary* shock) are

$$\rho_1 u_1 = \rho_2 u_2 \quad \text{and} \tag{9}$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \tag{10}$$

Dividing the momentum equation by the continuity equation gives

$$\frac{p_1}{\rho_1 u_1} + u_1 = \frac{p_2}{\rho_2 u_2} + u_2 \tag{11}$$

Using the ideal gas law ($p = \rho RT$), equation (11) can be written in terms of only temperature and

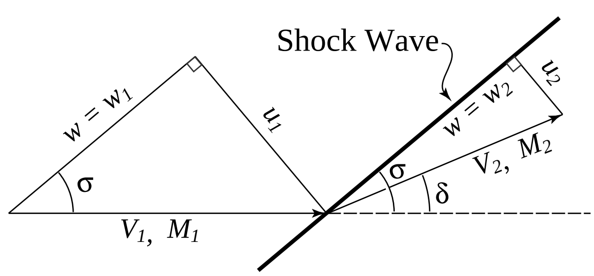


Figure 1. Geometric relationships of oblique shock waves.

normal velocity as

$$\frac{RT_1}{u_1} + u_1 = \frac{RT_2}{u_2} + u_2 \tag{12}$$

Substituting for u_1 and u_2 with equations (6) and (7), equation (12) becomes

$$\frac{RT_1}{V_1 \sin\sigma} + V_1 \sin\sigma = \frac{RT_2}{V_2 \sin(\sigma - \delta)} + V_2 \sin(\sigma - \delta) , \tag{13}$$

a function of shock angle σ, deflection angle δ, the upstream and downstream velocities V_1 and V_2, and the upstream and downstream static temperatures T_1 and T_2. However, the velocity of a thermally perfect gas may be expressed as a function of temperature[2]

$$V^2 = 2\int_T^{T_t} c_p dT \tag{14}$$

at any point in the flow field, whether upstream or downstream of the shock. Thus, the dependencies on velocity in equations (8) and (13) can actually be expressed as dependencies on temperature.

Assuming all upstream flow conditions are known (state *1*), and substituting equation (14) for V_1 and V_2, equations (8) and (13) represent a set of two nonlinear equations for three unknowns: σ, δ, and T_2. Given any one of these variables, the other two may be found numerically by means of Newton iteration[4]. If the shock angle σ is known, the tangential velocity component is

$$w = w_1 = w_2 = V_1 \cos\sigma \tag{15}$$

Then the downstream normal velocity can be defined as

$$u_2^2 = V_2^2 - w^2 = 2\int_{T_2}^{T_t} c_p dT - w^2 , \tag{16}$$

a function of T_2 only, instead of both T_2 and δ as in equation (7). Thus, instead of equation (13), equation (12) reduces to a function of T_2 only and can be solved independently of equation (8). For the case of known deflection angle δ, equations (8) and (13) must be solved simultaneously for T_2 and σ.

Once the primary variables of temperature T_2, σ, and δ are known, all other flow quantities may be computed.

$$\gamma_2 = \frac{c_{p_2}}{c_{p_2} - R} \tag{17}$$

$$a_2^2 = \gamma_2 R T_2 \tag{18}$$

$$M_2 = V_2 / a_2 \tag{19}$$

where V_2 is known from equation (14).

Pressure and density downstream of the shock wave can be calculated by the normal shock wave relations[2], noting that all velocity terms (including Mach number) are defined normal to the shock. The values of total pressure ratio $p_{t,2}/p_{t,1}$ and the ratio of upstream-static to downstream-total pressure $p_1/p_{t,2}$ can be calculated from combinations of static and total pressure ratios[2,4].

Figure 2 illustrates the relationships between M_1, σ, and δ for air at a sample T_t. For a given M_1 and δ, two solutions exist for σ, corresponding to what are commonly called 'weak' and 'strong' shock waves. A maximum flow deflection angle δ_{max} exists for any M_1, defined as the point at which the weak and strong shock solutions coincide. Strong shock waves always result in subsonic downstream Mach numbers and have shock wave angles approaching 90°. Weak shock waves are those for which the corresponding wave angle σ is less than that at which δ_{max} occurs, and usually result in supersonic downstream Mach numbers, except as σ approaches $\sigma(\delta_{max})$.

Oblique shock waves can only exist at Mach numbers above a limiting case, i.e., $M_1 > M_{1,lim}$. For a given σ, the limiting Mach number is that at which the Mach angle equals the shock angle, i.e., μ=σ, where the Mach angle μ is defined by

$$\sin\mu = \frac{1}{M_1} \tag{20}$$

At these conditions the shock strength and δ reduce to zero. For a given δ, the limiting case $M_{1,lim}$ corresponds to the Mach number for which $\delta = \delta_{max}$. From a physical perspective, this limit is the minimum Mach number at which an attached shock wave can occur at the leading edge of a wedge. Below $M_{1,lim}$ the flow results in a detached strong shock wave standing a finite distance upstream of the wedge leading edge, and the flow approaching the point of turning is subsonic, not supersonic.

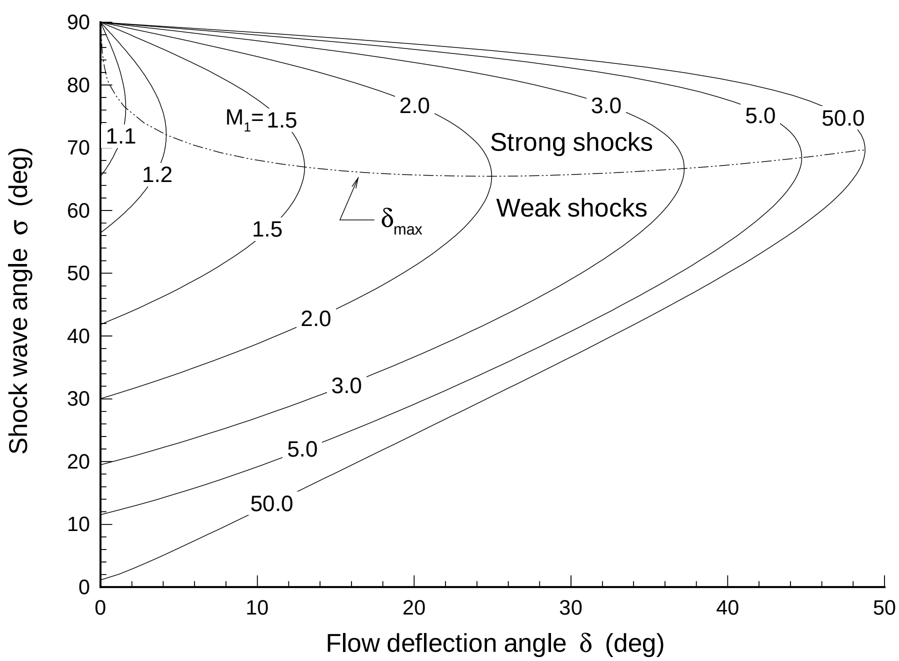


Figure 2. Contours of upstream Mach number M_1 for given shock wave angle σ and flow deflection angle δ; thermally perfect air at an arbitrary T_t=3000 K.

Oblique Shock Code Description

An interactive FORTRAN computer code, herein referred to as the TPG code, has been written based on the equations described herein and in previous work[2,3,4]. The code delivers a complete table of results within seconds when run on a computer workstation or personal computer. The purpose and primary output of the code is the creation of tables of compressible flow properties for a thermally perfect gas or mixture of gases (styled after those found in NACA Rep. 1135). In addition to isentropic flow and normal shock wave properties, the TPG code now computes properties across oblique shock waves, given either the shock wave angle σ or the flow deflection angle δ. Tabular entries may be based upon constant increments of Mach number, or constant decrements of static temperature from the total temperature. As in previous versions[2,3], the utility of the TPG code is its capability to generate tables of compressible flow properties of any gas, or mixture of gases, for any total conditions over any specified range of Mach numbers or static temperatures $T<T_t$. The code recognizes that the properties of thermally perfect gases vary with both total temperature T_t and static temperature T, rather than with only the ratio T/T_t. A complete description of the TPG FORTRAN code, Version 3.1, is given in NASA CR-4749[4] and NASA TP 3447[2], including the specification of a thermochemical data file for the gases of interest.

Sample Tabular Output

Table 1 shows a sample of the tabular output in the single table format for a shock angle of 30° in air at T_t=1500 K. Following a summary of the gas mixture definition are columns of data for the isentropic flow properties and the properties across the oblique shock wave. For a given shock angle, the minimum flow deflection is 0°, corresponding to a shock wave of zero strength, i.e., a Mach wave. Thus, the minimum Mach number of 2.0 for a 30° shock angle is determined by the equation for the Mach angle, equation (20). For all non-subsonic Mach numbers the code outputs an informative message stating the minimum $\sigma(=\mu)$ for that Mach number. At subsonic Mach numbers there is obviously no solution to the shock relations, as noted in the output.

Tables 2(a) and (b) illustrate the TPG tabular output for a constant flow deflection angle δ. Table 2(a) gives the weak shock solutions, and 2(b) gives the strong shock solutions (i.e., σ approaches 90° and M_2<1). In these cases the limiting Mach number is determined by the maximum flow deflection angle for which the flow would remain attached to the leading edge of a wedge with half-angle δ. That is, solutions to equations (8) and (13) only exist below some δ_{max}, and are double-valued in that regime. At Mach numbers below the corresponding limiting $M_{1,lim}$, an informative message notes the δ_{max}.

Oblique Shock Code Validation

The oblique shock wave capabilities within the TPG code were validated in the same manner as were the basic isentropic flow and normal shock wave methods[2,3], both in the calorically perfect and in the thermally perfect temperature regimes. In the current development, a normal shock wave is simply a special case of an oblique shock wave with σ=90°; i.e., the previous validations still hold for this special case.

Calorically Perfect Temperature Regime

The first validation test of the TPG code's oblique shock wave capability was the verification of accuracy in the calorically perfect temperature regime with air as the test gas. In this temperature regime, the specific heat of air is nearly constant and the TPG code results should be nearly identical to results obtained from the calorically perfect formulas of NACA Rep. 1135. For these test cases, data for standard four-species air was used along with the standard values for the mass fraction composition of air. The total temperature was set to 400 K, a temperature considered within the calorically perfect temperature regime for air. Properties were computed from stagnation conditions to Mach 10, at Mach number increments of 0.1. In the case of real air at T_t=400 K, liquefaction would occur well before Mach 10; the data is presented to that extreme herein merely for comparison with the calorically perfect gas tables of NACA Rep. 1135 (which, incidentally, extend up to Mach 100).

Figures 3 and 4 present TPG calculations of M_2, δ, p_2/p_1, ρ_2/ρ_1, T_2/T_1, and $p_{t,2}/p_{t,1}$ for air at shock wave angles of 30° and 50°, respectively, as ratios of the thermally perfect values (from TPG) to the calorically perfect values computed by the formulas of NACA Rep. 1135; each variable is plotted versus upstream Mach number M_1. The differences are less than 0.25% for all variables except total pressure ratio $p_{t,2}/p_{t,1}$. Even for this most sensitive variable, the differences are less than 1%, and that value is approached only at the largest shock angle and for Mach numbers approaching 10. These small differences actually represent the small amount of error associated with the calorically perfect gas assumption[2]. A slight variation with temperature actually exists in the heat capacities even at such a low T_t, and is the cause of the variations seen in figures 3 and 4.

Thermally Perfect Temperature Regime

Outside of the calorically perfect temperature regime, the TPG code was validated by comparisons with results obtained via the imperfect gas relations of NACA Rep. 1135 (i.e., the Θ-equations for a diatomic gas) for the properties of δ, M_2, p_2/p_1, T_2/T_1, ρ_2/ρ_1, and $p_{t,2}/p_{t,1}$. The test cases involved standard four-species air at total temperatures of 1500 K and 3000 K, and at shock wave angles of 30° and 50°.

The calculation for a total temperature of 3000 K is presented as an extreme case to illustrate application of the TPG code over an extended temperature range under the assumption of chemically frozen flow (i.e., frozen composition). The presentation is in the same spirit as that of previous works[6,7], where data is presented to 5000 K and 6000 K, respectively. As always, users must keep in mind the applicability of the assumption of frozen flow to a particular problem.

Figures 5(a)-(f) present ratios of the thermally perfect gas properties to the calorically perfect properties at identical values of M_1 to yield a measure of the imperfect gas effects. Results are shown for both total temperatures and both shock angles, for both the TPG code and the Θ-equation method of NACA Rep. 1135[1]. The two thermally perfect gas methods agree extremely well for this approximately-diatomic gas. Cursory examination of the plots shows that imperfect gas effects increase with both total temperature and shock angle. For some flow conditions the differences appear to be negligible, but, for other conditions, the differences can be large. Also, not all properties appear to be equally sensitive to caloric imperfections.

Differences due to caloric imperfections of 10% or greater are observed for temperature, density, and total pressure ratios at the higher total temperature and greatest shock angle. Caloric imperfection differences on the order of 4-5% are observed for all variables except static pressure ratio, even at the lower total temperature. Also, the magnitudes of the caloric imperfections do not vary uniformly with Mach number. The effects on δ are largest at lower M_1, but are larger for other variables at higher M_1. For static pressure ratio, the sign of the caloric imperfection effect changes as M_1 increases. Thus, the use of the calorically perfect relationships could result in substantial errors, particularly in the design or analysis of flows with a sequence of such shock waves.

The differences between the two thermally perfect gas methods can be seen to be small (typ-

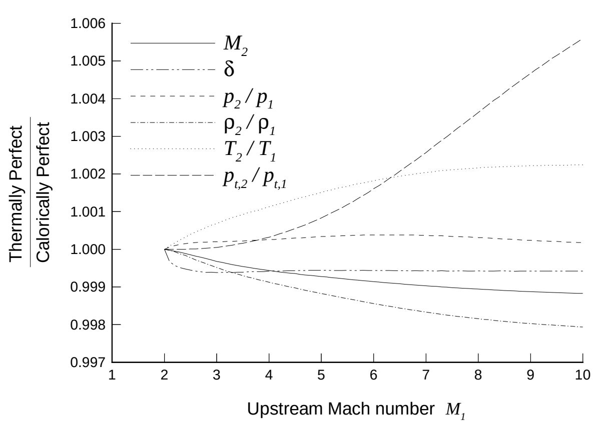


Figure 3. Effect of caloric imperfections on oblique shock wave properties within the calorically perfect temperature regime; air, T_t=400 K, σ=30°.

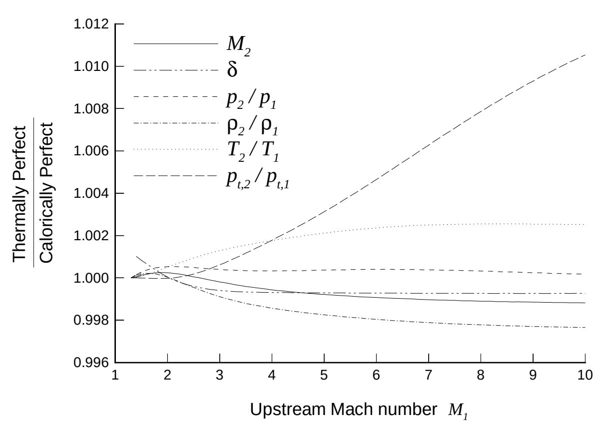
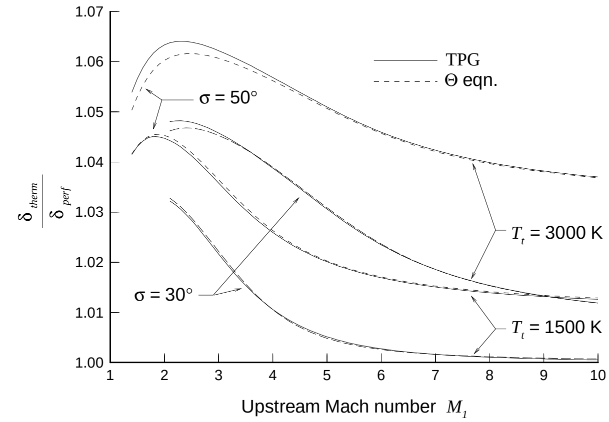
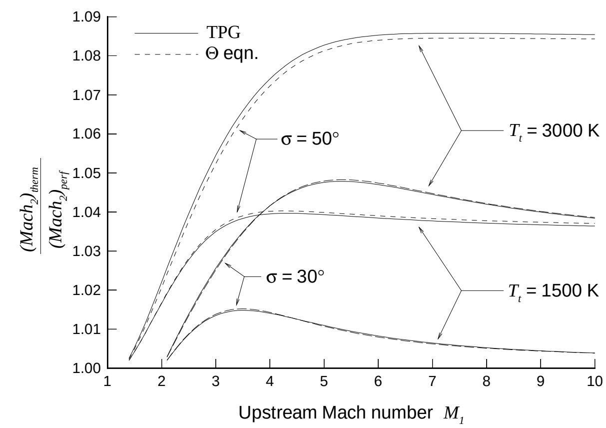


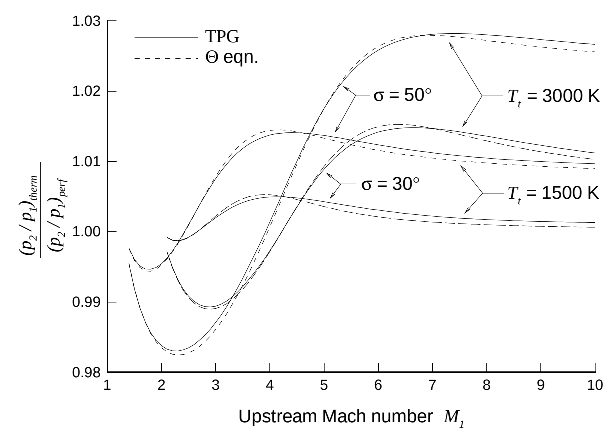
Figure 4. Effect of caloric imperfections on oblique shock wave properties within the calorically perfect temperature regime; air, T_t=400 K, σ=50°.



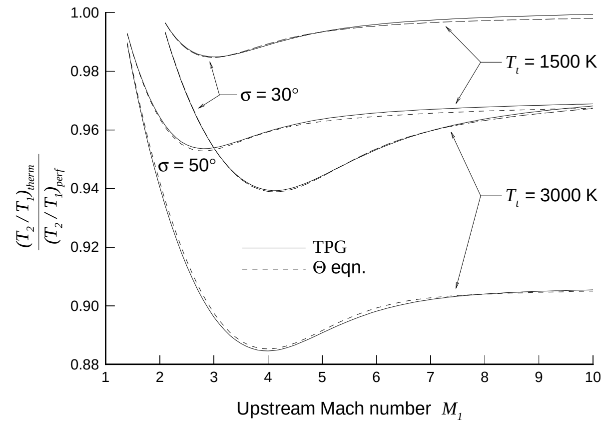
(a) Flow deflection angle δ



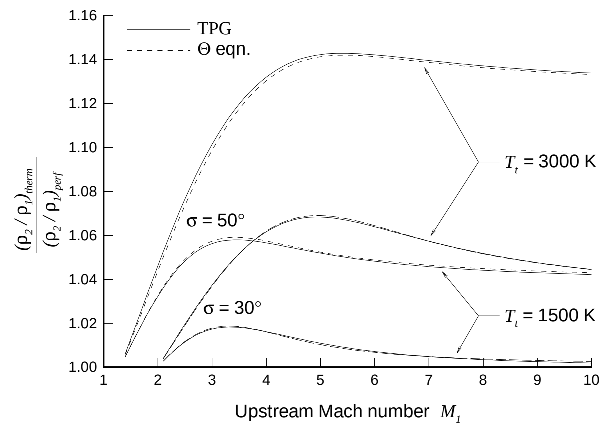
(b) Downstream Mach number M_2



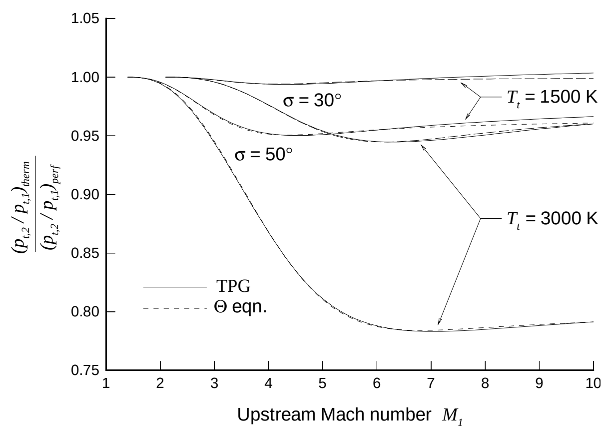
(c) Static pressure ratio p_2/p_1



(d) Static temperature ratio T_2/T_1



(e) Density ratio ρ_2/ρ_1



(f) Total pressure ratio $p_{t,2}/p_{t,1}$

Figure 5. Effect of caloric imperfections on oblique shock wave properties; comparisons between TPG and NACA Rep. 1135 for T_t=1500 K and 3000 K, and σ=30° and 50°.

ically less than 0.25%). This excellent agreement verifies the accuracy of the TPG code with the derived thermally perfect gas relations for oblique shock waves based upon polynomial expressions for c_p. Although these test cases were all for air, which is a primarily diatomic gas, the TPG code is also valid for polyatomic gases. The utilization of a polynomial curve fit for c_p makes the TPG code applicable to any molecular structure of the gas, not just the diatomic structure upon which the Θ-equations (of NACA Rep. 1135) are based.

Comparisons with CFD

For arbitrary mixtures of non-diatomic gases outside of the calorically perfect temperature regime, no exact method was available with which to validate the TPG code's oblique shock wave capability. A further illustration of the TPG code flexibility and robustness is shown by comparison with a computational fluid dynamics (CFD) Euler solution (i.e., inviscid flow) obtained using the General Aerodynamic Simulation Program (GASP)[11]. GASP solves the integral form of the governing equations, including the full time-dependent Reynolds-averaged Navier-Stokes equations and various subsets: the Thin-Layer Navier-Stokes equations, the Parabolized Navier-Stokes equations, and the Euler equations, including a generalized chemistry model and both equilibrium and non-equilibrium thermodynamics models. The current computations utilized space marching (i.e., totally supersonic flow) for the inviscid Euler equations. Third-order upwind inviscid fluxes were calculated using Roe's split flux normal to the flow direction with Min-Mod flux limiting. The NASA Lewis Research Center equilibrium curve fits for specific heat[8,9,10] of the same form employed within the TPG code defined the thermodynamic characteristics of the gases within GASP.

Since the Θ-equations of NACA Rep. 1135 are valid only for a single-species diatomic gas, CFD test case conditions were selected to highlight the flexibility of the TPG code. The gas chosen was a two-species mixture of 20% steam and 80% CO_2 by mass, neither species being diatomic. Upstream conditions were set at M_1=3.5, T_1=1200 K and p_1=101325 N/m^2 (1 atmosphere). A 2-D GASP grid was constructed over a rather severe wedge angle of 25° with 20 uniformly-spaced computational cells per unit length defined on a nondimensional domain (10 by 8.4 units). The domain height was chosen so that the resulting oblique shock wave would pass through the downstream boundary.

GASP required 282.4 cpu seconds to compute the solution on a Cray* Y-MP computer, not including grid generation and GASP input setup time (about 2 days). The TPG solution was practically instantaneous, computed on a Sun† Sparcstation 20 workstation. The resulting solutions are shown in figure 6, with the TPG solution (σ=37.3037°) overlaid as a thick dashed line on the GASP pressure ratio (p/p_1) contours. The magnified view in the inset confirms the excellent agreement of the shock positions, considering that GASP captures the shock over a number of cells and the TPG solution is a precise point solution. The line plots of M, p/p_1, and T/T_1 shown in figure 7(a)-(c) corroborate the accuracy of the TPG code for arbitrary mixtures of polyatomic gases. The data points were interpolated from the GASP solution (figure 6) along a horizontal line at z=5.0 units above the wedge leading edge, and the TPG solution is shown as a solid line with the discontinuous-shock position calculated at the same lateral location of 5 units.

Temperature Limits of the TPG Code

The TPG code provides valid results as long as its application is within the thermally perfect temperature regime for the gas of interest. Outside of the region for which c_p is a function of temperature only, the thermally perfect results produced by TPG will no longer accurately reflect what actually happens in nature. Dissociation will occur above some upper temperature limit, and will cause a deviation from thermally perfect theory due to a changing composition of the gas mixture. At the opposite extreme, below some lower temperature real gas effects will become important (i.e., intermolecular forces will not be negligible). The TPG code user must remain aware of these high and low temperature boundaries associated with the thermally perfect assumption for the particular gases under consideration. Note that these are boundaries associated with the physical properties of the gases, and are distinct from the upper and lower temperature limits associated with the polynomial curve fits utilized within the TPG code. These

* Cray Research, Inc., Minneapolis, MN 55402.

† Sun Microsystems, Inc., Mountain View, CA 94043.

latter curve fit limits are tracked within the code, and warnings are output by the TPG code when these limits are exceeded. The limits of the thermally perfect assumption are the user's responsibility, and are dependent upon the specific gas properties and flow conditions[2].

Conclusions

A set of compressible flow relations describing flow properties across oblique shock waves has been derived for a thermally perfect, calorically imperfect gas, and applied within the existing thermally perfect gas (TPG) computer code. The relations are based upon the specific heat expressed as a polynomial function of temperature. The code produces tables of compressible flow properties of oblique shock waves, as well as the properties of normal shock waves and basic isentropic flow, in a format similar to the tables for normal shock waves found in NACA Rep. 1135. The code results were validated in both the calorically perfect and in the calorically imperfect, thermally perfect temperature regimes through comparisons with the theoretical methods of NACA Rep. 1135. The TPG code is applicable to any type of gas or mixture of gases; it is not restricted to only diatomic gases as are the thermally perfect methods of NACA Rep. 1135. This utility is illustrated in comparison with a state-of-the-art computational fluid dynamics code.

The TPG code computes properties of oblique shock waves for given shock wave angles, or for given flow deflection (wedge) angles, including both strong and weak shock waves. Both tabular output and output for plotting and post-processing are available. Typical computation time is on the order of 1-5 seconds for most computer workstations or personal computers, and the user effort required is minimal. Thermally perfect properties of flows through oblique shock waves may be computed with less effort than has traditionally been expended to compute calorically perfect properties. Errors incurred from using calorically perfect gas relations, instead of the thermally perfect gas equations, in the thermally perfect temperature regime have been shown to approach 10% for some applications.

Acknowledgment: *This work was performed under NASA Langley Research Center contract NAS1-96014 by Lockheed Martin Engineering and Sciences Company.*

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Table 1: Sample TPG tabular output for constant shock wave angle

```
-------------------------------------------
| Thermally Perfect Gas Properties Code |
|           TPG, Version 3.1.0            |
|                                         |
|      NASA  Langley Research Center      |
-------------------------------------------

Table of Thermally Perfect Compressible Flow Properties
Gaseous Mixture:   Air: 4-Species Mixture of N2, O2, Argon, and CO2
Database file name: [ Default database of Air Mixture ]
Species Names are:
              N2   ,    O2   ,    Argon,    CO2  ,
Species Mass Fractions are:
             0.75530   0.23140   0.01290   0.00040
Species Mole Fractions are:
             0.78092   0.20946   0.00935   0.00028
Mixture Properties:
                    Molecular Weight =  28.9663
                        Gas Constant = 2.87035E+02 J/(kg*K)
           Polynomial Coefficients : cp/R = Sum[A(I)*T^(I-2)]
              80.0 < T <  1000.0 degrees K
     -3.73198210+00   5.41967010-01   3.46935860+00   3.83537980-04
     -2.76531300-06   8.18861420-09  -7.73686900-12   2.43487230-15
            1000.0 < T <  6000.0 degrees K
      2.37698510+05  -1.24405270+03   5.12666900+00  -2.04006440-04
      6.83218010-08  -1.05535420-11   6.64500710-16   0.00000000+00

Total Temperature =  1500.000 K
```

ISENTROPIC FLOW PROPERTIES --->									OBLIQUE SHOCK WAVE FLOW PROPERTIES (2=downstream, 1=upstream) --->						
M	T(K)	Gamma	P/Pt	RHO/RHOt	T/Tt	q/Pt	A/A*	V/a*	ShokAngl	FloDflec	M2	P2/P1	RHO2/RHO1	T2/T1	Pt2/Pt1
0.000	1500.0	1.3107	1.000E+00	1.000E+00	1.0000	0.000E+00	infinite	0.00000	**	Subsonic: Not Applicable --->					
0.250	1485.6	1.3112	9.600E-01	9.694E-01	0.9904	3.934E-02	2.426E+00	0.26693	**	Subsonic: Not Applicable --->					
0.500	1443.7	1.3127	8.513E-01	8.845E-01	0.9625	1.397E-01	1.348E+00	0.52659	**	Subsonic: Not Applicable --->					
0.750	1378.5	1.3152	7.015E-01	7.634E-01	0.9190	2.595E-01	1.064E+00	0.77258	**	Subsonic: Not Applicable --->					
1.000	1295.6	1.3187	5.422E-01	6.277E-01	0.8637	3.575E-01	1.000E+00	1.00000	**	Minimum Oblique Shock Wave Angle = 90.000					
1.250	1201.4	1.3234	3.974E-01	4.962E-01	0.8009	4.109E-01	1.049E+00	1.20580	**	Minimum Oblique Shock Wave Angle = 53.130					
1.500	1101.7	1.3291	2.794E-01	3.805E-01	0.7345	4.178E-01	1.188E+00	1.38864	**	Minimum Oblique Shock Wave Angle = 41.810					
1.750	1001.5	1.3360	1.907E-01	2.856E-01	0.6677	3.901E-01	1.419E+00	1.54868	**	Minimum Oblique Shock Wave Angle = 34.850					
2.000	904.6	1.3437	1.277E-01	2.117E-01	0.6031	3.431E-01	1.758E+00	1.68691	30.0000	0.0000	2.000	1.000E+00	1.000E+00	1.000E+00	1.000E+00
2.250	813.5	1.3522	8.460E-02	1.560E-01	0.5423	2.896E-01	2.229E+00	1.80531	30.0000	4.6888	2.086	1.308E+00	1.220E+00	1.073E+00	9.979E-01
2.500	729.6	1.3611	5.593E-02	1.150E-01	0.4864	2.379E-01	2.864E+00	1.90595	30.0000	8.2210	2.188	1.655E+00	1.445E+00	1.145E+00	9.866E-01
2.750	653.8	1.3697	3.713E-02	8.518E-02	0.4359	1.923E-01	3.701E+00	1.99099	30.0000	10.9419	2.294	2.040E+00	1.671E+00	1.221E+00	9.630E-01
3.000	586.4	1.3774	2.488E-02	6.364E-02	0.3909	1.542E-01	4.782E+00	2.06264	30.0000	13.0501	2.399	2.463E+00	1.894E+00	1.300E+00	9.276E-01
3.250	526.8	1.3839	1.687E-02	4.805E-02	0.3512	1.233E-01	6.154E+00	2.12301	30.0000	14.7063	2.500	2.923E+00	2.111E+00	1.385E+00	8.826E-01
3.500	474.6	1.3889	1.160E-02	3.668E-02	0.3164	9.872E-02	7.873E+00	2.17404	30.0000	16.0269	2.596	3.420E+00	2.320E+00	1.474E+00	8.307E-01
3.750	428.9	1.3928	8.094E-03	2.831E-02	0.2859	7.927E-02	1.000E+01	2.21739	30.0000	17.0954	2.684	3.953E+00	2.520E+00	1.569E+00	7.746E-01
4.000	388.9	1.3956	5.725E-03	2.208E-02	0.2593	6.391E-02	1.261E+01	2.25444	30.0000	17.8721	2.767	4.522E+00	2.710E+00	1.668E+00	7.165E-01

Table 2: Sample TPG tabular outputs for constant flow deflection angle

(a) Weak shock wave solutions

```
-------------------------------------------
| Thermally Perfect Gas Properties Code |
|           TPG, Version 3.1.0            |
|                                         |
|      NASA  Langley Research Center      |
-------------------------------------------

Table of Thermally Perfect Compressible Flow Properties
Gaseous Mixture:   Air: 4-Species Mixture of N2, O2, Argon, and CO2
Database file name: [ Default database of Air Mixture ]
Species Names are:
              N2   ,    O2   ,    Argon,    CO2  ,
Species Mass Fractions are:
             0.75530   0.23140   0.01290   0.00040
Species Mole Fractions are:
             0.78092   0.20946   0.00935   0.00028
Mixture Properties:
                    Molecular Weight =  28.9663
                        Gas Constant = 2.87035E+02 J/(kg*K)
           Polynomial Coefficients : cp/R = Sum[A(I)*T^(I-2)]
              80.0 < T <  1000.0 degrees K
     -3.73198210+00   5.41967010-01   3.46935860+00   3.83537980-04
     -2.76531300-06   8.18861420-09  -7.73686900-12   2.43487230-15
            1000.0 < T <  6000.0 degrees K
      2.37698510+05  -1.24405270+03   5.12666900+00  -2.04006440-04
      6.83218010-08  -1.05535420-11   6.64500710-16   0.00000000+00

Total Temperature =  1500.000 K
```

ISENTROPIC FLOW PROPERTIES --->									OBLIQUE SHOCK WAVE FLOW PROPERTIES (2=downstream, 1=upstream) --->						
M	T(K)	Gamma	P/Pt	RHO/RHOt	T/Tt	q/Pt	A/A*	V/a*	ShokAngl	FloDflec	M2	P2/P1	RHO2/RHO1	T2/T1	Pt2/Pt1
0.000	1500.0	1.3107	1.000E+00	1.000E+00	1.0000	0.000E+00	infinite	0.00000	**	Subsonic: Not Applicable --->					
0.250	1485.6	1.3112	9.600E-01	9.694E-01	0.9904	3.934E-02	2.426E+00	0.26693	**	Subsonic: Not Applicable --->					
0.500	1443.7	1.3127	8.513E-01	8.845E-01	0.9625	1.397E-01	1.348E+00	0.52659	**	Subsonic: Not Applicable --->					
0.750	1378.5	1.3152	7.015E-01	7.634E-01	0.9190	2.595E-01	1.064E+00	0.77258	**	Subsonic: Not Applicable --->					
1.000	1295.6	1.3187	5.422E-01	6.277E-01	0.8637	3.575E-01	1.000E+00	1.00000	**	Maximum Attached-flow Shock Deflection Angle = 0.000					
1.250	1201.4	1.3234	3.974E-01	4.962E-01	0.8009	4.109E-01	1.049E+00	1.20580	**	Maximum Attached-flow Shock Deflection Angle = 5.554					
1.500	1101.7	1.3291	2.794E-01	3.805E-01	0.7345	4.178E-01	1.188E+00	1.38864	**	Maximum Attached-flow Shock Deflection Angle = 12.803					
1.750	1001.5	1.3360	1.907E-01	2.856E-01	0.6677	3.901E-01	1.419E+00	1.54868	**	Maximum Attached-flow Shock Deflection Angle = 19.218					
1.784	988.0	1.3370	1.807E-01	2.743E-01	0.6586	3.845E-01	1.459E+00	1.56887	65.4776	20.0000	0.919	2.898E+00	2.156E+00	1.340E+00	8.800E-01
2.000	904.6	1.3437	1.277E-01	2.117E-01	0.6031	3.431E-01	1.758E+00	1.68691	51.7181	20.0000	1.280	2.696E+00	2.050E+00	1.315E+00	9.013E-01
2.250	813.5	1.3522	8.460E-02	1.560E-01	0.5423	2.896E-01	2.229E+00	1.80531	45.8418	20.0000	1.513	2.866E+00	2.126E+00	1.348E+00	8.844E-01
2.500	729.6	1.3611	5.593E-02	1.150E-01	0.4864	2.379E-01	2.864E+00	1.90595	42.0239	20.0000	1.715	3.101E+00	2.228E+00	1.392E+00	8.603E-01
2.750	653.8	1.3697	3.713E-02	8.518E-02	0.4359	1.923E-01	3.701E+00	1.99099	39.2678	20.0000	1.898	3.376E+00	2.339E+00	1.443E+00	8.317E-01
3.000	586.4	1.3774	2.488E-02	6.364E-02	0.3909	1.542E-01	4.782E+00	2.06264	37.1736	20.0000	2.066	3.682E+00	2.454E+00	1.500E+00	7.997E-01
3.250	526.8	1.3839	1.687E-02	4.805E-02	0.3512	1.233E-01	6.154E+00	2.12301	35.5277	20.0000	2.223	4.015E+00	2.570E+00	1.562E+00	7.653E-01
3.500	474.6	1.3889	1.160E-02	3.668E-02	0.3164	9.872E-02	7.873E+00	2.17404	34.2010	20.0000	2.368	4.374E+00	2.688E+00	1.629E+00	7.291E-01
3.750	428.9	1.3928	8.094E-03	2.831E-02	0.2859	7.927E-02	1.000E+01	2.21739	33.1098	20.0000	2.503	4.757E+00	2.800E+00	1.699E+00	6.918E-01
4.000	388.9	1.3956	5.725E-03	2.208E-02	0.2593	6.391E-02	1.261E+01	2.25444	32.1973	20.0000	2.629	5.163E+00	2.913E+00	1.773E+00	6.540E-01

Table 2: Sample TPG tabular outputs for constant flow deflection angle

(b) Strong shock wave solutions

```
---------------------------------------------
| Thermally Perfect Gas Properties Code     |
|            TPG, Version 3.1.0             |
|                                           |
|     NASA  Langley Research Center         |
---------------------------------------------

Table of Thermally Perfect Compressible Flow Properties
Gaseous Mixture:   Air: 4-Species Mixture of N2, O2, Argon, and CO2
Database file name: [ Default database of Air Mixture ]
Species Names are:
                 N2    ,    O2    ,    Argon,    CO2   ,
Species Mass Fractions are:
              0.75530   0.23140   0.01290   0.00040
Species Mole Fractions are:
              0.78092   0.20946   0.00935   0.00028
Mixture Properties:
                    Molecular Weight =  28.9663
                         Gas Constant = 2.87035E+02 J/(kg*K)
            Polynomial Coefficients : cp/R = Sum[A(I)*T^(I-2)]
              80.0 < T <  1000.0 degrees K
     -3.73198210+00   5.41967010-01   3.46935860+00   3.83537980-04
     -2.76531300-06   8.18861420-09  -7.73686900-12   2.43487230-15
              1000.0 < T <  6000.0 degrees K
      2.37698510+05  -1.24405270+03   5.12666900+00  -2.04006440-04
      6.83218010-08  -1.05535420-11   6.64500710-16   0.00000000+00

Total Temperature =  1500.000 K
```

ISENTROPIC FLOW PROPERTIES ---> OBLIQUE SHOCK WAVE FLOW PROPERTIES (2=downstream, 1=upstream) --->

M	T(K)	Gamma	P/Pt	RHO/RHOt	T/Tt	q/Pt	A/A*	V/a*	ShokAngl	FloDflec	M2	P2/P1	RHO2/RHO1	T2/T1	Pt2/Pt1
0.000	1500.0	1.3107	1.000E+00	1.000E+00	1.0000	0.000E+00	infinite	0.00000	**	Subsonic: Not Applicable --->					
0.250	1485.6	1.3112	9.600E-01	9.694E-01	0.9904	3.934E-02	2.428E+00	0.26693	**	Subsonic: Not Applicable --->					
0.500	1443.7	1.3127	8.513E-01	8.845E-01	0.9625	1.397E-01	1.348E+00	0.52659	**	Subsonic: Not Applicable --->					
0.750	1378.5	1.3152	7.015E-01	7.634E-01	0.9190	2.595E-01	1.064E+00	0.77258	**	Subsonic: Not Applicable --->					
1.000	1295.6	1.3187	5.422E-01	6.277E-01	0.8637	3.575E-01	1.000E+00	1.00000	**	Maximum Attached-flow Shock Deflection Angle = 0.000					
1.250	1201.4	1.3234	3.974E-01	4.962E-01	0.8009	4.109E-01	1.049E+00	1.20580	**	Maximum Attached-flow Shock Deflection Angle = 5.554					
1.500	1101.7	1.3281	2.794E-01	3.805E-01	0.7345	4.178E-01	1.189E+00	1.38864	**	Maximum Attached-flow Shock Deflection Angle = 12.803					
1.750	1001.5	1.3360	1.907E-01	2.856E-01	0.6677	3.901E-01	1.419E+00	1.54868	**	Maximum Attached-flow Shock Deflection Angle = 19.218					
1.784	988.0	1.3370	1.807E-01	2.743E-01	0.6586	3.845E-01	1.459E+00	1.56887	65.4776	20.0000	0.919	2.889E+00	2.156E+00	1.340E+00	9.800E-01
2.000	904.6	1.3437	1.277E-01	2.117E-01	0.6031	3.431E-01	1.758E+00	1.68691	76.3155	20.0000	0.695	4.220E+00	2.737E+00	1.542E+00	7.315E-01
2.250	813.5	1.3522	8.460E-02	1.560E-01	0.5423	2.896E-01	2.229E+00	1.80531	79.5417	20.0000	0.620	5.542E+00	3.186E+00	1.740E+00	5.980E-01
2.500	729.6	1.3611	5.593E-02	1.150E-01	0.4864	2.379E-01	2.864E+00	1.90595	81.2798	20.0000	0.574	6.985E+00	3.572E+00	1.955E+00	4.825E-01
2.750	653.8	1.3697	3.713E-02	8.518E-02	0.4359	1.923E-01	3.701E+00	1.99099	82.3730	20.0000	0.543	8.573E+00	3.909E+00	2.193E+00	3.846E-01
3.000	586.4	1.3774	2.488E-02	6.364E-02	0.3909	1.542E-01	4.782E+00	2.06264	83.1176	20.0000	0.520	1.031E+01	4.200E+00	2.455E+00	3.051E-01
3.250	526.8	1.3839	1.687E-02	4.805E-02	0.3512	1.233E-01	6.154E+00	2.12301	83.6516	20.0000	0.502	1.220E+01	4.452E+00	2.739E+00	2.421E-01
3.500	474.6	1.3889	1.160E-02	3.668E-02	0.3164	9.872E-02	7.873E+00	2.17404	84.0498	20.0000	0.489	1.423E+01	4.669E+00	3.047E+00	1.926E-01
3.750	428.9	1.3928	8.094E-03	2.831E-02	0.2859	7.927E-02	1.000E+01	2.21739	84.3554	20.0000	0.478	1.640E+01	4.857E+00	3.377E+00	1.538E-01
4.000	388.9	1.3956	5.725E-03	2.208E-02	0.2593	6.391E-02	1.261E+01	2.25444	84.5963	20.0000	0.469	1.872E+01	5.021E+00	3.729E+00	1.235E-01

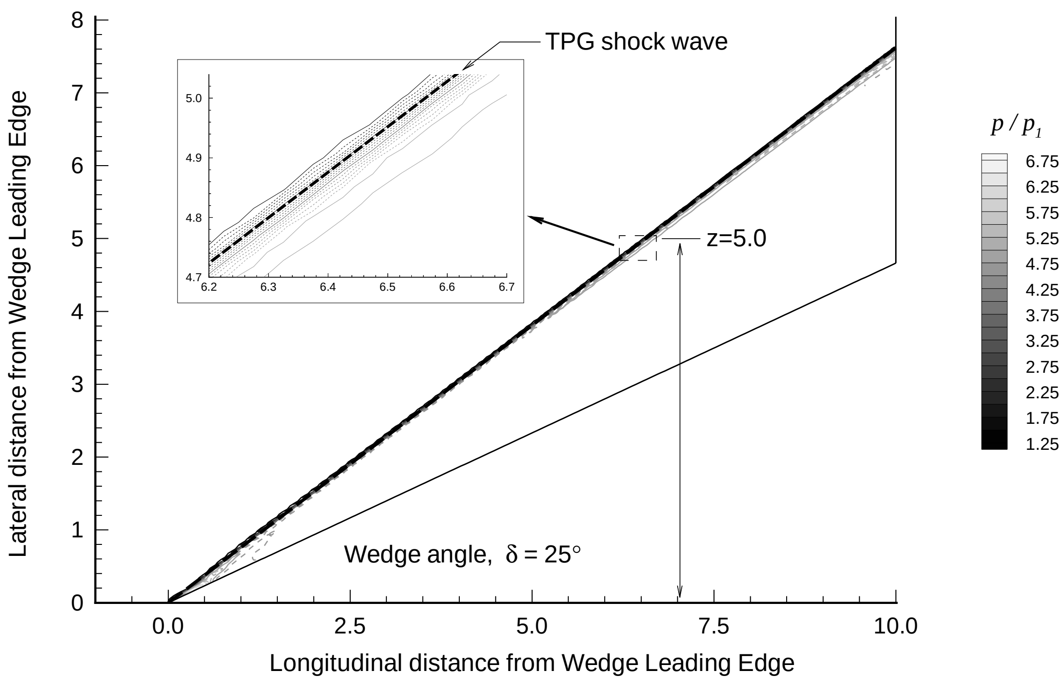
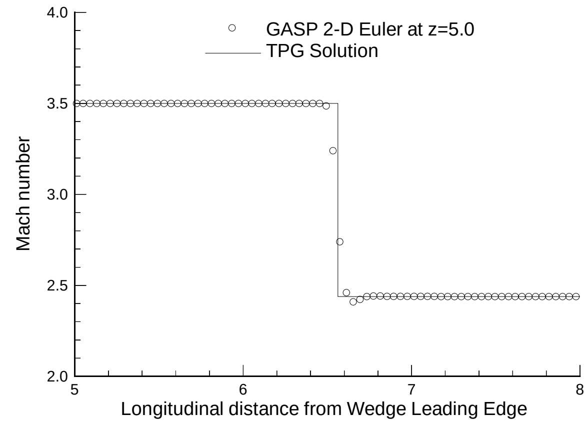
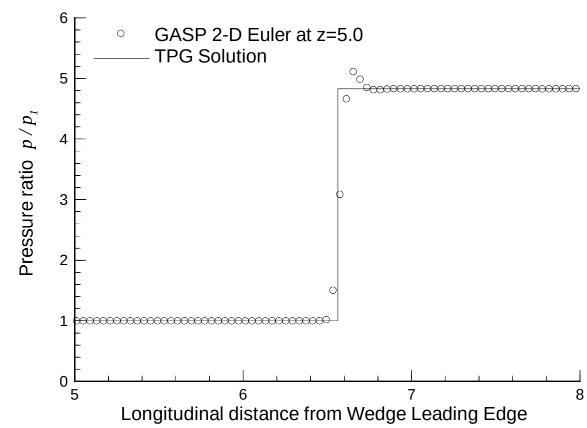


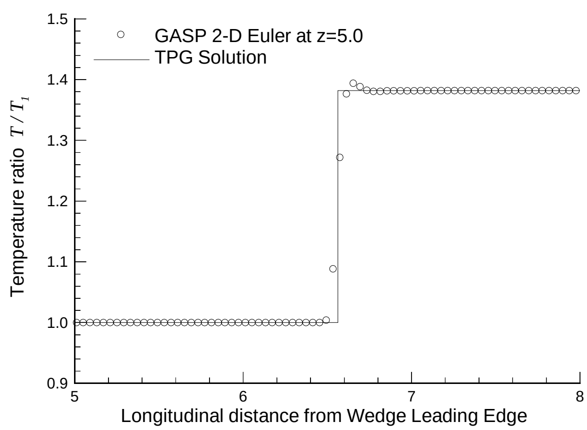
Figure 6. GASP 2-D Euler solution pressure ratio contours and TPG oblique shock wave for 20% Steam/80% CO_2, by mass; M_1=3.5, T_1=1200 K over a 25° wedge.



(a) Mach number M



(b) Static pressure ratio p/p_1



(c) Static temperature ratio T/T_1

Figure 7. GASP 2-D Euler and TPG oblique shock wave calculations for 20% Steam/80% CO_2, by mass; M_1=3.5, T_1=1200 K over a 25° wedge: at z=5.0 units above the wedge leading edge.