A computational technique for high enthalpy shock tube and shock tunnel flow simulation

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Abstract. A contact discontinuity tracking method with a specially designed moving grid is developed to eliminate the interface smearing completely. In order to precisely locate the contact surface, an updated Riemann solver for unsteady one-dimensional inviscid flows is also developed to allow consideration of the specific heat ratio change across the shock wave. These two new computational techniques are illustrated in a high Mach number shock tube flow field computation.

Key words: Shock tube, Shock tunnel, Riemann solver

Nomenclature

C: sound speed C_p : specific heat at constant pressure C_v : specific heat at constant volume e: internal energy e_{vi} : vibrational energy of species i h: enthalpy p: pressure q_i : mass fraction of species i R_i : gas constant of species i t: time T: temperature u: velocity U: general variable W: shock Mach number x: coordinate along the shock tube

Greek symbols

 $(\Delta h_i^f)_T$: standard heat of formation of species i at temperature T ϕ_i : net production rate of species i γ : specific heat ratio, C_p/C_v μ_i : molecular weight of species i θ_{vi} : characteristic vibrational temperature of species i ϱ : density τ_{vi} : characteristic relaxation time of species i

Superscript

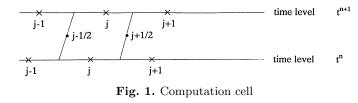
*: intermediate states
': first order derivative
'': second order derivative
Subscript
l: left side
r: right side

1 Introduction

Renewed interest in hypersonics has created a demand for short duration high-enthalpy ground test facilities which are confined to hypervelocity flight regions. This special requirement has spawned a number of exotic facilities which represent in essence various extensions of the basic shock tube flow. The present work investigates shock tube and shock tunnel (without piston) flows, which represent only a few of many different types of impulse facilities. Numerical simulations of such flows are required to better understand the test flow conditions, to determine test duration time and supplement the results of experiments. It is also useful to improve the shock tunnel operation characteristics.

However, flow conditions in a shock tunnel are very severe and put enormous strain on the accuracy and stability of the current numerical techniques. The unsteady flow inside a high enthalpy shock tube and shock tunnel is significantly influenced by very strong shock waves, chemically reacting and inert gas interfaces (contact discontinuities), high temperature effects, chemical reactions

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and viscous interactions. These important flow features take place in a few millimeters in the axial direction in a facility that can be tens of meter long.

A number of researchers (see, for example, Refs. 1-4) have performed numerical simulations of high enthalpy pulse facilities to tackle the above mentioned challenges. Cambier et al. (1992) describe the computational work on the flow simulation of the NASA Ames 16" Shock Tunnel Facility and describe the numerical problems encountered during the computation of various flow transients and the methods used to resolve them. Particular attention is given to problems arising from extremely stiff chemistry. Wilson (1992) presents a quasi-one-dimensional methodology for numerically simulating the flow inside high-enthalpy pulse facilities. The numerical approach uses a finite volume TVD scheme for the Euler equations coupled with finite- rate chemistry on a moving mesh. A Riemann solver is incorporated for tracking contact discontinuities. A 4th order non-oscillatory scheme and flow loss models are used by Itoh et al (1993) to study the tuned operation of a free piston shock tunnel. The aim of the present paper was to develop a numerical simulation technique for shock tube and shock tunnel flows with particular emphasis on predicting accurate test times by accurately determining the contact surface motion separating the chemically active region of the flow from the cold flow and taking into account the real gas effects on the shock wave strengths with an improved Riemann solver.

The numerical approach taken in the present work has been to solve the unsteady quasi- one-dimensional Euler equations coupled to a detailed finite rate chemistry model for high temperature air. The numerical scheme employed is a modified version of the two-dimensional Godunov type upwind non-oscillatory Euler solver proposed by Rodionov (Rodionov 1987) for transient flows. Second order spatial accuracy of smooth solutions is obtained by linear approximation of the conservative variables within the control volumes. The corresponding gradient of the flow variables in the control volume determined by one sided derivatives is chosen as the minimum of average gradients for neighbouring control volumes (Colgan 1972). Second order accuracy with respect to time is achieved by a two step predictor-corrector technique. In the predictor step, intermediate values at grid points are determined following the above mentioned one-sided derivatives in conjunction with the principle of minimum derivative. Using the arithmetic average of the known variable value and the corresponding intermediate value to replace the known value of grid points an exact Riemann solver is used in the corrector step to determine the flow variables at the control volume

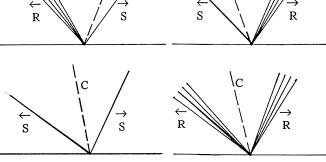
Fig. 2. Four available wave patterns in the Riemann problem solution S - shock wave R - rarefaction wave C - contact surface

interfaces. Note that the predictor step of the scheme involves no Riemann solver and hence contributes to the efficiency of the employed computational technique.

Two numerical issues are the focus of the present work. The first issue relates to the solution of the exact Riemann problem for very high Mach number shock tube or shock tunnel flows involving very strong discontinuities when the specific heat ratio becomes a function of temperature. In these cases, it is inconsistent to use an exact Riemann solver based on constant specific heat ratio when chemical reactions are treated as temperature dependent. An improved exact Riemann solver for unsteady one dimensional flows is presented which takes into account the change of the specific heat ratio across shock waves.

The second issue concerns the smearing of cold and very hot gas interfaces by numerical diffusion. This smearing increases as the distance the interface travels becomes greater. This is the case when the length of the shock tunnel being simulated becomes large. This large smearing results in non-physical mass transfer of chemical species and in non-physical chemical reactions across the interface. Moreover, the performance of the shock tube and the available maximum test time in the test section of the shock tunnel are very closely related to the interaction between the reflected shock wave from the end of of the driven section and the contact discontinuity, the interface between cold and reacting hot gases. Therefore, it is imperative to precisely locate the contact discontinuity at any instant of time in the shock tube.

Tracking the contact discontinuity eliminates the interface smearing completely. A contact discontinuity tracking method is proposed in the present work by applying the above described computational technique to a specially designed moving grid, resulting in sharp, step-like variations of the flow parameters across it.



2 An updated Riemann solver

Consider the grid shown in Fig. 1 with U_j as the known value of the general variable U at grid point x_j , and time level t_n . In order to find the value of U_j at time level t^{n+1} , U_i^n , with a finite volume method, a certain discretization scheme is needed to determine the values of the variable Uat the cell boundaries, $U_{j-1/2}$ and $U_{j+1/2}$. However, while discontinuities exist in the flow field, the discontinuity between two adjacent points, say U_j at x_j and U_{j+1} at x_{j+1} , will break into leftward and rightward moving waves separated by a contact surface. Each wave can be either a shock wave or a rarefaction wave and the physically available combinations produce four wave patterns as shown in Fig. 2. The problem of determining the wave patterns and the flow field in each region is called a Riemann problem and the algorithm to solve this problem is called a Riemann solver. Therefore, while discontinuities exist in the flow field, in order to determine the variable values at the cell boundary, a Riemann problem must be solved. Thus an efficient and precise Riemann solver is an important part of a CFD method for supersonic and hypersonic flows where the flow discontinuities must be considered.

Riemann problems were first introduced into computational fluid dynamics by Godunov (Godunov 1976). Since then, various approximate solvers and "exact" solvers were developed (see for example, Gottlieb, Groth 1988).

The exact Riemann solver developed by Gottlieb and Groth is demonstrated to be an efficient and robust one. The central concept of the solver is to choose the common flow velocity of the intermediate state (u^*) as the iterate and the pressure difference $(p_l^* - p_r^*)$ across this contact discontinuity is made equal to zero.

The initial guess (n=0) for the flow velocity u^* is given by $u_0^* = \frac{u_l^* Z + u_r^*}{1 + Z}$

where

$$\begin{split} u_l^* &= u_l + \frac{2C_l}{\gamma_l - 1} \\ u_r^* &= u_r + \frac{2C_r}{\gamma_r - 1} \\ Z &= \frac{\gamma_l - 1}{\gamma_r - 1} \frac{C_r}{C_l} \left(\frac{p_l}{p_r}\right)^{\frac{\gamma - 1}{2\gamma}} \\ if \quad p_l < p_r, \quad \gamma = \gamma_r \\ p_l \ge p_r, \quad \gamma = \gamma_l. \end{split}$$

By using the standard Newton iteration procedure the successive iterates of u^* are given by

$$u_{n+1}^* = u_n^* - \frac{p_l^*(u_n^*) - p_r^*(u_n^*)}{p_l^{*'}(u_n^*) - p_r^{*'}(u_n^*)}$$
(2)

where the prime denotes the first derivative with respect to u^* . The values of $p_l^*(u_n^*)$, $p_r^*(u_n^*)$, $p_l^{*!}(u_n^*)$, $p_r^{*!}(u_n^*)$ are determined based on the wave patterns. The iteration ends when the following convergence criterion is satisfied:

$$\left|\frac{2(p_l^* - p_r^*)}{(p_l^* + p_r^*)}\right| < \varepsilon_p,\tag{3}$$

where ε_p is a prescribed infinitesimal (1e-7 in the present work). In order to improve the convergence rate, second order derivatives are also included in the Newton iterative procedure. The successive iterates of u^* will then be:

$$u_{n+1}^{*} = u_{n}^{*} - \frac{p_{l}^{*}(u_{n}^{*}) - p_{r}^{*}(u_{n}^{*})}{p_{l}^{*'}(u_{n}^{*}) - p_{r}^{*'}(u_{n}^{*})} - \frac{(p_{l}^{*}(u_{n}^{*}) - p_{r}^{*}(u_{n}^{*}))^{2}(p_{l}^{*''}(u_{n}^{*}) - p_{r}^{*''}(u_{n}^{*}))}{2(p_{l}^{*'}(u_{n}^{*}) - p_{r}^{*''}(u_{n}^{*}))^{3}},$$

$$(4)$$

where the double prime denotes the second derivative with respect to u^* .

The detailed expressions for the four wave patterns in Fig. 2 are given in [8] (Gottlieb, Groth 1988). These expressions are derived based on the assumption that the specific heat ratio γ is constant across the shock wave. In high Mach number shock tube and shock tunnel or any other flow field with strong discontinuities, the temperature variation in the field is large, and the specific heat ratio γ can not be considered constant as it is a function of temperature. Sometimes, even the chemical reactions must be considered. It is inconsistent to use the Riemann solver based on constant specific heat ratio assumption while the main program considers chemical reactions and treats the thermodynamic properties as a function of temperature. As an update to the mentioned Riemann solver, further iteration is introduced to consider the specific heat ratio change across the shock wave, if the shock wave strength in the Riemann problem solution is very strong, for example, the pressure ratio across the shock is greater than 10 in the present work.

For non-constant specific heat ratio, we have

$$\begin{array}{ll} \text{if} \quad p^* > p_r, \qquad T_r^* = T_r \frac{\frac{\gamma_r + 1}{\gamma_r - 1} + \frac{p^*}{p_r}}{\frac{(2A - 1)\gamma_r + 1}{\gamma_r - 1} + \frac{p_r}{p^*}}, \\ \\ \text{where} \quad A = \frac{\gamma_r^*}{\gamma_r} \frac{\gamma_r - 1}{\gamma_r^* - 1}, \end{array}$$

otherwise

(1)

$$T_{r}^{*} = T_{r}(\frac{p^{*}}{p_{r}})^{\frac{\gamma-1}{\gamma}}, \text{ where } \gamma = \frac{\gamma_{r} + \gamma_{r}^{*}}{2},$$

if $p^{*} > p_{l}, \quad T_{l}^{*} = T_{l}\frac{\frac{\gamma_{l}+1}{\gamma_{l}-1} + \frac{p^{*}}{p_{l}}}{\frac{(2A-1)\gamma_{l}+1}{\gamma_{l}-1} + \frac{p_{l}}{p^{*}}},$
where $A = \frac{\gamma_{l}^{*}}{\gamma_{l}}\frac{\gamma_{l}-1}{\gamma_{l}^{*}-1},$

otherwise

$$T_l^* = T_l(rac{p^*}{p_l})^{rac{\gamma-1}{\gamma}}, \quad ext{where} \quad \gamma = rac{\gamma_l + \gamma_l^*}{2}.$$

Fewer mathematical operations will be needed for iterations to consider the effect of non-constant specific heat ratio, if the common pressure of the intermediate states (p^*) is chosen as an iterate. The initial guess of pressure p^* should obviously be

$$p^* = (p_l + p_r)/2 \tag{1'}$$

For the guessed p^* , based on constant γ calculate an assumed T^* and then find the guessed γ^* . Once the guessed p^* and γ^* are prescribed, the T^* can then be recalculated. The successive iterates of p^* is as follows.

$$p_{n+1}^{*} = p_{n}^{*} - \frac{u_{l}^{*}(p_{n}^{*}) - u_{r}^{*}(p_{n}^{*})}{u_{l}^{*'}(p_{n}^{*}) - u_{r}^{*'}(p_{n}^{*})} - \frac{(u_{l}^{*}(p_{n}^{*}) - u_{r}^{*}(p_{n}^{*}))^{2}(u_{l}^{*''}(p_{n}^{*}) - u_{r}^{*''}(p_{n}^{*}))}{2(u_{l}^{*'}(p_{n}^{*}) - u_{r}^{*'}(p_{n}^{*}))^{3}},$$

$$(4')$$

The iteration ends when a certain convergence criterion is satisfied:

$$\left|\frac{2(u_l^* - u_r^*)}{(u_l^* + u_r^*)}\right| < \varepsilon_u,\tag{3'}$$

where ε_u is a prescribed infinitesimal (0.001 in the present work). All the corresponding terms involved in the calculation for the four wave patterns can be written as follows when the specific heat ratio change across the waves is considered.

1. In the case of rightward moving shock for which $p^* > p_r$,

$$\begin{split} u_r^* &= u_r + \frac{C_r(\frac{p^*}{p_r} - 1)}{\gamma_r W_r}, \\ u_r^{*\prime\prime} &= \frac{C_r}{\gamma_r p_r W_r} [1 - p_r(\frac{p^*}{p_r} - 1) \frac{W_r^{\prime}}{W_r}], \\ u_r^{*\prime\prime} &= 2 \frac{C_r}{\gamma_r W_r^3} (\frac{p^*}{p_r} - 1) W_r^{\prime 2} - 2 \frac{C_r}{\gamma_r p_r W_r^2} W_r^{\prime} \\ &- \frac{C_r}{\gamma_r W_r^2} (\frac{p^*}{p_r} - 1) w_r^{\prime\prime}, \end{split}$$

where

$$\begin{split} W_r &= [\frac{D_1(\frac{p^*}{p_r})^2 + (1-D_1)\frac{p^*}{p_r} - 1}{D_2\frac{p^*}{p_r} - D_3}]^{\frac{1}{2}}, \\ W_r' &= \frac{2D_1\frac{p^*}{p_r} + 1 - D_1 - D_2W_r^2}{2p_r(D_2\frac{p^*}{p_r} - D_3)w_r}, \\ W_r'' &= \frac{\frac{D_1}{p_r} - 2D_2W_rW_r' - p_r(D_2\frac{p^*}{p_r} - D_3)w_r'^2}{p_r(D_2\frac{p^*}{p_r} - D_3)w_r}, \\ D_1 &= \frac{(2A-1)\gamma_r + 1}{\gamma_r - 1}, \\ D_2 &= \frac{2\gamma_r[(A-1)\gamma_r + 1]}{\gamma_r - 1}, \\ D_3 &= \frac{2\gamma_r}{\gamma_r - 1}, \\ A &= \frac{\gamma_r^*}{\gamma_r}\frac{\gamma_r - 1}{\gamma_r' - 1}. \end{split}$$

2. In the case of leftward moving shock for which $p^* > p_l$,

$$u_l^* = u_l + \frac{C_l(\frac{p^*}{p_l} - 1)}{\gamma_l W_l},$$
$$u_l^{*\prime} = \frac{C_l}{\gamma_l p_l W_l} [1 - p_l(\frac{p^*}{p_l} - 1)\frac{W_l'}{W_l}],$$

$$\begin{split} u_l^{*\prime\prime} &= 2 \frac{C_l}{\gamma_l W_l^3} (\frac{p^*}{p_l} - 1) W_l^{\prime 2} - 2 \frac{C_l}{\gamma_l p_r W_l^2} W_l^{\prime} \\ &- \frac{C_l}{\gamma_l W_l^2} (\frac{p^*}{p_l} - 1) w_l^{\prime\prime}, \end{split}$$

where

$$W_{l} = -\left[\frac{D_{1}(\frac{p^{*}}{p_{l}})^{2} + (1 - D_{1})\frac{p^{*}}{p_{l}} - 1}{D_{2}\frac{p^{*}}{p_{l}} - D_{3}}\right]^{\frac{1}{2}},$$

$$W_{l}^{'}=rac{2D_{1}rac{p^{*}}{p_{l}}+1-D_{1}-D_{2}W_{l}^{2}}{2p_{l}(D_{2}rac{p^{*}}{p_{l}}-D_{3})w_{l}},$$

$$W_{l}^{''} = \frac{\frac{D_{1}}{p_{l}} - 2D_{2}W_{l}W_{l}^{'} - p_{l}(D_{2}\frac{p^{*}}{p_{l}} - D_{3})w_{l}^{'2}}{P_{l}(D_{2}\frac{p^{*}}{p_{l}} - D_{3})w_{l}},$$
$$D_{1} = \frac{(2A - 1)\gamma_{l} + 1}{\gamma_{l} - 1},$$
$$D_{2} = \frac{2\gamma_{l}[(A - 1)\gamma_{l} + 1]}{\gamma_{l} - 1},$$

$$D_3 = rac{2\gamma_l}{\gamma_l - 1},
onumber \ A = rac{\gamma_l^*}{\gamma_l} rac{\gamma_l - 1}{\gamma_l^* - 1}.$$

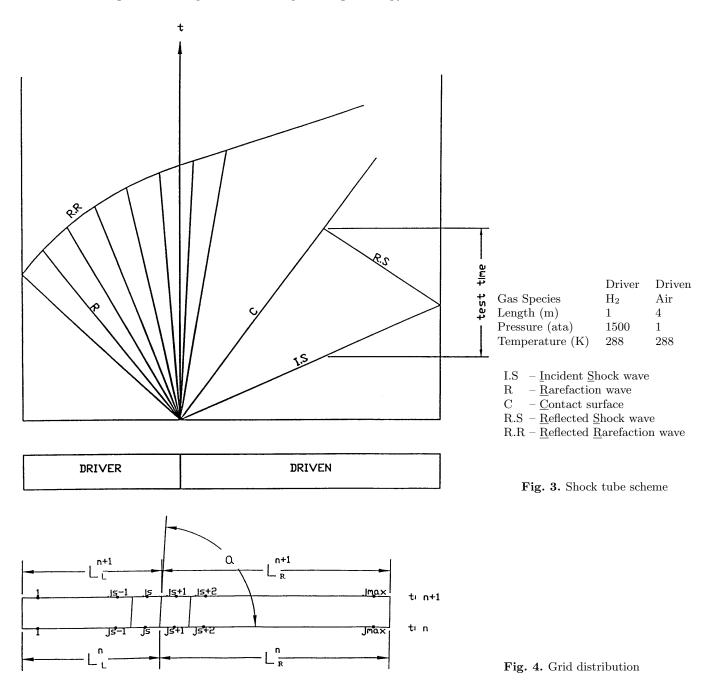
For the cases of rarefaction waves, the arithmetic average specific heat ratio is used and the terms involved in the calculation are shown in case 3 and 4.

3. In the case of right rarefaction wave with $p^* \leq p_r$,

$$u_r^* = u_r + \frac{2}{\gamma - 1} (C_r^* - C_r),$$
$$u_r^{*\prime} = \frac{C_r^*}{\gamma p^*},$$
$$u_r^{*\prime\prime} = -\frac{\gamma + 1}{2\gamma} \frac{u_r^{*\prime}}{p^*},$$
$$C_r^* = C_r (\frac{T_r^*}{T_r})^{\frac{1}{2}}.$$

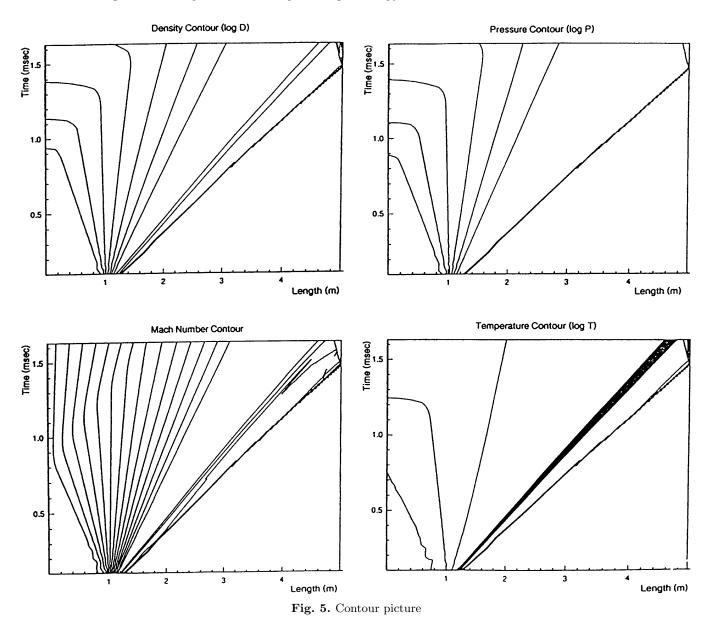
4. In the case of left rarefaction wave with $p^* \leq p_l$,

$$\begin{split} u_{l}^{*} &= u_{l} - \frac{2}{\gamma - 1} (C_{l}^{*} - C_{l}), \\ u_{l}^{*\prime\prime} &= -\frac{C_{l}^{*}}{\gamma p^{*}}, \\ u_{l}^{*\prime\prime\prime} &= -\frac{\gamma + 1}{2\gamma} \frac{u_{l}^{*\prime}}{p^{*}}, \\ C_{l}^{*} &= C_{l} (\frac{T_{l}^{*}}{T_{l}})^{\frac{1}{2}}. \end{split}$$



3 Shock tube flow field numerical simulation

In shock tube flow field analysis, it is important to precisely locate the contact surface. A sketch of a shock tube is shown in Fig. 3. When the diaphragm breaks, a strong incident shock followed by a contact surface is produced by the moving high pressure gas in the driver towards the lower pressure driven tube. This shock wave travels down to the end of the driven tube and then reflects back to interact with the contact surface. The available maximum test time is closely related to the interaction between the reflected shock wave and the contact surface. In order to obtain high Mach number and stagnation temperature in the test section, hydrogen (or helium) with high pressure is used as the driver gas; the driven gas is air (78.084% N_2 , 20.946% O_2 , 0.97% A_r) at standard atmosphere pressure. In such a case, the incident shock may be very strong, and the temperature behind the shock is high enough that the chemical reactions and non-constant thermal property effect must be considered. A Riemann solver based on constant specific heat ratio assumption is not acceptable. In order to illustrate the appropriateness of the updated Riemann solver, a high Mach number shock tube flow is numerically solved. The shock tube scheme and detailed input data are shown in Fig. 3.



3.1 Governing differential equations

Since the incident shock wave is quite strong, chemical reactions must be considered for the driven gas. In this work, five species in air (O_2, N_2, NO, N, O) are involved and seventeen chemical reactions are considered. The related thermodynamic data and chemical reaction information are taken from Ref. 9 and Ref. 10. The governing differential equations for a non-equilibrium unsteady one dimensional flow in a shock tube problem can be written as follows:

$$\frac{\partial \varrho}{\partial t} + \frac{\partial \varrho u}{\partial x} = 0, \tag{5}$$

$$\frac{\partial(\varrho u)}{\partial t} + \frac{\partial(p + \varrho U^2)}{\partial x} = 0, \tag{6}$$

$$\frac{\partial}{\partial t} [\varrho(h + \Sigma q_i e_{vi} + \frac{u^2}{2}) - p] + \frac{\partial}{\partial t} [\rho u(h + \Sigma q_i e_{vi} + \frac{u^2}{2})] = 0.$$
(7)

$$\frac{\partial x}{\partial t}(\varrho q_i) + \frac{\partial}{\partial x}(\varrho u q_i) = \varrho \Phi_i, \tag{8}$$

$$\frac{\partial}{\partial t}(\varrho q_i e_{vi}) + \frac{\partial}{\partial x}(\varrho u q_i e_{vi}) = \varrho e_{vi})\Phi_i
+ \varrho q_i \frac{[\theta_{vi} R_i]/[\exp(\frac{\theta_{vi}}{T}) - 1] - e_{vi}}{\tau_{vi}},$$
(9)

where

$$h = 8314.0\Sigma_i \frac{q_i}{\mu_i} [a_{i1}T + \frac{a_{i2}}{2}T^2 + \frac{a_{i3}}{3}T^3 + \frac{a_{i4}}{4}T^4 + \frac{a_{i5}}{5}T^5 + a_{i6} + 298.15C_{pi} - ([\Delta h_i^f]_{298.5} - [\Delta h_i^f]_0)$$

	$A(i,\!m)X(i)$	+ A(i,m)X(i)	$== B(i,\!m)X(i)$	+B(i,m)x(i)	+B(i,m)X(i)
1	O_2	+ N	== 20	+ N	
2	O_2	+ NO	== 20	+ NO	
3	O_2	$+ O_2$	== 20	$+ O_2$	
4	O_2	$+ N_{2}$	== 20	$+ N_{2}$	
5	O_2	+ O	== 20	+ O	
6	N_2	+ N	== 2N	+ N	
7	N_2	+ NO	== 2N	+ NO	
8	N_2	$+ O_2$	== 2N	$+ O_2$	
9	N_2	$+ N_{2}$	== 2N	$+ N_2$	
10	N_2	+ O	== 2NO	+ O	
11	NO	$+ N_{2}$	== N	+ O	$+ N_{2}$
12	NO	+ N	== N	+ 0	+ N
13	NO	$+ O_2$	== N	+ O	$+ O_2$
14	NO	+ O	== N	+ O	+ O
15	NO	+ NO	== N	+ 0	+ NO
16	Ο	+ NO	== N	$+ O_2$	
17	Ο	$+ N_{2}$	== N	+ NO	

Table 1. Chemical reactions involved

$$C_{pi} = 8314.0(a_{i1} + a_{i2}T + a_{i3}T^2 + a_{i4}T^3 + a_{i5}T^4),$$

$$\Phi_i = \frac{\varrho}{1000} \mu_i \Sigma_m [(B(i,m) - A(i,m))(AFR(m)T^{BFR(m)}) + A(i,m)](AFR(m)T^{BFR(m)}) + A(i,m)$$

$$\exp(-\frac{DFR(m)}{T})\Pi_i (\frac{1000\mu_i q_i}{\varrho})^{A(i,m)}$$

$$\tau_{vi} = \frac{\sum_{k \frac{q_k}{\mu_k} \exp(A_i[T^{-\frac{1}{3}} - 0.015(\frac{\mu_i \mu_k}{\mu_i + \mu_k})^{\frac{1}{4}}] - 18.42)}{\frac{p}{1.033e5}\sum_k \frac{q_k}{\mu_k}}$$

Constants in the vibrational energy equations are as follows:

Species	N_2	O_2	NO
A_i	220	129	168
θ_{vi}	3390	2270	2740
<i>a</i>	1 . 1 .	1 .	1 .

Constants related to chemical reactions see tables and other data can be found in [9] (Sagnier, Marraffa 1991) and [10] (Gupta, Yos, Thompson, Lee 1990).

3.2 Contact surface tracking

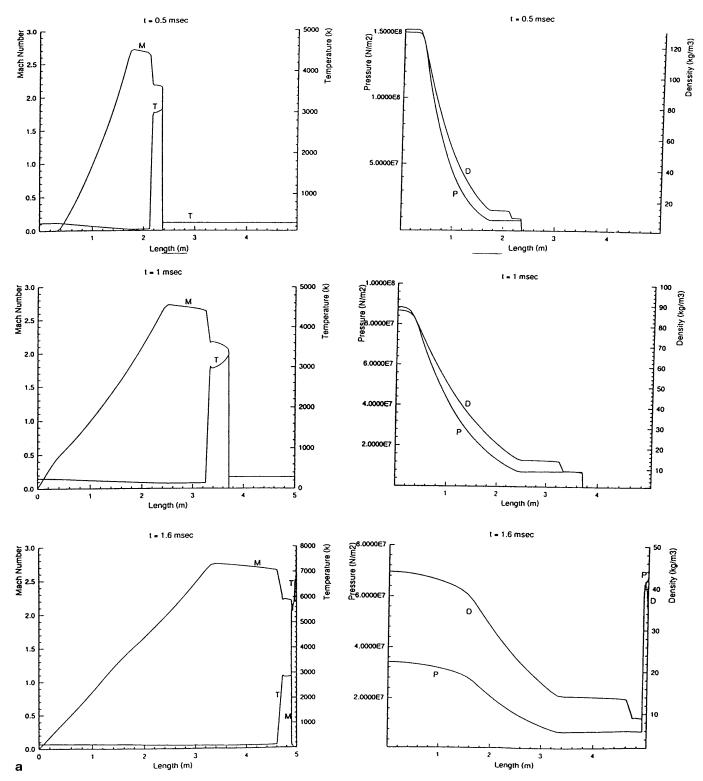
In a shock tube or a shock tunnel, the driver and the driven gases are usually different. When the diaphragm breaks, a contact surface separates the two different gases. Tracking the contact surface to divide the computational domain into two parts with two different gas species can greatly simplify the computation work. It is especially important when the incident shock is strong and the temperature is high enough behind the incident shock wave that the real gas effect must be considered. When the incident shock reaches the tube end and a reflected shock wave is developed, the whole driven gas is under high temperature, the

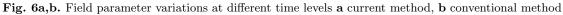
Table 2. Chemical reaction rate coefficients

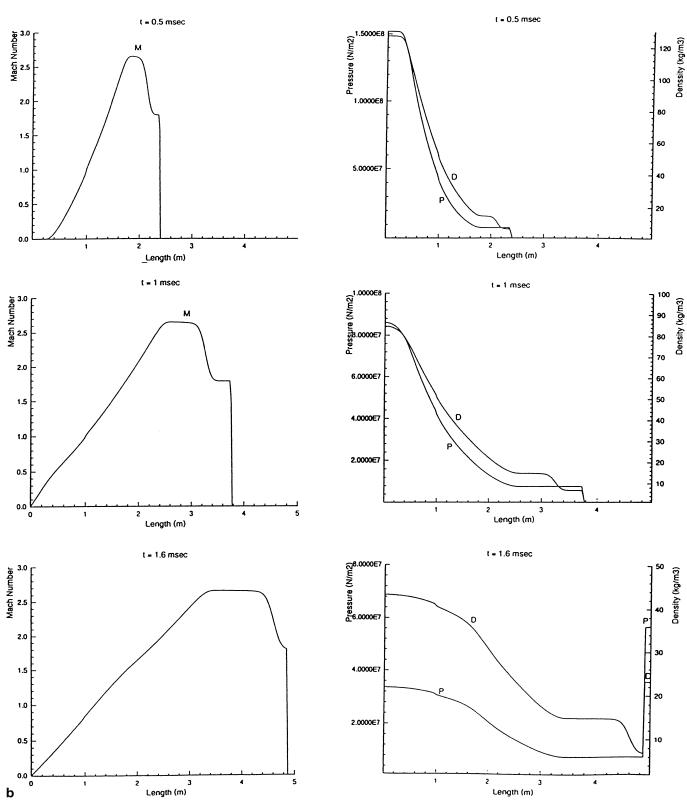
	AFR	BFR	DFR	ABR	BBR	DBR
1	3.6e18	-1	0.595e5	3.0e15	-0.5	0.0
2	3.6e18	-1	0.595e5	3.0e15	-0.5	0.0
3	3.249e19	-1	0.595e5	2.7 e16	-0.5	0.0
4	7.2e18	-1	0.595e5	6.0e15	-0.5	0.0
5	9.0e19	-1	0.595e5	7.5e16	-0.5	0.0
6	4.08e22	-1.5	1.132e5	2.27e21	-1.5	0.0
7	1.9e17	-0.5	1.132e5	1.1e16	-0.5	0.0
8	1.9e17	-0.5	1.132e5	1.1e16	-0.5	0.0
9	4.7 e17	-0.5	1.132e5	2.72e16	-0.5	0.0
10	1.92 e17	-0.5	1.132e5	1.1e16	-0.5	0.0
11	3.97 e20	-1.5	0.755e5	1.0e20	-1.5	0.0
12	7.8e20	-1.5	0.755e5	2.0e20	-0.5	0.0
13	3.97 e20	-1.5	0.755e5	1.0e20	-1.5	0.0
14	7.8e20	-1.5	0.755e5	2.0e20	-1.5	0.0
15	7.8e20	-1.5	0.755e5	2.0e20	-1.5	0.0
16	3.18e9	1.0	1.968e4	1.3e10	1.0	3.58e3
17	7.0e13	0.0	3.8e4	1.56e13	0.0	0.0

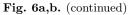
real gas effects and the chemical reactions must be considered for the whole region. In the meantime, the driver gas is under low temperature, even though the starting temperature may be higher than the one in driven gas because of the rarefaction wave caused by the breakdown of the diaphragm. The chemical reactions there can be neglected. Tracking the contact surface to separate these two regions can limit the consideration of real gas effects to the driven gas only. In addition, the performance of the shock tube and the available maximum test time, are closely related to the interaction between the reflected shock wave and the contact surface. Therefore, it is also important to precisely locate the contact surface.

Obviously, at time level $t^0 = 0$, the starting point of the contact surface is at the location of the diaphragm,









 $x = x_{js+1/2} = x_{js} + \Delta x/2$ as shown in Fig. 4. On the left side is the uniform driver gas and on the right side is the uniform driven gas; solving the Riemann problem gives the location of the contact surface, the angle, α , in the Fig. 4. Once the time interval, τ , is set, the starting point for the new time level $t^1 = t^0 + \tau$ is determined. At this new time level, the left-hand side and the right-hand side of the contact surface are not uniform any longer. The initial values of the Riemann problem with no consideration of gradients on both sides of the discontinuity are determined by the discretization scheme. Solving the Riemann problem will give the location of the contact surface (angle α) at the new time level. In this way, the contact surface can be tracked for all time levels. The precision of the contact surface depends on the precision of the Riemann solver and the discretization scheme.

3.3 Grid distribution and discretization

The whole solution domain is divided into cells as shown in Fig. 4.

For each cell, the differential equations can be converted to algebraic equations using Green's theorem. Arranging the grid line distribution by tracking the contact surface can greatly improve the computational precision. Obviously, at time level $t^n = 0$, the starting point of the contact surface is at the location of the diaphragm, $x = x_{js+1/2} = x_{js} + \Delta x/2$ as shown in Fig. 4. The grid intervals in the driver section and the driven section are equal, $\Delta x_L = \Delta x_R = \Delta x$. According to the Godunov-Colgan method (Colgan 1972), an approximation using one-sided derivatives in conjunction with the principle of the minimum derivative provides a correct distribution of variables in the cells when discontinuities are present, and is of $0(h^2)$ accurate for smooth solutions. Based on the principle of the minimum derivative, the independent variable values U at the cell boundary js + 1/2 from the left cell , js, should be

$$U_{js+1/2} = U_{js} + K_{js} * \Delta x_L/2;$$

$$K_{js} = \min\left(\left|\frac{u_{js+1} - u_{js}}{X_{js+1} - X_{js}}\right|, \left|\frac{u_{js} - u_{js-1}}{X_{js} - X_{js-1}}\right|\right)$$

The independent variable values U at the cell boundary js + 1/2 from the right cell, js + 1, should be

$$U_{js+1/2} = U_{js+1} - K_{js+1} * \Delta x_R/2;$$

$$K_{js+1} = \min\left(\left|\frac{u_{js+2} - u_{js+1}}{X_{js+2} - X_{js+1}}\right|, \left|\frac{u_{js+1} - u_{js}}{X_{js+1} - X_{js}}\right|\right).$$

Thus, a discontinuity exists at the cell boundary. A Riemann problem based on these initial values with no consideration of gradients on both sides of the discontinuity is solved to determine the contact surface location angle, α , and the cell boundary value. The maximum velocity of propagation of disturbances generated in the Riemann problem, C_w , is also recorded for the purpose of determining the time interval, τ . This discretization scheme is proved to be first order accurate in marching direction (time in this work) and second order accurate in the coordinate x. It is stable if the following criterion is satisfied.

$$\tau/\Delta x \ll 0.5/C_w$$

where C_w is the maximum velocity of propagation of disturbances generated in the Riemann problem and τ is the permissible time interval. Once the contact surface location angle, α , and the time interval, τ , are determined, the grid distribution for the new time level $t^{n+1} = t^n + \tau$ can be found geometrically as shown in Fig. 4.

In order to improve the accuracy in the marching direction, a modification developed by Rodionov is introduced (Rodionov 1987). According to Rodionov, intermediate values at grid points are determined following the above mentioned one-sided derivatives in conjunction with the principle of the minimum derivative before solving the Riemann problem. Then the arithmetic average of the known variable value and the corresponding intermediate value is used to replace the known value at grid points and to discretize the equations. This new scheme can provide an accuracy close to second order in the marching direction. When the grid distribution is determined, one follows the same procedure to solve the Riemann problems for all the cell boundaries to determine the cell boundary values and the maximum velocity of propagation of disturbances generated in the Riemann problems, C_w . The final discretized equations can be written as follows:

$$\varrho_{j}^{n} = \frac{1}{c} \left(\varrho_{j} + \frac{\tau}{h_{x}} \left(\left[\varrho(u - W^{*}) \right]_{j - \frac{1}{2}} - \left[\varrho(u - W^{*}) \right]_{j + \frac{1}{2}} \right) \right),$$
(5')

$$\begin{aligned} (\varrho u)_{j}^{n} &= \frac{1}{c} \bigg((\varrho u)_{j} + \frac{\tau}{h_{x}} \Big(\big[p + \varrho u (u - W^{*}) \big]_{j - \frac{1}{2}} \\ &- \big[p + \varrho u (u - W^{*}) \big]_{j + \frac{1}{2}} \Big) \bigg), \end{aligned}$$
(6')

$$\begin{split} &8341C \varrho_{j}^{n} \Sigma_{i} \{ \frac{q_{ji}^{n}}{\mu_{i}} (a_{i1}T_{j}^{n} + \frac{a_{i2}}{2}T_{j}^{n2} + \frac{a_{i3}}{3}T_{j}^{n3} \\ &+ \frac{a_{i4}}{4}T_{j}^{n4} + \frac{a_{i5}}{5}T_{j}^{n5} + a_{i6} + 298.15C_{pi} \\ &- [(\Delta h_{i}^{f})_{298.15} - (\Delta h_{i}^{f})_{0}]) \} \\ &- 8341C \varrho_{j}^{n} T_{j}^{n} \Sigma_{i} \frac{q_{ji}^{n}}{\mu_{i}} + C \varrho_{j}^{n} \Sigma_{i} q_{ij}^{n} e_{vij}^{n} \\ &- [\varrho h + \varrho \frac{u^{2}}{2} + \varrho \Sigma_{i} q_{i} e_{vi} - p]_{j} \\ &+ \frac{\tau}{h_{x}} \{ [(\varrho h + \varrho \frac{u^{2}}{2} + \varrho \Sigma_{i} q_{i} e_{vi})(u - W^{*}) \\ &+ pW^{*}]_{j - \frac{1}{2}} - [(\varrho h + \varrho \frac{u^{2}}{2} \\ &+ \varrho \Sigma_{i} q_{i} e_{vi})(u - W^{*}) + pW^{*}]_{j + \frac{1}{2}} \} = 0 \end{split}$$

$$\begin{split} q_{ij}^{n} &- \frac{\left[(1-S_{2}) \frac{1+h_{x}^{n}/h_{x}}{2} \tau \right] \frac{(\varrho_{j}^{n})^{2}}{1000} \mu_{i}}{\varrho_{j}^{n}C} \\ \Sigma_{m} \left[B(i,m) - A(i,m) \right] \left[AFR(m) T_{j}^{n \; BFR(m)} \right. \\ &\left. \exp\left(- \frac{DFR(m)}{T_{j}^{n}} \right) \Pi_{i} \left(\frac{1000\mu_{i}q_{ij}^{n}}{\varrho_{j}^{n}} \right)^{A(i,m)} \right. \\ &\left. - ABR(m) T_{j}^{n \; BBR(m)} \exp\left(- \frac{DBR(m)}{T_{j}^{n}} \right) \right. \\ &\left. \Pi_{i} \left(\frac{1000\mu_{i}q_{ij}^{n}}{\varrho_{j}^{n}} \right)^{B(i,m)} \right] \\ &\left. - \frac{1}{\varrho_{j}^{n}C} \left(\left(\varrho_{i} q_{i} \right) + \frac{\tau}{h_{x}} \left\{ \left[\varrho_{i} (u - W^{*}) \right]_{j - \frac{1}{2}} \right. \\ &\left. - \left[\varrho_{i} (u - W^{*}) \right]_{j + \frac{1}{2}} \right\} \right) \right. \\ &\left. + \frac{1}{\varrho_{j}^{n}C} \left(\varrho_{i} \phi_{ij} \left[S_{2} \frac{1 + h_{x}^{n}/h_{x}}{2} \tau \right] \right) = 0, \end{split}$$

$$\left. \left\{ \frac{\tau}{h_{x}} \left(\left[\varrho_{i} e_{vi}(u - W^{*}) \right]_{j - \frac{1}{2}} - \left[\varrho_{i} e_{vi}(u - W^{*}) \right]_{j + \frac{1}{2}} \right) \right\} \\ &\left. + \frac{1}{\varrho_{j}^{n}C} \left\{ \left(\varrho_{i} e_{vi} (u - W^{*}) \right]_{j - \frac{1}{2}} - \left[\varrho_{i} e_{vi}(u - W^{*}) \right]_{j + \frac{1}{2}} \right) \right\} \end{split}$$

$$\left\{ \frac{h_x}{h_x} \left(\left[\varrho q_i e_{vi}(u - W^*) \right]_{j - \frac{1}{2}} - \left[\varrho q_i e_{vi}(u - W^*) \right]_{j + \frac{1}{2}} \right) \right\} \\
+ \frac{1}{\varrho_j^n C} \left\{ (\varrho q_i e_{vi})_j + \left(\frac{1 + h_x^n / h_x}{2} \tau \right) (\varrho e_{vi} \Phi_i)_j \right\} \\
+ (\varrho q_i)_j \left(\frac{1 + h_x^n / h_x}{2} \tau \right) \frac{1}{\varrho_j^n C \tau_{vij}} \\
\left\{ \frac{\theta_{vi} R_i}{exp(\theta_{vi} / T_j) - 1} - e_{vij} \right\} = 0.$$
(9)

Where

$$h_{x} = x_{j+1/2} - x_{j-1/2},$$

$$h_{x}^{n} = x_{j+1/2}^{n} - x_{j-1/2}^{n},$$

$$w_{j-1/2}^{*} = (x_{j-1/2}^{n} - x_{j-1/2})/\tau,$$

$$w_{j+1/2}^{*} = (x_{j+1/2}^{n} - x_{j+1/2})/\tau,$$

$$C = (w_{j+1/2}^{*} - w_{j-1/2}^{*})\tau/h_{x},$$

$$S = 0.5,$$

$$S_{1} = 0.5,$$

$$S_{2} = 0.4.$$

3.4 Computational results

The high Mach number shock tube problem outlined in Fig. 3 is solved with the contact discontinuity tracking method and the updated Riemann solver. The results are summarized in Fig. 5 and Fig. 6. Figure 5 shows the contour picture of pressure, temperature, density and Mach number. In order to assess the quantitative variations in flow variables along the shock tube, the parameter variations at three typical time levels are shown in Fig. 6A. The time level t= 0.5 msec. corresponds to the stage when the incident shock and the rarefaction waves have not reached the tube end; Time level t= 1 msec. corresponds to the stage after the rarefaction waves have reached the tube

end, but the incident shock has not. Time level t = 1.6msec. displays the case after the incident shock reaches the wall and reflects from there. The same shock tube problem is also solved by a conventional method with no contact surface tracking and no chemical reaction considered. The specific heat ratio is considered to be constant both in the main flow field computation and in the Riemann solver. The results are shown in Fig. 6B. Comparing these results, it can be seen that both methods can predict the incident shock by the sharp jump of pressure and density profiles. However, only the present method can locate the contact surface by the sharp jump of the density profile. There is a large smeared region around the contact surface which makes it difficult to locate the contact surface when the conventional method is used. Since the real gas effects are considered in the current method, there is no sharp jump for the reflected shock wave. The reflected shock wave travels in a non-uniform reacting fluid intermedium, no sharp jump across the reflected shock will appear. The sharp jump shown in Fig. 6B is caused by the perfect gas assumption, it does not mean the conventional method can precisely locate the reflected shock wave. For the field behavior, the shock wave strength and location, there are significant differences between the predicted results by these two methods. This is caused by real gas effects considered in the present method. The computational technique such as the contact discontinuity tracking method and the Riemann solver can change the solution precision and the computation cost; however, only the equations, including the chemistry models, viscous models will influence the field behavior. Therefore, the detailed discussion of the field behavior is beyond the scope of this article.

4 Conclusions

The Riemann solver developed by Gottlieb and Groth in 1987 is demonstrated to be an efficient and robust one. Since it is based on constant specific heat ratio assumption across the shock wave, it is not acceptable when a strong discontinuity is present in the flow field. Especially, when chemical reactions are considered and thermodynamic properties are treated as functions of temperature in the main code, it is inconsistent to take the constant specific heat ratio assumption in the Riemann solver subroutine. An update to consider the specific heat ratio change across shocks in the solver must be introduced. However, even if there are strong multi-discontinuities in the whole flow field, most calls for the Riemann solver in the code only handle a weak shock in the Riemann problem, therefore, the update is introduced in the solver as an option only when it is necessary. This treatment can keep the merit of the original solver and simplify the modification. The solver starts with the constant specific heat ratio assumption and then processes further iterations to consider the effect of variable specific heat ratio across the shock wave when it is necessary. In this part of further iterations, the conventional way of choosing the common pressure of the intermediate states (p^*) as the iterate is more convenient.

In shock tube or shock tunnel, the smearing of cold and hot gas interfaces by numerical diffusion increases as the distance that the interface travels becomes greater. Tracking the contact discontinuity can eliminate the interface smearing completely so that the simulation precision is greatly improved. Besides, in high Mach number shock tube or shock tunnel, the driver gas and the driven gas are usually different. When the diaphragm breaks, a contact surface separates the two different gases. Tracking the contact surface to divide the computational domain into two parts with two different gas species can greatly simplify the computational work. It is especially important when the incident shock is strong so the real gas effects and the chemical reactions must be considered. Tracking the contact surface to separate these two regions can limit the consideration of real gas effect in the driven gas only. Obviously, similar tracking methods based on the perfect gas assumption [11][12] do not provide this advantage and their applications are therefore limited.

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