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SHOCK

A PROGRAM FOR PREDICTING CHEMICAL KINETIC BEHAVIOR BEHIND INCIDENT AND REFLECTED

Reaction Design

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Reaction Design cautions that some of the material in this manual may be out of date. Updates will be available periodically on Reaction Design's web site. In addition, on-line help is available on the program CD. Sample problem files can also be found on the CD and on our web site at www.ReactionDesign.com.

SHO-036-1

SHOCK: A PROGRAM FOR PREDICTING CHEMICAL KINETIC BEHAVIOR BEHIND INCIDENT AND REFLECTED SHOCKS

ABSTRACT

SHOCK is a CHEMKIN Application that predicts the chemical changes that occur after the shock heating of reactive gas mixtures. The program is designed to handle both incident and reflected shock waves. It makes allowances for real-gas behavior, boundary layer effects and detailed finite-rate chemistry. The program is intended for use in conjunction with shock tube experiments. Computer simulation of such experiments is valuable to the interpretation of the experimental results and to the understanding of the chemical kinetic behavior.

CONTENTS

			Page
LIS	ST OF	FIGURES	5
NC	OMEN	ICLATURE	7
1.	INTF	RODUCTION	
2.	THE	ORETICAL DEVELOPMENT	
	2.1	Boundary Layer Effects	
	2.2	Laboratory Time and Gas-particle Time	
	2.3	Incident SHOCK Initial Conditions	
	2.4	Reflected SHOCK Initial Conditions	
3.	PRO	GRAM STRUCTURE	
	3.1	Optional User Programming	
4.	PRO	GRAM INPUT	
	4.1	Keyword Syntax and Rules	
	4.2	Problem Type (Must choose only one)	
	4.3	Solution Method Options	
	4.4	Conditions Before an Incident SHOCK	
	4.5	Conditions After an Incident SHOCK	
	4.6	Conditions After a Reflected SHOCK	
	4.7	Initial Species Mole Fractions	
	4.8	Additional Input for Boundary Layer Corrections	
	4.9	Miscellaneous	
	4.10	Comparing SHOCK with Experiments	
	4.11	The Save File	
5.	POS	T PROCESSING	
	5.1	CHEMKIN Graphical Post-processor	
	5.2	Configurable Command-line Post-processor	
6.	SAM	IPLE SHOCK PROBLEM	
	6.1	Input to the CHEMKIN Interpreter	
	6.2	Output from the CHEMKIN Interpreter	
	6.3	Input to the SHOCK Program	
	6.4	Output from the SHOCK Program	
7.	REFE	ERENCES	

LIST OF FIGURES

Figure 1.	A distance-time diagram shows the movements of the shock front, contact surface, rarefaction wave, and reflected shock wave	10
Figure 2.	Laboratory and gas-particle times.	15
Figure 3.	Laboratory-fixed and Incident-shock-fixed coordinate systems.	17
Figure 4.	Laboratory-fixed and reflected-shock-fixed coordinate systems	21
Figure 5.	Relationship of the SHOCK Program to the CHEMKIN Preprocessor, and to the Associated Input and Output files.	23

Page

NOMENCLATURE

		CGS Units
Α	Cross-sectional area available for flow downstream of the shock wave	cm ²
С	Ratio defined by Eq. (17)	
c_p	Specific heat at constant pressure of gas mixture	ergs∕(g K)
C_{pk}	Specific heat at constant pressure of the <i>k</i> th species	ergs∕(g K)
d	Hydraulic diameter (4 times the ratio of the cross-sectional area of the	
	tube to the perimeter of the tube)	cm
h	Specific enthalpy of the mixture	ergs/g
h_k	Specific enthalpy of the <i>k</i> th species	ergs/g
l_m	Distance between the shock and the contact surface at infinite distance	
	from the diaphragm	cm
M_1	Mach number of the incident shock	
p	Pressure	dynes/cm²
R_u	Universal gas constant	ergs/(mole K)
Т	Temperature	K
t	Time	sec
t_l	Laboratory time	sec
t_p	Gas-particle time	sec
и	Gas velocity in shock-fixed coordinates	cm/sec
U	Gas velocity in laboratory-fixed coordinates	cm/sec
U_{rs}	Reflected shock velocity	cm/sec
U_s	Incident shock velocity	cm/sec
v	Velocity	cm/sec
W	Ratio u_w/u_2 used in Eqs. (15) and (16)	
W_k	Molecular weight of <i>k</i> th species	g/mole
z	Distance	cm
Ζ	Ratio $(\gamma + 1)/(\gamma - 1)$ used in Eq. (16)	

GREEK

CGS Units

α	Temperature ratio across the incident shock, T_2/T_1	
α'	Temperature ratio across the reflected shock, T_5/T_1	
β	Temperature ratio across the incident shock, p_2/p_1	
β'	Temperature ratio across the reflected shock, p_5/p_1	
γ	Specific heat ratio	
η	Density ratio across the incident shock, ρ_2 / ρ_1	
μ	Viscosity	g∕(cm sec)
V	Kinematic viscosity	cm²/sec
ξ	Density ratio, $\rho \neq \rho_I$	
ρ	Mass density of the gas mixture	g/cm ³
$\dot{\omega}_k$	Production rate of the <i>k</i> th species from gas-phase reactions	mole/(cm ³ sec)

SUBSCRIPTS

k	Denotes species k
W	Denotes condition at the wall
0	Denotes reference condition
1	Denotes condition before the incident shock
2	Denotes condition immediately behind the incident shock
5	Denotes condition immediately behind the reflected shock

1. INTRODUCTION

The shock tube has found widespread use as an experimental device in which to investigate chemical kinetic behavior in reactive gas mixtures. Much can be learned by experiment alone, however such investigations are enhanced considerably when done in concert with computer simulations. To this end, SHOCK simulates the chemical changes that occur after the shock heating of a reactive gas mixture. The program is designed to account for both incident and reflected normal shock waves. It makes allowances for the non-perfect gas behavior, boundary layer effects and detailed finite-rate chemistry.

SHOCK provides flexibility in describing a wide variety of experimental conditions. Often people who perform shock-tube experiments report their experimental conditions differently. The SHOCK simulator allows input of these different conditions directly, without requiring hand calculations to prepare the input. In addition to this flexibility, SHOCK works together with the CHEMKIN Gas-phase Utility package.

The input options to SHOCK coincide with the parameters most likely to be measured in shock tube experiments. For incident shock cases, the incident shock velocity and any two of the density, temperature and pressure, either before or behind the shock, can be specified. For reflected shocks, any two of the density, temperature and pressure behind the shock can be specified or conditions for the incident shock can be given. If the reflected shock velocity is specified, it is used in determining the temperature and pressure of the gas mixture behind the shock. Otherwise, the program determines that reflected shock velocity (and associated temperature and pressure) which renders the gas behind the shock at rest. Whenever gas conditions before the shock are given, SHOCK calculates conditions behind he shock from the Rankine-Hugoniot equations using real gas thermodynamic properties for the test gas mixture.

The SHOCK Application makes use of the CHEMKIN Thermodynamic Database of thermodynamic property fits and uses the Gear-Hindmarsh² numerical algorithm for solving sets of stiff ordinary differential equations.

This manual presents a complete description of the SHOCK program. Chapter 2 states the governing conservation equations and then describes the derivation of the set of ordinary differential equations (ODEs) for the distributions of the flow variables behind the shock. Chapters 3 through 5 give instructions for setting up and using the program. Finally, in Chapter 6 we present a sample problem demonstrating the use of SHOCK.

2. Theoretical Development

A shock tube is a device in which a gas at high pressure (the driver gas) is initially separated from a gas at lower pressure (the test gas) by a diaphragm. When the diaphragm is suddenly burst, a plane shock wave propagates through the test gas raising it to new temperature and pressure levels. At the elevated temperature and pressure, chemical reaction commences. As the shock wave moves through the test gas, a rarefaction wave moves back into the high-pressure gas at the speed of sound. The test gas and the driver gas make contact at the "contact surface", which moves along the tube behind the shock front. Conventional notation represents the conditions in the unperturbed, low-pressure test gas by the subscript 1, so that the initial temperature and pressure in this region are denoted as p_1 and T_1 , respectively. The region between the shock front and the contact surface is denoted by 2; the region between the contact surface and the rarefaction wave by 3. The initial conditions on the high-pressure side are given the subscript 4. If the shock wave is allowed to undergo reflection at the end of the tube, the pressure conditions in this region are given the subscript 5. Figure 1 shows the ideal movement of the shock front, the contact surface, the rarefaction wave and the reflected shock wave in a distance-time diagram.

The set of equations, which describe the concentration, velocity and temperature distributions downstream of the shock, are derived from the well-established conservation laws of mass, momentum and energy transfer.



Figure 1. A distance-time diagram shows the movements of the shock front, contact surface, rarefaction wave, and reflected shock wave.

The flow is assumed to be adiabatic; transport phenomena associated with mass diffusion thermal conduction and viscous effects are assumed to be negligible. Test times behind shock waves are typically on the order of a few hundred microseconds; hence, neglect of these transport processes is of little consequence. Initial conditions for the governing equations are derived from the Rankine-Hugoniot relations for flow across a normal shock. The conservation equations for one-dimensional flow through an arbitrarily assigned area profile are stated below:

Continuity:

$$\rho vA = \text{constant}$$
 (1)

Momentum:

$$\rho v \frac{dv}{dz} + \frac{dp}{dz} = 0 \tag{2}$$

Energy:

$$\frac{dh}{dz} + v\frac{dv}{dz} = 0 \tag{3}$$

Species:

$$\rho v \frac{dY_k}{dz} = \dot{\omega}_k W_k \tag{4}$$

Temperature is related to the specific enthalpy of the gas mixture through the relations:

$$h = \sum_{k=1}^{K} h_k Y_k \tag{5}$$

and

$$h_{k} = (h_{k})_{0} + \int_{T_{0}}^{T} c_{pk} dT$$
(6)

The net molar production rate of each species due to chemical reaction is denoted by $\dot{\omega}_k$. A detailed description of this term is given in the CHEMKIN Thermodynamics Database manual. The equations of state relating the intensive thermodynamic properties is given by:

$$p\overline{W} = \rho R_u T \tag{7}$$

where the mixture molecular weight is determined from the local gas concentration via:

$$\overline{W} = \frac{1}{\sum_{k=1}^{K} Y_k / W_k}$$
(8)

In the shock tube experiments, the usual measurable quantities are density, species concentration, velocity and temperature as functions of time. It is therefore desirable to have time as the independent variable and not distance. Employing the relation

$$\frac{d}{dt} = v \frac{d}{dz} \tag{9}$$

differentiating Eqs. (5), (6), (7), and (8), and combining the equations results in the following set of coupled, ordinary differential equations:

$$\frac{d\rho}{dt} = \left(\frac{1}{p + pv^2/c_p T - \rho v^2}\right) \left(\frac{R_u \rho}{\overline{W}c_p} \sum_{k=1}^K \dot{\omega}_k W_k \left(h_k - \frac{\overline{W}c_p T}{W_k}\right) + \frac{\rho^2 v^3}{A} \left(1 - \frac{R_u}{c_p \overline{W}}\right) \frac{dA}{dz}\right)$$
(10)

$$\frac{dY_k}{dt} = \frac{\dot{\omega}_k W_k}{\rho} \tag{11}$$

$$\frac{dv}{dt} = -\frac{v}{\rho}\frac{d\rho}{dt} - \frac{v^2}{A}\left(\frac{dA}{dz}\right)$$
(12)

$$\frac{dT}{dt} = -\frac{v^2}{\rho c_p} \frac{d\rho}{dt} - \frac{1}{\rho c_p} \sum_{k=1}^K h_k \dot{\omega}_k W_k + \frac{v^3}{A c_p} \left(\frac{dA}{dz}\right)$$
(13)

The time-histories of the measurable flow quantities should satisfy these relations.

2.1 Boundary Layer Effects

In a shock tube, the presence of the wall boundary layer causes the shock to decelerate, the contact surface to accelerate and the flow behind the shock to be non-uniform. In this one-dimensional analysis, we must account empirically for effect that the flow of mass into the cold boundary layer has on the free-stream variables. We take the approach developed by Mirels.³ Assuming a laminar boundary layer, Mirels proposed treating the flow as quasi-one-dimensional with the variation of the free-stream variables calculated from

$$\frac{\rho_V}{(\rho_V)_2} = 1 - (z/l_m)^{1/2} , \qquad (14)$$

where l_m is the distance between the shock and contact surface at infinite distance from the diaphragm and the subscript 2 denotes conditions immediately behind the shock. He then obtained an expression for l_m by considering the simultaneous boundary layer development and change in free-stream conditions external to the boundary layer. This expression is

$$l_m = \frac{d^2}{16\beta^2} \left(\frac{\rho_2}{\rho_w}\right)^2 \frac{1}{(W-1)} \left(\frac{u_2}{v_w}\right),$$
(15)

where

$$\beta = 1.59C \left(1 + \frac{1.796 + 0.802W}{(ZW - 1)} \right), \tag{16}$$

with $Z = (\gamma + 1)/(\gamma - 1)$ and $W = u_w/u_2$. The effect of variable viscosity is accounted for by *C*, where

$$C = \left[\left(\frac{\rho_2}{\rho_w} \right) \left(\frac{\mu_2}{\mu_w} \right) \right]^{0.37}.$$
 (17)

The wall is assumed to remain at its initial temperature, while the pressure at the wall changes to p_2 after passage of the shock. The viscosity correction is based on numerical solutions for air. For the purposes of the boundary layer corrections, we take the viscosity to be that of the diluent gas.

Hirschfelder, Curtiss and Bird⁴ give the viscosity of a pure gas as

$$\mu = \frac{2.6693 \times 10^{-5} \sqrt{WT}}{\sigma^2 \Omega^{(2,2)^*} T^*} \,. \tag{18}$$

where μ is the viscosity in gm/cm-sec; σ , the low-velocity collision cross-section for the species of interest in Angstroms; *W*, the molecular weight; *T*, the temperature in Kelvin; and $\Omega^{(2,2)*}$, the reduced collision integral, a function of the reduced temperature T^* ($T^* = T/(\varepsilon/k)$ where (ε/k) is the potential parameter for the species of interest). The reduced collision integral represents an averaging of the collision crosssection over all orientations and relative kinetic energies of colliding molecules. Tabulated values of this integral at various reduced temperatures are given in reference 6. The values can be fit to within 2% for $T^* > 2.7$ by the expression:

$$\Omega^{(2,2)^*} = 1.2516 \left(T^* \right)^{-0.1756}.$$
(19)

Using this in the expression for the viscosity yields:

$$\mu = \left[\frac{2.1327 \times 10^{-5} \sqrt{W}}{\sigma^2 (\varepsilon/k)^{0.1756}}\right] T^{0.6756} .$$
⁽²⁰⁾

Evaluating the above equation at 300K and using this as a reference point results in the following expression for the viscosity:

$$\mu = \mu_0 (T/300)^{0.6756} \,. \tag{21}$$

A value for μ_0 for the diluent gas must be specified by the user when considering boundary layer effects.

To derive an equation for the area variation, we first combine Eqs. (1) and (14) to yield

$$\frac{A_2}{A} = 1 - \left(z/l_m\right)^{1/2}.$$
(22)

Then, the change in cross-sectional area with distance downstream of the shock is given by

$$\frac{1}{A}\frac{dA}{dz} = \frac{(z/l_m)^{-1/2}}{2l_m \left(1 - (z/l_m)^{1/2}\right)}.$$
(23)

This expression is used in Eqs. (10), (12) and (13). Equation (23) allows us to account for the boundary layer effects by computing the "effective" area through which the gas must flow. The distance of a fluid element from the shock, z, follows from Eq. (9) and is given by

$$\frac{dz}{dt} = v . (24)$$

2.2 Laboratory Time and Gas-particle Time

The experimentalist records changes in the test gas conditions (be it pressure, temperature, density or species concentration) after passage of the shock at some observation point. The time recorded on some external recording device is referred to as the laboratory time, t_l . Since the test gas is flowing however, it has been at the post-shock conditions for some time longer than the laboratory time. This longer time is referred to as the gas-particle time, t_p and is the time of interest with respect to rate processes in the test gas. A relationship between t_l and t_p can be derived. To do so, begin by considering the distance-time diagram in Figure 2. When the shock arrives at the observation point, measurements are made on the test gas for a period Δt_l . The test gas has been at the shock-heated conditions for a time Δt_p and has traveled a

distance Δz since being shocked. The time that it took the shock wave to travel this same distance is ($\Delta t_p - \Delta t_l$). Hence, from the relationship between distance and time



$$\Delta z = U_s \left(\Delta t_p - \Delta t_l \right) = U \Delta t_p .$$
⁽²⁵⁾

Figure 2. Laboratory and gas-particle times.

Taking the limit as Δz approaches zero results in the following ordinary differential equation relating gas particle and laboratory times:

$$\frac{dt_l}{dt_p} = 1 - \frac{U}{U_s}.$$
(26)

For mass continuity across the shock wave, it can be shown that

$$\rho_1 A_1 / \rho A = 1 - U / U_s . \tag{27}$$

and, therefore, Eq. (26) can be written as

$$\frac{dt_l}{dt_p} = \rho_1 A_1 / \rho A .$$
⁽²⁸⁾

Thus, when rate processes are measured, the time as measured must be multiplied by the density-area ration across the shock to obtain the true rate referred to the test gas. In SHOCK, Eq. (28) is integrated along with the other ODEs so that laboratory time as a function of gas-particle time is available.

SHOCK solves the coupled set of ODEs for either an incident or reflected shock problem. These ODEs, Eqs. (10), (11), (12) and (13), are integrated along with Eq. (24), for distance from the shock, and (28) for laboratory time, when gas-particle time is the independent variable. Values of the pressure, mean molecular weight and area as a function of gas-particle time are also given.

The initial time for a problem, $t_p = 0$, is taken as the time immediately after the shock wave has elevated the test gas to new levels of temperature and pressure. The incident shock wave is assumed to instantaneously raise the test gas from initial conditions 1 to conditions 2; the reflected shock is assumed to instantaneously raise the test gas from conditions 2 to conditions 5. Gas composition immediately after passage of the shock is assumed to remain unchanged from the initial conditions. Vibrational and rotational energy relaxation processes are neglected.

2.3 Incident SHOCK Initial Conditions

In relating the pressures, temperatures and densities immediately across the shock, it is conventional to consider the gas motion in relation to the shock front. In such a frame of reference, the gas enters the shock at a relative velocity u_1 , and leaves with a relative velocity u_2 . In shock tube jargon, the shock is then considered to be at rest; u is the gas velocity measured in shock-fixed coordinates and U is that measured in laboratory-fixed coordinates. These two frames of reference are related by:

$$u_1 = U_s \,. \tag{29}$$

$$u_2 = U_s - U_2. (30)$$

where U_s is the shock velocity. Gas conditions associated with the incident shock in the two coordinate systems are shown in Figure 3. The Rankine-Hugoniot relations for properties across the incident shock front are

$$\rho_1 u_1 = \rho_2 u_2 \,. \tag{31}$$

$$p_1 + \rho_1 u_1^2 = p_2 + \rho_2 u_2^2 \,. \tag{32}$$

$$h_1 + u_1^2/2 = h_2 + u_2^2/2$$
. (33)

Utilizing the equation of state and Eq. (31) to eliminate the velocity u_2 from Eqs. (32) and (33) results in the following expressions for the pressure and temperature ratios across the incident shock:

$$1 + \rho_1 u_1^2 / p_1 [1 - (T_2/T_1)(p_1/p_2)] - p_2/p_1 = 0.$$
(34)

$$h_1 + u_1^2 / 2 \left[1 - (p_1/p_2)^2 (T_2/T_1)^2 \right] - h_2 = 0.$$
(35)



SHOCK--FIXED COORDINATES

Figure 3. Laboratory-fixed and Incident-shock-fixed coordinate systems.

Since we assume no change in gas composition across the shock, *h* is a function of temperature alone and, hence, Eqs. (34) and (35) represent a system of two equations in two unknowns. The solution gives p_2 and T_2 when conditions before the incident shock are specified. Knowing these, ρ_2 is determined from the equation of state and u_2 from Eq. (31).

An iterative procedure is employed to solve Eqs. (34) and (35) for p_2 and T_2 . Letting α and β be the temperature and pressure ratios, respectively, across the shock, Eq. (34) can be solved for β in terms of α to yield

$$\beta = \frac{1}{2} \left[\left(1 + \frac{\rho_1 u_1^2}{p_1} \right) + \sqrt{\left(1 + \frac{\rho_1 u_1^2}{p_1} \right)^2 - \frac{4\rho_1 u_1^2 \alpha}{p_1}} \right].$$
(36)

This expression is then substituted into Eq. (35) to yield one equation with one unknown, α . Within the SHOCK program, a routine called ZEROIN⁵, which finds the zeros of functions, is employed to determine the value of α that satisfies this equation. An initial guess for α is provided by assuming that the test gas is ideal (c_p and c_v are constant and independent of temperature). For ideal gases

$$\alpha = \frac{T_2}{T_1} \frac{\left(\gamma M_1^2 - \frac{\gamma - 1}{2}\right) \left(\frac{\gamma - 1}{2} M_1^2 + 1\right)}{\left(\frac{\gamma + 1}{2}\right)^2 M_1^2}.$$
(37)

where is the specific heat ratio and M_1 is the Mach number of the incident shock.

$$M_1 = U_s \left(\frac{\rho_1}{\gamma p_1}\right)^{1/2}.$$
 (38)

Many times the experimentalist reports the incident shock speed, U_s , and temperature and pressure behind the shock, T_2 and p_2 , respectively. Before the experiment can be modeled, however, the gas velocity behind the shock must be determined. Employing the equation of state in Eq. (34) to eliminate ρ_1/p_1 results in

$$1 + \frac{\rho_2 u_1^2}{p_2} (T_2/T_1) [1 - (T_2/T_1)(p_1/p_2)] - (p_2/p_1) = 0.$$
(39)

This equation and Eq. (35) again represent two equations in two unknowns. The solution gives T_1 and p_1 and from these the density in region 1 is determined from the equation of state. The velocity behind the shock, u_2 , is determined from Eq. (31). The solution to Eqs. (39) and (35) is analogous to that already described for Eqs. (34) and (35).

2.4 Reflected SHOCK Initial Conditions

For reflected shocks, shock-fixed and laboratory-fixed coordinates are again employed, but now shock-fixed coordinates refer to the reflected shock, which moves at velocity U_{rs} . Considering the reflected shock to be at rest, gas at condition 2 flows into the shock front and gas at condition 5 flows out. The velocities in the two coordinate systems are related by:

$$u_2' = U_{rs} + U_2 , (40)$$

and

$$u_5 = U_{rs} - U_5. (41)$$

The gas velocity measured in shock-fixed coordinates with respect to the reflected shock is u'. Gas conditions associated with the reflected shock in the two coordinate systems are shown in Figure 4. The Rankine-Hugoniot relations for properties across the reflected shock are

$$\rho_2 u_2' = \rho_5 u_5, \tag{42}$$

$$p_2 + \rho_2 (u'_2)^2 = p_5 + \rho_5 (u_5)^2, \qquad (43)$$

and

$$h_2 + (u'_2)^2 / 2 = h_5 + (u_5)^2 / 2$$
. (44)

By analogy with Eqs. (31), (32) and (33), the solution to the above set of coupled equations is found by finding the values of T_5 and p_5 which satisfy

$$1 + \frac{\rho_2 (u_2')^2}{p_2} [1 - (T_5/T_2)(p_2/p_5)] - (p_5/p_2) = 0, \qquad (45)$$

and

$$h_2 + \frac{(u_2')^2}{2} \left[1 - (p_2/p_5)^2 (T_5/T_2)^2 \right] - h_5 = 0, \qquad (46)$$

where

$$u_2' = U_{rs} + U_2 = U_{rs} + U_s - u_2.$$
(47)

When the gas is assumed to be at rest behind the reflected shock (i.e., $U_5 = 0$), then the reflected shock velocity, U_{rs} , is given by

$$U_{rs} = \frac{(p_2/p_5)(T_5/T_2)(U_s - u_2)}{[1 - (p_2/p_5)(T_5/T_2)]}.$$
(48)

Only in the ideal case is the gas behind the reflected shock at rest, however. Non-idealities cause the gas to move in the same direction as the incident shock and, hence, at conditions different from those calculated assuming $U_5 = 0$. Therefore, often the velocity of the reflected shock, as well as that of the incident shock, is measured. Then the values of T_5 and p_5 are computed so as to satisfy the Rankine-Hugoniot relationships using these measured velocities. Having determined T_5 and p_5 , the density of the gas at condition 5 can be determined from the equation of state and u_5 , from Eq. (42).

Initial estimates for T_5 and p_5 can be obtained by again assuming ideal gas behavior. The temperature ration across the incident shock when c_p and c_v are constant is given by Eq. (37) and the pressure ratio by

$$p_2/p_1 = \frac{2\gamma_1 M_1^2 - (\gamma_1 - 1)}{(\gamma_1 + 1)}.$$
(49)

Letting η and ξ be defined as the following density ratios:

$$\eta = \rho_2 / \rho_1 \,, \tag{50}$$

$$\xi = \rho_5 / \rho_1 \,. \tag{51}$$

then the equation of state, Eq. (37) and Eqs. (45) to (49) can be combined to show that for temperatureindependent specific heats

$$\eta = \frac{M_1^2(\gamma_1 + 1)}{(\gamma_1 - 1)M_1^2 + 2},$$
(52)

$$\xi = \frac{\eta \left[M_1^2 (\eta - 1) \gamma_1 + \eta \right]}{M_1^2 (\eta - 1) (\gamma_1 - 1) + \eta},$$
(53)

$$p_5/p_1 = 1 + \frac{\gamma_1 M_1^2 (\eta - 1)(\xi - 1)}{(\xi - \eta)},$$
(54)

$$T_5/p_1 = 1 + \frac{M_1^2(\gamma_1 - 1)(\eta - 1)(\xi - 1)}{\eta(\xi - \eta)},$$
(55)

and

$$U_{rs} = \frac{U_s(\eta - 1)}{(\xi - \eta)}.$$
 (56)

Even in the event that U_{rs} is specified, and hence U_5 is not necessarily zero, we still assume that the gas is at rest when solving the conservation equations. Only the initial state of the gas is modified by the nonideal reflected shock velocity. Because of this, for reflected shock problems, we find it more convenient to use laboratory-time as the independent variable, since then the boundary layer effects are of no consequence. For such cases, laboratory-time and gas-particle time are the same.



SHOCK--FIXED COORDINATES

Figure 4. Laboratory-fixed and reflected-shock-fixed coordinate systems.

3. PROGRAM STRUCTURE

The CHEMKIN Application User Interface runs the SHOCK program automatically through a mousedriven interface and then allows the user to directly launch visualization of solution results using the CHEMKIN Graphical Post-processor. The SHOCK program has a modular structure with interfaces to the CHEMKIN Utility package for obtaining kinetic and thermodynamic parameters. In addition to input directly from the user, SHOCK depends on data obtained from the CHEMKIN Gas-phase package. Therefore, to solve a SHOCK problem the user must first execute the preprocessor program, "chem", which has access to a thermodynamic database (e.g. "therm.dat"). SHOCK then reads input from the user (described in Chapter 4), solves the specified problem, and prints out the solution. The CHEMKIN Graphical Post-processor can then be launched from the Application User Interface to plot solution data. Figure 5 shows the relationships between these components. For more information about the CHEMKIN Application User Interface or Graphical Post-processor, please see the CHEMKIN Getting Started manual.

The first step is to execute the CHEMKIN Interpreter, "chem". The CHEMKIN Interpreter first reads usersupplied information about the species and chemical reactions for a particular reaction mechanism. It then extracts further information about the species' thermodynamic properties from a database file (e.g. "therm.dat"). The user may also optionally input thermodynamic property data directly in the input file to the CHEMKIN Interpreter to override or supplement the database information. The information from the user input and the thermodynamic properties is stored in the CHEMKIN Linking File, "chem.asc"; a file that is later required by the CHEMKIN subroutine library, which will be accessed from the SHOCK program.

SHOCK makes appropriate calls to the CHEMKIN library to initialize the species- and reaction-specific information. The purpose of the initialization is to read the Linking File and set up the internal working and storage space required by all subroutines in the libraries.

SHOCK next reads the input that defines a particular problem and any other needed parameters in a Keyword format from the input file (e.g. "shock.inp"). SHOCK produces printed output (e.g. "shock.out") and it saves the solution in a binary Save File, "save.bin". The Save File is used to post-process the solution, as discussed in Chapter 5.

3.1 Optional User Programming

In addition to using SHOCK through the CHEMKIN Application User Interface, users have the flexibility to write their own interface to SHOCK. To facilitate this, the SHOCK program itself is written as a FORTRAN subroutine that may be called from a user-supplied driver routine. We provide examples of

such driver routines as part of the SHOCK software distribution, written in both C++ and FORTRAN. The driver routine performs the function of allocating total memory usage through definition of array sizes, as well as opening input and output files. SHOCK checks internally to make sure that the allocated work arrays are sufficiently large to address the problem described by the input files. Programs can be linked to the SHOCK subroutine by following the examples in the makefiles provided in the sample driver subdirectories ("drivers_f77" or "drivers_cpp") of the standard distribution. Users taking advantage of this flexibility should be experienced with compiling and linking program files on their operating system and must have either a C++ or FORTRAN compiler installed.



Figure 5. Relationship of the SHOCK Program to the CHEMKIN Preprocessor, and to the Associated Input and Output files.

4. PROGRAM INPUT

4.1 Keyword Syntax and Rules

The SHOCK program's input is in a Keyword format. On each input line an identifying Keyword must appear first. For some Keywords only the Keyword itself is required, while for others, additional information is required. Some Keywords have default values associated with them and in such cases the Keyword line need not be included. In the case of restarts or continuation problems, some of the Keywords can be changed. If not changed, they retain their former values. In each Keyword description, we note whether or not it can be changed upon a restart or continuation. The order of the Keyword inputs is generally unimportant, except in the case of some grouped lists that must be ordered. The rules governing the syntax of the Keyword images are listed below:

- 1. The first four characters of the line are reserved for the Keyword, and it must begin at the first column.
- 2. Any further input associated with the Keyword can appear anywhere in columns 5 through 80. The specific starting column is not important.
- 3. When more than one piece of information is required, the order in which the information appears is important.
- 4. When numbers are required as input, they may be stated in either integer, floating point, or "E" format. The program converts the numbers to the proper type. The double precision specification is not recognized; however, conversion to double precision is done internally as necessary.
- 5. When species names are required as input, they must appear exactly as they were specified in the CHEMKIN input. This input is case sensitive.
- 6. When more than one piece of information is required, the pieces are delimited by one or more blank spaces.
- 7. If more information is input than required, then the inputs that are read last are used. For example, if the same Keyword is encountered twice, the second one read is taken.
- 8. A "comment" line can be inserted by placing either a period (.) or a slash (/) in the first column. Such a line is ignored by the program, but it is echoed back in the printed output. In addition, on any Keyword line, any input that follows the required input and is enclosed in parentheses is taken as a comment.
- 9. The Keyword END must be the last input line.

4.2 Problem Type (Must choose only one)

- **ISHK** Inclusion of this keyword designates an incident shock problem without boundary layer correction. No further information is required for this keyword.
- **ISKB** Inclusion of this keyword designates an incident shock problem with boundary layer correction. No further information is required for this keyword.
- **RSHK** Inclusion of this keyword designates a reflected shock problem. No further information is required for this keyword.

4.3 Solution Method Options

TSTR — Starting time for the problem. Units — sec.

Default—0.0 sec Example: TSTR 0.0

- **TEND** Ending time for the problem. Units — sec. Default—none; required input Example: TEND 1.E-3
- DT Time increment for printed output. Units – sec. Default – 1.0e-6 sec. Example: DT 1.E-5
- LGDT Logarithmic time increment for printed output. If this option is invoked, the starting time is taken as 0.0, and the number given on the TSTR input is taken as the first output time. For example, if the input on this line was 1.0 the output time would be incremented by one order of magnitude after each print until TEND is reached. Note that TSTR may not be 0.

Units — ALOG10(sec) Default — none Example: LGDT 1.0

ATOL — Absolute error tolerance for the ODE integration by LSODE. The local truncation errors are maintained below RTOL z(k) + ATOL, where z(k) are the dependent variables.

Units — none Default — 1.0E-10 Example: ATOL 1.E-8 RTOL — Relative error tolerance for the ODE integration by LSODE. The local truncation errors are maintained below RTOL z(k) + ATOL, where z(k) are the dependent variables. Units — none Default — 1.0E-6 Example: RTOL 1.E-3

4.4 Conditions Before an Incident SHOCK

(The shock velocity and any two of temperature, pressure, or density must be specified)

VSHK — Incident shock velocity. This input is required for all incident shock problems, and may be used for some reflected shock problems.

Units — cm/sec Default — none Example: VSHK 3000.

- T1 Temperature before the incident shock. Units — K Default — none Example: T1 300.
- P1A Pressure before the incident shock. Units — atm. Default — none Example: P1A 1.0
- RHO1 Mass density before the incident shock. Units — gm/cm³ Default — none Example: RHO1 1.E-4

4.5 Conditions After an Incident SHOCK

(The shock velocity and any two of temperature, pressure, or density must be specified)

VSHK — Incident shock velocity. This input is required for all incident shock problems, and may be used for some reflected shock problems.

Units — cm/sec Default — none Example: VSHK 3000.

T2 — Temperature after the incident shock. Units — K Default — none Example: T2 1500.

- P2A Pressure after the incident shock. Units — atm. Default — none Example: P2A 2.3
- RHO2 Mass density after the incident shock. Units — gm/cm³ Default — none Example: RHO2 1.E-4

4.6 Conditions After a Reflected SHOCK

(The shock velocity and any two of temperature, pressure, or density must be specified)

VSHK — Incident shock velocity. As an optional input, the incident shock velocity may be specified. If the reflected shock velocity is not specified, the incident shock velocity is used to determine the reflected shock velocity that causes the gas behind the reflected shock to be at rest. However, if both shock velocities are given, then they are both used to determine the state of the gas behind the reflected shock.

> Units — cm/sec Default — none Example: VSHK 3000.

- VRS —Reflected shock velocity. If specified, it is used to determine the state of the gas after the shock.
The reflected shock velocity is never used unless the incident shock velocity is also given.
Units cm/sec
Default No shock velocities are computed, but $U_5 = 0$.
Example: U5 100
- **T3** Temperature after the reflected shock, given as T_5 in the equations. Units — K Default — none Example: T5 1500.
- **P3A** Pressure after the reflected shock, given as p_5 in the equations Units — atm. Default — none Example: P3A 2.3
- RHO3 Mass density after the reflected shock. Units — gm/cm³ Default — none Example: RHO3 1.E-4

4.7 Initial Species Mole Fractions

INIT — Initial unshocked species mole fraction. This keyword must be followed by a species name and then a mole fraction for that species. One species is entered per line. Species not explicitly entered are taken as having a mole fraction of 0. There may be as many INIT lines as there are species in the problem. The mole fraction for all the species must add up to 1.0 plus or minus 1.0E-6.

> Units — none Default — 0.0 Example: INIT N2 0.76

4.8 Additional Input for Boundary Layer Corrections

- DIA Shock tube diameter. Required input for boundary layer corrections. Units — cm Default — 1.0 cm Example: DIA 2.0
- VISC Viscosity of the mixture at 300K. Required input for boundary layer corrections. Units — gm sec/cm2 Default — none Example: VISC 2.65E-4

4.9 Miscellaneous

- TITL Text characters for a problem title. Example: "My reflected shock case #1"
- **CONC** If this keyword is used, the printed output will appear in molar concentration (moles/cc) rather than mole fraction. No further input is required on this line.
- CNTN If this keyword is used, the program will look for a new set of shock conditions following the END keyword. A continuation case will be run with the new conditions specified. Note that full specification of the shock conditions is required for each solution and the solutions are unrelated.
- **END** This keyword must be the last one read. Any input following the END will be ignored.

4.10 Comparing SHOCK with Experiments

It may be helpful to discuss a number of possibilities for simulating a given experiment. Consider a situation in which more than the minimum information has been measured. Take, for example, a reflected shock problem in which conditions are known before the incident shock and after the reflected shock, and both the incident and reflected shock speeds are measured. The user must input initial mole

fractions of the unshocked gas with the INIT keyword. In addition the user should specify a print output increment, DT, and an ending time for the problem with the TEND keyword. The RSHK keyword is needed to identify the reflected shock problem. In the case that the problem is set up using the information before the incident shock, ant two of T1, P1A, or RHO1 are required input. In addition, the incident shock speed must be specified with the VSHK keyword. The reflected shock speed could be specified with the VRS keyword. If VRS is omitted, the reflected shock speed will be computed by the program. As an alternative, the user could have decided not to use the measured conditions before the incident shock. Instead, one can just as readily specify conditions after the reflected shock, using two of the keywords: T3, P3A, or RHO3. In this case, the user may not specify the measured reflected shock speed. In all reflected shock problems, the gas behind the reflected shock is assumed to be at rest, i.e., a constant pressure process. The various combinations of shock velocity inputs are used only to determine the state of the gas behind the reflected shock.

4.11 The Save File

In addition to printed output the program produces a binary Save File ("save.bin") that contains the solution data. The binary solution file is used to post-process the solution. Further information on this subject can be found in Chapter 5.

5. POST PROCESSING

5.1 CHEMKIN Graphical Post-processor

The CHEMKIN Graphical Post-processor provides a means for quick visualization of results from SHOCK. Launched from the CHEMKIN Application User Interface, the Graphical Post-processor will automatically read in the solution date from the "save.bin" file in the working directory. Alternatively, the post-processor may be launched independently and a solution file may be opened from within the Post-processor. The user may open one or more solution files in the Post-processor and may also import external data for comparisons with the simulation results. In addition, the Graphical Post-processor can be used to export all of the solution data into comma-, tab-, or space-delimited text for further analysis with other software packages. For more information on the Graphical Post-processor, please see the CHEMKIN Getting Started manual.

5.2 Configurable Command-line Post-processor

In addition to the CHEMKIN Graphical Post-processor representation of solution data, we provide the user with a FORTRAN post-processor called SHOCK_POST. This program reads the binary solution file and prints selected data to text files, which can then be imported by many other graphics programs. The full source-code, shock_post.f, is provided in the CHEMKIN "post_processors" subdirectory. Also in this directory is a makefile script for re-building the SHOCK_POST program, in case the user makes changes to the source code. In this way, users may easily configure SHOCK_POST for their own analysis needs.

To run SHOCK_POST from the command-line, you will need to do the following:

- 1. Open a MS-DOS Prompt (PC) or shell (UNIX).
- 2. Change directories to your working directory, where your "save.bin" solution file resides.
- 3. Run SHOCK_POST from the command-line, specifying the full path to the CHEMKIN "bin" directory where the "shock_post" executable resides, unless this is already in your environment "path" variable:

shock_post < shock_post.inp > shock_post.out

Here, "shock_post.inp" is an input file that contains keywords described below. The output "shock_post.out" will contain diagnostics and error messages for the SHOCK_POST run. SHOCK_POST will also create text files containing comma-separated values. The names for these files use a suffix (extension) of ".csv".

SHOCK_POST uses keyword input. The available keywords are printed as a banner when the program is invoked; they are also described briefly here:

- **PREF** A character-string prefix used to name output files. Default — "shock".
- **SPEC** List of the names of species for which fractions are output. Default — No species fractions will be printed. Example: SPEC H2 O2 H2O H O OH
- MASS— Print species fractions as mass fractions Default — Mole fractions are printed.
- **SMIN** Minimum species fraction quantity of interest. Default —0.0, all species fractions listed. Example: SMIN 1.0E-3
- RATE List of the names of species for which production rates are listed. Default — No species production rates will be printed. Example: PROD H2 O2 H2O H O OH
- DROP Filter out lowest reaction rates, by percent. Default — 10., lowest 10% of reaction rates and sensitivity coefficients are not printed. Example: DROP 15
- **HELP** List descriptions of the keywords available.
- END Must be the last keyword in the input

6. SAMPLE SHOCK PROBLEM

The sample problem corresponds to the experimental work of Camac and Feinberg,⁶ who studied the formation of NO in shock-heated air. The purpose here is not to discuss air chemistry, but only to illustrate the use of the SHOCK on a problem that has a relatively simple chemical reaction mechanism. We use the reaction mechanism recommended by Camac and Feinberg. Sections 6.1 through 6.4 show the input and output files from each of the programs needed to run the problem.

6.1 Input to the CHEMKIN Interpreter

This input is used to describe the chemical reaction set to the CHEMKIN Interpreter. Required entries are the elements, species and reactions, which are to be considered by the SHOCK program. The form of the input is described in detail in the CHEMKIN documentation. However, we point out here a method for describing reactions that have different temperature dependencies for different third bodies. In this example, we have excluded N from participating as a third body in the reaction $N_2 + M = N + N + M$; i.e., the effective third body efficiency for N is set to zero. The next reaction $N_2 + N = N + N + N$ accounts for the different temperature dependence of the nitrogen atom as a third body.

ELEMENTS	O N	AR	END						
SPECIES	02	N2	NO	N	0	AR I	END		
REACTION	S								
N2+02=NO	+NO				9.3	LE24		-2.5	128500.
N2+O=NO+I	N				7.0	DE13		0.	75000.
02+N=NO+0	C				1.3	34E1	0	1.0	7080.
02+M=O+O	+M				3.6	52E1	8	-1.0	118000.
N2/2/ 02	2/9/	С)/25/						
N2+M=N+N-	+M				1.9	92E1	7	-0.5	224900.
N2/2.5/	N/0/	/							
N2+N=N+N	+N				4.2	LE22		-1.5	224900.
NO+M=N+O+M 4.0E20 -1.5 150000.									
NO/20/ 0)/20/	' N	1/20/						
END									

6.2 Output from the CHEMKIN Interpreter

This file is the printed output returned from the CHEMKIN Interpreter. If the "No errors were encountered..." message is not printed, then an error was detected and the linking file was not created. Hence, the problem cannot proceed until the indicated corrections are made.

CHEMKIN-III GAS-PHASE MECHANISM INTERPRETER: DOUBLE PRECISION Vers. 6.24 2000/06/18 Copyright 1995, Sandia Corporation. The U.S. Government retains a limited license in this software. _____ ELEMENTS ATOMIC CONSIDERED WEIGHT _____ 15.9994 1. 0 2. N 14.0067 14.000 39.9480 3. AR _____ _____ С P H H A A R SPECIESSGMOLECULARTEMPERATUREELEMENTCOUNTCONSIDEREDEEWEIGHTLOWHIGHONAR _____ _____ G031.99880300500020G028.013403005000020G030.006103005000110G014.006703005000010 1. 02 2. N2 3. NO 4. N G 0 15.99940 300 5000 1 0 G 0 29.04000 200 5. O G 0 39.94800 300 5000 0 0 1 6. AR

						(k = A	T**b exp) (-E/RT)
	REACTIONS CONSI	DERED				А	b	E
1.	N2+O2=NO+NO				9	.10E+24	-2.5	128500.0
2.	N2+O=NO+N				7	.00E+13	0.0	75000.0
3.	O2+N=NO+O				1	.34E+10	1.0	7080.0
4.	O2+M=O+O+M				3	.62E+18	-1.0	118000.0
	N2	Enhanced	by	2.000E+00				
	02	Enhanced	by	9.000E+00				
	0	Enhanced	by	2.500E+01				
5.	N2+M=N+N+M				1	.92E+17	-0.5	224900.0
	N2	Enhanced	by	2.500E+00				
	N	Enhanced	by	0.000E+00				
б.	N2+N=N+N+N				4	.10E+22	-1.5	224900.0
7.	NO+M=N+O+M				4	.00E+20	-1.5	150000.0
	NO	Enhanced	by	2.000E+01				
	0	Enhanced	by	2.000E+01				
	N	Enhanced	by	2.000E+01				

NOTE: A units mole-cm-sec-K, E units cal/mole

NO ERRORS FOUND ON INPUT: ASCII Vers. 1.1 CHEMKIN linkfile chem.asc written. WORKING SPACE REQUIREMENTS ARE

INTEGER: 259 REAL: 217 CHARACTER: 9 Total CPUtime (sec): 0.125

6.3 Input to the SHOCK Program

This file is the keyword input to SHOCK. The descriptions for each of the possible keywords are given in the previous two sections of the manual. In this example, we are considering an incident shock problem with boundary layer corrections. The unshocked temperature is 296K, the pressure is 6.58E-3 atm, and the shock velocity is 2.8E5 cm/sec. The initial mole fractions are 0.78118 N₂, 0.20948 O₂, and 0.00934 Ar. The output time interval is 10 microseconds, and the problem will terminate at 310 microseconds. The shock tube diameter is 3.81 cm, and the viscosity of the gas at 300K is 1.777E-4 gm/cm-sec; these parameters are used for the boundary layer corrections. The relative and absolute error tolerances for the numerical integration are 1.0E-4 and 1.0E-8, respectively. Finally, the CONC keyword indicates that the results will be printed in molar concentration units rather than mole fraction.

```
TITL SHOCK TUBE CODE TEST
P1A 6.58E-3 ! ATM
           ! K
т1
     296
VSHK 2.8E5
             ! CM/SEC
INIT N2 0.78118 ! MOLE FRACTION
INIT 02 0.20948 ! MOLE FRACTION
INIT AR 0.00934 ! MOLE FRACTION
TSTR 0.
TEND 310.E-6
DT
     10.E-6
                  !CM**2
    3.81
DIA
VISC 177.7E-6
RTOL 1.E-4
ATOL
     1.E-8
CONC
ISKB
END
```

6.4 Output from the SHOCK Program

The first page of the output simply echoes the keyword input. The second page prints the integration control parameters and the initial gas composition. The third page gives the before-shock and after-shock conditions. The after-shock conditions are the initial conditions from which the shock tube equations are integrated. The final pages give the state of the gas as a function of time for the requested output times. The times in the left columns are the gas-particle times, however the laboratory times are also reported at the end of the first row.

SHOCK: CHEMKIN-III Shock Tube Code, DOUBLE PRECISION Vers. 2.11 2000/07/30 Copyright 1995, Sandia Corporation. The U.S. Government retains a limited license in this software.

CKLIB: CHEMKIN-III GAS-PHASE CHEMICAL KINETICS LIBRARY, DOUBLE PRECISION Vers. 5.28 2000/08/05 Copyright 1995, Sandia Corporation. The U.S. Government retains a limited license in this software.

KEYWORD INPUT:

TITL SHOCK TUBE CODE TEST P1A 6.58E-3 ! ATM 296. ! K т1 VSHK 2.8E5 ! CM/SEC INIT N2 0.78118 ! MOLE FRACTION INIT 02 0.20948 ! MOLE FRACTION INIT AR 0.00934 ! MOLE FRACTION TSTR 0. TEND 310.E-6 DT 10.E-6 DIA 3.81 !CM**2 VISC 177.7E-6 RTOL 1.E-4 ATOL 1.E-8 CONC ISKB END

INCIDENT SHOCK WITH BOUNDARY LAYER PROBLEM CORRECTION

INTEGRATION PARAMETERS:

RTOL	1.0000E-04
ATOL	1.0000E-08
T1	0.0000E+00
т2	3.1000E-04
DT	1.0000E-05

MOLE FRACTIONS

02	2.0948E-01
N2	7.8118E-01
NO	0.0000E+00

N	0.0000E+00
0	0.0000E+00
AR	9.3400E-03

	CONDITONS BEFORE THE SHOCK	CONDITONS AFTER THE SHOCK
PRESSURE (atm)	6.5800E-03	5.2445E-01
TEMPERATURE (K)	2.9600E+02	3.4650E+03
DENSITY (g/cc)	7.8453E-06	5.3417E-05
VELOCITY (cm/s)	2.8000E+05	4.1124E+04
MACH NO.	8.1140E+00	3.6419E-01

GAS VISCOSITY BEFORE SHOCK (q/cm/s) 1.7610E-04 BOUNDARY LAYER PARAMETER BETA 1.3728E+00 LIMITING SEPARATION BETWEEN SHOCK AND CONTACT SURFACE (cm) 8.8315E+01 PRES(atm) RHO(g/cc) MEAN WT AREA(cm**2)VEL(cm/s) LAB TIME(sec) 1 T(sec) TEMP(K) 02 N2 NO Ν 0 AR 0.000E+00 3.465E+03 5.245E-01 5.342E-05 2.896E+01 1.140E+01 4.112E+04 0.000E+00 3.864E-07 1.441E-06 0.000E+00 0.000E+00 0.000E+00 1.723E-08 1.000E-05 3.464E+03 5.297E-01 5.394E-05 2.895E+01 1.222E+01 3.863E+04 1.395E-06 3.886E-07 1.454E-06 1.177E-09 5.552E-13 1.889E-09 1.740E-08 2.000E-05 3.460E+03 5.324E-01 5.425E-05 2.893E+01 1.258E+01 3.731E+04 2.727E-06 3.893E-07 1.462E-06 2.426E-09 1.135E-12 3.789E-09 1.750E-08 3.000E-05 3.454E+03 5.344E-01 5.452E-05 2.892E+01 1.287E+01 3.631E+04 4.019E-06 3.896E-07 1.469E-06 3.726E-09 1.719E-12 5.672E-09 1.758E-08 4.000E-05 3.448E+03 5.360E-01 5.475E-05 2.890E+01 1.311E+01 3.547E+04 5.280E-06 3.897E-07 1.474E-06 5.070E-09 2.303E-12 7.528E-09 1.766E-08 5.000E-05 3.442E+03 5.374E-01 5.496E-05 2.889E+01 1.333E+01 3.475E+04 6.513E-06 3.897E-07 1.479E-06 6.451E-09 2.885E-12 9.353E-09 1.773E-08 6.000E-05 3.436E+03 5.386E-01 5.516E-05 2.888E+01 1.354E+01 3.409E+04 7.722E-06 3.895E-07 1.484E-06 7.864E-09 3.465E-12 1.114E-08 1.779E-08 7.000E-05 3.429E+03 5.397E-01 5.535E-05 2.886E+01 1.373E+01 3.349E+04 8.909E-06 3.893E-07 1.489E-06 9.304E-09 4.042E-12 1.290E-08 1.785E-08 8.000E-05 3.423E+03 5.407E-01 5.553E-05 2.885E+01 1.391E+01 3.296E+04 1.008E-05 3.890E-07 1.493E-06 1.077E-08 4.614E-12 1.462E-08 1.791E-08 9.000E-05 3.417E+03 5.415E-01 5.570E-05 2.884E+01 1.408E+01 3.249E+04 1.123E-05 3.886E-07 1.496E-06 1.225E-08 5.180E-12 1.630E-08 1.796E-08 1.000E-04 3.410E+03 5.423E-01 5.586E-05 2.883E+01 1.424E+01 3.203E+04 1.236E-05 3.882E-07 1.500E-06 1.374E-08 5.745E-12 1.794E-08 1.802E-08 1.100E-04 3.404E+03 5.431E-01 5.602E-05 2.881E+01 1.440E+01 3.158E+04 1.347E-05 3.878E-07 1.504E-06 1.525E-08 6.303E-12 1.955E-08 1.807E-08 1.200E-04 3.398E+03 5.438E-01 5.618E-05 2.880E+01 1.456E+01 3.117E+04 1.458E-05 3.874E-07 1.507E-06 1.677E-08 6.856E-12 2.112E-08 1.812E-08 1.300E-04 3.392E+03 5.445E-01 5.632E-05 2.879E+01 1.471E+01 3.077E+04 1.566E-05 3.869E-07 1.510E-06 1.830E-08 7.404E-12 2.266E-08 1.817E-08 1.400E-04 3.386E+03 5.451E-01 5.647E-05 2.878E+01 1.485E+01 3.040E+04 1.674E-05 3.865E-07 1.513E-06 1.983E-08 7.947E-12 2.416E-08 1.821E-08

	1.500E-04	3.380E+03 3.860E-07	5.457E-01 1.516E-06	5.661E-05 2.136E-08	2.877E+01 8.483E-12	1.499E+01 2.563E-08	3.005E+04 1.826E-08	1.780E-05		
	1.600E-04	3.374E+03 3.855E-07	5.463E-01 1.519E-06	5.674E-05 2.290E-08	2.876E+01 9.014E-12	1.513E+01 2.707E-08	2.970E+04 1.830E-08	1.884E-05		
	1.700E-04	3.369E+03 3.850E-07	5.468E-01 1.522E-06	5.688E-05 2.443E-08	2.875E+01 9.540E-12	1.527E+01 2.847E-08	2.937E+04 1.834E-08	1.988E-05		
1	T(sec)	TEMP(K) O2	PRES(atm) N2	RHO(g/cc) NO	MEAN WT N	AREA(cm**2 0)VEL(cm/s) AR	LAB TIME(sec)		
	1.800E-04	3.363E+03 3.845E-07	5.474E-01 1.525E-06	5.701E-05 2.596E-08	2.874E+01 1.006E-11	1.540E+01 2.984E-08	2.905E+04 1.839E-08	2.090E-05		
	1.900E-04	3.358E+03 3.840E-07	5.479E-01 1.527E-06	5.714E-05 2.748E-08	2.873E+01 1.057E-11	1.553E+01 3.118E-08	2.874E+04 1.843E-08	2.192E-05		
	2.000E-04	3.352E+03 3.834E-07	5.483E-01 1.530E-06	5.726E-05 2.900E-08	2.872E+01 1.108E-11	1.566E+01 3.250E-08	2.844E+04 1.847E-08	2.292E-05		
	2.100E-04	3.347E+03 3.829E-07	5.488E-01 1.533E-06	5.738E-05 3.051E-08	2.871E+01 1.158E-11	1.578E+01 3.378E-08	2.816E+04 1.851E-08	2.391E-05		
	2.200E-04	3.342E+03 3.824E-07	5.492E-01 1.535E-06	5.750E-05 3.201E-08	2.871E+01 1.207E-11	1.591E+01 3.504E-08	2.788E+04 1.854E-08	2.490E-05		
	2.300E-04	3.337E+03 3.819E-07	5.497E-01 1.537E-06	5.761E-05 3.350E-08	2.870E+01 1.255E-11	1.603E+01 3.627E-08	2.762E+04 1.858E-08	2.587E-05		
	2.400E-04	3.331E+03 3.813E-07	5.500E-01 1.540E-06	5.773E-05 3.498E-08	2.869E+01 1.303E-11	1.615E+01 3.747E-08	2.736E+04 1.862E-08	2.683E-05		
	2.500E-04	3.327E+03 3.808E-07	5.504E-01 1.542E-06	5.784E-05 3.644E-08	2.868E+01 1.350E-11	1.627E+01 3.865E-08	2.711E+04 1.865E-08	2.779E-05		
	2.600E-04	3.322E+03 3.803E-07	5.508E-01 1.544E-06	5.794E-05 3.789E-08	2.867E+01 1.397E-11	1.639E+01 3.980E-08	2.686E+04 1.869E-08	2.873E-05		
	2.700E-04	3.317E+03 3.798E-07	5.512E-01 1.546E-06	5.805E-05 3.933E-08	2.867E+01 1.443E-11	1.651E+01 4.093E-08	2.662E+04 1.872E-08	2.967E-05		
	2.800E-04	3.312E+03 3.793E-07	5.516E-01 1.548E-06	5.816E-05 4.075E-08	2.866E+01 1.488E-11	1.662E+01 4.204E-08	2.638E+04 1.876E-08	3.060E-05		
	2.900E-04	3.308E+03 3.788E-07	5.519E-01 1.550E-06	5.826E-05 4.216E-08	2.865E+01 1.532E-11	1.674E+01 4.312E-08	2.615E+04 1.879E-08	3.152E-05		
	3.000E-04	3.303E+03 3.783E-07	5.522E-01 1.552E-06	5.836E-05 4.355E-08	2.865E+01 1.576E-11	1.685E+01 4.418E-08	2.594E+04 1.882E-08	3.243E-05		
	3.100E-04	3.299E+03 3.777E-07	5.525E-01 1.554E-06	5.845E-05 4.492E-08	2.864E+01 1.618E-11	1.697E+01 4.522E-08	2.574E+04 1.885E-08	3.334E-05		
	Total CPUtime (sec): 0.04687									

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