PROJECT SQUID

TECHNICAL REPORT PSU-7-P

CONTACT SURFACE TAILORING IN A CHEMICAL SHOCK TUBE

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THE PENNSYLVANIA STATE UNIVERSITY
University Park, Pennsylvania

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JAMES FORRESTAL RESEARCH CENTER
PRINCETON UNIVERSITY
PRINCETON, NEW JERSEY

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IN A CHEMICAL SHOCK TUBE

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For the study of gaseous kinetics using a single-pulse (or "chemical") shock tube, it has been found very desirable to "tailor" the driver-driven gas interface (or "contact surface") to prevent multiple shock reflections or rarefactions (1). If one is not interested in producing extreme temperatures in the reflected shock, it is possible to achieve tailoring over a range of reflected shock conditions by varying the composition of the driver gas at room temperature.

Many gaseous reactions can be studied conveniently at temperatures below 2000°K; i.e., the reaction time available -- typically, a few milliseconds in a laboratory-size single-pulse shock tube -- will be sufficient to produce a measurable change in the reacting mixture, which is quenched by a rarefaction and then analyzed. A typical system might employ a driver gas composed of He and Ar and a driven gas consisting of Ar plus a few percent of the gas or mixture to be reacted. The large excess of Ar is used to minimize aerodynamic problems of the sort described by Strehlow and Cohen (2). Thus, for computing the tailoring conditions, the driven gas may be treated as pure Ar. No further refinement is justified because ideal bursting of the diaphragm is assumed in the calculations.

Since we have computed a set of tailoring conditions for changing driver gas composition, and since we have not been able to find any previous publication of the results of such computations, our results are presented in the hope that they will be useful to others making use of single-pulse shock tubes for studying gaseous reactions under moderate temperature conditions.

The requirement for tailoring the interface is that the specific internal energy ratio in gases 2 and 3 (see Figure 1) be unity (3); i.e.,

$$E_{32} = e_3/e_2 = [\tilde{C}_{v_3} T_3/\tilde{M}_3] \; / \; [\tilde{C}_{v_2} T_2/\tilde{M}_2] = 1 \qquad (1)$$

When $\tilde{C}_{v_3} = \tilde{C}_{v_2}$, the requirement leads to the condition, $\rho_2 = \rho_3$, which is sometimes cited as an approximate rule for tailoring. However, for present purposes, equation (1) is preferable. This can be rewritten as

$$\tilde{M}_1/\tilde{M}_4 = T_{21} \; T_{43} \; \tilde{C}_{v_1}/\tilde{C}_{v_4} \quad , \qquad (2)$$

since $\tilde{M}_1 = \tilde{M}_2$, $\tilde{M}_3 = \tilde{M}_4$, $\tilde{C}_{v_1} = \tilde{C}_{v_2}$, $\tilde{C}_{v_3} = \tilde{C}_{v_4}$, $T_{23} = (T_{21} \; T_{14} \; T_{43})$, and $T_{14} = 1$ (both driver and driven gases start at room temperature). Heat capacities are assumed to be independent of temperature.

Glass (3) shows that

$$T_{43} = [P_{41} \; P_{12}]^{2\beta_4} \qquad (3)$$

and

$$T_{21} = P_{21} \; (\alpha_1 + P_{21}) \; / \; (\alpha_1 \; P_{21} + 1) \quad . \qquad (4)$$

P_{41} is related to P_{21} by the ideal bursting equation,

$$P_{41} = P_{21} \; / \; [1 - (P_{21} - 1)(\beta_4 \; E_{14} / \; [\alpha_1 \; P_{21} + 1] \;)^{\frac{1}{2}}]^{\,1/\beta_4} \quad . \qquad (5)$$

E_{14} may be replaced by $(\tilde{C}_{v_1} \tilde{M}_4 / \; \tilde{C}_{v_4} \tilde{M}_1)$ since $T_1 = T_4$. The combination of equations (2), (3), (4), and (5) yields $(\tilde{M}_1/\tilde{M}_4)$ as a function of P_{21} and $(\tilde{C}_{v_1}/\tilde{C}_{v_4})$. When the driver gas is a mixture of He and Ar, $\tilde{C}_{v_1} = \tilde{C}_{v_4}$. Computations are made by expressing $(\tilde{M}_1/\tilde{M}_4)$ as a function of X_{He}, and solving for X_{He} for various assumed P_{21}'s.

The other driver gas combination that we have computed is H_2-N_2, chosen because the $\tilde{C}_v$'s of these two gases are approximately equal, yielding a β_4 that is independent of X_{H_2}. Without this condition the computation would be very tedious. Again, constant $\tilde{C}_v$'s are assumed. This is not very accurate for H_2-N_2 drivers, but since tailoring computations serve merely as a guide to experiment, the simplification is warranted. Achievement of tailoring can only be established by observation of a pressure record, or the equivalent, in the actual experimental run.

Once the driver gas compositions are computed, the other shock conditions follow. Of particular interest are

$$\rho_{21} = P_{21} / T_{21} \quad , \tag{6}$$

$$P_{52} = (\alpha_1 + 2 - P_{12})/(\alpha_1 P_{12} + 1) \quad , \tag{7}$$

$$T_{52} = P_{52}\,(\alpha_1 + P_{52})/(\alpha_1 P_{52} + 1) \quad , \tag{8}$$

$$T_{51} = T_{52}\,T_{21} \quad , \tag{9}$$

$$\rho_{52} = P_{52}/T_{52} \quad , \tag{10}$$

$$\rho_{51} = \rho_{52}\,\rho_{21} \quad , \tag{11}$$

and the incident shock velocity,

$$U_s = a_1\,[\beta_1(\alpha_1 P_{21} + 1)]^{\frac{1}{2}} \quad . \tag{12}$$

In Figure 2, those variables which seem most important in chemical kinetic studies are plotted over a reflected shock temperature range of 700° to 2000°K.

SYMBOLS USED

X = mole fraction

$\tilde{M}$ = molecular weight

$\tilde{C}_v$ = constant-volume heat capacity per mole

e = internal energy per unit mass

$\alpha = (\gamma + 1)/(\gamma - 1)$

$\beta = (\gamma - 1)/2\gamma$

ρ = density

T = absolute temperature

P = pressure

a = velocity of sound

$\gamma = \tilde{C}_p/\tilde{C}_v$

$T_{ij} = T_i/T_j$

$P_{ij} = P_i/P_j$

$\rho_{ij} = \rho_i/\rho_j$

$E_{ij} = e_i/e_j$

Table I.

Tailoring conditions using He-Ar or H_2-N_2 mixtures as driver gas.
Initial conditions: $T_1 = T_4 = 298.2°K$.

P_{21}	X_{He} (He-Ar)	P_{41} (He-Ar)	X_{H_2} (H_2-N_2)	P_{41} (H_2-N_2)	ρ_{51}	T_5 (°K)	$U_s \times 10^{-4}$ (cm/sec)
3.00	.629	7.30	*	*	3.096	702	5.19
3.50	.683	9.38	.032	11.63	3.500	795	5.58
4.00	.725	11.63	.131	14.44	3.863	888	5.94
4.50	.759	13.89	.212	17.24	4.193	979	6.28
5.00	.788	16.34	.279	20.75	4.486	1071	6.60
5.50	.815	18.58	.337	23.81	4.755	1161	6.90
6.00	.832	21.20	.385	27.40	5.000	1252	7.20
7.00	.866	26.45	.4675	35.00	5.435	1431	7.75
8.00	.892	31.87	.531	41.45	5.792	1614	8.27
9.00	.914	37.35	.582	50.30	6.100	1792	8.76
10.00	.930	43.10	.623	59.17	6.368	1973	9.22
17.35	1.000	86.32	.798	123.0	7.586	3292	12.08

P_{21}	ρ_{21}	T_{21}	ρ_{52}	P_{52}	T_{52}	T_{51}	P_{51}
3.00	1.857	1.615	1.667	2.430	1.457	2.353	7.29
3.50	2.000	1.750	1.750	2.667	1.524	2.667	9.33
4.00	2.125	1.882	1.818	2.875	1.582	2.977	11.50
4.50	2.235	2.013	1.876	3.059	1.631	3.283	13.77
5.00	2.333	2.143	1.923	3.222	1.675	3.590	16.11
5.50	2.421	2.272	1.964	3.367	1.714	3.894	18.52
6.00	2.500	2.400	2.000	3.499	1.749	4.198	20.99
7.00	2.635	2.657	2.061	3.733	1.810	4.805	26.13
8.00	2.750	2.909	2.106	3.917	1.860	5.411	31.34
9.00	2.850	3.160	2.140	4.070	1.902	6.011	36.63
10.00	2.929	3.415	2.174	4.214	1.938	6.618	42.14
17.35	3.297	5.261	2.301	4.831	2.099	11.04	83.82

* Will not tailor.

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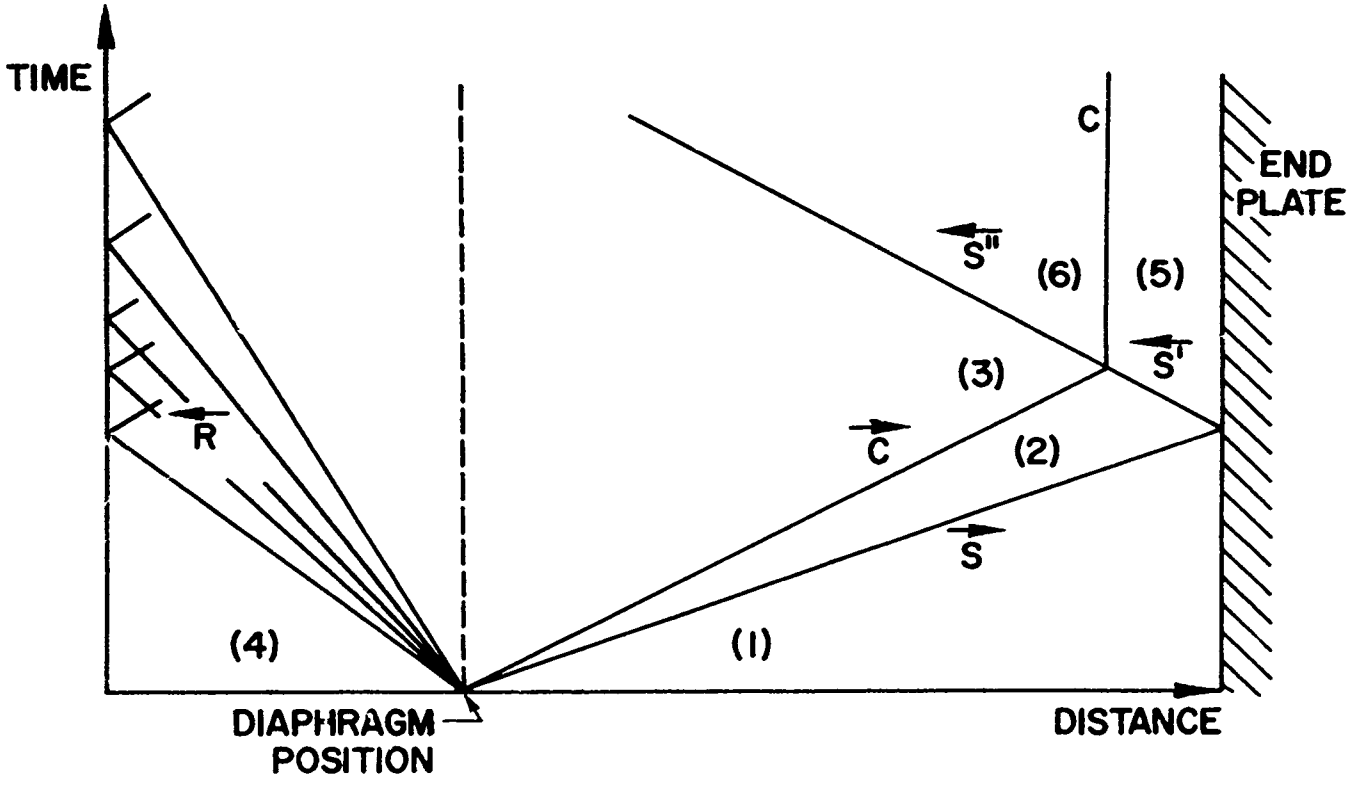
2. R. A. Strehlow and A. Cohen, J Chem. Phys., 30, 257 (1959)

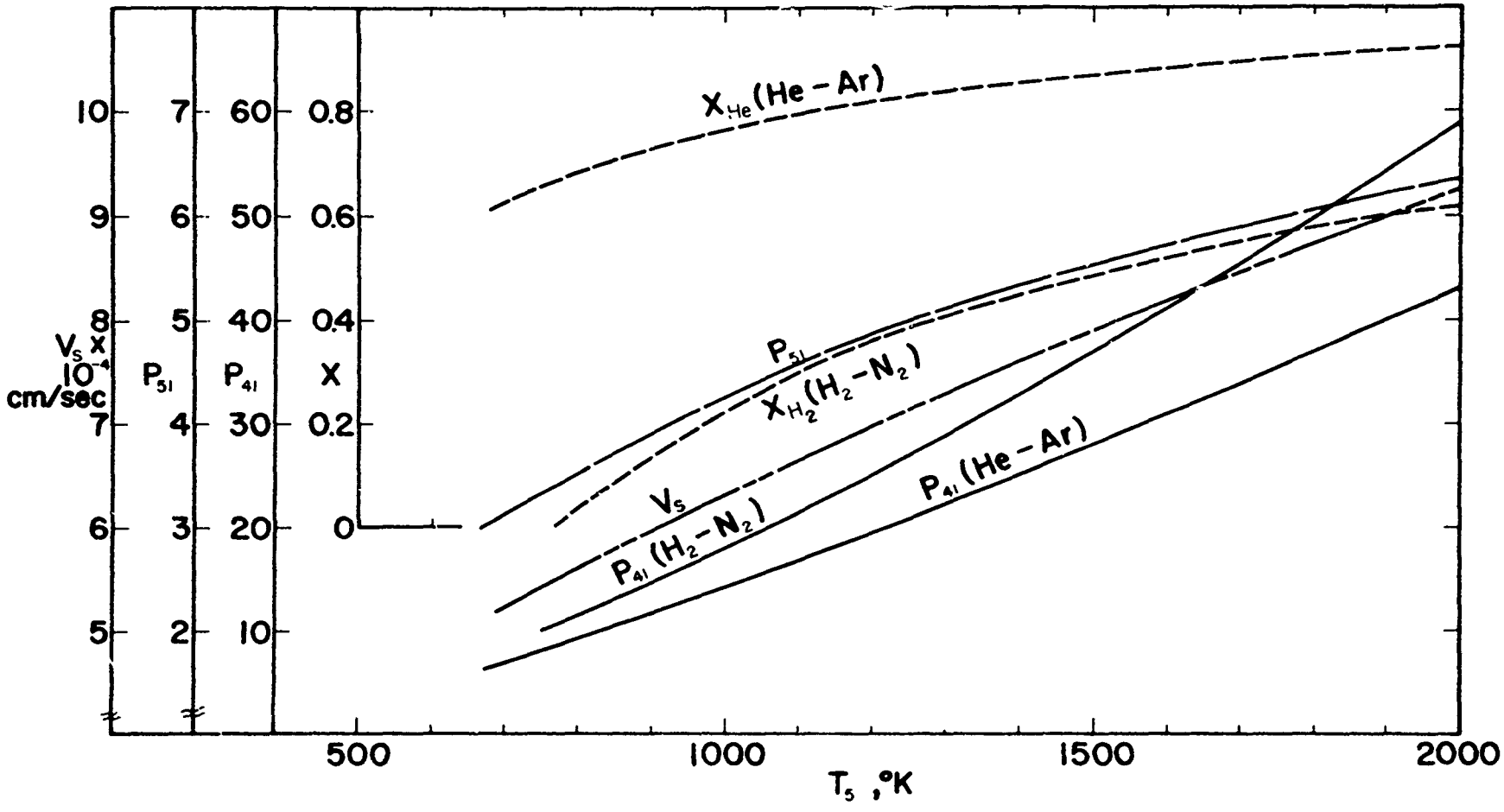
3. I. I. Glass, UTIA Review No. 12, Part I, Institute of Aerophysics, University of Toronto, May, 1958

FIGURE TITLES

Figure 1. Typical x-t diagram for a single pulse shock tube under "tailored" interface conditions. $\overleftarrow{R}$ = rarefaction fan; $\overrightarrow{S}$ = primary shock; $\overleftarrow{S}'$ = reflected shock; $\overleftarrow{S}''$ = reflected shock after transmission through contact surface; $\overrightarrow{C}$ = contact surface; C = stationary contact surface. The various gas regions are numbered.

Figure 2. Computed tailoring conditions for reflected shocks in argon, using as a driver gas He-Ar or H_2-N_2 mixtures, for the temperature range 700° to 2000°K.


TIME
C
END
PLATE
S''
(6)
(5)
S'
(3)
R
C
(2)
S
(4)
(1)
DIAPHRAGM
POSITION
DISTANCE


X_{He} (He – Ar)
P_{51}
X_{H_2} (H_2 – N_2)
V_s
P_{41} (H_2 – N_2)
P_{41} (He – Ar)
V_s x 10^{-4} cm/sec
P_{51}
P_{41}
X
10
9
8
7
6
5
7
6
5
4
3
2
60
50
40
30
20
10
0.8
0.6
0.4
0.2
0
500
1000
1500
2000
T_5 , °K