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Abstract

An explosion in a space causes an increase in temperature and pressure. To quantify the challenge that will be presented to essential components in a ventilation system, it is necessary to analyze the dynamics of a shock wave generated by an explosion, with attention directed to the propagation of such a wave in a duct.

Using the equations of unsteady flow and shock tube theory, a theoretical model has been formulated to provide flow properties behind moving shock waves that have interacted with various changes in duct geometry. Empirical equations have been derived to calculate air pressure, temperature, Mach number, and velocity in a duct following an explosion.

I. Introduction

A comprehensive safety analysis should evaluate the effects of a localized detonation on essential air-cleaning components in an exhaust system. The analysis should predict the capability of critical air-cleaning apparatus to remain functional following a detonation, even if the location of the actual incident is distant from those components and connected to them by a complex path. In order to describe an explosion, it will be necessary to differentiate between normal burning and detonation.

Description of Explosions

Normal burning is a result of heating an optimal volume of a combustible gas mixture to the ignition temperature by an external source, after which the flame propagates through the entire volume.[1] The maximum flame front speed for normal burning of a hydrogen-air mixture is 320 cm/sec, and the maximum post- to precombustion pressure ratio is 8.[2,3] However, detonation differs from normal burning in that the velocity of flame propagation and pressure ratio are significantly higher (e.g., for a 40% hydrogen-air mixture the detonation wave velocity is 2100 m/sec, and the pressure ratio is approximately 20).[4,5] Although the phenomenon is not completely understood at present, the steady detonation wave has been modeled as a shock front, followed, after a short time interval, by a combustion zone, and then a region of hot gases in equilibrium. This model has been

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used successfully to predict the detonation wave velocities for various gas mixtures.[7] Detonation velocity depends on the reaction-kinetic properties of the mixture. Because of the tremendous pressures that such equipment would experience upon wave impact, detonation can be more damaging to air-cleaning components than normal burning.

Initiation and Propagation of Detonation

If an explosive mixture is present in a duct system, there exists the possibility of spontaneous transition from normal burning to detonation at some "*induction distance*."[8,9] This phenomenon occurs because, as a flame propagates down a duct, the burning rate increases continuously due to the turbulence of the mixture in front of the flame and the increase in flame surface area. The rapid burning creates a shock wave in the unburned mixture, which ignites the gas downstream from the flame front.

Of particular interest also is the likelihood of detonation waves propagating from a smaller duct to a larger one. From generalizations of earlier experiments,[10,11] it was erroneously concluded that it is impossible for a detonation wave to propagate to the larger duct.[7] However, if a detonation wave is transmitted to a large volume or duct from a smaller duct or tube whose cross section is sufficiently large, the detonation wave can propagate into the large duct. For example, Zel'dovich has shown experimentally that the *initiation of spherical detonation* in an explosive gas mixture is possible by means of a plane detonation wave from a tube, only if the tube diameter is equal to or greater than a certain critical diameter (e.g., for a hydrogen-air mixture, the critical diameter is 19 mm).[12] If the diameter of the tube is less than the critical diameter, a plane detonation wave collapses, and normal burning of the gas takes place. Zel'dovich thus concluded that, at a point where the tube diameter changes, a plane detonation wave can either be attenuated, transformed to slow burning, or transformed to a spherical wave that will propagate within the volume, with all the consequences that follow.

The conclusion concerning attenuation has led to a proposed detonation-control measure by placing orifices with diameters less than the critical diameter for detonation at intervals in a duct less than the "*induction distance*."[8] In this paper, less consideration is given to the probability of occurence of a detonation than to the effects produced by such a phenomenon.

Hydrogen-Air Mixtures

Because a hydrogen-air mixture has so many prevalent possible sources (e.g., radiolytic or thermal disassociation of water, metal fires in the presence of water, sodium-water reaction, etc.) its detonation properties are of major interest. The actual explosive mixture might be air-hydrogen-steam, and a theoretical phase diagram for such a mixture is presented in Figure 1. Theoretically, in an air-hydrogen-steam mixture, 11% steam is sufficient to suppress any detonation.[13] However, using a "third explosion limit theory", Mathews shows that the water molecule is only as effective as the hydrogen molecule in suppressing the active radicals in a hydrogen-air mixture.[14] Thus the effectiveness of water vapor in suppressing detonations is still open to question, and experimental verification is lacking. In the present analysis, the effect of steam is neglected, and since the water molecule is more effective than the nitrogen molecule in suppressing the active radicals in the hydrogen-air mixtures,[14] an air-hydrogen mixture should have a more destructive potential.

Experimental data for the detonation properties of hydrogen-air mixtures for various percentages of hydrogen are used in the analysis given here. The molecular weight of the mixture, the detonation velocity, the Mach number, and the Mach number based on 100% air are given in Table I.[12,4] The detonation wave Mach number is defined as the ratio of the wave velocity to the speed of sound in the gas ahead of the wave. The effect of a shock wave passing through a duct containing a nonexplosive gas is independent of the explosive mixture at the initiation of the explosion and

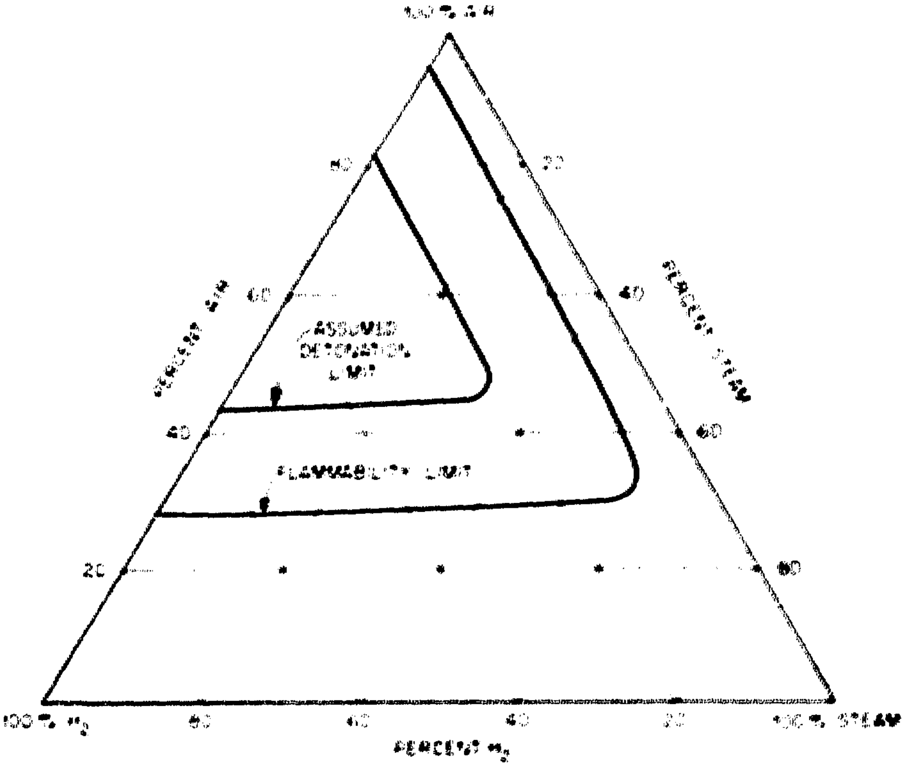

Figure 1: Detonation and flammability limits for air-hydrogen-steam mixtures (ref. 15).

Table 1. Detonation data for hydrogen-air mixtures
(1 atm; 300 K)

H_2 (percent by volume)	Mixture molecular wt.	Detonation velocity m/sec	Wave Mach Number (based on mixture)	Wave Mach Number (based on 100% air)
18.5[a]	23.98	1300	4.11	3.74
18.8[b]	23.90	1483	4.70	4.27
19.0[a]	23.85	1480	4.70	4.26
19.9[a]	23.60	1650	5.26	4.75
35[a]	19.53	1950	6.84	5.62
42[a]	17.64	2100	7.75	6.05
55[b]	14.14	2200	9.07	6.34
58.9[b]	13.08	2190	9.39	6.31

[a] R. Wendlandt, *Z. Physik Chem.*, 110, 637 (1924).

[b] J. Brenton, *Ann. Office Nat'l. Combustibles Liquids*, 11, 487 (1936).

depends only on the incident shock wave Mach number and the gas-mixture properties and configuration within the duct.

II. The Duct-Detonation Wave Model

For the theoretical model, it is assumed that detonation occurs in a localized section of a duct where a hydrogen-air mixture is present. The blast wave is established and advances with a velocity corresponding to the hydrogen composition as given in Table I. It is assumed that in the duct there exists an imaginary plane which divides the detonable mixture from 100% air. As the detonation wave crosses this plane into the air, combustion ceases, and the shock wave is then governed by those equations applicable to moving shock systems. Therefore, the Mach number of the wave as it travels in the noncombustible region is based on the speed of sound in 100% air. The variation of Mach number with hydrogen composition is presented in Figure 2. As predicted by this assumption, the values of pressure, temperature, and density behind the wave would be those related to the von Neumann "spike" and are consistent with the assumed model of the detonation wave (i.e., a shock front, followed by a combustion zone, and then a region of hot gases in equilibrium).[2]

The interactions of the moving shock wave with sudden or gradual duct contractions or enlargements are calculated by utilizing a shock-tube digital-computer program in which the area ratio between duct stages is an independent variable. The program employs the unsteady flow and shock tube equations to determine by an iterative technique the flow conditions as the duct area changes.[10-12] A variety of flow conditions may be established after the passage of the shock wave. Once the area ratio and gas properties are fixed, the computer program will provide the flow condition that reflects what actually occurs. The program is limited to the unsteady one-dimensional flow of real and ideal gases. The energy- and momentum-dissipative effects of heat transfer and friction at the duct walls have not been considered in the calculation of shock wave properties. Since these effects tend to weaken the wave, neglecting them provides conservative results. Also, for the same reason, the possibility of reflected rarefaction waves overtaking and weakening the shock system has not been included in the model.

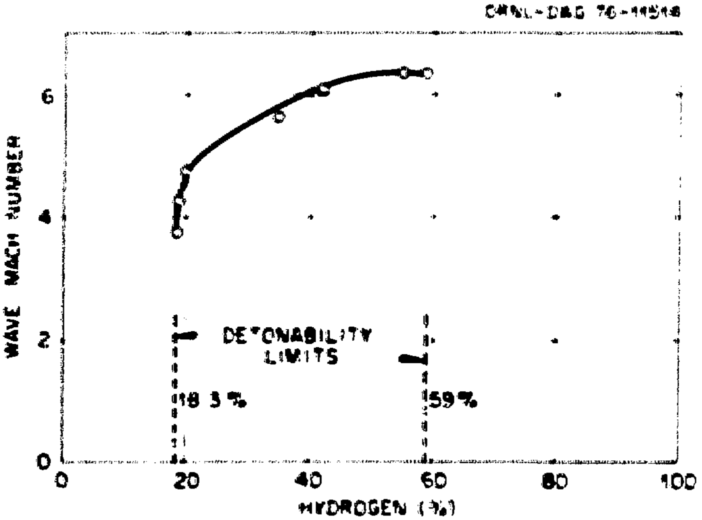

Figure 2: Detonation wave Mach numbers for hydrogen-air mixtures (refs. 4 and 12).

A time-displacement diagram for a typical sudden contraction is presented in Figure 3. As the incoming shock impinges upon the area change, another shock wave is reflected upstream while a stronger shock (i.e., higher Mach number) is transmitted downstream in the smaller duct. A contact surface and an unsteady expansion follow the transmitted wave. For a sudden enlargement, a typical time-displacement diagram is given in Figure 4. As the incident shock wave encounters the sudden

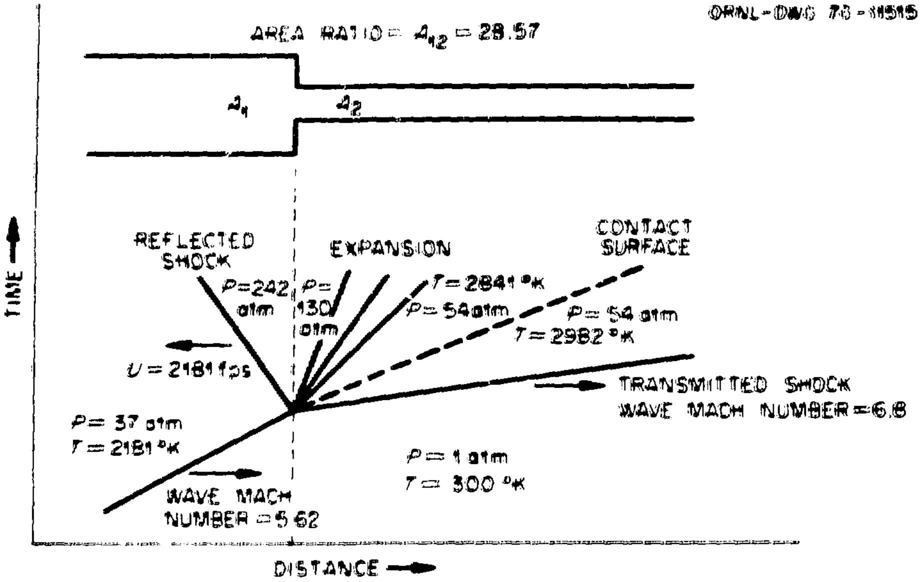

Figure 3: Shock wave interaction with sudden contraction.

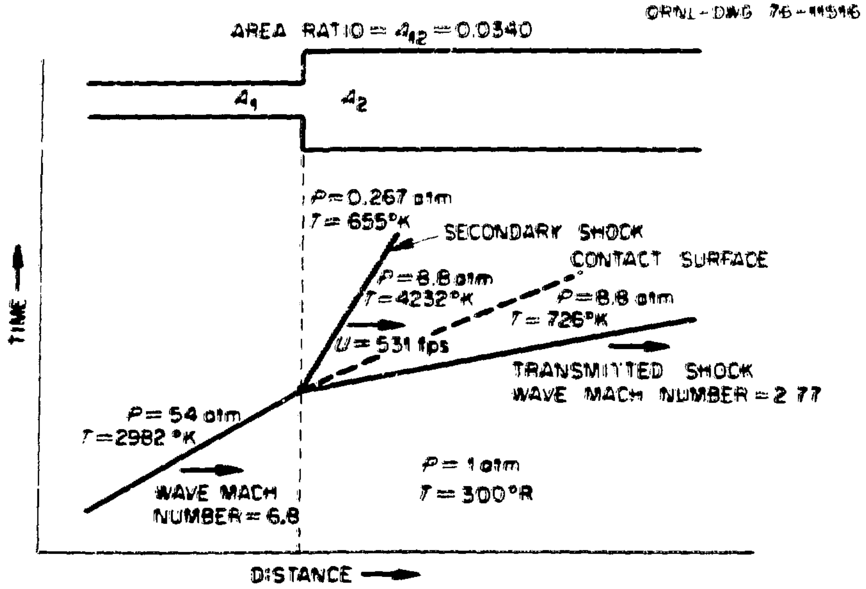

Figure 4: Shock wave interaction with sudden enlargement.

enlargement, a weaker shock wave is transmitted which is followed by a contact surface and a secondary shock that is swept downstream. With assumed ideal air and by utilizing the computer program, surfaces may be constructed in a three-dimensional plot of area ratio vs incident Mach number vs transmitted Mach number, static pressure, static temperature, or velocity. Empirical equations for these surfaces have been derived and are given below for a sudden area contraction or enlargement:

$$M_1 = M_s(1 + a_1 \ln A_{12}) \tag{1}$$

$$P_1 = a_2 + (M_s)^2[b_2 + c_2(\ln A_{12}) + d_2(\ln A_{12})^2] \tag{2}$$

$$T_1 = a_3 + b_3(M_s) + c_3(M_s)^2 + (\ln A_{12})[d_3 + e_3(M_s)] + (\ln A_{12})^2[f_3 + g_3(M_s)^2] \tag{3}$$

$$U_1 = a_4 + b_4(M_s) + c_4(M_s)^2 + (\ln A_{12})[d_4 + e_4(M_s)] + (\ln A_{12})^2[f_4 + g_4(M_s)^2] \tag{4}$$

where

dependent variables are:

M_1 = transmitted shock wave Mach number;
P_1 = transmitted static pressure behind wave, atm;
T_1 = transmitted static temperature behind wave, °K;
U_1 = transmitted velocity behind wave, fps;

and independent variables are

M_s = incident shock wave Mach number,
A_{12} = area ratio, upstream area/downstream area

The coefficients and range of applicability for the appropriate geometry are given in Table II. It must be emphasized that these equations are empirical, and no inference concerning property functional

Table II. Coefficients and limits for transmitted flow property equations [eqns. (1) to (4)]

Transmitted property	Eqn. no. and subscript	Coefficients						
		a	b	c	d	e	f	g
For sudden contraction limit of applicability: $A_{12} > 1.0$, $M_s > 2.1$								
Mach No., M_1	1	0.070						
Pressure, P_1	2	−0.728	1.19	0.362	−0.066			
Temperature, T_1	3	277	58.7	13.0	−14.7	18.2	2.66	−3.23
Velocity, U_1	4	108	950	−1360	227	91.1	−156	143
For sudden enlargement limit of applicability: $A_{12} > 0.13$, $M_s > 2.5$								
Mach No., M_1	1	0.182						
Pressure, P_1	2	−0.120	1.16	0.443	0.046			
Temperature, T_1	3	288	58.1	−64.1	1.76	22.1	−1.02	2.32
Velocity, U_1	4	19.1	947	−970	72.4	175	37.1	−142

relationships is intended. All the properties behind the shock wave may be determined from the above equations. The equations apply only to ideal air ahead of the shock wave (though the computer program can apply to other ideal and real gases) and are presented in order to facilitate design and safety analyses. The results from the equations agree within about 5% of the computer results.

If a sudden enlargement results in a secondary shock which attempts to propagate upstream (i.e., $A_r < 0.13$ and $M_s > 2.5$), the computer program will not calculate the flow-field properties. For such cases, three-dimensional flow-field effects are significant but are beyond the scope of the assumed model. However, if these sudden enlargements are modeled as gradually expanding channels with pre- to post-enlargement ratios equal to that of the actual sudden enlargements, the expansion properties may be estimated for the actual cases. In this model, a stationary shock wave is allowed to stand at some calculated area ratio in the diverging duct, and its presence will adjust the downstream properties to match the flow requirements for the primary shock wave. Specifically, the solution for such a case may be constructed on a pressure-velocity (P-U) diagram in the following way:

1. A stationary normal shock is assumed to stand at a given duct area ratio.
2. An isentropic, steady expansion is assumed up to the shock.[15]
3. The normal shock relations are used to calculate flow properties across the shock.[16]
4. An isentropic steady expansion is assumed downstream of the shock until the final area is traversed. The pressure and velocity at the final area are plotted on the P-U diagram.
5. By assuming different shock locations, a locus of points may be constructed.
6. The pressure and velocity behind the primary shock wave are given in terms of conditions ahead of the wave by the following relation:[16]

$$\frac{U_t}{C_1} = \frac{\dfrac{P_t}{P_1} - 1}{\gamma\sqrt{1 + \dfrac{\gamma + 1}{2\gamma}\left(\dfrac{P_t}{P_1} - 1\right)}} \tag{5}$$

   Also the upstream or transmitted pressure behind the shock wave, P_t, is given in terms of the shock wave Mach number as:[2]

$$\frac{P_t}{P_1} = \frac{2\gamma M_t^2 - (\gamma - 1)}{(\gamma + 1)} \tag{6}$$

where

γ = specific heat ratio, C_P/C_V;
M_t = transmitted shock wave Mach number;
U_t = transmitted velocity behind shock wave, fps;
C_1 = speed of sound in gas downstream, fps;
P_1 = pressure in gas downstream, atm;
P_t = transmitted static pressure behind shock wave, atm.

   By assuming various values of P_t when P_1 and C_1 are given, a shock polar may be constructed on the P-U diagram.

7. The intersection of the shock polar with the previously constructed curve will give the pressure and velocity behind the primary shock wave.

An example of this procedure applied to a specific duct enlargement is presented in Figure 5. Because the assumption of a gradual enlargement should yield a stronger transmitted shock than that formed in a sudden enlargement, this formulation is conservative (as desired in a safety analysis).

The limits of applicability for a sudden contraction are $A_{12} > 1.0$ and $M_s > 2.1$. Cases for $M_s < 2.1$ are being investigated. Since sudden contractions always produce a stronger transmitted wave, a conservative estimate is made for cases where $M_s < 2.1$ if the incident Mach number is assumed to be 2.1.

The flow properties should also be affected by other geometrical duct arrangements such as bends, tees, valves, or long runs of straight duct. However, in an experimental study of detonation in hydrogen-air mixtures in Savannah River process equipment, Porter found that pipe bends up to 90° had no apparent effect on the formation or propagation of detonation waves.[5] In addition, a combination of 1½- and 2-in. pipe in a "Y" configuration had no significant effect on the detonation process. Similar results were found by Hishida and Hori for the propagation of pressure waves in water in pipes of various geometries.[1] Thus, experimentally, there appears to be no measurable shock-wave suppression effects in bends or tees. Even though these geometries must have flow losses associated with them, the effects cannot be calculated with the present model; and since these losses appear to be experimentally insignificant, they will be neglected in the present analysis.

As an example, a duct system consisting of contractions and enlargements (Figure 6) will be analyzed for detonation effects. It is assumed that a detonation wave is established near the entrance of the duct and enters a nondetonable mixture (i.e., air) as shown. A sudden contraction at *a* and sudden enlargements at *b* and *c* are encountered. The time-displacement conditions are shown in Figure 6. At point *c* the gradual enlargement assumption is invoked. It is observed that such a duct

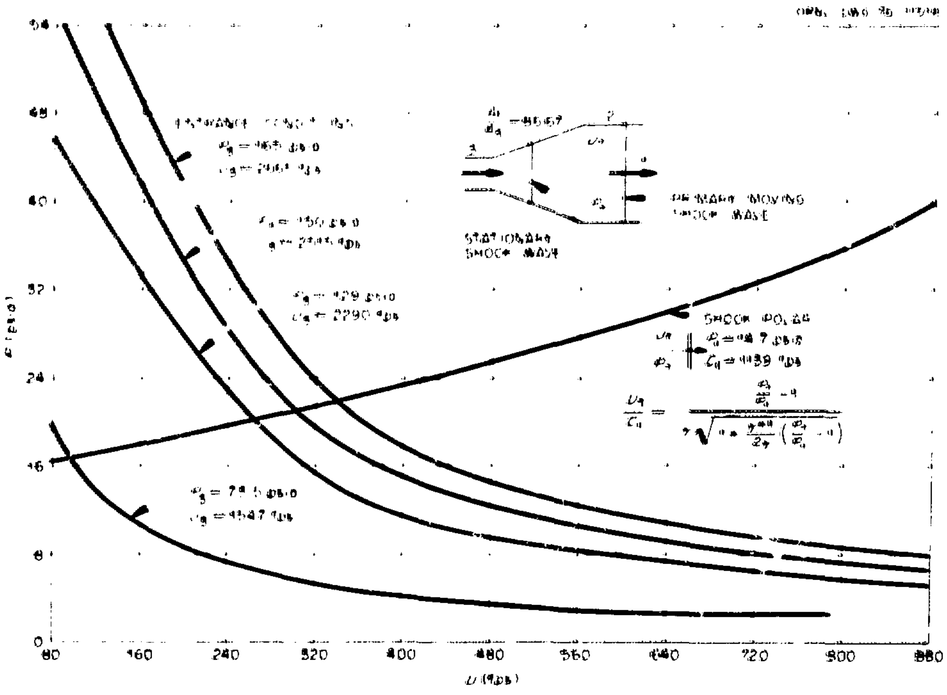

Figure 5: Estimation of conditions behind shock wave propagating through a gradual duct enlargement.

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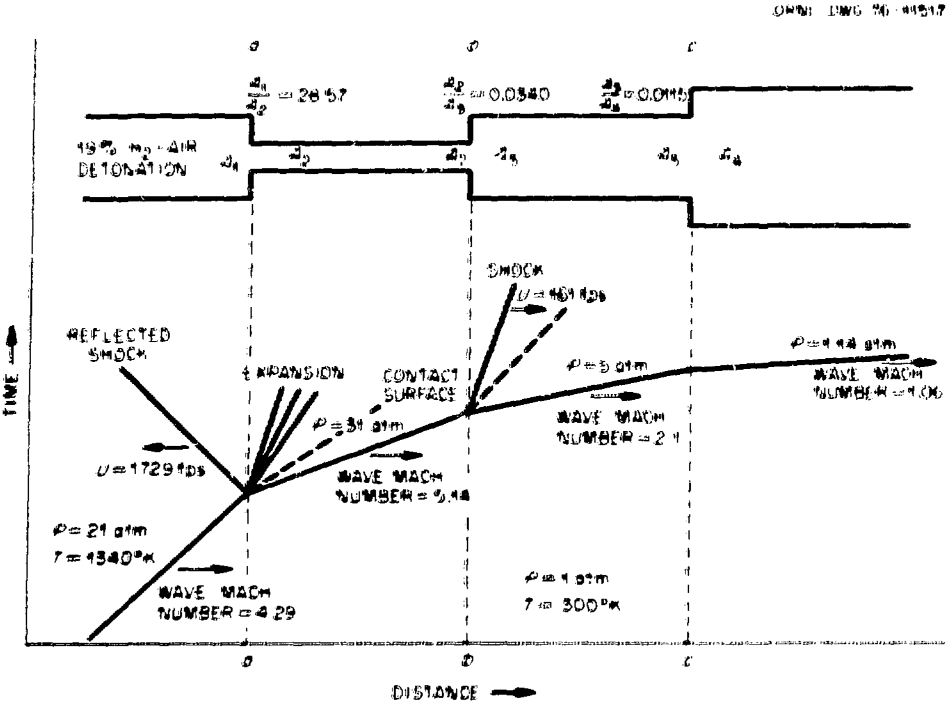

Figure 6: Duct system analysis.

arrangement for the given initial shock condition (i.e., a shock of $M_s = 4.29$ moving into air at 1 atm and 300° K) would produce a pressure drop from 21 to 1.14 atm. Any number of such duct contractions or enlargements may be joined together and analyzed for the final flow properties.

III. Conclusions

A theoretical model has been presented which should aid in a comprehensive safety analysis of explosion-induced shock waves in ducts of various geometries. Empirical equations for a range of sudden duct contractions and enlargements virtually eliminate the necessity of computer computations for the flow-field properties behind the primary shock wave. Also, a method has been presented which can conservatively estimate the flow properties for enlargements outside the range of the computer model applicability. Damage to air-cleaning components in duct systems due to wave impact can be estimated.

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