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Informal Report

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**Analysis of Ventilation Systems Subjected to
Explosive Transients
Initial Analysis and Proposed Approach**

University of California



LOS ALAMOS SCIENTIFIC LABORATORY

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Analysis of Ventilation Systems Subjected to Explosive Transients

Initial Analysis and Proposed Approach

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ABSTRACT

This report describes our initial study of explosive pressure transients and their propagation through ventilation systems. The objective of this study is to organize the required calculations into a computer code that is highly user-oriented and will predict explosive-induced gas dynamics within a ventilation system. The explosive process is subdivided into three regimes--deflagration, detonation, and transition from deflagration to detonation. Equations describing each process and suggested procedures for solving these equations are presented. The proposed organization of the explosion code capitalizes on the desirable aspects of the previously developed TVENT code, which predicts tornado-induced pressure transients within ventilation systems. The explosion code will include both near- and far-field analyses. The near-field analysis will use detailed models to describe the combustion process near the explosive event, and provide parametric driving potentials for flow in the regions that are removed from the explosive event (far-field). The far-field analysis will include the combustion wave as it propagates through the rest of the system.

I. INTRODUCTION

The possibility and resulting consequences of an explosion within a facility, especially its ventilation system, is of utmost importance to facility designers and to analysts responsible for safety evaluations. Their chief concern is the propagation of explosively driven pressure waves throughout a facility such that the physical integrity of the ventilation system and other interior components is compromised. This is always a concern with many industrial processes, but it becomes even more important when hazardous material is involved. Our emphasis in this program will be upon those Department of Energy facilities that handle hazardous material and especially those involved in the nuclear fuel cycle.

For existing or planned nuclear fuel cycle facilities, the common practice is to make estimates of the atmospheric dispersion of material from the ventilation system exhaust effluent for normal operating conditions. Further, analysts are required to estimate the atmospheric dispersion of potential exhaust material under accident conditions. An important aspect of these estimates is the modification in the atmospheric source term produced by the ventilation system. For an explosion accident, this term is impossible to estimate unless the gas dynamic variables can be predicted.

Strehlow and Baker state that much of the information pertaining to internal explosions is scattered throughout the literature.¹ Reference 2 substantiates this claim, and after the initial phases of our investigations, we also believe it to be true. In Ref. 1 an attempt was made to bring together a comprehensive review of this literature. However, we find that much of the information deals with explosions in the unconfined atmosphere, and very little pertains to explosions within structures. Strehlow and Baker explain that explosions within buildings usually result from the following scenarios.

1. A spill of some combustible material occurs, and a slow fire causes a build-up of pressure.
2. A piece of equipment explodes producing a blast wave inside the building.
3. A leak occurs, and the combustible material ignites.

Other scenarios can include runaway chemical reactions, nuclear excursions, and liquid vaporization processes.

In this initial study we have performed a preliminary analysis of explosive phenomena noting that most combustion processes are involved. This analysis permits us to categorize combustion processes as deflagrations, detonations, or deflagrations that transform into detonations. Using this approach, we analyze each condition, and several analytical descriptions of the processes have evolved. Possible solution routines using these procedures are outlined.

Our proposed approach is based upon using the computer code TVENT that was developed to analyze tornado-induced pressure transients within ventilation systems.³ We review this code and evaluate it in relation to the requirements for modeling explosive phenomena.

Finally, we present our proposed organization of the explosion code that will feature many applicable aspects of the TVENT code. Our approach subdivides the problem into near- and far-field analyses. For processes near the explosion, we propose analyses that model the combustion process in detail. This provides parameters that can be used to drive the flow in the far-field analysis, that is, in regions of the system that are relatively independent of the characteristics of the explosive event.

This approach is highly preliminary, and many changes may evolve. Many aspects of the analyses cannot be determined until they are attempted and evaluated in more detail.

II. OBJECTIVES

The main objective of this study is to develop a method to predict air flow and pressures within facilities subjected to internal explosions. The computer code developed will have particular applicability to nuclear fuel cycle facilities, but it can also be applied to other facilities such as synthetic fuel plants. Emphasis will be placed on facility ventilation systems, but the code will also be applicable to other flow pathways within structures. A further objective of this study is to capitalize upon the capabilities of the computer code TVENT, which predicts air flows and pressures within facilities subjected to tornado depressurization. The most important task is to develop a computer code that has the capabilities noted above but is flexible enough to be highly user-oriented and portable.

III. EXPLOSIVE PHENOMENA

A. General

The types of explosive phenomena we will consider are those that can result from combustible processes in most industrial operations, especially those in nuclear fuel cycle facilities. Many industrial operations use a wide variety of combustible materials in liquid, solid, powder, or gaseous form. The explosive nature of these materials is highly variable, but they are generally considered low-order. That is, they generate lower pressures and pressurization rates when compared to high explosives. The pressure wave duration associated with these low-order explosions can vary from several microseconds to hundreds of milliseconds.⁴ Most low-order explosions originate from fine particulate matter (dust), liquid vaporization, solid and liquid fires, and volatile gases.

Dust explosibility is affected by so many chemical and physical factors that only empirical relationships have been developed. Dust explosions have been defined as a rapid combustion of particulate matter in a confined space where heat is generated at a much higher rate than it is dissipated.⁵ Reference 5 contains a comprehensive list of materials and their explosive characteristics, and a condensed version of this list is outlined by H. E. Hesketh.⁶ Minimum explosive concentration, maximum explosive pressure, and average rate of pressure rise are given in the above references.

A preliminary survey of the Atomic Energy Commission's serious accident reports for 1943-1975 has been performed to identify the cause of explosive accidents.⁷ A chemical reaction between mixtures of liquids and/or solids was identified as the cause of approximately 40% of these explosions. In many cases the initiating event was an explosion followed by a fire.

Further examination of the serious accident statistics revealed that approximately 50% of the explosions originated from volatile gases.⁷ Hydrogen gas was involved in most of these accidents. In other cases, high pressure nitrogen or air, methane, or oil vapors were involved.

After considering materials in powder, solid, liquid, and gaseous form, we concluded that in most cases our analyses should handle explosions that evolve from gases. However, considering gaseous explosions adds complexity to the analyses required. This is because the spatial extent of the gas mixture must

be considered, whereas explosions that originate from powders, solids, or liquids can usually be considered as point sources. Therefore, we believe that approaching the explosion process by considering gas mixtures will encompass the most difficult analysis required and also be representative of most explosions in nuclear-related facilities. The first step taken in understanding gas explosions can be obtained by considering the general gas combustion process.

B. Combustion

Combustion can be defined as a chemical reaction (usually oxidation) producing heat. Pressure waves can be generated from the combustion process. A combustion wave will propagate into the unburned reactants leaving combustion products behind the wave. Two types of combustion pressure waves have been observed: deflagrations that propagate at subsonic speeds and detonations that propagate at supersonic speeds. Peak pressures for gaseous deflagration waves have been reported to be 130 psi or less in a closed vessel, whereas detonation waves may reach several thousand psi.⁴ Generation of a deflagration wave or a detonation wave depends on several factors, but of primary importance are the composition of the gaseous reactants and the ability of the combustion wave to propagate in more than one direction.

Combustion wave velocities and the flow properties associated with the waves are typical parameters of interest. Also of interest are density, temperature, and pressure across the wave. For a detonation wave, the wave propagation speed is called detonation velocity, and for a deflagration wave, it is called the flame speed.

The combustion wave is an unsteady flow process with respect to a stationary reference system. However, if the reference system moves at the same speed as the combustion wave, we can consider the process with steady-state analyses. This procedure is similar to that used in analysis of normal shock waves.⁸ Treating the combustion wave as a steady process is valid only as long as its propagation velocity is constant. An accelerating combustion wave can only be treated as an unsteady-state phenomenon. This process will occur if a deflagration wave undergoes transition to a detonation wave. The accelerating motion is attributed to an expanding burning mixture that is ahead of the combustion wave. This motion tends to compress the waves ahead of the unburned mixture until they coalesce to produce a shock wave. If the shock wave is strong enough, it will compress the reacting mixture until a rapid chemical reaction

occurs and a detonation wave forms.⁹ Therefore, only an unsteady-state analysis in which both spatial and time effects are considered can be used to accurately describe this process.

This brief discussion of explosive phenomena indicates that consideration of the combustion process can offer a viable approach to a better understanding of the gas dynamic effects associated with explosions. Our investigation shows that we must consider three types of pressure wave conditions: detonation, deflagration, and transition from deflagration to detonation. In the following sections we will outline the analytical considerations for each wave condition.

1. Detonation Equations.⁸⁻¹⁰ We will consider that combustion can occur within two primary ventilation system components, as shown in Fig. 1, that is, within a duct or in a large volume, such as a room.

The detonation wave will move faster than the speed of sound into the undisturbed air ahead of it. Ahead of the detonation waves in the region undisturbed by the initial explosion, the air flow continues as if nothing happened. But the equations must be developed to describe the flow behind the wave.

For a detonation to occur, a detonable mixture must be present, as shown in Fig. 2. As the wave moves through this mixture, it is sustained by the energy released from the chemical reaction occurring in the wave front. Once the detonation wave overruns the region that contains the detonable mixture, it is no longer sustained by an energy release but begins to be attenuated by frictional effects and by trailing rarefaction waves that move faster than the shock front. When the rarefaction wave does overtake the detonation wave, the two travel forward together as a sound wave.

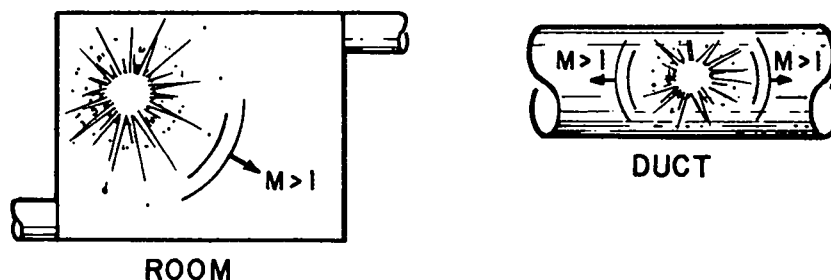


Fig. 1.
Detonation within a system component.
Note: M = Mach number

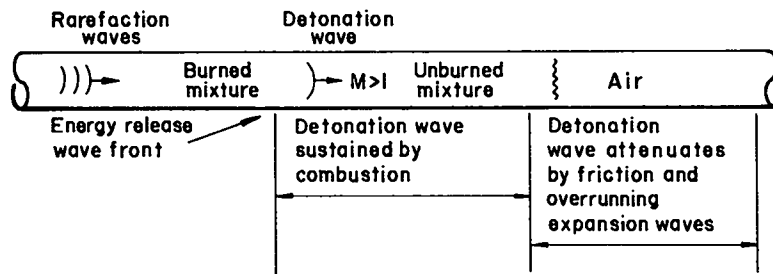


Fig. 2.
Regions through which a detonation wave moves.

Because detonation waves are shock waves sustained by the energy of a chemical reaction that is initiated by the shock compression, a theory of their propagation can be developed based upon hydrodynamics alone.⁸ This theory allows the computation of wave velocity and particle velocity behind the wave if the physical properties of the explosive medium are known.

Consider the steady, one-dimensional motion of a shock wave moving into an undisturbed fluid (Fig. 3). Ahead of the wave, the pressure of a unit mass is P_1 , the density ρ_1 , the specific volume v_1 , and the temperature T_1 . Behind the wave, the pressure is P_2 , the density ρ_2 , the specific volume v_2 , and the temperature T_2 . U_1 is the velocity of the shock wave, and w is the velocity of the fluid particles behind the shock wave.

If we consider a coordinate system moving with the shock front, then assuming a perfect gas, the continuity equation is

$$U_1 \rho_1 = U_2 \rho_2 \quad , \quad (1)$$

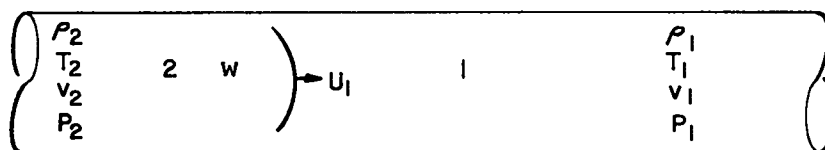


Fig. 3.
Motion of a shock wave.

or

$$\frac{U_1}{\rho_2} = \frac{U_2}{\rho_1} , \quad (2)$$

where $U_2 = U_1 - w$.

The momentum equation is

$$\frac{U_1^2}{v_1} + P_1 = \frac{U_2^2}{v_2} + P_2 , \quad (3)$$

and the energy equation is

$$E_1 + \frac{U_1^2}{2} + P_1 v_1 = E_2 + \frac{U_2^2}{2} + P_2 v_2 , \quad (4)$$

where E_1 and E_2 are the internal energies per unit mass.

From Eqs. (2) and (3) we obtain

$$U_1 = v_1 \sqrt{\frac{P_2 - P_1}{v_1 - v_2}} \quad (5)$$

as the propagation velocity of the shock wave. Also because $w = U_1 - U_2$, we can show that the particle velocity of the gas behind the shock wave is

$$w = (v_1 - v_2) \sqrt{\frac{P_2 - P_1}{v_1 - v_2}} . \quad (6)$$

Further, the change in internal energy is, combining Eqs. (2), (3), and (4)

$$E_2 - E_1 = \Delta E = 1/2(P_1 + P_2)(v_1 - v_2) \quad . \quad (7)$$

The change in internal energy across the shock wave will be due to the compression of the gas plus the energy release ΔE_c , where ΔE_c is the energy release from the chemical reaction taking place. Thus

$$\Delta E = \bar{C}_v(T_2 - T_1) - \Delta E_c \quad , \quad (8)$$

where \bar{C}_v is the mean specific heat at constant volume of the burned gas between T_1 and T_2 .

If we assume the burned gas to be a perfect gas, then the equation of state is

$$P_2 v_2 = RT_2 \quad . \quad (9)$$

Equations (5) through (9) contain six unknowns: U_1 , w , P_2 , v_2 , T_2 , and ΔE . Here we have assumed that the undisturbed properties v_1 , ρ_1 , T_1 , the energy release ΔE_c , and the near specific heat at constant volume \bar{C}_v are all known.

Because there are six unknowns but only five equations, an additional relationship is necessary. This necessary relationship is found by considering a P-v diagram.

By combining Eqs. (7), (8), and (9), the P-v diagram of Fig. 4 can be constructed. This diagram is called a Hugoniot curve and relates all pairs of values of P_2 , v_2 for a given pair of values P_1 , v_1 . The values v_1 and w corresponding to any pair of values P_2 , v_2 are obtained as follows. Consider the angle $P_1 AB = \alpha$.

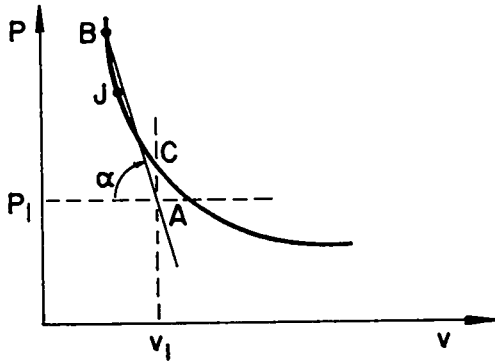


Fig. 4.
A P-v diagram for detonation.

From Fig. 4,

$$\tan \alpha = \frac{P_2 - P_1}{v_1 - v_2} \quad (10)$$

But Eq. (5) gives

$$U_1 = v_1 \sqrt{\frac{P_2 - P_1}{v_1 - v_2}} = v_1 \sqrt{\tan \alpha} \quad (11)$$

and Eq. (6) gives

$$w = (v_1 - v_2) \sqrt{\frac{P_2 - P_1}{v_1 - v_2}} = (v_1 - v_2) \sqrt{\tan \alpha} \quad (12)$$

At any point but the point J, two states appear possible behind the detonation wave. However, above the point J the detonation wave is mechanically unstable. The rarefaction wave tends to overtake the detonation wave. Further, points below J have lower entropy than points above J, and therefore these states are statistically less likely to occur than states above J. Therefore, we are led to the Chapman hypothesis that the wave will only find it possible to travel at a speed corresponding to state J. State J is also known as the Chapman-Jouguet state.

From Eq. (7) we can find the derivative of E with respect to v at state J.

$$\lim_{v \rightarrow 0} \frac{\Delta E}{\Delta v} = \lim_{\Delta v \rightarrow 0} \frac{1/2(P_1 + P_2)(v_1 - v_2)}{(v_2 - v_1)} \quad (13)$$

and

$$\lim_{\Delta v \rightarrow 0} \frac{\Delta E}{\Delta v} = - \lim_{\Delta v \rightarrow 0} \frac{1/2(P_1 + P_2)}{\Delta v} \quad (14)$$

But from Eq. (10)

$$P_1 = P_2 - (v_1 - v_2) \tan \alpha \quad . \quad (15)$$

So

$$\begin{aligned} \lim_{\Delta v \rightarrow 0} \frac{\Delta E}{\Delta v} &= - \lim_{v \rightarrow 0} \left\{ \frac{1}{2} P_2 + P_2 - (v_1 + v_2) \tan \alpha \right\} \\ &= - \lim_{\Delta v \rightarrow 0} \left\{ P_2 - \frac{1}{2}(v_1 - v_2) \tan \alpha \right\} \\ &= - P_2 \quad ; \end{aligned} \quad (16)$$

and in general,

$$\frac{dE}{dv} = -P \quad ,$$

or

$$dE = -Pdv \quad , \quad (17)$$

which is the energy equation for isentropic compression within gas 2. This provides us with our needed sixth relationship. In gas 2,

$$dE = C_v dT_2 = -P_2 dv_2 \quad . \quad (18)$$

From the equation of state for a perfect gas

$$P_2 v_2 = RT_2 \quad . \quad (19)$$

So differentiating Eq. (19) gives

$$P_2 dv_2 + v_2 dP_2 = R dT_2 \quad . \quad (20)$$

Hence,

$$C_V dT_2 = \frac{C_V P_2 dv_2 + v_2 dP_2}{R} \quad , \quad (21)$$

or

$$C_V dT_2 = \frac{1}{(k_2 - 1)} (P_2 dv_2 + v_2 dP_2) \quad , \quad (22)$$

and from Eq. (18)

$$C_V dT_2 = -P_2 dv_2 \quad , \quad (23)$$

where $k_2 = C_p/C_V$ the specific heat ratio for gas 2. Rearranging

Eq. (23) gives

$$\frac{dP_2}{dv_2} = \frac{-k_2 P_2}{v_2} \quad . \quad (24)$$

Eqs. (5) through (9) and (24) are now deterministic, and from them we can solve for v_1 , w , P_2 , v_2 , T_2 , and ΔE .

The analysis given above assumes that complete combustion takes place with the attainment of peak pressure.

2. Deflagration Equations.¹¹⁻¹³ As stated earlier, deflagrations propagate at a much smaller velocity than a detonation wave. For this reason the deflagration wave is, in many ways, much more complex than a detonation wave. This could be due to the greater velocity of the detonation wave such that it is relatively independent of external disturbances.¹⁰ Owczarek states that only limited success has been achieved in describing the deflagration process.⁹

Several theories have been developed for predicting speeds of deflagration waves: (1) thermal, (2) diffusion, and (3) a combination of thermal and diffusion. The analyses, based on thermal theory, put forth by Zeldovich-Frank-Kamenetski will be described here.¹⁰

Kanury notes that flame propagation is strongly dependent upon whether the flow is laminar or turbulent.¹¹ First, we will consider laminar flame propagation and then extend this to turbulent flame propagation.

a. Laminar Combustion. If one considers the quasi-steady combustion of a premixed mixture in a constant area duct from a one-dimensional viewpoint, then a relationship between flame speed and reaction rate can be deduced.

The energy equation is

$$K \frac{d^2 T}{dx^2} - (\rho u) C_p \frac{dT}{dx} - \dot{W}_f''' \Delta H = 0$$

with boundary conditions

$$x = -\infty, T = T_f, \frac{dT}{dx} = 0$$

$$x = +\infty, T = T_s, \frac{dT}{dx} = 0 \quad . \quad (25)$$

The chemical reaction rate is

$$\dot{W}_f''' = -k_n C_o^{n-j} C_f^j e^{-E/RT} \quad . \quad (26)$$

In these equations

- C_p = specific heat at constant pressure (mean),
- n = overall order of the reaction,
- j = order with respect to reactants,
- C_o = concentration of oxidant,
- T = temperature,
- C_f = concentration of reactant,
- ΔH = heat of combustion,
- ρ = density,
- u = fluid velocity,
- K = mean conduction coefficient,
- R = gas constant,
- E = activation energy,
- k = reaction rate constant, and
- \dot{W}_f''' = combustion reaction rate.

The combustion process proceeds as shown in Fig. 5.

The problem is simplified by dividing it into two zones: (1) a preheat zone, and (2) a reaction zone. For the preheat zone, the reaction rate is assumed negligible, so the energy equation reduces to

$$K \frac{d^2 T}{dx^2} - (\rho u) C_p \frac{dT}{dx} = 0 \quad (27)$$

with boundary conditions

$$x = -x_i, \quad T = T_i$$

$$x = +\infty, \quad T = T_s, \quad \frac{dT}{dx} = 0 \quad (28)$$

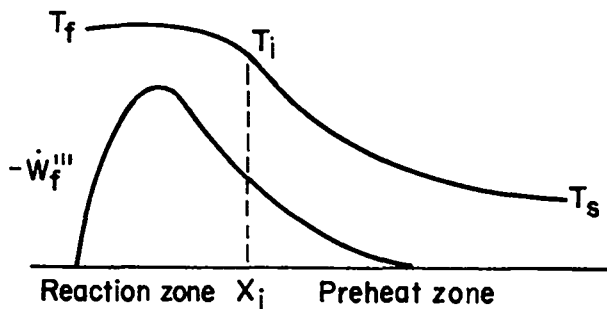


Fig. 5.

Thermal theory of flame propagation.

The first integral of this equation is, assuming steady flow ($\rho u = \text{constant}$),

$$\frac{dT}{dx} \Big|_i = (\rho u) \frac{C_p}{K} (T_i - T_s) \quad . \quad (29)$$

In the reaction zone, as T_i is approximately equal to T_f , the gradient dT/dx can be neglected in this region. The energy equation in this case becomes

$$K \frac{d^2 T}{dx^2} - \dot{W}''' \Delta H = 0 \quad . \quad (30)$$

Now

$$\frac{d^2 T}{dx^2} = \dot{W}''' \frac{\Delta H}{K} \quad , \quad (31)$$

and

$$d\left(\frac{dT}{dx}\right) = \dot{W}_f''' \frac{\Delta H}{K} dx \quad . \quad (32)$$

Multiplication by dT/dx gives

$$\frac{dT}{dx} d\left(\frac{dT}{dx}\right) = \dot{W}_f''' \frac{\Delta H}{K} dT \quad . \quad (33)$$

Integration gives

$$\frac{1}{2} \left(\frac{dT}{dx}\right)^2 \Big|_{T_i}^{T_f} = \int_{T_i}^{T_f} \dot{W}_f''' \frac{\Delta H}{K} dT \quad (34)$$

or

$$\frac{1}{2} \left(\frac{dT_f}{dx} \right)^2 - \frac{1}{2} \left(\frac{dT_i}{dx} \right)^2 = \int_{T_i}^{T_f} \dot{w}'''' \frac{\Delta H}{K} dT \quad (35)$$

Thus,

$$\frac{dT_i}{dx} = \left(\frac{2\Delta H}{K} \int_{T_i}^{T_f} (-\dot{w}_f'''') dT \right)^{1/2} \quad (36)$$

Notice from Eq. (26) that $\dot{w}_f'''' < 0$, so we can replace $-\dot{w}_f''''$ by $|\dot{w}_f''''|$ in Eq. (36).

We now equate Eqs. (29) and (36) to obtain

$$(\rho u) C_p \frac{(T_i - T_s)}{K} = \left(\frac{2\Delta H}{K} \int_{T_i}^{T_f} |\dot{w}_f''''| dT \right)^{1/2} \quad (37)$$

But $T_i = T_f$ and from Fig. 5 we see that the reaction rate is negligible from T_s to T_i , so

$$\rho u = \left\{ \frac{2\Delta HK}{C_p^2 (T_f - T_s)^2} \int_{T_s}^{T_f} |\dot{w}_f''''| dT \right\}^{1/2} \quad (38)$$

By the mean value theorem for integrals,

$$\frac{1}{T_f - T_s} \int_{T_s}^{T_f} |\dot{w}_f''''| dT = \overline{|\dot{w}_f''''|} \quad (39)$$

so

$$\rho u = \left\{ \frac{2\Delta HK}{C_p^2 (T_f - T_s)} \left| \dot{w}_f \right| \right\}^{1/2} . \quad (40)$$

Usually the constant 2 is replaced by $\frac{1}{\Lambda}$ where Λ is called the flame speed eigenvalue. So, in general,

$$\rho u = \left\{ \frac{\Delta HK}{C_p^2 \Lambda (T_f - T_s)} \left| \dot{w}_f \right| \right\}^{1/2} . \quad (41)$$

If the gas velocity ahead of the flame front is taken to be zero, then the flame velocity can be calculated from Eq. (41) as

$$u_0 = \left\{ \frac{\Delta HK \left| \dot{w}_f \right|}{\rho_s^2 C_p^2 \Lambda (T_f - T_s)} \right\}^{1/2} , \quad (42)$$

where u_0 is the speed of the flame relative to the unburned gas.

A relation between the pressures before and after the flame front can be found assuming an incompressible one-dimensional flow. The momentum equation is

$$\rho u \frac{du}{dx} = - \frac{dp}{dx} , \quad (43)$$

or

$$-dP = \rho u du . \quad (44)$$

Integration of Eq. (44) gives

$$- (P_f - P_s) = \rho_s u_s (u_f - u_s) \quad (45)$$

or

$$-(P_f - P_s) = \rho_s u_s^2 \left(\frac{\rho_s}{\rho_f} - 1 \right) . \quad (46)$$

So,

$$P_s = P_f + \rho_s u_s^2 \left(\frac{\rho_s}{\rho_f} - 1 \right) . \quad (47)$$

If u_s is taken to be the burning velocity, then

$$P_s = P_f + \rho_s \left\{ \frac{K\Delta H |\dot{W}_f|}{\Lambda \rho_s^2 C_p^2 (T_f - T_s)} \right\} \left(\frac{\rho_s}{\rho_f} - 1 \right) \quad (48)$$

$$= P_f + \frac{K\Delta H |\dot{W}_f|}{\Lambda C_p^2 (T_f - T_s)} \left(\frac{1}{\rho_f} - \frac{1}{\rho_s} \right) . \quad (49)$$

Equation (49) along with the equation of state allows determination of the pressure in front of the combustion wave if the temperature there is known:

$$P_s = \rho_s R T_s . \quad (50)$$

The fluid velocity behind the combustion wave is determined through the continuity equation

$$u_f = \frac{\rho_s u_0}{\rho_f} . \quad (51)$$

b. Turbulent Combustion. Turbulent combustion, like turbulent flow, is approached in a semiempirical fashion. Several models exist that relate the turbulent flame speed to laminar flame speed. Because flows through buildings and their ventilation systems have fairly low velocities and turbulence is at a low level, a model like that of Karlovitz can be used.¹²

$$u_{oT} = u_{oL} + u' \quad (52)$$

where

$$u' = \frac{u_{oL}}{3} \left(\frac{\rho_s}{\rho_f} - 1 \right) , \quad (53)$$

and u_{oL} and u_{oT} are the laminar and turbulent flame speeds, respectively.

The pressure given by Eq. (49) is modified by substituting u_{oT} from Eq. (52) into Eq. (49).

3. Transition from Deflagration to Detonation Waves.¹⁴⁻¹⁸ If combustion is rapid, then the quasi-steady state treatment of the above section is not sufficient to determine the wave velocity. Compressibility must be accounted for in addition to time dependence. The energy equation for nonsteady compressible one-dimensional flow is

$$K \frac{d^2 T}{dx^2} - \left\{ \frac{\partial}{\partial t} \left[\rho \left(c_v T + \frac{u^2}{2} \right) \right] + \frac{\partial}{\partial x} \left[\left(c_p T + \frac{u^2}{2} \right) \rho u \right] \right\} - \dot{W}_f'' \Delta H = 0 , \quad (54)$$

where C_v and C_p are the specific heats at constant volume and pressure, respectively. Now, from the perfect gas laws

$$C_v = \frac{R}{k-1} \quad (55)$$

and

$$C_p = \frac{kR}{k-1} \quad (56)$$

So,

$$C_v T = \frac{RT}{k-1} = \frac{kRT}{k(k-1)} = \frac{a^2}{k(k-1)}, \quad (57)$$

and

$$C_p T = \frac{kRT}{k-1} = \frac{a^2}{k-1}, \quad (58)$$

where $k = C_p/C_v$ and $a^2 = kRT$ is the square of the speed of sound. Thus Eq. (54) becomes

$$\frac{k}{kR} \frac{d^2 a^2}{dx^2} - \left\{ \frac{\partial}{\partial t} \left[\rho \left(\frac{a^2}{k(k-1)} + \frac{u^2}{2} \right) \right] + \frac{\partial}{\partial x} \left[\left(\frac{a^2}{k-1} + \frac{u^2}{2} \right) \rho u \right] \right\} - \dot{w}_f'''' \Delta H = 0 \quad (59)$$

The nonsteady continuity equation is

$$\frac{\partial \rho}{\partial t} = - \frac{\partial(\rho u)}{\partial x} \quad (60)$$

After taking the indicated derivatives of Eq. (59) and using Eq. (60), the energy equations become

$$\begin{aligned} \frac{k}{kR} \frac{\partial^2 a^2}{\partial x^2} - \rho \left\{ \frac{2a}{k(k-1)} \frac{\partial a}{\partial t} + \frac{2au}{k-1} \frac{\partial a}{\partial x} \right\} - \rho \left\{ u \frac{\partial u}{\partial t} + u^2 \frac{\partial u}{\partial x} \right\} \\ - \frac{a^2}{k} \frac{\partial(\rho u)}{\partial x} - \dot{w}_f'''' \Delta H = 0 \quad (61) \end{aligned}$$

The momentum equation for nonsteady one-dimensional compressible flow is

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = - \frac{1}{\rho} \frac{\partial P}{\partial x} \quad (62)$$

From the equation of state for a perfect gas,

$$P = \rho RT = \frac{\rho kRT}{k} = \frac{\rho a^2}{k} \quad (63)$$

Therefore, the momentum equation becomes

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = - \frac{1}{k\rho} \frac{\partial(\rho a^2)}{\partial x} = - \frac{1}{k} \left\{ \frac{\partial a^2}{\partial x} + \frac{a^2}{\rho} \frac{\partial \rho}{\partial x} \right\} \quad (64)$$

Multiplying Eq. (64) by u and using the result in Eq. (61) yields

$$\begin{aligned} \frac{k}{kR} \frac{\partial^2 a^2}{\partial x^2} - \rho \left\{ \frac{\partial a}{k(k-1)} \frac{\partial a}{\partial t} + \frac{\partial au}{k-1} \frac{\partial a}{\partial x} \right\} \\ - \rho \left\{ - \frac{u}{k} \left[\frac{\partial a^2}{\partial x} + \frac{a^2}{\rho} \frac{\partial \rho}{\partial x} \right] \right\} - \frac{a^2}{k} \frac{\partial(\rho u)}{\partial x} - \dot{w}_f''' \Delta H = 0 \end{aligned} \quad (65)$$

and, with further simplification,

$$\frac{k}{kR} \frac{\partial^2 a^2}{\partial x^2} - \rho \left\{ \frac{1}{k(k-1)} \frac{\partial a^2}{\partial t} + \frac{u}{k(k-1)} \frac{\partial a^2}{\partial x} + \frac{a^2}{k} \frac{\partial u}{\partial x} \right\} - \dot{w}_f''' \Delta H = 0 \quad (66)$$

The continuity equation, Eq. (60), the equation of state, Eq. (63), the momentum equation, Eq. (62), and the energy equation, Eq. (66), constitute a set of four simultaneous differential equations in the four unknowns, a^2 , u , ρ , and P . We must assume that \dot{w}_f''' is known.

The solution of these equations will reveal whether a shock wave will form and whether the combustion wave overtakes it to form a detonation wave. If it does, then the detonation wave will travel at a constant velocity and can be treated by the equations given for detonation waves.

IV. REVIEW OF THE TVENT COMPUTER CODE

A perception of the relationship of explosive phenomena to the explosion analysis objectives can be obtained by a brief discussion of the TVENT code.

TVENT was developed at Los Alamos Scientific Laboratory over a period of approximately three years. Its main purpose was to predict the flow rates and pressures that would exist within the ventilation systems of a building if a tornado passed over that building. This is a complex problem because the ventilation systems of large buildings are very intricate. These systems consist of many branching and looping ducts, large volumes such as rooms and gloveboxes, many blowers, dampers, filters, etc. Furthermore, the flow through the ventilation system is not steady but changes with time because the pressure pulse caused by the tornado passage over the building changes with time. An additional complication is the compressible nature of the air flowing through the system.

As we developed TVENT, we could see that because of the relatively small peak pressures expected from tornadoes (3 psi) and the relatively slow occurrence of the pressure pulse, we could make several simplifying assumptions. These assumptions are listed below.

- One-dimensional, incompressible flow
- Isothermal (constant temperature) flow
- System components treated as lumped parameters
- Fluid storage or compressibility allowed only at rooms or gloveboxes
- Inertial effects and shock formation are neglected

The equations that govern flow through the system are the momentum equation, the continuity equation (conservation of mass), the energy equation, and the equation of state of the fluid. For a one-dimensional, incompressible, quasi-steady flow, the momentum equation and the energy equation integrate to the same equation. Hence, for all components except large volumes, the equation of motion and energy equation can be replaced by a relationship between the flow rate through the component and the pressure drop across the component. The continuity equation is satisfied by demanding that mass be conserved at each node between components.

When a component has a large volume, we assume that there is no pressure drop across it because the velocity within the volume is small. However, mass storage can occur within the volume so that its pressure does change with time. The time derivative of the equation of state for a perfect gas coupled with the conservation of mass allows this change in pressure to be calculated.

Thus the numerical solution technique conceptionally appears fairly simple. At a given instant in time, the nonlinear equations for flow rate as a function of pressure through each component are solved in an iterative manner until conservation of mass is attained at each node. Time is then incremented, the tornado pressure value is changed, and once again the pressures at each node are adjusted in an iterative procedure that assures conservation of mass. This stepping in time continues until the pressure pulse has ended and the system has returned to its nominal steady-state operation.

The application of TVENT to various ventilation systems has been quite successful. When applied to steady-state conditions, it closely predicts the actual performance of the building's ventilation systems. Transient performance will soon be verified by construction of a small-scale ventilation system where tornado pressure pulses can be modeled. In general, instability of the numerical solutions has not been a difficulty with TVENT.

V. TVENT AND EXPLOSIVE PHENOMENA

The above discussions of explosive phenomena and the structure of TVENT allow us to outline some general considerations in extending TVENT to modeling explosions within structures. TVENT appears to be a good starting point for a code that will predict the flow rates and pressures within a building ventilation system caused by an explosion within the system. But how can TVENT be modified to handle this event? Let us return to the assumptions made for TVENT.

An explosion-induced flow cannot be assumed isothermal or incompressible. Shock formation cannot be ignored and there is a possibility that inertial effects may not be negligible. Furthermore, because of the relatively high velocities of explosion wave fronts (faster than the speed of sound for detonation waves), the lumped parameter techniques may be invalid. Finally, if the explosion initiates within a large volume, the flow within that volume cannot be considered one-dimensional. Thus most of the assumptions made for TVENT seem, on the surface, to be questionable.

Other difficulties that explosions add include the following.

1. We must predict burned gases (constituents).
2. We must determine energy release quantities.
3. The perfect gas law does not hold.
4. A large pressure pulse may cause interaction between fluid and flexing ductwork.

5. Many components of the system (blowers, etc.,) may be damaged, and their pressure drop vs flow rate relationship may change.
6. A deflagration wave may undergo transition to a detonation wave.
7. Pulsating and spinning propagation waves are possible near the limits of detonability.
8. Heat transfer and mass diffusion processes within mixtures may need to be considered.
9. Thermodynamic equilibrium may not be present behind a detonation wave.
10. The potential user of the code may not know many of the parameters required for input for the code.
11. The code may prove too complex for HVAC designers and analysts.
12. Deflagration and detonation limits have to be considered.

Within the ducts of the ventilation system, the one-dimensional approximation can probably be retained. Further, because explosions of the type that would probably occur within a facility are of fairly low energy, we may need to take into account the three-dimensional nature of the blast only within the system component where it initiates, with one-dimensional flow assumed everywhere else. Thus the one-dimensional assumption can possibly be retained for the major portion of the system.

Theory indicates that time-dependent effects should be small for deflagrations and detonations as long as the source mass is of the same order of magnitude as the driven mass within the ventilation system.^{11,13} This has been borne out by experiment. We must be careful, however, because neglecting inertia in time-dependent, one-dimensional compressible flows removes one of our most important tools--the method of characteristics.

For detonations, shock waves cannot be neglected. However, except within the component where the detonation takes place, the shock wave can be considered a planar wave. The propagation of the wave can be analyzed using the hydrodynamic equations discussed earlier. Its strength and velocity will depend upon the physical properties of the explosive media. The flows on either side of the detonation wave can be coupled or patched through the Rankine-Hugoniot equations.¹⁵ Expansion waves trail the moving shock waves and tend to overtake them. Also, the relative position of the expansion waves and the shock waves effects the reaction of the burning gases.¹³ Ahead of the shock wave the flow is the undisturbed steady flow of the ventilation system.

Deflagration waves, as noted earlier, travel more slowly than the speed of sound and propagate by the process of heat transfer and diffusion. Treatment of the flow behind deflagration waves is inherently more difficult than treatment of detonation waves. However, because the waves move slower than the speed of sound, air ahead of a wave is set in motion by precompression. Therefore, in the regions of the system ahead of deflagration waves, TVENT can be used to predict pressure and flow rates with some modification. These modifications will include complete compressible flow in connecting ducts and addition of inertia effects. Note that compressibility effects are accounted for at specified points in TVENT.

Because a lumped-parameter approach cannot be used for all regions of the system, we must express the governing differential equation of fluid motion as functions of time and displacement along the axes of ducts and other system components. Any approach that adds the effects of inertia, such as method of characteristics or incompressible subelement, will require incremental calculations along the axis of propagation.^{14,19} However, time and spatially dependent differential equations add complexity to the numerical solution and numerical stability is sometimes difficult to achieve.²⁰ Very large volumes where the explosion does not initiate can perhaps still be treated as in TVENT because the flow will expand and become very slow.

We believe that much or all of the TVENT code will be directly usable in the explosion code, at least for some regions of the ventilation system. The steady-state solution for flow and pressure given by TVENT is essential for initial conditions for any transient and would be coupled to any shock wave calculation. Subdivision of the analysis into regions may prove to be a viable approach. Regions near the explosive event will be treated with analyses that use detailed information to describe the fluid motion. As the flow develops and moves to other regions of the ventilation system, the present TVENT equations for fluid motion will be used to propagate the pressure pulse through the remainder of the system. Of course, these equations will have to be modified for compressibility and inertia effects.

Clearly, much new analysis and programming must be done if explosions are to be treated successfully. The added complexity of shock waves, expansion waves, deflagration waves, space- and time-dependent flows, and compressibility is enormous. If we also add to this the need to predict burned gas constituents, the energy release of the explosion, the possible damage to structures,

nonequilibrium states, etc., then the task becomes even greater. Therefore we recommend that the explosion computer code be attacked in stages.

In the first stage we will assume that the problem is simply a gas dynamics problem with the explosion modeled parametrically. For example, energy release, rate of energy release, mass and extent of explosive media, burned constituents, etc., will all be given as input to the computer code. Further, we will assume that the flow structure is completely rigid and cannot be harmed by the explosions. Equilibrium thermodynamics will be used, and both burned and unburned gases will be assumed perfect. After the code has been proven in this form, it could then be gradually modified to include theoretical prediction of detailed explosion parameters.

VI. EXPLOSION CODE ORGANIZATION

A. General

Our organization of the explosion computer code is expected to evolve from the established TVENT code. The input format for the TVENT code will be retained along with the steady-state portion of the code. However, the transient analysis portion of code will require extensive work. We propose to subdivide the transient analysis into two major categories as shown in Fig. 6. These two categories are called near- and far-field and apply to regions of the ventilation system that are both near or far away from the explosive event.

We believe that the near-field analysis should consist of three main segments, as shown in Fig. 6. Depending upon the characteristics of the explosive event, a deflagration, detonation, or transition to detonation will take place. As shown in earlier sections, each type of phenomenon requires different solution routines.

TVENT is now initiated by describing a pressure pulse at some point within the system or at a system boundary. For a detonation or deflagration taking place somewhere within the system, pressure and temperature changes persist not only in time, but also in space. Thus we must know the extent of the explosive medium as well as its location within the system. The computer code will consider these to be parameters so that events of any magnitude and any location can be studied.

In many cases, especially within a large building and ventilation system, deflagrations and detonations can be relatively unconfined. Experimental

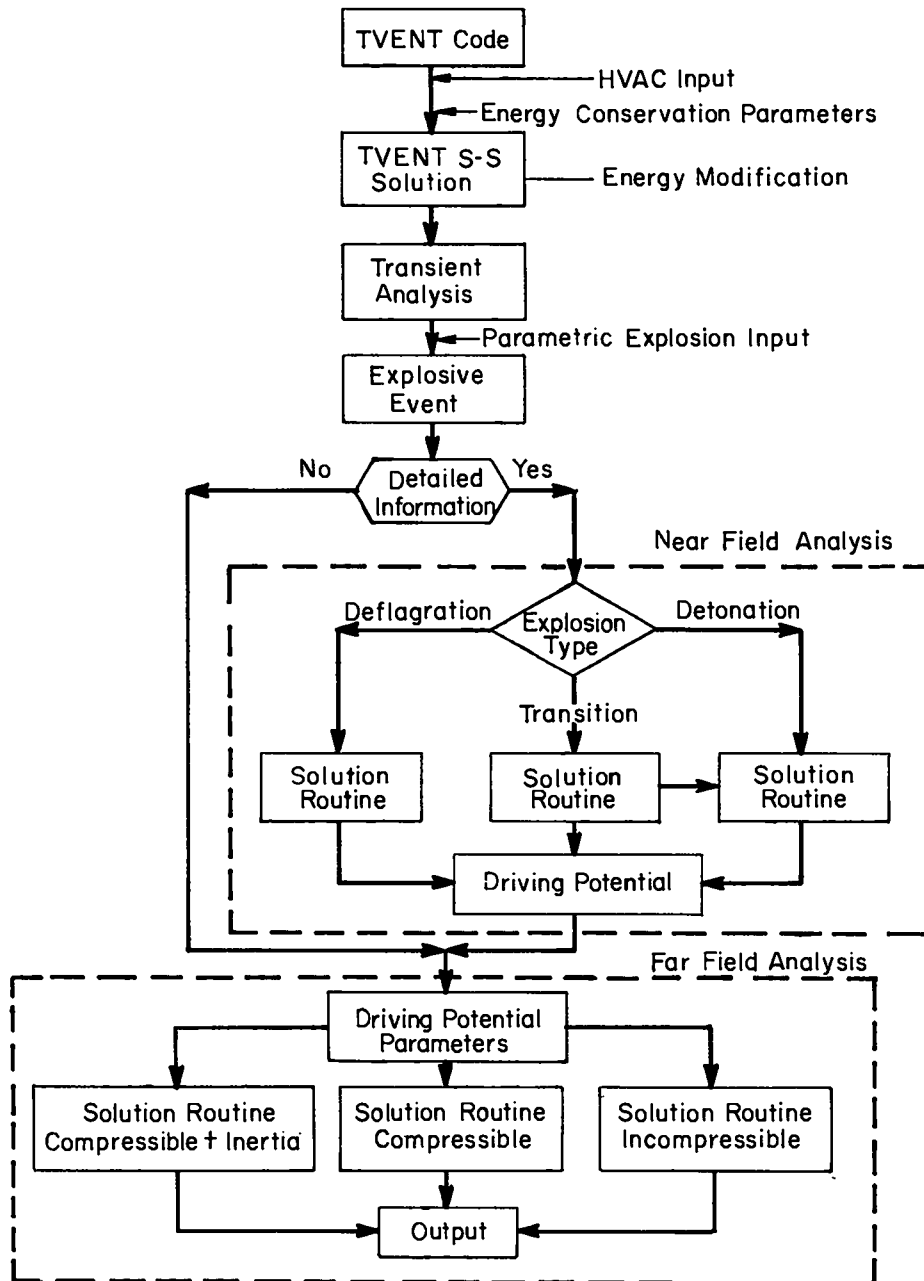


Fig. 6. Explosion code organization.

evidence shows that, in this case, these explosive events will be stationary or their wave velocity propagation will be constant.^{11,13} Thus, as shown in Fig. 6, these events will be treated using steady-state theory developed in earlier sections. However, under certain conditions deflagrations will tend to evolve toward detonations. In these explosions, unsteady-state theory must be used.

The output from the near-field analyses will be the driving potential for the rest of the system. We believe that less complicated analyses can be used in the far-field regions of the system. These regions are far removed from the explosive event and are thus relatively independent of the explosive event characteristics. Only the driving parameters such as pressure, temperature, and velocity are important to the fluid motion in the remainder of the system.

Using these driving potentials we can return to the existing TVENT code. In some cases TVENT's way of describing fluid motion as incompressible may be appropriate and thus can be used to propagate the flow through the system. However, for other cases we must modify TVENT to treat compressible flow and also include inertia effects.

We must point out that this approach is proposed without our having done any of the analyses outlined above. As the program progresses, we expect that our development will be flexible enough to accommodate required changes. For example, we may find that using the method of characteristics is suitable for the entire explosion computer code. Another possibility is that not enough information is known about the explosive event to warrant the near-field analysis outlined above. In this case, the far-field analyses may be the only recourse that can be used. Other uncertainties involve the three-dimensional nature of an explosion within a chamber. Further, separation of the code into distinct near- and far-field analyses may not be possible. In some flow region cases, we may desire to mix far-field and near-field calculations. Only additional work will determine this.

Another aspect that could greatly affect the above approach is the user-oriented nature of the code desired. Analysis complexity, large computational time, nonportability, and machine dependence may require many tradeoffs in the desired approach.

In any case we will outline in the sections that follow how the solution routines shown in Fig. 6 would evolve.

B. Near-Field Analyses

1. Solution Routine for Detonation. Because the detonation wave moves into the undisturbed flow at a speed faster than the speed of sound, the flow ahead of the detonation wave can be treated using TVENT.

Behind the detonation wave, the flow is subsonic but compressible. Particle velocity and pressure immediately behind the wave are given by the solution of Eqs. (5) through (9) and (24). Flow behind the detonation wave can be analyzed using shock tube relations.^{8,15,21} A procedure similar to this is suggested in Ref. 20 for instantaneous combustion.

Because the ventilation system is open, initially we can assume that there are no shock or expansion wave reflections. When an expansion wave overtakes a shock wave, the wave will collapse to a sound wave and from that point onward will travel at the local speed of sound.

After the detonation has overrun the detonable media, it becomes a shock wave, and it will be attenuated by friction and expansion waves that overtake it.

2. Solution Routine for Subsonic Deflagration. Because subsonic deflagration takes place at a rate that causes combustion waves to travel slower than the speed of sound, we believe that most of the TVENT code can be used. The solution routine could develop as follows.

- (a) An explosive medium is hypothesized at some location within the ventilation system.
- (b) The extent of the explosive medium is known.
- (c) The final temperature and reaction rate are known.
- (d) The flame velocity can be calculated using Eq. (42) for laminar combustion. Equation (52) can be used if the combustion process is turbulent.
- (e) The length of time for combustion to be completed can be calculated using the extent of the explosive medium and the flame velocity.
- (f) Pressure ahead of the combustion wave can be calculated using Eq. (49). Again, if the flow is turbulent, Eq. (52) will be substituted into Eq. (49).
- (g) The fluid velocity behind the combustion wave can be calculated using Eq. (51).
- (h) The calculations in steps (d) through (g) are used to propagate the combustion wave in the near-field region and also provide the driving potential for the remainder of the system.
- (i) The existing TVENT equations for fluid motion or modification of these equations for compressible flow and inertia are then used to calculate the wave propagation in the far-field region.

3. Solution Routine for Transition to Detonation¹⁴⁻¹⁷ The continuity, momentum, and energy equations (Eqs. (59), (61), (66)) are hyperbolic and can be solved using the method of characteristics. Typically, these solutions reveal Mach lines that may or may not coalesce into shock waves. The method is outlined by Shapiro.¹⁴ The characteristic curves are defined as curves where the derivatives of the fluid properties are indeterminate. The derivatives in this case are, $\partial u/\partial x$, $\partial u/\partial t$, $\partial/\partial x$, $\partial/\partial t$, $\partial a^2/\partial x$, and $\partial a^2/\partial t$. We must assume that $\partial a^2/\partial x^2$ is known (as Shapiro does) or approximate it in terms of the first derivative or a^2 itself¹⁴.

Equations (60), (62), and (66) can be solved first and then Eq. (63). In addition to Eqs. (60), (62), and (66), we define by the chain rule

$$du = dx \frac{\partial u}{\partial x} + dt \frac{\partial u}{\partial t} \quad , \quad (67)$$

$$da^2 = dx \frac{\partial a^2}{\partial x} + dt \frac{\partial a^2}{\partial t} \quad , \quad \text{and} \quad (68)$$

$$d\rho = dx \frac{\partial \rho}{\partial x} + dt \frac{\partial \rho}{\partial t} \quad . \quad (69)$$

If we now solve for any one of the derivatives $\partial u/\partial x$, $\partial u/\partial t$, etc., from Eqs. (60), (62), (66), (67), (68), and (69) using Cramer's rule, then two equations are obtained corresponding to setting both the determinate in the denominator and the numerator equal to zero. One of these equations defines the characteristic lines in the physical plane, whereas the other defines the characteristics of the physical properties ρ , u , and a^2 . The solution is completed by incrementing along the characteristic lines in a manner similar to finite difference solutions.

Once the solution algorithm is completed, frictional effects can be added with little effort.

C. Far-Field Analyses

1. Solution Routine for Compressible Flow with Inertia.²² A lumped-parameter or control-volume approach will be used for the far-field analysis.

The lumped parameter technique is used in the present transient portion of TVENT. We propose to extend this technique to treat compressible flow and include inertia effects. Our experience using TVENT leads us to believe that the computational cost of this method will be low. Reference 22 states that the computational cost will definitely be low when compared to finite difference methods that are necessary when using method of characteristics.

However, detailed information about the propagation of the waves cannot be obtained. Also the accuracy is less with the lumped parameter method than with finite difference methods.

For some conditions the incompressible approach used in TVENT will be suitable. However, for other conditions compressible flow and inertia will have to be included.

Consider the one-dimensional unsteady momentum equation:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{1}{\rho} \frac{\partial P}{\partial x} - \frac{Fu^2}{\partial L}, \quad (70)$$

where F is a dimensionless coefficient and L is the duct length. Neglecting the second term in Eq. (70) and multiplying Eq. (70) by the density, ρ , and duct cross sectional area A gives

$$\rho A \frac{\partial u}{\partial t} = - A \frac{\partial P}{\partial x} - \frac{F \rho A u^2}{2L}. \quad (71)$$

Now for a duct length, L ,

$$- \frac{\partial P}{\partial x} = \frac{\Delta P}{L}. \quad (72)$$

Substituting and expressing as mass flow rate, Eq. (72) becomes

$$\frac{d(\rho Au)}{dt} = \frac{A}{L} \Delta P - \frac{F \rho^2 A^2 u^2}{2L \rho A}. \quad (73)$$

Noting that the mass flow rate, \dot{m} , is equal to ρAu , Eq. (73) can be rewritten as

$$\frac{d\dot{m}}{dt} = \frac{A\Delta P}{L} - \frac{F \dot{m} |\dot{m}|}{2L\rho A} \quad (74)$$

At the nodes in the lumped parameter approach, the energy and continuity equations can be written

$$\frac{dE_j}{dt} = \sum_i H_i \dot{m}_i - \sum_o H_o \dot{m}_o + Q_j \quad (75)$$

$$\frac{dM_j}{dt} = \sum_i \dot{m}_i - \sum_o \dot{m}_o \quad (76)$$

where

- E_j = internal energy at node j,
- H_i, H_o = inlet and outlet enthalpies,
- \dot{m}_i, \dot{m}_o = inlet and outlet as flow,
- M_j = mass of fluid at node j, and
- Q_j = energy release at node j.

After the internal energy and the mass of each node are known, the pressure and temperature at the nodes can be calculated using the equation of state and definition of enthalpy:

$$T = E_j C_v / M_j \quad (77)$$

$$P = R M_j T_j / V_j \quad (78)$$

where V_j = volume of node j.

Equations (74) through (78) can be used to evaluate all of the flow properties throughout the system provided driving parameters such as energy release, pressure, mass release, etc., are given.

VII. SUMMARY

We have described our initial study of explosive phenomena and how it relates to the previously developed TVENT code. This work has led us to put forth a proposed approach and organizational plan for an explosion computer code patterned after TVENT.

The explosion process was subdivided into three areas--deflagration, detonation, and transition from deflagration to detonation. Governing equations were written for each process, and potential solution routines for these equations were outlined.

The organization of the explosion code can evolve from the steady-state portion of the TVENT code. Further, the explosion code can be subdivided into a near- and far-field analysis. In the near-field, or near the explosive event, detailed combustion equations would be used to describe the flow dynamics. This analysis would also provide parametric driving potential for flow in the remainder of the ventilation system. The far-field applies to those regions that are somewhat insensitive to the characteristics of the explosive event. Given a proper driving potential for the flow, from the near-field analysis, the existing TVENT equations or modifications to these equations can be used to propagate the pressure waves through the remainder of the system.

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