Estimation of Peak Pressure for Sonic-Vented Hydrocarbon Explosions in Spherical Vessels

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Two closed-form approximate solutions are presented for the final pressure produced by a hydrocarbon explosion in a spherical vessel with sonic venting. A constant factor which multiplies the ideal spherical flame velocity is used to describe the effect of flame acceleration. One of the solutions is a simple, easy-to-use equation which may appeal to vent designers; it agrees well with reported results from a comprehensive computer model and correlates available experimental data as well as previous models involving several variable turbulence factors.

INTRODUCTION

A substantial body of experimental data exists on sonic-vented deflagrations of hydrocarbon–air mixtures in high pressure vessels up to 60 m^3 in volume. To interpret the observed peak pressures correctly, it is, of course, necessary to have a theoretical model of the chemistry and dynamics of such vented deflagrations, and this has typically been done by recourse to computer simulation (see, e.g., [1-4]). The purpose of this paper is to exploit analytical techniques developed in the field of vented deflagration research to obtain approximate closed-form expressions for the pressure in a sonic-vented vessel at the completion of a transient, spherical deflagration. While these results cannot be used for accurate vent design, they should prove valuable for understanding quantitative features of vented deflagrations, inferring approximate scaling laws, and developing a methodology for the selection of "safe" vent areas for pressure relief. Moreover, the expressions correlate the available experimental data as well as previously reported numerical models with some pretense of accuracy regarding the treatment of flame acceleration mechanisms.

ANALYSIS

We treat here the particular case of "sonic-vented" deflagrations, in which the vent opening pressure (or set pressure) is sufficiently high and the rate of burning is greater than the rate of venting so that the gas discharge through the vent is choked (sonic) throughout the duration of the combustion process. The wholly sonic venting regime is typical of explosion venting of high pressure storage or process vessels. It is assumed that the fuel and oxidizer gases are uniformly mixed and contained within a rigid spherical vessel of radius R.[1] The gases are centrally ignited and the pressure in the vessel begins to rise at a rate proportional to the product of deflagration flame speed and area. The corresponding model of the deflagration in a spherical vessel is depicted in Fig. 1. The behavior of the spherical reaction front

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[1] For the purpose of treating a nonspherical vessel, R is the radius that a sphere would attain if it had the same volume as the nonspherical vessel.

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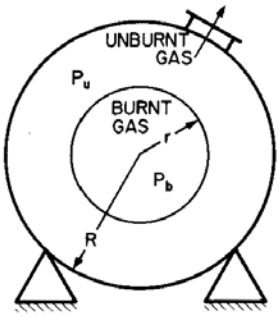

Fig. 1. Configuration and notation: flame propagation in a spherical vented container.

itself constitutes the first and most important assumption:

1. The reaction or flame front speed is sufficiently rapid to cause the thickness of the reaction zone to be small compared with the (as yet undetermined) flame radius, r. The flame front is spherical and propagates outward from the center of the vessel without any significant distortion due to natural convention or venting. Finally, it is assumed that a constant factor ϕ which multiplies the burning velocity S_u adequately describes the effects of increased burning rate due to both small-scale turbulence and flame wrinkling (large-scale turbulence). Yao et al. [1] assumed this to account for flame acceleration effects.

Other important assumptions invoked to obtain simple analytical results are

2. The ideal gas law is applicable to both the unburned and burned gases, with the ratio of specific heats (or polytropic exponents) and the molecular weights for each gas characterized by known constants. The burned and unburned gases are compressed isentropically.
3. The temperature of the burned gas region is uniform in space.
4. Energy losses to the vessel wall are negligible and the pressure P is uniform throughout the vessel.
5. When venting occurs only the unburned gases are vented.

We now consider the fully transient combustion-venting problem of predicting the maximum pressure reached in the vessel at the instant when the flame arrives at the wall (i.e., when $r = R$).

The mass rate of production of burned gas is given by the familiar formula for spherical flame growth,

$$\frac{dm_b}{dt} = 4\pi r^2 \phi \rho_u S_u, \tag{1}$$

where S_u is the burning velocity and ϕ is the turbulence correction factor (to be determined from experimental data). The mass rate of loss of the unburned gas is given by

$$\frac{dm_u}{dt} = -4\pi r^2 \phi \rho_u S_u - A_v G. \tag{2}$$

The first term on the right-hand side of the above equation represents the rate of loss of unburned gas due to flame propagation and the second term represents the escape of unburned gas through the vent. Assumptions (2) and (3) imply

$$\frac{\rho_u}{\rho_{u,0}} = \left(\frac{P}{P_0}\right)^{1/\gamma_u} \quad \text{and} \quad \frac{\rho_b}{\rho_{b,0}} = \left(\frac{P}{P_0}\right)^{1/\gamma_b}, \tag{3}$$

where the subscript 0 refers to conditions in the vessel at ignition. In writing the second of Eqs. (3) we are assuming that the burned gas density does not depend on whether the gas is first compressed and subsequently burned, or first burned and then compressed. The burned gas density at ignition, $\rho_{b,0}$, is unknown; it can be estimated, however, from a knowledge of the vessel pressure following an explosion in a closed vessel (see below). It follows from (3) that the instantaneous mass of burned gas is given by

$$m_b = \frac{4}{3}\pi r^3 \rho_b = \frac{4}{3}\pi r^3 \rho_{b,0}\left(\frac{P}{P_0}\right)^{1/\gamma_b} \tag{4}$$

and that the total volume of the vessel, V, is

$$V = \frac{m_u}{\rho_u} + \frac{m_b}{\rho_b} = \frac{m_u}{\rho_{u,0}}\left(\frac{P}{P_0}\right)^{-1/\gamma_u} + \frac{m_b}{\rho_{b,0}}\left(\frac{P}{P_0}\right)^{-1/\gamma_b}. \tag{5}$$

Differentiating Eq. (5) with respect to time, using Eqs. (11 and 12) to eliminate dm_u/dt and dm_b/dt, and solving the result for dP/dt, yields

$$\frac{1}{\gamma_b}\frac{d \ln P}{dt} = \frac{4\pi r^2 \phi(\rho_u/\rho_b - 1)S_u - A_v G/\rho_u}{(\gamma_b/\gamma_u)m_u/\rho_u + m_b/\rho_b}. \tag{6}$$

Simplification of this equation is possible if we can put $\gamma_b = \gamma_u$ in the denominator. The denominator is then constant and equal to the volume of the vessel [see Eq. (5)]. Making this approximation, Eq. (6) becomes

$$\frac{V}{\gamma_b}\frac{d \ln P}{dt} = 4\pi r^2 \phi(\rho_u/\rho_b - 1) S_u - A_v G/\rho_u. \quad (7)$$

Differentiating Eq. (4) with respect to time and using Eq. (7) to eliminate dP/dt gives the following differential equation for the burn radius r:

$$4\pi r^2 \frac{dr}{dt} = 4\pi r^2(\rho_u/\rho_b)\phi S_u - 4\pi r^3/(3V) \times [4\pi r^2(\rho_u/\rho_b - 1)\phi S_u - A_v G/\rho_u]. \quad (8)$$

Dividing Eq. (7) by Eq. (8), we have

$$\frac{1}{\gamma_b}\frac{d \ln P}{dZ} = \frac{(\phi S_u \rho_u A_s/GA_v)[(\rho_u/\rho_b) - 1)] Z^{2/3} - 1}{(\phi S_u \rho_u A_s/GA_v)\{(\rho_u/\rho_b) - [(\rho_u/\rho_b) - 1] Z\} Z^{2/3} + Z}, \quad (9)$$

where A_s is the surface area of the spherical vessel, equal to $4\pi R^2$, and Z is a dimensionless burn volume:

$$Z \equiv \frac{(4/3)\pi r^3}{V}. \quad (10)$$

Equation (9), when integrated, gives the variation of pressure within the vessel as a function of the volume of the flame "ball." Of course, the maximum or final pressure, P_f, is reached when $Z = 1$, i.e., when the flame ball occupies the entire vessel volume. Equation (9) shows that P_f depends only on the dimensionless groups ρ_u/ρ_b and $\phi S_u \rho_u A_s/(GA_v)$.

The burning velocity S_u for most hydrocarbons is linked empirically to pressure and unburned gas temperature by the power law

$$\frac{S_u}{S_{u,0}} = \left(\frac{T_u}{T_{u,0}}\right)^2 \left(\frac{P_0}{P}\right)^{1/2}. \quad (11)$$

The sonic mass rate of discharge per unit area of vent is

$$\frac{G}{G_0} = \left(\frac{P\rho_u}{P_0\rho_{u,0}}\right)^{1/2}. \quad (12)$$

Using the laws of isentropic compression, the group $S_u\rho_u/G$ may be expressed in terms of pressure only:

$$\frac{S_u\rho_u/G}{(S_u\rho_u/G)_0} = \left(\frac{P}{P_0}\right)^{1-3/(2\gamma_u)} \quad (13)$$

Since for most hydrocarbon–air mixtures $\gamma_u \simeq 1.36$, the exponent on the pressure ratio is only -0.1. We can conclude that the group $S_u\rho_u/G$ is not greatly dependent on pressure during an isentropic compression and for all practical purposes is constant. The assumption that $S_u\rho_u/G$ is constant is used here. From Eq. (3) we note that the density ratio ρ_u/ρ_b is related to pressure by

$$\frac{\rho_u}{\rho_b} = \frac{\rho_{u,0}}{\rho_{b,0}}\left(\frac{P}{P_0}\right)^{1/\gamma_u - 1/\gamma_b}. \quad (14)$$

The specific heat ratio for the burned gases is approximately 1.08 (see below) and thus the exponent $(1/\gamma_u - 1/\gamma_b) \simeq -0.2$, so we can assume that ρ_u/ρ_b is also uninfluenced by changes in pressure and is a known constant.

The dimensionless group $\phi S_u\rho_u A_s/(GA_v)$ that appears in Eq. (9) is the ratio of the maximum burning rate to the sonic discharge rate. To simplify the notation we will denote it by B and call it the burning number, viz.,

$$B \equiv \frac{\phi S_u \rho_u A_s}{GA_v}. \quad (15)$$

Most hydrocarbon–air mixtures have effectively the same value of the group $S_u\rho_u/G$, so that in reality the burning number B is only a function of the area ratio A_s/A_v and the turbulence correction factor ϕ.[2] Previous analyses [1, 3] and experimen-

[2] For hydrocarbon–air mixtures and a venting discharge coefficient of 0.7 $S_u\rho_u/G$ has the value of approximately 0.0032. For laminar burning ($\phi = 1$) the burning number is related to the Bradley-Mitcheson [3] dimensionless venting parameter: $\bar{A}/\bar{S}_0$ by $B = (\bar{A}/\bar{S}_0)^{-1}(\rho_{u,0}/\rho_{b,0} - 1)^{-1}/[(\gamma_u + 1)/2]^{(1/2)} \cdot (\gamma_u + 1)/(\gamma_u - 1)$.

tal work [1, 5] suggest that explosion venting data in terms of peak pressure should be specified as a function of the ratio A_s/A_v. Measured peak pressures within vessels discharging gas in subsonic flow have been found to compare well with numerical results calculated by using constant turbulent correction factors ϕ in the range 2-3 [1].

Before the vent opens $G = 0$ and Eq. (9) simplifies to

$$\frac{1}{\gamma_b}\frac{d\ln P}{dZ}=\frac{\rho_u/\rho_b-1}{\rho_u/\rho_b-(\rho_u/\rho_b-1)Z}. \tag{16}$$

Equation (16) can be readily integrated, leading to an expression between the vessel pressure and the dimensionless burn volume when the vent opens:

$$\frac{P_{set}}{P_0}=\left[\frac{\rho_u/\rho_b}{\rho_u/\rho_b-(\rho_u/\rho_b-1)Z_{set}}\right]^{\gamma_b}. \tag{17}$$

If the flame reaches the vessel wall without the vent opening, $Z_{set} = 1$ and Eq. (17) then has its maximum value corresponding to an explosion in a closed vessel:

$$\frac{P_{max}}{P_0}=\left(\frac{\rho_u}{\rho_b}\right)^{\gamma_b}. \tag{18}$$

Since P_{max}/P_0 and ρ_u/ρ_b are frequently tabulated quantities for combustible mixtures, Eq. (18) serves as a means for evaluating the effective constant exponent γ_b. For most hydrocarbon–air mixtures we find $\gamma_b = 1.08$.

At this point it is desirable to express Z_{set} in terms of P_{max}/P_0. From Eqs. (17) and (18)

$$Z_{set}=\frac{1-(P_{set}/P_0)^{-1/\gamma_b}}{1-(P_{max}/P_0)^{-1/\gamma_b}}. \tag{19}$$

Integrating Eq. (9) from $P = P_{set}$ at $Z = Z_{set}$ to $P = P_f$ at $Z = 1$, using Eq. (18) to eliminate ρ_u/ρ_b, results in the following integral for the peak (final) pressure:

$$\ln\frac{P_f}{P_{set}}=\gamma_b\int_{Z_{set}}^{1}\frac{[(P_{max}/P_0)^{1/\gamma_b}-1]\cdot B\cdot Z^{2/3}-1}{\{(P_{max}/P_0)^{1/\gamma_b}-[(P_{max}/P_0)^{1/\gamma_b}-1]Z\}\cdot B\cdot Z^{2/3}+Z}\cdot dZ. \tag{20}$$

It is not possible to do anything analytical with this equation as it stands. We can, however, find analytic expressions for P_f which are upper bounds to the set of solutions to Eq. (20). The larger the value of B inserted into Eq. (20), the higher is the corresponding final pressure P_f. Thus, if we ignore the variation of $Z^{2/3}$ which multiplies B, a useful upper limit to P_f is obtained by setting $Z^{2/3}$ equal to its maximum value of unity. This substitution allows Eq. (20) to be integrated in closed form, with the result

$$\frac{P_f}{P_0}=\frac{P_{max}}{P_0}\left[\frac{\lambda+B}{1+B}\right]^{\gamma_b}, \tag{21}$$

where λ is a dimensionless vent opening pressure defined by

$$\lambda\equiv\frac{(P_{set}/P_0)^{1/\gamma_b}-1}{(P_{max}/P_0)^{1/\gamma_b}-1}. \tag{22}$$

Interestingly enough, the values of P_f calculated from Eq. (21) are not too much larger than those calculated from Eq. (20). The error associated with Eq. (21) is largest when the set pressure is low and approximately equal to P_0, but even in this limit the error is tolerable. For example, the error is less than 30% for $P_{set}/P_0 = 1.3$. Clearly, the integral in Eq. (20) is not greatly dependent on the value of $Z^{2/3}$, because an increased value of this quantity raises the numerator and denominator of the integral almost proportionately.

It should be noted that Eq. (21) is the solution for the final pressure produced in a one-dimensional vessel (cylinder) with ignition at the closed end and a vent in the vessel opposite the plane of ignition. In particular, it is the exact solution to Eqs. (1)-(5) with the flame front area $4\pi r^2$ constant and equal to the cross-sectional area of the cylindrical vessel ("flat flame approximation"). Thus the simpler one-dimensional model can be used without too much loss in accuracy to predict the final pressure in a vented spherical vessel. However, when the initial pressure and the set pressure are nearly equal, Eq. (21) overestimates the final explosion pressure in a spherical vessel by about a factor of two.

An accurate closed-form approximation for P_f over the entire range of P_{set} values, $P_0 \leq P_{set} \leq P_{max}$, can be obtained by substituting $Z^{1/2}$ for $Z^{2/3}$ in Eq. (20). It is obvious that this substitution will introduce a smaller error than that caused by replacing $Z^{2/3}$ by unity. Integrating Eq. (20) with $Z^{2/3}$ now $Z^{1/2}$ yields

$$\frac{P_f}{P_{set}} = \left[\frac{Z_{set}{}^{1/2}(1 - BZ_{set}{}^{1/2}) + \epsilon B(1 - Z_{set})}{1+B}\right]^{\gamma_b} \cdot \left[\frac{2(\epsilon-1)BZ_{set}{}^{1/2} + \beta - 1}{2(\epsilon-1)B + \beta - 1}\right]^{\gamma_b/\beta} \times \left[\frac{-2(\epsilon-1)B + 1 + \beta}{-2(\epsilon-1)BZ_{set}{}^{1/2} + 1 + \beta}\right]^{\gamma_b/\beta}, \quad (23)$$

where we have introduced the definitions

$$\epsilon \equiv \left(\frac{P_{max}}{P_0}\right)^{1/\gamma_b}, \quad (24)$$

$$\beta \equiv [1 + 4\epsilon(\epsilon-1)B^2]^{1/2}. \quad (25)$$

This result accurately predicts the final explosion pressure. In the limit $P_{set}/P_0 \to 1.0$ the results are especially encouraging, with Eq. (23) representing the numerical solutions of Eq. (20) to better than 10%.

Equation (23) for the final explosion pressure is more complex than the proceding equation for the flat flame, viz., Eq. (21). Fortunately accurate predictions can be made with Eq. (21) as long as $P_{set}/P_0 > 1.3$. This is usually the case in practice. In the next section we compare the predictions of Eq. (21) with available numerical and experimental results.

DISCUSSION

Bradley and Mitcheson [3] have provided computer solutions of laminar (ϕ = 1) spherical burning within a vented vessel which are free from many of the approximations invoked here. Their analysis included a reaction zone of finite thickness, equilibrium chemistry calculations of the burned gas properties allowing for twelve chemical species, and a spatially nonuniform temperature of the burned gas behind the deflagration zone. The calculated peak pressures for a methane–air explosion are plotted in Fig. 2 in a manner suggested by Eq. (21). The accurate computer solution results of Bradley and Mitcheson [3] appear as data points which were read off the theoretical curves provided in their paper for the sonic venting regime. The fact that all their numerical data approximately collapse to a single line close to the straight line represented by Eq. (21) suggests a sound basis for the simple theory presented here.

Chippett [4] carried out an experimental and theoretical investigation of pressures developed in methane- and propane–air mixtures in spheres ranging from 0.65 to 3.8 m³ in size under sonic venting conditions. Figure 3 shows the comparison of Chippett's experimentally determined peak pressures for propane explosions in the 0.65 m³ vessel with his model of vented deflagrations and with Eq. (21). The dark squares in Fig. 3 represent Chippett's data plotted against peak pressures predicted with his model while the open circles represent his measurements positioned according to Eq. (21) with a turbulent correction factor ϕ = 5. Thus, it is necessary to introduce a fivefold increase in burning velocity above that of the laminar values to bring the experimental data into

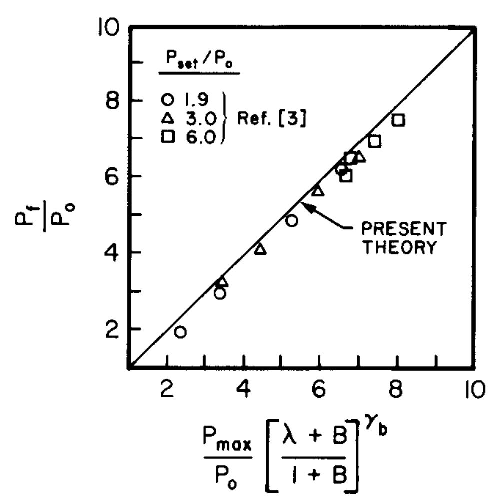

Fig. 2. Peak combustion pressure: comparison of present result and numerical solutions reported in [3].

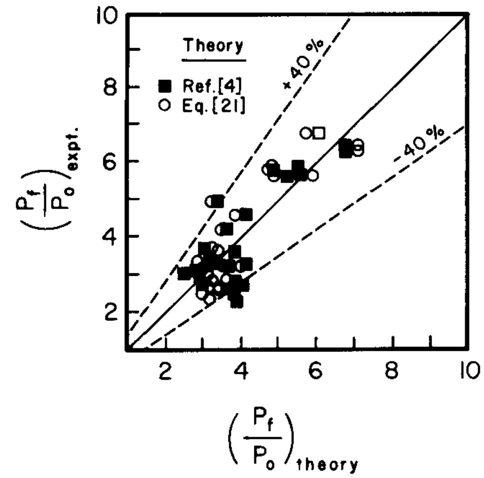

Fig. 3. Peak propane–air measured explosion pressures of Ref. [4] plotted against the predictions of Ref. [4] and against Eq. (21) with $\phi = 5$.

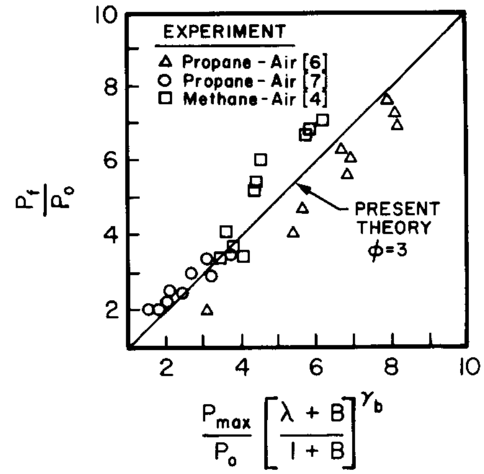

Fig. 4. Peak combustion pressure: comparison of present result with experimental data for propane–air explosions [6, 7] and methane–air explosions [4]

line with the present theory. It is pertinent to note that Chippett presented a rather elaborate numerical model of vented deflagrations involving three empirical flame acceleration parameters that were determined from his experimental data. Despite the complexity of his model, it can be seen from Fig. 3 that it yields no better correlation of the peak pressure data than that obtained with the single ϕ-parameter model presented here.

Measurements of the pressure rise during pentane vapor–air explosions in vented containers having length-to-diameter ratios of order unity have been made by Cousins and Cotton [6] in a 0.032 m^3 vessel and by Donat [7] in vessels of 1, 10, and 60 m^3. Some of their results obtained in the sonic venting regime have been recast in the form of the foregoing theory and are plotted in Fig. 4, where they may be compared directly with Eq. (21). Also plotted in Fig. 4 are the peak pressures measured by Chippett [4] in his study of methane–air explosions in 1.9 m^3 and 3.8 m^3 spherical vessels. The experimental peak pressure data have been plotted by assuming $\phi = 3$. The circular data points were obtained from empirical curves reported by Donat [7]. The data from the Cousins and Cotton study fall somewhat below the theoretical curve, while that of Chippett's study lie somewhat above the theory; nevertheless, the data trends are parallel to the curve and, therefore, better agreement with Eq (21) can be achieved by simply assigning a lower value of ϕ to Cousins and Cotton's [6] data and a higher value of ϕ to Chippett's [4] methane–air data.

Clearly, a single value of the turbulence correction factor ϕ does not yield accurate values for the peak pressure measured in all the venting deflagration studies mentioned in the foregoing discussion. A possibly important parameter (that is not included in the model) is the vessel geometry, which was different in each of these experimental studies. In nonspherical vessels a part of the flame may contact the vessel wall, with a resulting heat loss and reduction in maximum pressure, well before the deflagration is completed. Quenching by vessel walls can also occur if the ignition position is noncentral. Indeed, Cousin and Cotton [6] ignited their hydrocarbon–air mixtures at the vessel wall and their measured peak pressures require the lowest value of ϕ to give agreement with the theory.

Differences in the required value of ϕ not only arise between peak pressure data taken by various investigators using different vessels, but also between data taken in the same vessel. Figure 3 shows the scatter in the peak pressure data obtained from Chippett's [4] study of propane–air flames. Turbulence correction factors that range between $\phi = 3$ and $\phi = 10$ are required to account for the different peak pressures measured under essentially fixed initial conditions in the same vessel. Chippett suggests that the poor reproducibility may be due to slight variations in the gas mixture composition, which presumably could influence the stability of the flame when the vent opens, and to incomplete vent openings when the set pressure is reached.

CONCLUDING REMARKS

A simple model of spherical, sonic-vented deflagrations in hydrocarbon–air mixtures has been pursued here to the point of yielding an approximate closed-form expression for the peak explosion pressure. This approximate expression offers a generally useful correlation of the results of numerical computations of laminar, sonic-vented deflagrations. The model incorporates turbulence by simply multiplying the laminar burning velocity by a constant turbulence correction factor ϕ. The difficulty of employing the model in practice derives from our ignorance of ϕ; it is required to obtain it for each system by experiment. The spherical flame model adopted here represents a considerable idealization of actual combustion venting conditions. Distortion of the flame shape is known to occur as a result of asymmetric venting and hydrodynamic instabilities. These phenomena are at present unquantifiable and, accordingly, in current *numerical* treatments of combustion venting involving variable turbulence factors it is also necessary to make parameter adjustments (see, e.g., [4]) or to choose an appropriate turbulent Reynolds number [2] to account for observed flame acceleration effects. In view of the fact that a quantitative description of flame acceleration effects is still far off,[3] it seems best to employ a constant turbulence correction factor and gain the corresponding simplicity, rather than to carry more elaborate equations through a train of numerical computations whose accuracy is also limited to only a narrow range of experimental conditions. Moreover, the present one-parameter result provides a convenient tool with which the magnitude of the deviation of actual behavior from idealized laminar combustion venting can be readily determined.

[3] The recent photographic study of venting gaseous explosions by McCann et al. [8] represents another step toward our understanding of the mechanisms that produce flame acceleration.

NOTATION

A_s	surface area of vessel ($4\pi r^2$); m^2
A_v	vent area; m^2
B	dimensionless burning number; Eq. (15)
G	sonic mass discharge flux of unburned gas; kg/(m^2 s)
m	mass of gas; kg
P	pressure; kg/(m s^2)
P_f	final peak pressure at the end of combustion; kg/(m s^2)
P_{max}	maximum combustion pressure in a closed vessel; kg/(m s^2)
P_{set}	set or bursting pressure of the vent; kg/(m s^2)
r	instantaneous radius of spherical deflagration wave; m
R	radius of (equivalent) spherical vessel; m
S_u	"laminar" burning velocity; m/s
t	time; s
T	absolute temperature of gas; K
V	volume of vessel ($4/3\pi r^3$); m^3
Z	dimensionless burn volume; Eq. (10)
Z_{set}	dimensionless burn volume when the vent opens
γ	ratio of specific heats
ρ	gas density; kg/m^3
ϕ	turbulence correction factor

Subscripts

b	refers to the burned gases
0	refers to conditions in the vessel at ignition
u	refers to the unburned gases

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