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# A computational platform for gas explosion venting

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ABSTRACT

Explosions occurring in enclosures can be found in many technological applications such as internal combustion engines and typical chambers contacting combustibles. However, it is also possible to reach these events in facilities and buildings because of the leakage of a flammable gas, with usually devastating consequences. In this respect, vents are designed to relief the explosion-associated overpressures by allowing part of the fuel mixture gas to evacuate as the flame propagates. In the present work, a computational model is developed to analyse such vented explosion scenarios. The model solves the corresponding governing equations in a single-zone approximation, including the external explosion produced once the vented mixture is ignited by the expanding flame, to calculate the attained overpressures in relation to the domain geometry and burning conditions. A parametric study is performed varying the container dimensions and shapes, given by cuboids and cylinders with central and rear ignition locations, as well as the concentrations of a hydrogen-air fuel mixture. Moreover, different flame velocity expressions are employed to account for a variety of effects influencing the flame dynamics. A mitigating effect of the vent on the enclosure explosion intensity is demonstrated, thereby relating the different conditions to the attained burning regime, essential for the establishment of safety considerations in these partially confined enclosures.

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## 1. Introduction

The damage produced by a gas explosion is related to the internal pressure rise resulting from the combustion process, which can be large enough to create catastrophic consequences (CNN, 2014). Procedures to mitigate this damage suggest incorporating vent areas, and associated construction standards have been developed therein (NFPA, 2013; European Standard, 2007). However, such procedures are mostly based on correlations, which result in questionable technical suggestions since some features of the burning process may not obey the statistical criteria used for their development (Tamanini and Valiulis, 1996). In turn, approaches based on numerical simulations should deal with large enclosures and with the turbulent burning regime related to these scales, making the simulations computationally expensive. In this study, a framework of governing equations describing vented explosions is developed and the resulting non-linear system of equations is solved in order to quantify the time evolution of the pressure rise in the enclosure. An illustrative sketch of the problem is shown in Fig. 1. Within a single-zone approximation, the physical, chemical and thermal processes are captured by solving a system of non-linear time-dependent conservation equations, to provide a description of the mass, temperature and pressure of burned and unburned gases at given geometry and fuel conditions. Moreover, the solver accounts for the effects produced

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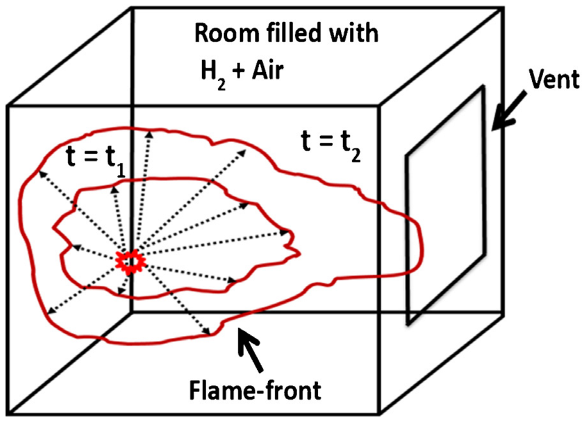

**Fig. 1 – Flame propagation taking place in a vented enclosure.**

by the asymmetric flame propagation and the external explosion, underestimated in previous mathematical descriptions, as discussed in Fairweather and Vasey, 1982.

The complexity of vented explosion events can be noticed by the non-monotonic nature of the process (Cooper et al., 1986). The internal pressure is permanently modified by the venting rate and confinement conditions, including the extinction of the flame at the walls. Multiple peak overpressures have been reported experimentally (Chao et al., 2011), which result from different physical causes. Namely, a peak overpressure is generated by the external explosion triggered once the flame reaches the vent area; a second peak may be produced by acoustic effects as a result of the interaction between the expanding burning material and the walls, and even a third peak can be attained if obstacles are included, namely, as a result of the enlargement of the flame surface when propagating within obstructed domains.

In this work, a parametric study of vented enclosures is performed. The investigated cases were set by considering multiple vent sizes, container shapes (given by parallel cuboids and cylinders of variable dimensions, including closed spheres for validation purposes), rear and central ignition locations, as well as different formulations to model a variety of effects influencing the flame velocity. While the present work is limited to hydrogen air combustion of variable concentrations, the analysis can readily be extended to other fuel mixtures, provided that the associated property data is available.

## 2. Mathematical formulation

In this section, a summary of the mathematical model is presented, starting with the model assumptions, and followed by the set of conservation equations and the auxiliary relations that are new to this work. The backbone of the formulation was proposed by Mulpuru and Wilkin (1982). Here, the analysis Mulpuru and Wilkin (1982) is modified and extended to address new elements regarding the flame shape, propagation velocity and enclosure shape, along with the effect of an external explosion. The set of assumptions constituting the present formulation are listed below.

### 2.1. *Model assumptions*

The model assumptions employed in the present formulation are

- Point-ignited combustion process
- Burned and unburned gases obey the ideal gas law.
- Compression and expansion of the unburned mixture are isentropic processes.
- The gas properties and pressure distribution are assumed to be spatially uniform.
- Potential acoustic effects are neglected (in the practical reality, the effect of acoustics can be mitigated, for example, by including corrugated walls (Harrison and Eyre, 1987)).
- The compartment does not have internal obstacles.

### 2.2. *Governing equations*

#### 2.2.1. *Mass balance*

The rate of change of the total mass can be considered as the sum of three components, namely:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m_u}{m_\mathrm{i}}\right)+\frac{\mathrm{d}}{\mathrm{d}t}(n)+\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m_v}{m_\mathrm{i}}\right)=0, \tag{1}$$

where $n = m_b/m_\mathrm{i}$ is the fraction of the initial mass burned, and the subscripts $u$, $b$, $v$ and $i$ designate unburned, burned, vented and initial conditions. The first term in parenthesis can be modified by using the isentropic relation $P/\rho^{\gamma_u} = \text{const}$ as

$$\frac{m_u}{m_\mathrm{i}}=\bar{\mathrm{P}}^{1/\gamma_u}\left(1-\bar{\mathrm{V}}\right), \tag{2}$$

where $\bar{\mathrm{P}}=\mathrm{P}/\mathrm{P}_\mathrm{i}$ is the current to initial pressure ratio, $\gamma_u = (\mathrm{C_P}/\mathrm{C_V})_u$ the unburned gas specific heat ratio, and $\bar{\mathrm{V}}=\mathrm{V}_b/\mathrm{V}_\mathrm{i}$ the fraction of initial volume currently occupied by the burned gas. The vented mass rate, defined by the last term in Eq. (1), is given by the orifice discharge relations (Bradley and Mitcheson, 1978) as:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m_v}{m_\mathrm{i}}\right)=\mathrm{C}_d\frac{\mathrm{A}_v\rho}{m_\mathrm{i}}\left[\frac{\mathrm{P}}{\rho}\left(\frac{\gamma+1}{2}\right)^{((\gamma+1)/(\gamma-1))}\right]^{1/2}, \tag{3}$$

for the choked condition $\left(\mathrm{P}_a/\mathrm{P}\le 1/\bar{\mathrm{P}}_\mathrm{critical}\right)$, and

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m_v}{m_\mathrm{i}}\right)=\frac{\mathrm{C}_d\mathrm{A}_v}{m_\mathrm{i}}\left[\frac{2\gamma\mathrm{P}\rho}{\gamma-1}\left(\frac{\mathrm{P}_a}{\mathrm{P}}\right)^{2/\gamma}\left[1-\left(\frac{\mathrm{P}_a}{\mathrm{P}}\right)^{(\gamma-1)/\gamma}\right]\right]^{1/2} \tag{4}$$

for the subsonic condition $\left(\mathrm{P}_a/\mathrm{P}>1/\bar{\mathrm{P}}_\mathrm{critical}\right)$, where $\mathrm{C}_d$ is the coefficient of discharge, $\mathrm{A}_v$ the vent area, $\rho$ and $\gamma$ the density and specific heat ratio of the venting gas (either burned or unburned gas), and the critical pressure given by:

$$\bar{\mathrm{P}}_\mathrm{critical}=\left(\frac{\gamma+1}{2}\right)^{\gamma/(\gamma-1)}. \tag{5}$$

The exit pressure, $P_a$, remains constant at the atmospheric value until the occurrence of the external explosion, as will be discussed in Section 2.3.3.

#### 2.2.2. *Burning rate*

The burned mass formation, $n = m_b/m_\mathrm{i}$, is formulated according to the definition of burning velocity as

$$\frac{\mathrm{d}n}{\mathrm{d}t}=\frac{1}{m_\mathrm{i}}\rho_u\mathrm{S_T}A, \tag{6}$$

where $\mathrm{S_T}$ is the flame velocity with respect to the fuel mixture and $A$ represents the flame surface area. Similar to Eq. (2), the

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