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Simplified multiple equations' inverse problem of vented vessels subjected to internal gas explosions

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ABSTRACT

This paper analyses the experimental data reported by Höchst and Leuckel (1998) for combustion in partially confined vessels and uses the data from these experiments to establish the burning rate based on a simplified model for the combustion process in such vessels. The model establishes three fundamental parameters which are necessary in characterizing the combustion process. These are: i) the burning rate, ii) the fraction of vent area occupied by burnt gas (or discharge sub-model), and iii) the vent area model (if cover mechanisms with variable vent areas are utilized). A set of independent equations is derived to determine the burning rate according to conservation of mass and volume for each gas fraction separately along with a general equation based on general volume conservation. Using this method we are able to describe the combustion process and examine the effect of various discharge models. The advantages of the model presented here include rapid applicability and a valuable analysis to derive mass burn rate and other useful parameters using experimental data from vented explosions with reasonable residual reactant values. Based on these results, the correct interpretation of the obtained burning rate can be used in order to explain the correct prediction of flame velocity and position according to a reasonable discharge model. The paper also evaluates the suitability of several discharge models for phenomenological models of vented explosions. The most appropriate is a Heaviside step function which considers that only unburnt gas is initially expelled, with that component decreasing and the burnt gas component increasing until finally only burnt gas is expelled. The obtained results in this study can be used to predict the burning rate behavior and the combustion process of similar problems.

1. Introduction

Venting is a widely applied method to mitigate consequences of internal explosions in vessels. Hence, methods to predict venting effects with reasonable accuracy and speed are important in order to derive an appropriate design. In general, studies of vented gas explosions have shown that the evolution of pressure with time depends on the nature and state of the initial fuel/oxidant mixture (composition, initial pressure and temperature), the vessel characteristics (dimension, shape and flexibility), the vent features (locations, areas, strengths, weights, shapes and mechanisms), the pre-ignition turbulence, the presence of obstacles (positions, distribution, sizes, shapes), location of the ignition source and other combined effects (Razus and Krause, 2001).

In general, gas explosion models can be divided into three categories: i) Venting Guidelines, ii) Computational Fluid Dynamics (CFD) models, and iii) Phenomenological models (Zalosh, 2008).

Venting guidelines are empirical and semi-empirical equations which are commonly used to determine the required vent area in order that the maximum internal pressure can be restricted to a pre-defined design value (e.g., [4–7]). In general, venting guidelines are the most widely used models due to the fact that they provide simplest design procedure, are not time consuming, do not require sophisticated and complex modeling or a profound knowledge of the physical process. However, these formulas are valid only within the conditions covered by the experiments used to fit these semi-empirical curves (restricted to certain limits of parameters associated with the vessel, the vent and the explosive mixture characteristics). Also, these equations do not provide information about

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the pressure time-history (duration, distribution, shape and impulse) acting on the enclosure's walls. As a consequence, chambers are usually designed through equivalent static methods based on conservative dynamic load factors (NFPA 68, 2007 Edition).

Computational Fluid Dynamics (CFD) models are based on the fundamental partial differential equations which describe the explosion phenomenon. That is, conservation equations of mass, momentum and energy (i.e. Navier–Stokes) as well as additional parameters for chemistry and shock waves where applicable are utilized to describe the fluid behavior, and are combined with physical models to include the effects of turbulence. Indeed, equations are discretized and solved for finite volumes or cells. Several CFD software packages are currently available to simulate gas explosions such as EXSIM, FLACS, AutoReaGas, CFX-4, COBRA. In general, CFD models provide detailed information and they are able to predict more accurate results over a wider range of geometries and conditions than guidelines or phenomenological models if they are properly applied. However, CFD models have not been widely tested against experimental data for confined vessels. For practical purposes, the detailed modeling of vented explosions through CFD models can be excessively sophisticated and time consuming and even not feasible for large and complex geometries (Razus and Krause, 2001).

Phenomenological models such as Yao's model (Yao et al., 1969), CINDY (Molkov et al., 2004b), SCOPE3 (Puttock et al., 2000) or CLICHE (Chippett, 1984) are simplified physical models based on pseudo-empirical sub-models. These are valid for some particular idealized conditions, i.e., the vent models, combustion models, the turbulent and laminar flame velocity models and flame shape modes are idealized depending on the geometry, the mixture conditions and the turbulence caused by repeated obstacles and their respective interactions. Phenomenological models are based on a set of coupled time dependent differential equations which are solved numerically to obtain the deflagration pressure as a function of time. These models can give reasonable results when simple geometries are under consideration (similar to the predefined model geometry; for example, large vessels with repeated obstacles). In fact, these models have been successfully calibrated and validated against hundreds of explosion experiments (Zalosh, 2008). The computational times used for phenomenological model solutions are commonly low (of the order of a few seconds), and in fact far lower than the computational requirements of CFD software packages. However, phenomenological models may be inaccurate when more complex geometries are under consideration or sub-model assumptions are insufficiently validated.

In general, phenomenological models and venting guidelines can be used as a benchmarking guideline prior to carrying out detailed CFD simulations. Phenomenological models depend on the burning rate model and the venting model. Indeed, phenomenological models determine the burning rate from sub-models which take into account several effects on the flame area and the flame velocity based on simplified empirical and logical correlations. Examples of this include the flame self-acceleration, the turbulent burning velocity, the flame shape mode, and other effects (Puttock et al., 2000). However, these models are accurate for certain simplified conditions and valid for limited ranges of parameters associated to conditions employed to determine these empirical approaches. Therefore, the burning rate can be erroneously predicted if conditions are different to experimental ones and/or their related parameters are outside of their validation ranges.

The burning rate for phenomenological models has been indirectly determined from experimental data through the inverse problem (e.g., Yao et al., 1969; Molkov et al., 2004b; Molkov et al., 2003). That is, the turbulent to laminar flame speed ratio (called also stretch function) is determined assuming a spherical flame mode and simplified models of the burning velocity in order that the pressure time-history obtained by the model is fitted to the experimental data. However, the stretch function is constrained to be a constant factor or a monotonic growing sequence, which does not always fit the experimental data (Yao et al., 1969). For example, the flame deceleration cannot be modeled by a mere constant or growing stretch function. As a result, the radical changes on the flame shape can be misinterpreted as the flame velocity varies if the assumed propagation mode (e.g. spherical or hemispherical) differs from the actual case.

The vent model used by most of the phenomenological models uses classical equations for ventilation through orifices (or valves) of pressurized vessel filled with quiescent gases. Venting occurs without any disturbance to the gas in the vessel. For this, isentropic processes are assumed and sonic or subsonic mass flow regimes are considered (Ferguson and Kirkpatrick, 2001). In general, the effective vent area is estimated from a discharge coefficient which takes into account the reduction of vent area downstream of the orifice. The discharge coefficient is assumed equal to experimental values obtained for pressurized tanks with individual gases depending on the geometry and mechanism of the vent (Yao et al., 1969); alternatively, more accurate models consider a variable discharge coefficient depending on the vent mechanism and the flow regime (e.g. the Reynolds number) (Ferguson and Kirkpatrick, 2001). The venting process of vessels subjected to internal deflagrations involves the discharge of two different gaseous mixtures (the burnt and unburnt gas fractions). Thus, a discharge sub-model which defines the fraction of reactants and products which are been vented is required in order to establish the expelled mass for each gas which are at different densities and temperatures. In general, the discharge sub-model is defined as a variable temporal function which states the fraction of the total vent area through which burnt gas flows (Yao et al., 1969; Molkov and Nekrasov, 1981). In particular, some simplified assumptions about the sub-charge model has been utilized: i) only the unburned gas is flowing out (e.g., Yao et al., 1969; Molkov and Nekrasov, 1981; Molkov et al., 1997b); ii) the amount of the out-flowing gases is directly proportional to the ratio of burned and unburned gases remaining inside the vessel (Yao et al., 1969); and iii) a joint discharge of the fresh mixture and combustion product: $A = r^2 = (V_b/V)^{2/3}$, where A is the portion of the discharge cross-sectional area occupied by combustion product, and r is the relative radius of the flame (e.g., Molkov and Nekrasov, 1981; Molkov et al., 1997a; Molkov et al., 1999). However, the consequences of different discharge sub-models have not been deeply studied and not well explained.

This article presents a simplified phenomenological model based on the same principle that other models have described before (e.g., Molkov's model). However, the treatment of equations is used in a different manner than previous studies. In general, the main advantage of the method is related to the direct derivation of the burning rate from experimental pressure time-history data relying on an appropriate vent model which is consequently disaggregated. As a consequence, the burning rate is a function variable with time, i.e., the turbulence function is not restrained to be described by a constant turbulence factor or a monotonic growing sequence. Finally, the accuracy of the ventilation model can be studied depending on the interpretation of results. That is, the coherency between results obtained for each individual equation and the explanation of the results such as the residual unburnt mass gas fraction are employed as indexes to calibrate and chose an appropriate ventilation model.

The simplified phenomenological model relies on conservation of mass and volume, a general burning rate function, a classical venting model and assumption of ideal gas behavior for each individual gas fraction. A system of independent multiple equations