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Critical review of Molkov's phenomenological model and variable stretch/turbulence function

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ABSTRACT

A critical review of Molkov's phenomenological model including the model's assumptions and sub-models is presented in this article. First, the effect of an incorrect discharge sub-model is studied and it is concluded that the choice of discharge sub-model is crucial because it can substantially modify the turbulence/stretch function, the mass distributions and the flame position. Therefore, a discharge sub-model should only be chosen when the sub-model is in agreement with the flame position and the residual unburnt gas mass reaches a reasonable value. Second, the equivalent flame radius and the apparent flame velocity (computed internally by Molkov's model) are found to depend on three different effects: the free flameball expansion, the adiabatic compression/extension and the venting process. Third, the interpretation of the turbulence function should account for the effect of the propagation mode and the spatial variation of the local flame speed. Fourth, the jet effect model related to hinge panels can be improved; therefore, a new model is presented. Fifth, the universal correlation and the two-lumped-parameter model are studied. Despite the high correlation reported in previous publications, it is concluded that the two-lumped-model has significant limitations and should be improved if a variable stretch/turbulence function is utilized, which will require the utilization of "usual" discharge coefficients. Finally, it is shown that the inverse problem with a variable stretch/turbulence function and a reasonable discharge coefficient can be utilized to accurately backfit experimental data.

1. Introduction

Venting is one of the most effective techniques used to reduce damage in vessels subjected to internal gas explosions. Therefore, methods to predict vent effects are essential if partially confined vessels are to be built to withstand these gas explosions. These models aim to restrict the maximum pressure (impulse, or pressure time-history) during an accidental explosion to within an acceptable range.

Molkov's phenomenological model of vented explosions was originally derived for partially confined vessels with a unique opening and filled with a flammable homogeneous gas/oxidant mixture (Molkov and Nekrasov, 1981). Molkov et al. subsequently extended the model to include vessels with multiple vents and/or different vent mechanisms (which have been generally described by SDoF systems) (Molkov, Eber, Grigorash, Tamanini and Dobashi, 2003), (Molkov et al., 2004b), (Molkov et al., 2005b). Molkov's model assumes that unburnt and burnt gas fractions can be described separately by the ideal gas Equation of State (EOS), with both gasses following adiabatic processes. Thus, the model depends on several thermodynamic and combustion coefficients related to the unburnt and burnt mixtures. Molkov's model also assumes that the flame is propagates laminarly following a spherical surface mode. The model's derivation relies on conservation of mass, volume and energy (Molkov et al., 2004a,b) and assumes that pressure is uniform throughout the enclosure but varies with time. Outflow gas mass rates are determined from classical equations of pressurized vessels assuming isentropic gas flows through the valves or orifices. The model is described by a set of three ordinary differential equations (the dimensionless pressure, the dimensionless burn mass and the dimensionless unburnt mass, appendix) and another second order differential equation related to the SDoF mechanism which describes the vent system and/or variation in the vent area.

Overall, Molkov's model depends on three transient functions

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that relate the rate of change of the burnt and unburnt gases. They are: i) the discharge model, ii) the vent area model (for variable vent areas), and iii) the burning rate. The implications of these three functions for the model are discussed in the following sections. Possible improvements include: i) extension of equations after combustion has finished, ii) a variable stretch/turbulence function which is not restrained to a monotonic growing sequence, and iii) vent model improvements associated with more accurate jet effect coefficients for hinge covers and inclusion of dynamic effects resulting from arresting and/or cover activation. Finally, the inverse problem with a non-monotonic stretch/turbulence function and a constant reasonable discharge coefficient has been studied based on numerical optimization tools in order that the simulated pressure time-history is backfitted by small time segments to the experimental data, obtaining a more accurate burning rate function which is similar to results obtained through the multiple equations inverse problem (Hernandez, Abdel-jawat, & Hao, 2015).

2. Discharge model

Discharge models are used to estimate the amount of gas expelled from a vessel through vent devices due to the difference between the internal and the external pressure (i.e., the overpressure) attained during the deflagration process. These discharge models are based on outflow mass discharge rates calculated according to traditional backfitted theoretical equations derived for pressurized vessels ventilated by orifices or valves (or the standard orifice equation). That is, the mass flow is computed assuming an isentropic mass flux and described by the following equation (Ferguson and Kirkpatrick, 2001),

$$\left.\frac{dm}{dt}\right|_{out} = \mu \cdot F(t) \cdot G(t) \tag{1}$$

where, $G(t)$ = the mass flow rate per unit area or mass flux (kg/m^{2}*s), μ = discharge coefficient, $F(t)$ = vent area (m^2) (related to the vent area model).

The mass flow rate ($G(t)$) depends on the expelled gas mixture, the overpressure and the outflow velocity (sonic or subsonic regimes). This quantity is described in the appendix and not discussed further in this article. The variation of the vent area with time ($F(t)$) is determined by a system of differential equations which describe the dynamic behavior of the vent mechanism as a function of the overpressure-time history. This mechanism is defined as the vent area model and is discussed in the following section.

2.1. Discharge coefficient

The discharge coefficient (μ) takes into account the Venturi effect and the energy losses due to turbulence that arise during the ventilation process. In other words, the discharge coefficient can be understood as a factor that accounts for the effective vent area ($\mu \cdot F(t)$) through which pressurized gases are discharged without energy loss. Therefore, the discharge coefficient should be less than or equal to one. Bradley and Mitcheson (1978) recommend that a constant discharge coefficient of $\mu = 0.6$ be used for vessels with sharp edges depressurized by vents whose areas are smaller than the cross-section of the vessel. However, other discharge coefficient values have been recommended for other kinds of vent geometries and/or enclosure sizes and shapes. For instance, Yao et al. (1969) recommend ignoring energy losses and setting $\mu = 1.0$ when an entire end of an enclosure is used as vent. This group also suggested that the effective vent area is almost equal to the entire vent area ($\mu = 0.98$) when a rounded nozzle is utilized as an opening. Other studies have suggested considering the discharge coefficient variable with time; for example, approaches that change according to the flow regime or the Reynolds number (Annand and Roe, 1974). Overall, irrespective of the choice of discharge coefficient, either simple or complex discharge models (which consider several conditions such as the vent size, the kind of vent mechanism, the vent position, the enclosure geometry, the outflow velocity, the vent orientation and the induced ventilation turbulence) can be used indiscriminately without reducing generalization of Molkov's equations. In most cases, a constant discharge coefficient can be used without a significant reduction in the accuracy of the model.

In the situation that the vent area is variable with time, the discharge coefficient should be compatible with the vent area model in order that both can predict the effective vent area. When pressurized gases are discharged through valves (with variable vent areas), experimental studies have shown that the discharge coefficient ($\mu = 0.6$) does not change significantly if the vent area is calculated through the curtain area ($F(t) = min(Cover_{perimeter} \cdot u(t), F_N)$) rather than the full seat area (F_N) (Annand and Roe, 1974). Similarly, when pressurized gases are discharged through pull out panels the discharge coefficient does not change significantly because inertial vent panels have been found to behave in a similar way to valves.

Derivations of the mass flow expelled from a pressurized vessel through valves assume that the gas inside the vessel is resting (average velocity equal to zero). However, the combustion attained during the course of the flame triggers the expansion of gases which pushes the gas ahead of the flame, generating a velocity gradient just before the gas is expelled. To "compensate the difference between real and calculated mass out-flow rates, in particular due to the non-zero velocity of outflowing gases inside the enclosure proposed during deduction of standard orifice equations" (Molkov, Dobashi, Suzuki and Hirano, 2000), Molkov et al. justified the use of "unusual" discharge coefficient values (as high as $\mu = 1.50$ for vessels without obstructions (Molkov et al., 2000) and $\mu = 3.15$ for vessels with obstructions (Molkov et al., 1997a,b)).

The uniform pressure assumption, however, contradict the significant gas velocity statement. A uniform pressure implies that the dynamic pressure is insignificant. In contrast, a substantial gas velocity should be related to a gradient of pressure along the vessel. In cases where the combustion is described by a slow deflagration process (assuming that the gas velocity is slower than 25% of the sound speed and/or the Mach number is less than 0.25, $Ma = v_{gas}/v_{sound}$), the dynamic pressure is insignificant in comparison to the effect of overpressure caused by the explosion. This can be proved by estimating the dynamic pressure associated with the gas velocity based on the Bernoulli principle and equal to $\Delta P_{eq} = v_{gas}^2 \cdot \rho_{mix}/2 = Ma^2 \cdot \gamma_{mix} \cdot P/2$; thus, the equivalent pressure is only increased 4.4% ($\Delta P_{eq} = 0.25^2 \cdot 1.4 \cdot P/2 = 0.044 \cdot P$, and $\gamma_{mix} = 1.4$) when the gas travels with a hypothetical gas velocity associated with a Mach number of 25% ($v_{gas} \approx 88 m/s$ for stoichiometric methane/air mixtures), or increased 0.7% for Mach numbers lower than 10% ($v_{gas} \approx 35 m/s$). Therefore, the increase of dynamic pressure due to the gas velocity effect can be ignored in most cases. According to Molkov's method, this effect is ignored and the pressure is considered uniform throughout the enclosure space and variable in time, if the Mach number derived from the apparent flame velocity is less than 0.1 (Vladimir Molkov, Dobashi, Suzuki and Hirano, 1999) or 0.25 (Molkov et al., 1997a,b). As the uniform pressure assumption is essential for Molkov's model derivation, a flame Mach number equal to 0.10 (or 0.25) has been conventionally considered like the limit of application of Molkov's method. Observe that the gas velocity should be less than the flame velocity; therefore, the effect on the dynamic pressure was studied with the maximum