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Investigation of concentration effects on the flame acceleration in vented channels

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ABSTRACT

Propane–air gas explosion experiments were performed in two vented channels of dimensions 1.5 m × 0.3 m × 0.3 m (lab-scale) and 6 m × 1.2 m × 1.2 m (medium-scale). The pressure–time development and flame speed were recorded. Tests were performed with several obstacle configurations. The equivalence ratio ϕ was varied between 0.7 and 1.7, to study the corresponding effects on the flame acceleration and maximum explosion overpressure. The experimental results were compared to numerical simulations performed with the computational fluid dynamics (CFD) tool FLACS, employing two different burning velocity models: (i) the standard burning velocity model in FLACS, (ii) an alternative burning velocity model that incorporates Markstein number effects. Both models gave acceptable predictions of the experimental maximum overpressures for $\phi < 1.4$. For fuel-rich mixtures, $\phi > 1.4$, the standard burning velocity model in FLACS generally under-predicted the maximum overpressures. The Markstein number-dependent burning velocity model gave improved results, consistently predicting overpressures within ±10% of the experimental values.

1. Introduction

In order to predict the consequences of accidental gas explosions in realistic geometries, it is necessary to consider the small-scale interactions between the flame zone and the flow, and how they feed back to the larger scales. The use of computational fluid dynamics (CFD) for explosion consequence analysis in the process industries therefore increases. CFD software computes approximate solutions to a set of partial differential equations describing fluid flow in time and three-dimensional space. However, in order to carry out efficient gas explosion simulations for real process facilities, a range of sub-grid models must be invoked to allow for grid cell sizes of 1–2 m. These cell sizes are generally larger than the flame thickness, and are often larger than important geometry details and the turbulence length scales generated during the explosion. Extensive model validation is necessary to ensure that sub-grid models are appropriate for the applications where they are used (Skjold et al., 2013).

The majority of large-scale gas explosion experiments found in the literature have been performed using near-stoichiometric fuel–air mixtures, as these often have the highest laminar burning velocity and are assumed to lead to the most severe consequences. These experiments form the validation basis for the sub-grid models in CFD tools. To improve the validity of sub-grid models for more general scenarios, it is crucial to further extend the matrix of gas explosion experiments involving off-stoichiometric mixtures, complementing earlier studies (Wingerden and Zeeuwen, 1983; Hjertager et al., 1988; Skjold et al., 2014; Bauwens et al., 2015).

Bradley et al. (2013) recently proposed a correlation for the turbulent burning velocity in terms of the strain rate Markstein number Ma_{sr}, to account for the response of laminar flamelets to stretch rates in a turbulent flow. Markstein number effects are important also at low turbulence levels, e.g. for spherical flame propagation in the initial phase of gas explosions under initially quiescent conditions (Bradley, 1999; Bradley et al., 2001; Jomaas et al., 2007).

This paper presents results from 42 propane–air gas explosion experiments where the equivalence ratio ϕ of the homogeneous fuel–air mixture was varied between 0.7 and 1.7. The experiments

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were done primarily to produce additional validation data for numerical models, and to investigate whether a burning velocity model that incorporates Markstein number effects would be beneficial for predicting the consequences of gas explosions in lab-scale and medium-scale rigs with varying obstacle configurations. Overpressures and flame speeds were compared to numerical simulations performed with the CFD tool FLACS (GexCon AS, 2015).

2. The numerical model

The CFD tool FLACS solves the three-dimensional Favre-averaged conservation equations for the densities of mass ρ, momentum ρu_i, enthalpy ρh, turbulent kinetic energy ρk, rate of dissipation of turbulent kinetic energy $\rho\varepsilon$, mass-fraction of fuel ρY_f and mixture-fraction $\rho\xi$ on a structured Cartesian grid. The equations are closed by invoking the ideal gas equation of state and the standard $k-\varepsilon$ model for turbulence (Launder and Spalding, 1974). Boundary layers are not resolved in FLACS, instead wall-functions are used to compute turbulence production and drag forces for objects that are on-grid, i.e. larger than the size of a computational cell (GexCon AS, 2015).

Geometry is represented on the computational grid using the porosity/distributed resistance (PDR) concept (Hjertager, 1986; Bakke, 1986). A volume porosity β_v, denoting the ratio of open volume to the total volume of each computational cell, is computed prior to the simulation and defined at the respective grid cell centre. Similarly, area porosities β_j represents the ratio of the projected open area between two neighbouring cell centres to the total area of the respective control volume face. The general variable Φ (representing either ρ, ρu_i, ρh, ρk, $\rho\varepsilon$, ρY_f or $\rho\xi$) is thus integrated over the porous part of the control volume, and the flux terms in the conservation equation for Φ are weighted with the area porosity β_j:

$$\frac{\partial}{\partial t}(\beta_v\rho\Phi)+\frac{\partial}{\partial x_j}(\beta_j\rho u_i\Phi)-\frac{\partial}{\partial x_j}\left(\beta_j\rho\Gamma_\Phi\frac{\partial}{\partial x_j}\Phi\right)=\beta_v(S_\Phi-R_\Phi), \tag{1}$$

where Γ_Φ is the effective turbulent exchange coefficient; S_Φ is the source term for Φ; and R_Φ represents additional resistance, additional mixing, and/or additional heat transfer caused by solid obstructions in the flow. The $k-\varepsilon$ model is extended to have a source term for the turbulence generation due to sub-grid obstructions.

To model premixed combustion, FLACS applies the flamelet concept with one-step reaction kinetics. Empirical burning velocity expressions that depend on the local mixture reactivity, pressure, temperature and flow conditions are used to model the reaction rate. The reaction rate is coupled with the source term in the equation for ρY_f using a modified version of the eddy dissipation model of Magnussen and Hjertager (Magnussen and Hjertager, 1977; Arntzen, 1998). The flame zone, defined by the gradient of Y_f, is numerically thickened to cover approximately three control volumes.

2.1. Burning velocity correlations in standard FLACS

The laminar burning velocity u_ℓ used in FLACS is based on literature values. An empirical model for the quasi-laminar burning velocity $u_{q\ell}$ controls the phase of cellular flame propagation, accounting for flame acceleration due to hydrodynamic instabilities (Darrieus, 1945; Landau, 1944) and thermo-diffusive effects (Barenblatt et al., 1962; Sivashinsky, 1977):

$$u_{q\ell}=u_\ell\left(1+C_{q\ell}\sqrt{R_f}\right),$$

where $C_{q\ell}$ is an empirical constant defined for each fuel and R_f is the flame radius. The turbulent burning velocity u_t is based on the expression by Bray (1990), correlating the 1650 experiments presented by Abdel-Gayed et al. (1987) according to

$$u_t=0.875u'K^{-0.392}, \tag{2}$$

with the Karlovitz stretch factor $K=0.157(u'/u_\ell)^2R_l^{-0.5}$. Here, R_l is the turbulent Reynolds number based on the integral length scale l, and u' is the root mean square (rms) turbulence velocity. The correlation for u_t is valid for mixtures with Lewis numbers $Le\leq 1.3$ (Bray, 1990). Equation (2) in the form used in FLACS takes mixture reactivity into account only through u_ℓ.

2.2. A Markstein number-dependent burning velocity model

The Markstein number Ma quantifies the effect of flame stretch on the localized burning velocity (Markstein, 1951), and generally depends on the mixture composition, pressure and temperature (Bradley et al., 1998a; Bechtold and Matalon, 2001). The stretched laminar burning velocity u_n can be expressed in terms of the unstretched laminar burning velocity u_ℓ, the laminar Karlovitz stretch factor accounting for flow strain $K_{\ell s}$ and flame curvature $K_{\ell c}$, together with the corresponding Markstein numbers Ma_{sr} and Ma_c (Clavin, 1985; Bradley et al., 1996) as

$$\frac{u_\ell-u_n}{u_\ell}=K_{\ell s}Ma_{sr}+K_{\ell c}Ma_c. \tag{3}$$

It follows from Equation (3) that mixtures with low Ma have an increased effective laminar burning velocity when exposed to positive stretch rates, compared to mixtures with higher Ma. Davis et al. (2002) computed Markstein numbers relative to the burnt gases in counterflow propane–air flames ranging from 3.56 for $\phi=0.63$ to -0.46 for $\phi=1.50$.

The cellular pattern and corresponding flame acceleration appearing at a critical flame radius R_0 in a spherically expanding gas explosion will depend on the value of Ma (Bradley, 1999; Bradley et al., 2001). Assuming that the cellular flame surface follows a fractal pattern, the flame radius R_F for a freely propagating spherical flame as a function of time can be expressed as

$$R_F=R_0+At^b,$$

where A is a mixture specific constant and the time exponent b is related to the fractal dimension D of the flame surface by $D=(3b-1)/b$ (Gostintsev et al., 1988; Bauwens et al., 2015). Bauwens et al. (2015) combined new experimental findings with fractal considerations, and expressed the increase in flame velocity due to cell formation on the flame surface as

$$\frac{u_{q\ell}}{u_\ell}=\left(\frac{R_F}{R_0}\right)^\zeta. \tag{4}$$

The value for ζ in Equation (4) is derived from experimental observations.

Furthermore, the Markstein number affects how the burning rate of flamelets in turbulent premixed combustion responds to the flame stretch rate. In particular, the flamelets in mixtures with negative Ma appear to have significantly higher burning rates compared to mixtures with positive Ma, and are less likely to quench at high strain rates (Bradley et al., 2005). Bradley et al. (2013) expressed the turbulent burning velocity u_t in terms of an