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The role of turbulence in the validity of the cubic relationship

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ABSTRACT

The effect of turbulence on unsteady premixed flame propagation and associated pressure rise during explosion of stoichiometric CH_4/air in closed spherical vessels of different size was investigated by means of CFD simulation. Computations were run by varying the vessel volume from 20 l to 200 l and to 1 m^3.

Numerical results have shown that, at fixed initial conditions, the turbulence kinetic energy induced by the propagating flame increases with increasing vessel volume. It has been demonstrated that the cubic relationship does not apply. Under the conditions investigated, a correction to the cubic relationship has been proposed to take into account the effect of the vessel volume on turbulence.

1. Introduction

In chemical industrial processes, many accidents are due to explosion of flammable mixtures causing huge damages to people and surrounding environment. Prevention and mitigation measures are based on the knowledge of parameters that fully characterize the flammability and explosion features of flammable mixtures. These parameters include the maximum pressure, P_{max}, and the maximum rate of pressure rise, $(dP/dt)_{max}$.

For a given mixture, P_{max} is dependent on the initial conditions of temperature and pressure and on the temperature reached during the explosion. The final temperature is linked to the thermodynamic value and is affected by both, the adiabaticity of the explosion vessel and the nature of the reactive mixture. In vessels with different shapes and/or sizes, the same mixture will give exactly the same maximum pressure, provided that explosion occurs under adiabatic conditions.

Conversely, $(dP/dt)_{max}$ is a kinetic parameter and, as such, is strongly dependent on the flame propagation velocity. This latter is dependent not only on the mixture reactivity, but also on the turbulence level present in the vessel. $(dP/dt)_{max}$ is also dependent on the vessel scale. In particular, it decreases with increasing vessel size. In order to make $(dP/dt)_{max}$ independent of the vessel size, the cubic relationship was developed which allows scaling of the maximum rate of pressure rise, thus obtaining a vessel volume independent parameter, the deflagration index, K_{St} for dust and K_G for gases (Bartknecht, 1989). The deflagration index is the key parameter for design of explosion protection measures and for classification of dust hazard.

The measurement of $(dP/dt)_{max}$ for the evaluation of the deflagration index of dusts was initially performed in a 1 m^3 vessel, which was the only internationally accepted dust explosion testing device (ISO 6184/1, 1985). However, it required much labor and large amounts of powder. As a consequence, the 20 l sphere was tested as an alternative to the 1 m^3 vessel (Bartknecht, 1989; Siwek, 1977, 1988).

The acceptance of the 20 l sphere as a standardized dust explosion testing device was dependent on whether or not it was capable to give the same K_{St} values as the 1 m^3 vessel. The major issue afforded was the control of the turbulence of the dust clouds ignited in the test vessels. Indeed, flame propagation velocity is significantly increased by turbulence. Thus, it has been assumed that tests in vessels with different scales may be comparable only if the initial level of turbulence is the same. Turbulence is generated by the dust injection into the vessel and, as such, it has a transient nature decaying in time. As a consequence, the delay time between dust feeding and ignition definitely identifies a pre-ignition turbulence level.

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For the 1 m^3 vessel, the ignition delay time is 600 ms. This is the minimum amount of time to ensure all of the dust in the reservoir is injected into the chamber, thus allowing maximum turbulence. The ignition delay time in the 20 l sphere was calibrated so that K_{St} values corresponded with those obtained from the 1 m^3 chamber. In particular, it was observed that the 20 l sphere produced K_{St} values that were in agreement with those obtained within the 1 m^3 vessel when the ignition delay time in the former was set equal to 60 ms (Siwek, 1977, 1988). However, van der Wel et al. (1992) showed that the K_{St} values of potato starch, lycopodium and activated carbon measured in the 20 l vessel at 60 ms ignition delay time are significantly different from those measured in the 1 m^3 vessel at ignition delay time equal to 600 ms.

Direct measurements of turbulence in the 20 l vessel and comparison with results obtained in a 1 m^3 vessel showed that comparable turbulence levels are attained in the test vessels when the ignition delay time of the 20 l sphere is 165 ms (van der Wel et al., 1992) or 200 ms (Dahoe et al., 2001; Pu et al., 1990) instead of the standard 60 ms.

All these works are focused on finding the same initial conditions of turbulence for scaling up the results on the measurement of the maximum rate of pressure rise by simply applying the cubic relationship, which does not take into account the effect of turbulence. However, turbulence is also generated by the flame propagation itself inside the vessel. As a consequence, even if the initial level of turbulence is the same, the turbulence evolution may be influenced by the vessel scale, thus resulting in different flame acceleration. In this case, the calculation of the deflagration index as parameter independent of the vessel scale through the cubic relationship may be misleading.

The turbulence induced by the flame propagation is dependent on several parameters, like the vessel scale, the flame velocity, the nature of the combustible substance. As a consequence, in order to scale the maximum rate of pressure rise, the effect of the volume on the turbulence generation has to be taken into account.

The aim of the present work is to study the role of the turbulence induced by the flame propagation in the validity of the cubic relationship. To this end, we performed CFD simulations of unsteady premixed flame propagation during explosion of stoichiometric CH_4/air in closed spherical vessels of different volume (20 l, 200 l and 1 m^3). Simulations were run by setting the same initial turbulence level. The maximum rate of pressure rise was extracted from the computed pressure time histories. Thus, the values of the deflagration index were calculated, by using the cubic relationship, and compared in the light of the turbulence evolution inside the vessels.

2. Description of the model

CFD simulations were run of unsteady premixed flame propagation during explosion in closed spherical vessels of different volume (20 l, 200 l and 1 m^3). In each vessel, an homogeneous stoichiometric CH_4/air mixture was initially present. In all simulations, ignition was positioned at the center of the vessel.

2.1. Computational domain and mesh

The spherical vessels were modeled as tridimensional. In Fig. 1, for all vessels, a two-dimensional view of the computational domain is shown along with the unstructured mesh used. The optimal mesh was obtained by performing simulations at different cell number, converging to the lowest cell number with the highest accuracy. The cell number was equal to 146,000 for the 20 l vessel, 228,000 for the 200 l vessel, and 320,000 for the 1 m^3 vessel.

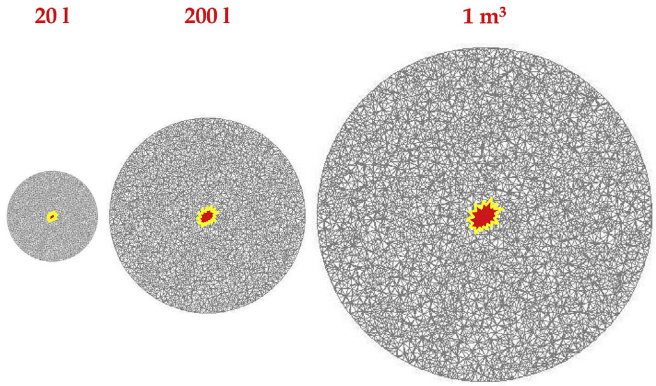

Fig. 1. Two-dimensional view of the computational domain with the unstructured mesh: Vessels of different sizes.

2.2. Equations

The model solves the unsteady time-averaged Navier-Stokes (URANS) equations, which express the conservation for mass, momentum, energy and chemical species. The species transport equation was recast in the form of a transport equation for the reaction progress variable, c ($c = 0$ within fresh reactants and $c = 1$ within burned products) (Libby and Williams, 1994). The URANS equation for c, written in vector form, reads as follows:

$$\frac{\partial \overline{\rho}\, \tilde{c}}{\partial t} + \nabla \cdot (\overline{\rho} \tilde{u} \tilde{c}) + \nabla \cdot [\overline{\rho}\, (\widetilde{uc} - \tilde{u} \tilde{c}\,)] = \overline{\nabla \cdot (\rho D \nabla \mathrm{c})} + \overline{\omega_c} \tag{1}$$

The model equations were solved by using the standard Shear Stress Transport (SST) k-ω model (Menter, 1994) as turbulence submodel. The Peters model was chosen as combustion sub-model to close $\overline{\omega_c}$ in Eq. (1) (Peters, 2000).

2.3. Numerics

The governing fluid flow equations were discretized using a finite-volume formulation on the three-dimensional unstructured grid shown in Fig. 1. The spatial discretization of the model equations used first order schemes for convective terms and second order schemes for diffusion terms. First-order time integration was used to discretize temporal derivatives with a time step of $1 \cdot 10^{-5}$ s. Adiabatic and no-slip wall boundary condition was applied at the solid interface (wall of the spherical chamber).

Parallel calculations were performed by means of the segregated pressure-based solver of the CFD code ANSYS Fluent 15.0 (ANSYS Fluent Theory Guide - Release 15.0, 2013). The Semi-Implicit Method for Pressure-linked Equations (SIMPLE) was used to solve the pressure-velocity coupling. In order to achieve convergence, all residuals were set equal to $1 \cdot 10^{-6}$.

2.4. Simulation conditions

The sphere was initially filled by a stoichiometric CH_4/air mixture. Two kind of simulations were performed: 1) starting from quiescent conditions (absence of turbulence); 2) starting from turbulent conditions. In this latter case, the initial value of turbulence kinetic energy, k^0, was set equal to 60 m^2/s^2. This value was chosen by looking at the turbulence kinetic energy maps obtained by our previous CFD simulations (Di Benedetto et al., 2013; Di Sarli et al., 2014). We found that, after dust injection in the 20 l sphere, the turbulence decays in time and that, at the ignition time (60 ms), the kinetic energy at the center of the sphere is equal to 60 m^2/s^2.