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A numerical approach to investigate the maximum permissible nozzle diameter in explosion by hot turbulent jets

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ABSTRACT

The ignition of a combustible environment by hot jets is a safety concern in many industries. In explosion protection concepts, for a protection of the type “flameproof enclosures” a maximum permissible gap is of major importance. In this work a numerical framework is described to investigate the ignition processes by a hot turbulent jet which flows out from such gaps. A Probability Density Function (PDF) method in conjunction with a reaction-diffusion manifold (REDIM) technique is used to model the turbulent reactive flow. In this paper the ignition of a stoichiometric mixture of hydrogen/air gas by a hot exhaust turbulent jet is examined. The impact of the nozzle diameter on the ignition delay time is investigated, too. The method is used to explore the maximum nozzle diameter for specific boundary conditions for which there is no ignition.

1. Introduction

Flameproof enclosures are used to encapsulate potential ignition sources in hazardous areas (IEC 60079-1, 2014). Due to an internal explosion in such an enclosure, hot exhaust gas may propagate, through a joint clearance or other (inevitable) gaps, into the combustible environment, which may cause an accidental explosion (Phillips, 1972; Hattwig and Steen, 2004). The investigation of the ignition by hot jets motivated by the explosion protection backgrounds has been studied by various authors (Phillips, 1972; Strehlow et al., 1979; Thibault et al., 1982; Djebaili et al., 1995; Larsen and Eckhoff, 2000; Sadanandan et al., 2007; Carpio et al., 2013). A semi-analytical approach is used by Phillips (1972) in order to approximate the minimum jet sizes for ignition by a number of fuels. In an experimental study conducted by Larsen and Eckhoff (2000) the transmission of an explosion from a virtually closed chamber into a combustible ambient was investigated. Larsen and Eckhoff (2000) studied the impact of the location of the ignition in the closed chamber on the re-ignition in the ambient. Sadanandan et al. (2007) conducted an extensive experimental measurement in order to obtain information about the spatial and temporal evolution of the ignition process. They employed simultaneous measurements of high-speed laser-induced fluorescence (LIF) of the hydroxyl radical (OH) and laser Schlieren methods. More recently, Carpio et al. (2013) investigated numerically the ignition by hot jets for various hydrogen–air concentrations.

We use a numerical approach to investigate the ignition of a premixed hydrogen/air mixture by a hot turbulent jet. In this regards, a stand-alone Probability Density Function (PDF) method (Ghorbani et al., 2015b) is used. The flow that is considered is a statistically transient reactive turbulent jet. In such a configuration chemical reactions occur at a small-scale which (in the presence of turbulence) makes it difficult to model. PDF methods, however, achieve closure at the level of one-point, one-time joint PDFs and have been used extensively to simulate combustion and reactive flows (Haworth, 2010). Simulations performed in the current study include hot turbulent jets at the inlet boundary which the hot jet is the combustion products of a stoichiometric mixture of hydrogen/air near equilibrium.

The principal objective of this study is to investigate the physico-chemical processes involved in the ignition processes mentioned. In the course of the current study some of the important influencing parameters have been quantified. This information can be used for the design and development of “flameproof enclosures” in order to prevent accidental explosions.

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2. Methodology

A statistical approach which is known as a PDF method (Pope, 1985) is used to model the turbulent reacting flow. In this approach a transport equation is solved for a joint velocity-turbulence frequency-composition PDF (Pope, 1985; Van Slooten and Pope, 1998). The transport equation for the modelled PDF is solved by a Monte Carlo technique (Van Slooten and Pope, 1998; Pope, 1981). In this technique, an ensemble of stochastic particles (known as notional particles) is used to represent statistics of the turbulent flow. Each notional particle is a realization of a possible flow event. To each notional particle a set of stochastic variables is attributed which is evolved by a set of modelled stochastic differential equations (SDEs). The ensemble of notional particles represents the joint PDF of the turbulent flow and the thermochemical quantities. In this work the same model equations and constants are used as in our previous work in Ghorbani et al. (2012, 2014). The position of each notional particle is evolved by its own velocity $\mathbf{U}^*$

$$\mathrm{d}\mathbf{x}^* = \mathbf{U}^*\mathrm{d}t. \tag{1}$$

The simplified Langevin model (SLM) (Pope, 1985) is used to model the particles velocity

$$\mathrm{d}U_i^* = -\nu^*\left(\frac{\partial\langle p\rangle}{\partial x_i}\right)^*\mathrm{d}t - \left(\frac{1}{2}+\frac{3}{4}C_0\right)\left(U_i^* - \widetilde{U}_i\right)\Omega\mathrm{d}t + \sqrt{C_0 k\Omega}\,\mathrm{d}W_i, \tag{2}$$

$$\Omega = C_\Omega\frac{\langle\rho^*\omega^*|\omega^*\geq\tilde{\omega}\rangle}{\langle\rho\rangle}, \tag{3}$$

where ν denotes the specific volume ($\nu = 1/\rho$, ρ is density), p the pressure, k the turbulent kinetic energy, ω the turbulent frequency, Ω the conditional turbulent frequency, $\mathbf{W}$ an isotropic Wiener process and C_0 and C_Ω are the model constants which are given in Table 1. In the above equations * indicates quantities attributed to the particles, $\langle\ \rangle$ a mean quantity and $\tilde{}$ a density-weighted mean quantity. The turbulence frequency of each notional particle is evolved according to the model that was developed in Van Slooten and Pope (1998) and is given by

$$\mathrm{d}\omega^* = -C_3(\omega^* - \tilde{\omega})\Omega\mathrm{d}t - \omega^* S_\omega\tilde{\omega}\mathrm{d}t + \sqrt{2C_3C_4\omega^*\tilde{\omega}\Omega}\mathrm{d}W, \tag{4}$$

where C_3 and C_4 are model constants. The values of the constants are specified in Table 1. S_ω represents the source term for the turbulent frequency and is given by (Hanjalic and Launder, 1972)

$$S_\omega = C_{\omega2} - C_{\omega1}\frac{\mathcal{P}}{k\Omega}, \tag{5}$$

where $C_{\omega1}$ and $C_{\omega2}$ are model constants also shown in Table 1. $\mathcal{P}$ is the turbulence production (Xu and Pope, 1999)

$$\mathcal{P} = -\widetilde{u_iu_j}\frac{\partial\widetilde{U}_i}{\partial x_j}, \tag{6}$$

where $\widetilde{u_iu_j}$ represent the Reynolds stresses. The evolution of each scalar ϕ_α^* is described by the following equation

$$\mathrm{d}\phi_\alpha^* = M_\alpha\omega_\phi\mathrm{d}t + S_\alpha^*(\phi^*)\mathrm{d}t, \tag{7}$$

where M_α represent a scalar mixing model, ω_ϕ is the scalar mixing frequency and $S_\alpha^*(\phi^*)$ is the chemical source term. In the above equation M_α is modelled by the interaction by exchange with the mean (IEM) model (Dopazo and O'Brien, 1974), thus,

$$M_\alpha = -\frac{1}{2}\left(\phi_\alpha^* - \widetilde{\phi_\alpha}\right), \tag{8}$$

and ω_ϕ is modelled based on a mechanical-to-scalar time scale ratio and is given by (Fox, 2003)

$$\omega_\phi = C_\phi\Omega, \tag{9}$$

where C_ϕ is a model constant which controls the molecular mixing rate. In this work a classical value of $C_\phi = 2$ is used. The impact of molecular mixing model parameter C_ϕ is investigated in Ghorbani et al. (2014). In Eq. (7) the last term corresponds to the chemical reactions which is closed using either a detailed or reduced kinetics. The mean pressure gradient in the velocity equation Eq. (2) appears in closed form. For low-Mach number flows, however, usually a Poisson equation has to be solved to obtain the mean pressure. In this work we use the PDF-PM algorithm (Ghorbani et al., 2015b) which is based on a projection method. This algorithm was designed for stand-alone PDF codes to simulate transient low-Mach number reactive flows.

To reduce the number of dependent variables in the simulation, a reduced description of the thermochemical state is applied using the REDIM method (Bykov and Maas, 2007). For the reactive case in the current work it is sufficient to describe the state with a two-dimensional manifold (Ghorbani et al., 2014). The manifold is parametrized with a chemical progress variable and a variable that represents mixing state of the two streams, i.e. exhaust gas and fresh unburnt gas. For hydrogen/air case the specific mole number of H_2O, ϕ_{H_2O}, is used as the progress variable. ϕ_{H_2O} is defined as w_{H_2O}/M_{H_2O}, where M_{H_2O} is the molar mass and w_{H_2O} is the mass fraction of H_2O. The state of mixing is represented by enthalpy, which also accounts for the heat losses due to nozzle walls (Ghorbani et al., 2014). Thus, ϕ_{H_2O} and enthalpy are the only additional variables that have to be solved in the reactive simulations. For the REDIM calculations the hydrogen mechanism from Warnatz et al. (2006) was applied.

Table 1
Model constants.

C_0	C_Ω	$C_{\omega1}$	$C_{\omega2}$	C_3	C_4	C_ϕ
2.1	0.6893	0.70	0.9	1.0	0.25	2.0

3. Computational setup

A sketch of the computational domain that is used in this work is shown in Fig. 1. The flow under consideration is a round jet of hot

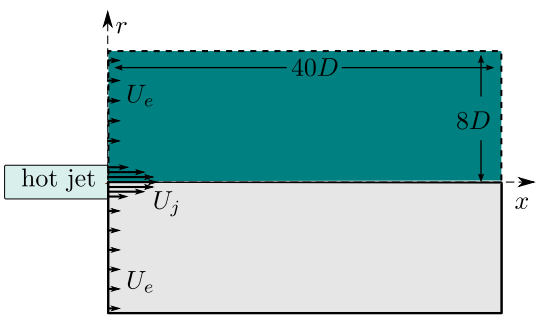

Fig. 1. A schematic sketch of the computational domain.

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