



The explosion characteristics of methane, hydrogen and their mixtures: A computational study



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ABSTRACT

The maximum pressure rise rate during gas explosions in enclosures and the deflagration index are important explosion characteristics of premixture. They can be used to quantify the potential severity of an explosion. However, there are large discrepancies in the deflagration index measured by different researchers for the same methane/air or hydrogen/air mixture. In this study, outwardly propagating spherical flames in a closed vessel are simulated by considering detailed chemistry as well as temperature-dependent thermal and transport properties. From simulation, the maximum pressure rise rate and deflagration index of methane, hydrogen and their mixtures are obtained. The influence of equivalence ratio, initial temperature and initial pressure on the maximum pressure rise rate and deflagration index is examined. It is found that the deflagration index has not been accurately measured in previous experiments, and that experiments conducted in cylindrical vessels have under-predicted greatly the deflagration index. For hydrogen/methane mixtures with hydrogen blending level above 70%, the deflagration index is observed to increase exponentially with hydrogen blending level. Moreover, the deflagration index is found to be greatly affected by initial pressure; while the initial temperature has little influence on deflagration index. Finally, based on theoretical analysis we propose a correlation to calculate the maximum pressure rise rate and deflagration index of methane at a broad range of initial pressure. The performance of this correlation is examined and it is demonstrated to provide accurate prediction.

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1. Introduction

Preventing unwanted explosion in fuels released into atmosphere is a crucial issue for fuel stocking and transportation. Therefore, the explosion characteristics of different fuels should be investigated thoroughly. The maximum pressure rise rate during gas explosions in enclosures, $(dP/dt)_{\max}$, and the deflagration index, K_G , are important explosion characteristics of premixture. They are popularly used to quantify the potential severity of an explosion. The maximum pressure rise rate, $(dP/dt)_{\max}$, depends not only on the mixture properties (such as mixture composition, initial temperature and initial pressure) but also on the volume of the vessel in which gas explosion takes place. Unlike $(dP/dt)_{\max}$, the deflagration index is an intrinsic property of the premixture and it is

independent of the volume of the vessel used in experimental measurements. The relationship between K_G and $(dP/dt)_{\max}$ is

$$K_G = (dP/dt)_{\max} \times V^{1/3} \quad (1)$$

in which V is volume of combustion vessel.

Since the deflagration index is an intrinsic property of a premixture at certain conditions (i.e., at specified initial temperature and pressure), experiments conducted by different groups should provide nearly the same value of K_G for the same premixture at the same condition. Unfortunately, due to different sources of uncertainty, there are substantial discrepancies in the deflagration index measured by different researchers for the same methane/air or hydrogen/air mixture (see Table 1 and Table 2 presented in Section 4).

Almost all the experiments for deflagration index measurements were conducted in cylindrical or spherical vessels (Cammarota et al., 2010; Dahoe, 2005; Dahoe and de Goey, 2003; Holtappels, 2002; Ma et al., 2014; Movileanu et al., 2013; Razus

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et al., 2011; Salzano et al., 2012). When a cylindrical vessel is used, the unburned mixture cannot be completely consumed by the propagating spherical flame as it reaches the inner wall of the vessel. Therefore, both maximum pressure rise rate and deflagration index are underestimated in experiments using a cylindrical chamber. Ideally, a spherical chamber should be used to measure the deflagration index. Other factors affecting the accuracy of deflagration index measurement include flame instability and turbulence, which increase flame propagation speed and pressure rise rate. Stable flame propagation and laminar flow need to be ensured so that the deflagration index is not over-predicted (Cammarota et al., 2010; Razus et al., 2011). However, in large vessels the flame may become unstable due to hydrodynamic or thermal-diffusion instability and the initial laminar flow may become turbulent during the spherical flame propagation. Consequently, experiments conducted in large vessels over predict K_G . Furthermore, since both maximum pressure rise rate and deflagration index are strongly correlated with the flame propagation speed, those factors (e.g., mixture preparation, ignition, buoyancy and radiation) affecting flame propagation speed can also cause uncertainty in deflagration index measurement.

In simulation, the influence of different factors on flame propagation speed can be circumvented or minimized (Chen, 2015). Therefore, accurate deflagration index can be obtained from direct numerical simulation. In this study, outwardly propagating spherical flames in a closed spherical vessel are simulated by considering detailed chemistry as well as temperature-dependent thermal and transport properties. From simulation, the maximum pressure rise rate and deflagration index of methane, hydrogen and their mixtures are obtained. Methane is the main component of natural gas which is one of the promising clean alternative fuels. However, the low flame speed and narrow flammability limits of methane pose challenges for its utilization in combustion engines. To solve this problem, hydrogen addition is popularly used (Chen, 2009; Shrestha and Karim, 1999). However, hydrogen addition also increases the probability and strength of explosion. In the literature, several studies were conducted to measure the maximum pressure rise rate and deflagration index of methane (Cammarota et al., 2010; Crowl, 2010; Salzano et al., 2012), hydrogen (Ma et al., 2014; Salzano et al., 2012; Tang et al., 2009) and methane/hydrogen mixtures (Ma et al., 2014; Salzano et al., 2012).

The objectives of this study are to obtain the deflagration index of hydrogen, methane, and their mixtures, and to examine the effects of initial temperature, initial pressure and equivalence ratio on the deflagration index of hydrogen/methane mixtures. Furthermore, a correlation is proposed to calculate the maximum pressure rise rate and deflagration index of methane at a broad range of initial pressures.

2. Numerical methods

To get the maximum pressure rise rate and deflagration index, we have simulated one-dimensional (1D) spherical flame propagation in a closed spherical vessel using the in-house code, A-SURF (Chen, 2010; Chen et al., 2009; Dai and Chen, 2015). A-SURF solves the following conservation equations (including the unsteady Navier–Stokes equations as well as the energy and species conservation equations) for 1D, adiabatic, multicomponent, reactive flow in a spherical coordinate (Chen, 2010; Chen et al., 2009; Dai and Chen, 2015):

$$\frac{\partial U}{\partial t} + \frac{1}{r^2} \frac{\partial F(U)}{\partial r} = \frac{1}{r^2} \frac{\partial F_v(U)}{\partial r} + S_R \quad (2)$$

in which t and r are the temporal and spatial coordinates,

respectively. In Eq. (2), the vectors U , $F(U)$, $F_v(U)$, and S_R are defined as:

$$U = \begin{pmatrix} \rho Y_1 \\ \rho Y_2 \\ \vdots \\ \rho Y_n \\ \rho u \\ E \end{pmatrix}, F(U) = \begin{pmatrix} r^2 \rho u Y_1 \\ r^2 \rho u Y_2 \\ \vdots \\ r^2 \rho u Y_n \\ r^2 (\rho u^2 + P) \\ r^2 (E + P)u \end{pmatrix}, F_v(U) = \begin{pmatrix} -r^2 \rho Y_1 V'_1 \\ -r^2 \rho Y_2 V'_2 \\ \vdots \\ -r^2 \rho Y_n V'_n \\ r^2 \tau_1 \\ r^2 q \end{pmatrix}, S_R = \begin{pmatrix} \omega_1 \\ \omega_2 \\ \vdots \\ \omega_n \\ -2\tau_2/r \\ 0 \end{pmatrix} \quad (3)$$

in which ρ , u , P , and E denote density, flow velocity, pressure and the total energy per unit mass, respectively. The quantities, Y_k , V'_k and ω_k , are the mass fraction, diffusion velocity and production rate of species k , respectively. The production rate ω_k due to chemical reaction is specified via collection of elementary reactions using a CHEMKIN compatible database (Kee et al., 1993). The mixture-averaged formula (Kee et al., 1985) is used to calculate diffusion velocity. In simulation the thermal diffusion of H and H₂ is considered since it affects the spherical flame propagation speed (Liang et al., 2013).

In the momentum equation, the viscous stresses, τ_1 and τ_2 , are:

$$\tau_1 = \frac{2\mu \partial u}{\partial r} - \frac{2\mu}{3r^2} \frac{\partial(r^2 u)}{\partial r}, \tau_2 = \frac{2\mu u}{r} - \frac{2\mu}{3r^2} \frac{\partial(r^2 u)}{\partial r} \quad (4)$$

where μ is the dynamic viscosity of the mixture.

In the energy conservation equation, the total energy, E , is defined through:

$$E = -P + \rho u^2 / 2 + \rho h, h = \sum_{k=1}^n (Y_k h_k), h_k = h_{k,0} + \int_{T_0}^T C_{P,k}(T) dT \quad (5)$$

where T is the temperature, h_k , the enthalpy of species k , $h_{k,0}$ the species enthalpy of formation at the reference temperature T_0 , and $C_{P,k}$ the specific heat of species k at constant pressure. The heat flux in the energy conservation equation is

$$q = \lambda \frac{\partial T}{\partial r} - \rho \sum_{k=1}^n (h_k Y_k V'_k) \quad (6)$$

where λ is the thermal conductivity of the gas mixture.

The finite volume method is used to solve the conservation governing equations listed above. The Strang splitting fractional-step procedure is used to separate the time evolution of the stiff reaction term S_R from that of the convection and diffusion terms. In the first fractional step, the non-reactive flow is solved. The Runge–Kutta, MUSCL–Hancock, and central difference schemes, all of second-order accuracy, are used to calculate the temporal integration, convective flux, and diffusive flux, respectively. In the second fractional step, the homogeneous reaction at constant volume is solved using the VODE solver (Brown et al., 1989). Detailed chemistry is considered in simulation: the mechanism developed by Li et al. (2004) for pure hydrogen, and GRI-Mech 3.0 (Smith et al., 1999) for methane and methane/hydrogen mixtures. The chemical reaction rates as well as the thermodynamic and transport

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