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Numerical simulation of auto-ignition induced by high-pressure hydrogen release with detailed reaction model: Fluid dynamic effect by diaphragm shape and boundary layer

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ABSTRACT

The effects of the diaphragm shape and boundary layer near walls on auto-ignition induced by high-pressure hydrogen release in a real size tube are numerically studied using the Navier–Stokes equations with multi-component gases. The numerical results show that there is a grid dependency that provides the optimal grid system via a comparison the theoretical boundary layer thickness. The validity of the present numerical system is confirmed by comparing the numerical and experimental precursor shock wave velocities. The initial diaphragm shape affects the hydrogen release flow structure and its auto-ignition mechanism. Two different auto-ignition styles are observed from the numerical results: one occurs near the boundary layer owing to the induction time effect and Kelvin-Helmholtz instability and another may occur near the center axis owing to the Rayleigh-Taylor instability.

Introduction

The features of flow pattern and auto-ignition characteristics of high pressure hydrogen release into air must be studied to handle hydrogen and to develop safety standards for its use at hydrogen stations. Under current safety provisions, high-pressure hydrogen might be accidentally released through a hole or tube. High-pressure hydrogen released in this manner poses a great risk because it can ignite without any ignition source.

Since the 1970s, many studies have focused on hydrogen auto-ignition. For example, Wolanski and Wójcicki (1972) [1], who were the first to study hydrogen auto-ignition, experimentally showed that ignition started in the local high-temperature region of oxygen behind a shock wave developed by high-pressure hydrogen released from a tube into a

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spherical chamber. They found that the shock wave's pressure is 3.8 MPa; temperature is 575 K; and Mach number, ~2.8.

Toward developing a safety standard, Dryer et al. (2007) [2] experimentally studied hydrogen release from a high-pressure tank with initial pressures of 2.0 and 8.6 MPa through an aluminum diaphragm with 76–229 μm thickness and reported that auto-ignition was caused by local reflected shock waves resulting from differences in the tube area, i.e., there is a bump in the tube for an initial pressure of 2.0 MPa. However auto-ignition occurred without such bumps in the tube when the initial high pressure was 8.6 MPa. They also explained that the curved shock wave due to diaphragm influenced on auto-ignition.

Golub et al. [3–5] studied high-pressure hydrogen ignition problem for rectangular and circular tubes both experimentally and numerically. Based on their experiments, they stated that hydrogen and air need to mix for a sufficiently long time and at sufficiently high temperature for auto-ignition. They also said that auto-ignition occurs more easily at high burst pressure and with a long tube. Their numerical analysis showed that auto-ignition did not occur with a hole with 2.6-mm diameter and that the flame jet became larger with a larger hole diameter. Furthermore, their calculation showed that when the burst pressure is high, the distance between the diaphragm and the location of auto-ignition is large.

Xu et al. [6–8] numerically demonstrated with and without a tube that a combustible mixture is produced at the contact area between hydrogen and air, where turbulence enhances their mixing, and that when the tube is sufficiently long, auto-ignition starts in the tube and the tube length plays an important role in producing mixing in the tube. They performed calculations for various cases, including diaphragm rupture, and showed that mixing at the contact surface curved by vortices plays an important role in auto-ignition.

Mogi et al. [9,10] experimentally studied auto-ignition occurring upon high-pressure hydrogen spurting out of a tube into the atmosphere. In perticular, they tested various tube lengths and initial burst pressures up to 20 MPa. They found that auto-ignition is related to the tube size and that it occurs at low pressure when tube length is longer. For high burst pressure, auto-ignition occurs even with a short tube.

However, recently, Kitabayashi et al. [11] experimentally showed that auto-ignition occurs again at high pressure when the tube length increases. This finding may be attributable to wall friction in the tube.

Most recently, Lee et al. and Kim et al. [12–14] experimentally showed that auto-ignition occurs near the wall immediately behind the precursor shock wave. They used a transparent 300-mm-long tube with a maximum burst pressure of 11.3 MPa to see the ignition point in the tube, especially in the boundary layer near the wall. They found that auto-ignition occurs more easily with higher burst pressure and a longer tube. However, even when using a transparent tube, they found it difficult to clarify the mechanism of high-pressure hydrogen auto-ignition in the tube.

The present study presents the effects of diaphragm shape and boundary layer on auto-ignition and mixing through a real-size analysis of high-pressure hydrogen auto-ignition in a tube using the compressible Navier–Stokes equations with a full hydrogen reaction mechanism.

Numerical method

The governing equations are the two-dimensional compressible Navier–Stokes equations (Eqs. 1 and 2) with a detailed hydrogen-air reaction mechanism.

$$\frac{\partial \mathbf{Q}}{\partial t}+\frac{\partial \mathbf{E}}{\partial x}+\frac{\partial \mathbf{F}}{\partial y}=\frac{\partial \mathbf{E}_d}{\partial x}+\frac{\partial \mathbf{F}_d}{\partial y}+\mathbf{S} \tag{1}$$

where

$$\mathbf{Q}=\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ e\\ \rho_i\end{pmatrix},\ \mathbf{E}=\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho uv\\ (e+p)u\\ \rho_i u\end{pmatrix},\ \mathbf{F}=\begin{pmatrix}\rho v\\ \rho uv\\ \rho u^2+p\\ (e+p)v\\ \rho_i v\end{pmatrix},\ \mathbf{E}_d=\begin{pmatrix}0\\ 0\\ 0\\ -q_x\\ \rho D_i\frac{\partial Y_i}{\partial x}\end{pmatrix},$$

$$\mathbf{F}_d=\begin{pmatrix}0\\ 0\\ 0\\ -q_y\\ \rho D_i\frac{\partial Y_i}{\partial y}\end{pmatrix},\ \mathbf{S}=\begin{pmatrix}0\\ 0\\ 0\\ 0\\ \dot{\omega}_i\end{pmatrix} \tag{2}$$

These equations are integrated explicitly and two-dimensionally in the x- and y- directions by the finite difference method: a Harten-Yee, second-order explicit non-MUSCL modified-flux-type total variation diminishing scheme [15] for the convective terms, a point-implicit method for the production terms, a central difference scheme for the diffusion terms, and a second-order Strang-type fractional step method for the unsteady term. Hong et al.'s Stanford model [16] is used for the chemical reaction system, which has 9 species – H_2, O_2, O, H, OH, HO_2, H_2O_2, H_2O, and Ar – and 20 elementary reactions, and is developed to consider the effect of high-pressure and high-temperature conditions. Chapman and Cowling's diffusion coefficient (Eq. 3) [17], Chapman and Enskog's molecular viscous coefficients (Eq. 7) [18], and Wike's law (Eq. 9) [19] are applied to calculate the transport coefficients as follows:

$$D_{ij}=1.8829\times10^{-2}\frac{\sqrt{T^3 m_{ij}}}{p\sigma_{ij}^2\Omega_D} \tag{3}$$

where m is the molar reduced mass; σ_{ij}, the collision diameter; and Ω_D, the diffusion collision integral:

$$m_{ij}=\frac{m_i m_j}{m_i+m_j} \tag{4}$$

$$\sigma_{ij}=\frac{1}{2}\left(\sigma_i+\sigma_j\right) \tag{5}$$

$$\Omega_D=\left(\frac{T}{T_{\varepsilon_{ij}}}\right)^{-0.145}+\left(\frac{T}{T_{\varepsilon_{ij}}+0.5}\right)^{-2.0} \tag{6}$$

and