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# Effects of initial diaphragm shape on spontaneous ignition of high-pressure hydrogen in a two-dimensional duct

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## ABSTRACT

A two-dimensional (2-D) simulation of spontaneous ignition of high-pressure hydrogen in a length of duct is conducted to explore ignition mechanisms. The present study adopts a 2-D rectangular duct and focuses on effects of the initial diaphragm shape on spontaneous ignition. The Navier–Stokes equations with a detailed chemical kinetics mechanism are solved in a manner of direct numerical simulation. The detailed mechanisms of spontaneous ignitions are discussed for each initial diaphragm shape. For a straight diaphragm, ignition only occurs near the wall owing to the adiabatic wall condition, while three ignition events are identified for a greatly deformed diaphragm: ignition due to reflection of leading shock wave at the wall, hydrogen penetration into shock-heated air near the wall, and deep penetration of hydrogen into shock-heated air behind the leading shock wave.

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## Introduction

When highly pressurized hydrogen is released into air, spontaneous ignition may occur owing to the production of shock-heated gas and sufficient mixing between hydrogen and air, which can potentially lead to significant hazardous incidences. Recently, storage pressures as high as about 700 atm have been considered for hydrogen fuel-cell vehicles. Thus, in order to establish reliable risk assessments or safety guidelines on the operation of high-pressure hydrogen, issues related to spontaneous ignition have to be clarified.

Following the pioneering experimental work by Wolanski and Wojcicki [1], several experimental studies [2–4] have examined spontaneous ignition of high-pressure hydrogen

released into air. The experimental data have generally confirmed that increasing the hydrogen pressure decreases the distance from the burst location to the point of the hydrogen ignition. Dryer et al. [2] demonstrated the occurrence of spontaneous ignition by releasing high-pressure hydrogen from a tube and provided potential scenarios of mixing phenomena that may result in spontaneous ignition. Golub et al. [3] identified the importance of the cross-sectional shape of the tube on hydrogen self-ignition. They also numerically simulated the influence of the boundary layer on governing ignition mechanisms. Mogi et al. [4] experimentally observed that the possibility of self-ignition increases with the length of the discharge tube. Kim et al. [5] provided flow visualization inside a tube using

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Shadowgraph in addition to measurement with pressure and light sensors.

While experimental works have been successfully dedicated to understand the spontaneous ignition mechanisms, increasing computational power has allowed numerical simulations to be conducted over the last five years to further identify detailed mechanisms of spontaneous ignition of high-pressure hydrogen inside a tube. Wen et al. [6] performed a parametric study on spontaneous ignition of pressurized hydrogen released through a length of tube by using two-dimensional (2-D) direct numerical simulation (DNS). The effects of rupture time, release pressure, and tube length and diameter on spontaneous ignition were comprehensively investigated. For example, slower rupturing process and smaller ratio of the tube length and diameter were suggested to help avoid the likelihood of spontaneous ignition. Following their previous study [6], Xu et al. [7] also determined the importance of the finite rupture process to numerically predicting the spontaneous ignition. The finite rupture process provides accurate predictions of the shock velocity and turbulent mixing at contact region, which influence the ignition mechanism.

Lee and Jeung [8] conducted 2-D DNS with detailed chemical kinetics using a realistic rupture process of the pressure boundary. They simulated the detailed mechanism of early ignition near the boundary layer and the following spontaneous ignition due to sufficient mixing of the expanding hydrogen jet and shock-heated air in the downstream region. Using 2-D DNS, Yamada et al. [9] indicated the possibility of auto-ignition induced by vortices behind the shock wave in a long tube, which suggests that understanding the phenomenon with vortices near the contact region is necessary.

A large-eddy simulation (LES) model [10] was applied to spontaneous ignition phenomena with a coarse grid resolution relative to the DNS studies [6,8,9]. The results agreed with the experimental data on the distance for spontaneous ignition from the rupture disk, which demonstrated the validity of their LES model with regard to predicting of spontaneous ignition, while the detailed unsteady flow structures were seemingly lost.

Following several successful numerical studies on spontaneous ignition of pressurized hydrogen released into tubes, in the present study, we numerically simulate spontaneous ignition of highly pressurized hydrogen inside a two-dimensional duct in a manner of DNS. We examine the effects of the initial diaphragm shape on spontaneous ignition mechanisms; in contrast, earlier relevant studies [6,8] investigated the effect of the rupture rate using only one initial diaphragm shape with curvature. A fully two-dimensional domain, i.e., no axisymmetric geometry is adopted in order to explore possible mechanisms of spontaneous ignition; this geometry differs from those used in most earlier studies [6–9].

## Numerical method

### Governing equations

The Navier–Stokes equations with the conservation equations of each chemical species are used as the governing equations and the thermally perfect gas equation of state is applied. The governing equations in this study are as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (1)$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \delta - \tau) = 0, \quad (2)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot ((E + p)\mathbf{u} - \tau \cdot \mathbf{u} - \mathbf{q}) = 0, \quad (3)$$

$$\frac{\partial (\rho Y_s)}{\partial t} + \nabla \cdot (\rho Y_s \mathbf{u}) - \nabla \cdot (\rho D_s \nabla Y_s) = \dot{\omega}_s, \quad (4)$$

where  $\rho$  is the density,  $\mathbf{u}$  is the velocity vector,  $p$  is the pressure,  $\delta$  is the unit tensor,  $\tau$  is the viscous stress tensor,  $E = \rho e + 1/2 \rho \mathbf{u} \cdot \mathbf{u}$  is the total energy, and  $\mathbf{q}$  is the heat flux vector.  $e$  is the internal energy per unit mass.  $Y_s$  is the mass fraction,  $D_s$  is the diffusion coefficient, and  $\dot{\omega}_s$  is the reaction rate of species. Here  $s=1 \sim N$  where  $N$  is the total number of species. The equation of state is

$$p = \rho R \sum_{s=1}^N \frac{Y_s}{W_s} T, \quad (5)$$

where  $R$  is the universal gas constant,  $W_s$  is the mole fraction of species  $s$ , and  $T$  is the temperature.

The viscous stress tensor  $\tau$  is represented by

$$\tau = \mu(2\mathbf{S}) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\delta, \quad (6)$$

where  $\mu$  is the viscosity for mixtures and  $\mathbf{S}$  is the symmetric strain rate tensor. The heat flux vector  $\mathbf{q}$  is

$$\mathbf{q} = -\kappa \nabla T - \rho \sum_{s=1}^N h_s D_s \nabla Y_s, \quad (7)$$

where  $\kappa$  is the thermal conductivity for mixtures and  $h_s$  is the enthalpy of species  $s$ .

The single component viscosities and binary diffusion coefficients are calculated by the standard kinetic theory expression of Hirschfelder [11], and Warnatz's model [12] is used for the single component thermal conductivity. The mixture-averaged viscosity is given by Bird's formula [13] and the mixture-averaged thermal conductivity is evaluated from Mathur et al.'s formula [14]. Bird et al.'s mixture-averaged model [13] is used for the mixture diffusion coefficient. The Soret effect for species transport and Dufour effect for heat transport are both neglected in this study.

The above Eqs. (1)–(4) are solved in the operator-splitting form in order to efficiently handle a wide range of time-scales in problems, i.e., the fluid and chemical reaction parts are solved separately in terms of the time integrations. The fluid part in Eqs. (1)–(4) is solved under the assumption that the chemical reactions are frozen, i.e.,  $\dot{\omega}_s = 0$ , while the chemical reaction is treated under the assumption that the volume and internal energy of fluids are constant. Spatial derivatives in Eqs. (1)–(4) are neglected. The governing equations for the chemical reactions are thus derived as follows:

$$\frac{dY_s}{dt} = \frac{\dot{\omega}_s}{\rho}, \quad (8)$$

$$\frac{dT}{dt} = -\frac{\sum_{s=1}^N e_s \dot{\omega}_s}{\rho c_v}, \quad (9)$$

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