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Numerical study of spontaneous ignition of pressurized hydrogen released by the failure of a rupture disk into a tube

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ABSTRACT

Recent experimental observations have shown that pressurized hydrogen may be spontaneously ignited in downstream tubes of sufficient length when it is released into the air due to the rapid failure of a pressure boundary. The mixing between hydrogen and shocked air within the downstream tubes is speculated to be a key process for the occurrence of spontaneous ignition of hydrogen. A direct numerical simulation has been conducted to analyze the processes of mixing and of spontaneous ignition of hydrogen within a tube after the rupture of a disk at a bursting pressure of 86.1 atm. A realistic assumption of the geometry of the pressure boundary at the moment of its failure is used for the initial condition of the numerical simulation to properly account for its effect on the mixing process. The present simulation results show that the mixing of shocked air and expanding hydrogen is enhanced by the transient multi-dimensional shock initiated by the failure of a rupture disk and by the following interactions during the flow development through the tube, thus causing spontaneous ignition of hydrogen within the tube.

1. Introduction

It is known that pressurized hydrogen released into the air by accident or during a technical operation can undergo spontaneous ignition. Hydrogen is considered to be a green energy carrier for a sustainable environment, and the industry of fuel-cell vehicles utilizing hydrogen is growing rapidly. Therefore, the safety issues related to the spontaneous ignition phenomena are significant, considering that the storage pressure of hydrogen for the operation of fuel-cell vehicles may be as high as 700 atm.

Astbury and Hawksworth [1] reviewed postulated mechanisms of high-pressure hydrogen leaks igniting for no apparent reason, such as the reverse Joule–Thomson effect, electrostatic charge generation, diffusion ignition, sudden adiabatic compression, and hot surface ignition. Among these, the diffusion ignition mechanism has been a primary interest of subsequent researchers. The diffusion ignition model was first established by Wolański and Wójcicki [2], who experimentally demonstrated spontaneous ignition at the contact region when piston-compressed hydrogen was released into the surrounding oxidizer. According to their model of diffusion ignition, the ignition was caused by an increase in the temperature of the combustible mixture produced by heat-flux-driven diffusion of the oxidizer heated by a leading shock wave.

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Recently, several experimental observations have been made to identify the limiting conditions of spontaneous ignition of pressurized hydrogen released through downstream tubes into air due to the failure of rupture disks. Dryer et al. [3] conducted more than 200 experiments on hydrogen, varying the downstream geometries and exploring failure pressures ranging from 11.2 atm to 113.25 atm. Their experiments showed that spontaneous ignition requires both a sufficiently high failure pressure and a downstream geometry for sufficiently fast mixing of the expanding hydrogen and shocked air. For example, when downstream tubes with a constant inner diameter of 12.7 mm were used, spontaneous ignition occurred at hydrogen pressures above 86 atm with tubes longer than 101.6 mm (4″). They postulated that since molecular diffusion across a contact surface is too slow to account for any significant formation of flammable mixture volumes, turbulent mixing and the heating of the mixture by the multi-dimensional shock-boundary and shock–shock interactions might play a significant role in the generation of sufficient volumes of flammable mixtures that could result in an ignition kernel. Mogi et al. [5] conducted similar experiments with downstream tube lengths varying from 3 mm to 300 mm and inner diameters of 5 mm and 10 mm, while the burst pressure was varied from 4 MPa to 30 MPa. They determined that the hydrogen jet showed an increasing tendency to ignite in the tube as the length of the tube increased, and did not ignite when short tubes were used. Golub et al. [4] used tubes of cylindrical and rectangular cross sections of lengths ranging from 65 mm to 185 mm and cross-sectional areas of 20 mm^2 for their experiments in discharging hydrogen through tubes into semi-confined air. In their experiments, the occurrence of spontaneous ignition within the tubes was detected using light sensors, at a pressure of 40 atm and higher.

There also have been several numerical studies of spontaneous ignition of pressurized hydrogen exiting from tubes into air [4,6,7]. However, the development of multi-dimensional transient flows and subsequent mixing process in the downstream tubes, associated with the failure of a rupture disk, have not been investigated in detail in most of these numerical studies.

In the present study, a direct numerical simulation with detailed reaction kinetics is conducted to investigate the transient flow development and the mechanism of spontaneous ignition when hydrogen is released into the air through a downstream tube by the failure of a rupture disk, with a realistic assumption of its failure geometry and conditions based on one of the experiments of Dryer et al., as an effort to demonstrate their postulation.

2. Numerical simulations

2.1. Numerical methods

The governing equations are the unsteady, compressible two-dimensional axi-symmetric Navier–Stokes equations for a chemically reactive multi-species mixture of ideal gases. The numerical scheme is based on the cell-centered finite volume method. The convective numerical fluxes are evaluated by the AUSM-DV scheme [8], which is accurate and robust for resolving shock and contact (stationary and moving) discontinuities. Second-order spatial accuracy is attained by using MUSCL extrapolation on primitive variables with limited slopes by the Superbee limiter for the Total Variation Diminishing (TVD) constraint. The viscous terms are evaluated by second-order central differencing discretization. For time integration, the second-order Strang-type method is employed, splitting convection–diffusion terms and chemical source terms. A memory-efficient type of four-step Runge–Kutta scheme [9] is used for the integration of convection and diffusion terms, while a stiff ODE solver named RADAU5 [10], an implicit Runge–Kutta method of order five with step size control, is used in order to overcome the stiffness caused by the chemical source terms. A comprehensive kinetic model of hydrogen combustion, recently updated by Li et al. [11] and based on the mechanism of Mueller et al. [12], is used for describing the reaction kinetics with nine species (H_2, O_2, H, O, OH, H_2O, HO_2, H_2O_2, N_2) and nineteen reactions. The evaluation of thermodynamic properties, transport properties, and chemical source terms is assisted by the Cantera [13] library with its interface for Fortran. Thermodynamic properties of the species are based on NASA polynomials [14]. The viscosity, thermal conductivity, and binary diffusion coefficients for each species are determined using Lennard–Jones potentials and kinetic theory. For mixture-averaged values, the formulae of Wilke [15] and Mathur et al. [16] are used.

2.2. Problem setup

For the present numerical simulation, conditions leading to spontaneous ignition in the experiments of Dryer et al. have been chosen. The bursting pressure of the rupture disk is 86.1 atm. The tube length from the plane of the rupture disk to the exit is 152.4 mm (6″), and the inner diameter is 12.7 mm (0.5″). While the minimum length of the tube required for the spontaneous ignition at the bursting pressure of 86.1 atm was 101.6 mm (4″) in their experiments, an increased length was used to ensure the observation of spontaneous ignition in the numerical simulation.

The computational domain is shown in Fig. 1 with the geometry of the pressure boundary that represents the concave shape of a type B rupture disk at the moment of its failure. The diameter of the hemispherical part of the rupture disk is assumed to be 10 mm. A small remaining part of the rupture disk is approximated as a thin vertical wall with a height of 1.35 mm. The dash–dot line in the figure represents the axi-symmetric line of the tube. The length of the upstream tube is arbitrarily chosen to be half of the downstream length, which is sufficient for the present simulation, since an expansion wave moves only to the left-hand side and does not

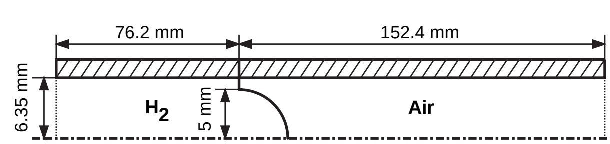

Fig. 1 – Computational domain and geometry of the pressure boundary.