Numerical simulations of spontaneous ignition of high-pressure hydrogen based on detailed chemical kinetics

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• Storage pressure of H\textsubscript{2} for the operation of fuel-cell vehicles: as high as 70 - 80 MPa

• Safety issues related to the spontaneous ignition of H\textsubscript{2} with air

• Need to establish reliable risk assessments and understand the mechanism of the spontaneous ignition

Schematic of spontaneous ignition

Hydrogen station in Japan (from Tokyo gas)
Several experimental and numerical studies conducted

- Lee and Jeung (2009)
- Yamada et al. (2011)
- Bragin and Molkov (2012)

Effects of initial diaphragm shape on spontaneous ignition
The compressible Navier-Stokes equations with a thermally perfect gas EoS

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \\
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho uu + p\delta - \tau) = 0, \\
\frac{\partial E}{\partial t} + \nabla \cdot ((E + p)u) = \nabla \cdot (\tau \cdot u - q), \\
\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho_k(u + V_k)Y_k) = \dot{\omega}_k
\]

- The operator-splitting form: **Fluid and Chemical reaction solved separately**
  - **Fluid**: chemistry frozen \( \dot{\omega}_k = 0 \)
  - **Chemical reaction**: internal energy and volume constant and spatial gradient terms neglected

\[
\begin{align*}
\frac{dY_k}{dt} &= \frac{\dot{\omega}_k}{\rho} \\
\frac{dT}{dt} &= -\sum e_k\dot{\omega}_k / (\rho c_v)
\end{align*}
\]
**Numerical methods**

- **Fluid**
  
  HLLC/HLL hybrid method (Kim et al. 2009) for numerical flux 3rd-order accuracy with MUSCL and Minmod limiter  
  Central differencing for viscous, heat source, and diffusion terms  
  3rd-order TVD Runge-Kutta method for time integration  
  
  - CHEMKIN-II library used for thermodynamic and transport properties

- **Chemical reaction**
  
  Dynamic multi-time scale (MTS, Gou et al. 2010) method for time integration  
  H₂ mechanism: UT-JAXA (Shimizu et al. 2011), 9 species and 34 reactions
Problem description

- 2-D rectangular duct of 10 cm × 0.5 cm

**Schematic of computational domain**

**High-pressure hydrogen**
- 10 MPa, 300 K

**Air**
- 0.1 MPa, 300 K

- Effects of initial diaphragm shape on spontaneous ignition

\[ x(y) = x_c - \delta \Delta h \cos\left(2\pi \frac{y}{\Delta h}\right) \]

\[ \delta = 0.0, 0.05, 0.1, -0.1 \]
Preliminary 0-D and 1-D studies

- 1-D shock tube problem

- Ignition delay using a 0-D computation

Profiles at $30.0 \times 10^{-6}$ s

- Pressure / atm
  - 80 µm
  - 40 µm
  - 20 µm

- Temperature / K
  - 1250 K
  - 1275 K
  - 1300 K

- H$_2$/O$_2$/N$_2$ = 2/1/3.76

No ignition in 1-D
Grid convergence study in 2-D


- 2000 K area rate defined as:

$$\bar{\mathcal{A}}_{2K}(t) = \frac{1}{\mathcal{A}_h} \sum_{i=1}^{\mathcal{A}} \sum_{k=1}^{T_{\geq 2000}} A_{i,k}$$
Straight diaphragm shape  \( \delta = 0.0 \)

- Temperature animation
Ignition near the wall due to adiabatic condition

Temperature distributions at $t = 32.1 \mu s$

- Temperature near the wall (1500 K) > Temperature behind the shock (1300 K)
Largely deformed diaphragm shape

- Temperature animation

$\delta = 0.1$
Three ignition events identified

First ignition

Temperature distributions at $t = 1.7 \mu s$

Time histories of 2000 K area rate

Schematic of the flow filed
Second ignition in largely deformed diaphragm shape $\delta = 0.1$

2. Second ignition

Enlarged view of temperature distributions at $t = 10.8 \mu s$

Schematic of the flow field

- Ignition near wall
- Hydrogen penetration
- Heated air
- Vorticity
- Deformed contact surface
- Shock wave
Third ignition in largely deformed diaphragm shape

δ = 0.1

③ Third ignition

Enlarged view of temperature distributions at $t = 29.3 \, \mu s$

Whole view

Schematic of the flow filed

Hydrogen penetration

Heated air

Shock wave

Large combustible area
Largely deformed diaphragm shape $\delta = 0.1$

- Temperature animation
Conclusions

- Spontaneous ignition of high-pressure hydrogen in a 2-D duct simulated using CFD with detailed chemical kinetics

- Effect of initial diaphragm shape on spontaneous ignition clarified

  - For the straight diaphragm, the ignition occurs near the wall

  - For the largely deformed diaphragm, three ignition events identified
    1. Ignition due to reflection of leading shock wave at the wall
    2. Hydrogen penetration into shock-heated air near the wall
    3. Deep penetration of hydrogen into shock-heated air
Largely deformed diaphragm shape in opposite direction

- Temperature animation
Mildly deformed diaphragm shape $\delta = 0.05$

- Temperature animation