Numerical Investigation on Self-Ignition Behavior of High Pressure Hydrogen Released from the Tube

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Introduction

Hydrogen is stored at high pressure in hydrogen station and fuel cell vehicle.

When hydrogen leaks from the tube, ignition occurs even without ignition source and causes damage to humans and properties.

Knowledge of self-ignition is required from the safety standpoint.
Objective

Mogi et al. (International Journal of Hydrogen Energy, 2009) :
confirmed that self ignition inside the tube did not occur
when the tube length was short.

From the previous study for inside the tube,
the factor and mechanism for self ignition have been clarified.

After leakage from the tube, the self ignition is quenched by
expansion unless hydrogen jet transits to jet fire.

There is little knowledge about the distance where self ignition is
sustained and factors that affect the distance.

Objective

To investigate the effective factor for self ignition of hydrogen
released from the tube using 2D axisymmetric simulation
Calculation target

Parameters:

- Tube length $L = 0, 30, 45, 60, 90$ mm
- Tube diameter $D = 3, 5, 10$ mm
- Release pressure $P_{H2} = 6.5, 10.0, 14.5, 20.0$ MPa

Minimum grid width: 10 μm (Max. grid points: 12726 x 2801)
Numerical method

◆ Governing equations:
  - 2D axisymmetric compressible Navier-Stokes equation
  - Conservation equation of chemical species
  - Ideal gas equation of state

◆ Discretization of convection term:
  - Yee’s non MUSCL type 2nd order TVD upwind explicit scheme

◆ Discretization of diffusion term:
  - 2nd order central differential scheme

◆ Reaction model (Hydrogen-Air):
  - Hong *et al.* (9 species and 20 elemental reactions)

◆ Time integration for chemical source term:
  - robust MTS method
Validation of present model

Present model can capture compressible flow and reaction correctly.
Results and discussions

• The effect of tube length and diameter (2D)
• The distance where the flame can be sustained (0D)
Flowfield (~ 68 μs after leakage)

Condition: \( L = 90 \text{ mm}, \ D = 10 \text{ mm}, \ P_{H2} = 20.0 \text{ MPa} \)
Self ignition of hydrogen released from tube

- Spherical shock wave compresses the ambient air and increases temperature, which sustains the chemical reaction.
- The self ignited hydrogen jet will be extinguished due to expansion as it goes away from the tube.
The effect of tube length ($D = 10\,\text{mm}$, $P_{\text{H}_2} = 20.0\,\text{MPa}$)

$L = 90\,\text{mm}$

Temperature [K]

$0\,\mu\text{s}$

Mass fraction of OH [-]

$0\,\mu\text{s}$

$L = 45\,\text{mm}$

Temperature [K]

$2000\,\mu\text{s}$

Mass fraction of OH [-]

$68\,\mu\text{s}$

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Reactivity by tube length

Longer tube length enhances the reactivity of self ignited hydrogen jet.

Production rate of OH

Time [µs]

Over 2000 K volume outside tube [mm³]

$L = 90$ mm
$L = 45$ mm
The effect of tube diameter ($L = 90$ mm, $P_{H2} = 14.5$ MPa)

68 $\mu$s after the leakage

![Diagram showing temperature and mass fraction of OH for $D = 3$ mm and $D = 10$ mm.](image)
Reactivity by tube diameter

Larger tube diameter enhances the reactivity of self ignited hydrogen jet.
Results and discussions

• The effect of tube length and diameter (2D)
• The distance where the flame can be sustained (0D)
Strength of spherical shock wave

The strength of spherical shock wave weaken as spherical shock wave propagates from the center.

The strength of spherical shock wave is enhanced by following factors.
1. Higher release pressure $P_{H2}$
2. Larger tube diameter $D$

$$\begin{align*}
    p_s &= \frac{2E_0}{\alpha} \delta^2 \frac{r_s^{-3}}{\gamma + 1} \\
    T_s &= \frac{2(\gamma - 1)}{R(\gamma + 1)^2} \delta^2 \frac{E_0}{\alpha \rho_0} r_s^{-3}
\end{align*}$$
Strength of spherical shock wave and induction time

Initial condition (0D): Shorter tube (After shock condition: $P_2$, $T_2$)
Longer tube ($P_2$, $T_2 + 100$ K, longer $L$)

Target mixture: $2\text{H}_2 + \text{O}_2 + 3.76\text{N}_2$

- The stronger the spherical shock wave becomes, the higher temperature after shock wave becomes, which leads to shorter induction time.
- Induction time becomes shorter due to higher initial temperature by longer tube length which produces larger ignited volume before leakage.
Distance where the self ignition is sustained

\( t_{\text{chem}} \) : the time required for the chemical reaction to occur
\( t_{\text{flow}} \) : the characteristic time of the flow to expand and extinguish the flame

\( t_{\text{chem}} \) (w/ larger \( D \), higher \( P_{\text{H2}} \), longer \( L \))

Condition for sustaining self ignition : \( t_{\text{chem}} < t_{\text{flow}} \)

Larger tube diameter, longer tube length and higher release pressure makes the characteristic time for chemical reaction short.
Conclusions

Self ignited hydrogen jet released from the tube is analyzed by two-dimensional axisymmetric numerical simulation and following knowledge is obtained.

• Reactivity and sustainability of self ignited hydrogen jet released from the tube is affected by tube length and tube diameter.

• In order for self ignition to be sustained outside the tube, the time required for the chemical reaction to occur needs to be shorter than the characteristic time of the flow to expand and extinguish the flame.

• Larger tube diameter, longer tube length and higher release pressure make the time for chemical reaction to occur short and increase the distance where the self ignited hydrogen jet is sustained.
Initial diaphragm shape affects the behavior of self ignition inside the tube.

Initial diaphragm shape is determined as following equation like Terashima et al.

\[ x_c = 0.05D \cos \left( \pi \frac{2y}{D} \right) \]

Trend for strength of spherical shock wave

The trend for strength of spherical shock wave from tube is approximated to a spherical shock wave generated from a point source.

\[ \gamma : \text{specific heat ratio} \]
\[ R : \text{gas constant} \]

\[
\begin{align*}
T_s &= 2 \left( \frac{\gamma - 1}{\gamma + 1} \right)^{2} \delta^2 \frac{E_0}{\alpha \rho_0 r_s^{-3}} \\
p_s &= 2E_0 \alpha^2 \delta^2 \frac{r_s^{-3}}{\gamma + 1}
\end{align*}
\]

\[
\alpha = 0.31246 (\gamma - 1)^{-1.1409 - 0.11735 \log(\gamma - 1)}
\]
\[ \delta = \frac{2}{5} \]
The effect of tube length ($D = 10 \text{ mm}, P_{\text{H}_2} = 20.0 \text{ MPa}$)

$L = 90 \text{ mm}$

- Temperature [K]
  - 200
  - 2000
  - $\sim 0 \mu s$

- Mass fraction of OH [-]
  - 0
  - 0.015

$L = 45 \text{ mm}$

- $\sim 0 \mu s$

68 $\mu s$
Calculation target

Parameters:
- Tube length \( L = 0, 30, 45, 60, 90 \) mm
- Tube diameter \( D = 3, 5, 10 \) mm
- Release pressure \( P_{H2} = 6.5, 10.0, 14.5, 20.0 \) MPa

Minimum grid width : 10 \( \mu \)m  (Max. grid points : 12726 x 2801)
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Distance where the self ignition is sustained

Characteristic time

Distance from tube exit

\( t_{\text{chem}} \) (w/ larger \( D \), higher \( P_{\text{H}2} \), longer \( L \))

\( t_{\text{flow}} \)

Flame holding distance

Condition for sustaining self ignition: \( t_{\text{chem}} < t_{\text{flow}} \)

- \( t_{\text{chem}} \): the time required for the chemical reaction to occur
- \( t_{\text{flow}} \): the characteristic time of the flow to expand and extinguish the flame

Larger tube diameter, longer tube length and higher release pressure makes the characteristic time for chemical reaction short.
Validation (Chemical reaction)

Calculation condition : $2\text{H}_2 + \text{O}_2 + 3.76\text{N}_2$, 2.5 atm

Induction time for hydrogen-air mixture shows good agreement with experimental results.

Reaction model used in present study can capture the chemical reaction of hydrogen-air mixture correctly.
Validation (Compressible flow)

Tube diameter : 10 mm

Shock wave propagation speed in present study shows good agreement with experimental and theoretical value.

Present model can capture compressible flow correctly.
The effect of tube length \((D = 10 \text{ mm}, P_{H_2} = 20.0 \text{ MPa})\)

\(L = 90 \text{ mm}\)

\[\begin{align*}
\text{Temperature [K]} & : 200 \rightarrow 2000 \\
\text{Mass fraction of OH [-]} & : 0 \rightarrow 0.015
\end{align*}\]

\(L = 45 \text{ mm}\)

\[\begin{align*}
\text{Temperature [K]} & : 200 \rightarrow 2000 \\
\text{Mass fraction of OH [-]} & : 0 \rightarrow 0.015
\end{align*}\]
Reactivity by tube length

Over 2000 K volume outside tube

From over 2000 K volume and production rate for OH, longer tube length enhances the reactivity of self ignited hydrogen jet.
Reactivity by tube diameter

Over 2000 K volume outside tube

From over 2000 K volume and production rate for OH, larger tube diameter enhances the reactivity of self ignited hydrogen jet.
Reactivity by tube diameter

From over 2000 K volume and production rate for OH, larger tube diameter enhances the reactivity of self ignited hydrogen jet.
Reactivity by tube diameter

From over 2000 K volume and production rate for OH, larger tube diameter enhances the reactivity of self ignited hydrogen jet.
円管直径による着火持続性

図：固定条件：L = 90 mm, P_{H2} = 14.5 MPa

- D = 10 mm
- D = 3 mm

温度が2000 Kを超える体積履歴およびOHの反応速度履歴より，円管直径が大きい場合では着火持続性が向上している。