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

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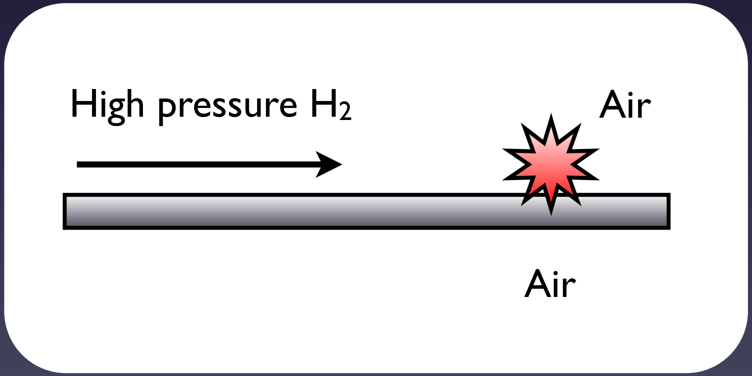
Backgrounds

- Storage pressure of H_2 for the operation of fuel-cell vehicles: as high as 70 - 80 MPa
- Safety issues related to the spontaneous ignition of H_2 with air
- Need to establish reliable risk assessments and understand the mechanism of the spontaneous ignition

Hydrogen station in Japan (from Tokyo gas)



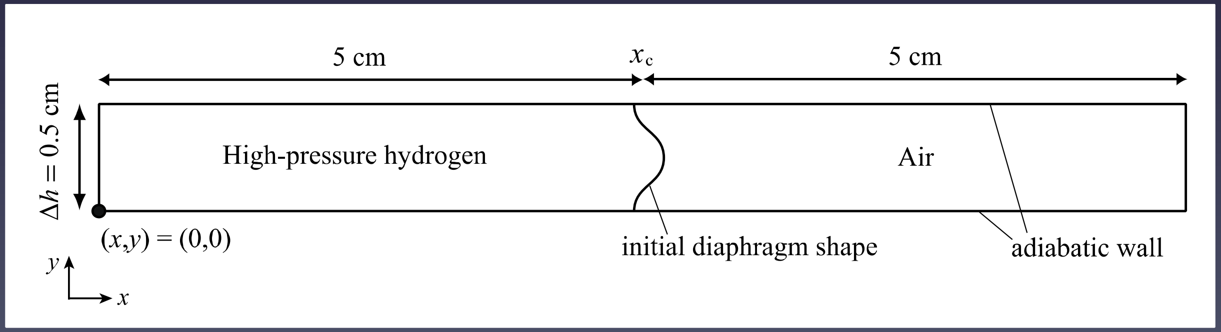
Schematic of spontaneous ignition

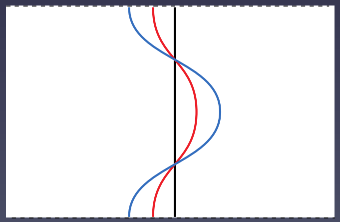
Purpose

- Several experimental and numerical studies conducted
  - Wen et al. (2008, 2009, 2012), Xu et al. (2009)
  - Lee and Jeung (2009)
  - Yamada et al. (2011)
  - Bragin and Molkov (2012)

from Lee and Jeung (2009

- Effects of initial diaphragm shape on spontaneous ignition





Governing equations

The compressible Navier-Stokes equations with a thermally perfect gas EoS

$$
\begin{aligned}
&\partial\rho/\partial t + \nabla\cdot(\rho\boldsymbol{u}) = 0,\\
&\partial(\rho\boldsymbol{u})/\partial t + \nabla\cdot(\rho\boldsymbol{u}\boldsymbol{u} + p\boldsymbol{\delta} - \boldsymbol{\tau}) = 0,\\
&\partial E/\partial t + \nabla\cdot((E+p)\boldsymbol{u}) = \nabla\cdot(\boldsymbol{\tau}\cdot\boldsymbol{u} - \boldsymbol{q}),\\
&\partial(\rho Y_k)/\partial t + \nabla\cdot(\rho_k(\boldsymbol{u}+\boldsymbol{V}_k)Y_k) = \dot{\omega}_k
\end{aligned}
$$

☐ 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

$$
\begin{aligned}
&\mathrm{d}Y_k/\mathrm{d}t = \dot{\omega}_k/\rho\\
&\mathrm{d}T/\mathrm{d}t = -\sum e_k\dot{\omega}_k/(\rho c_v)
\end{aligned}
$$

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

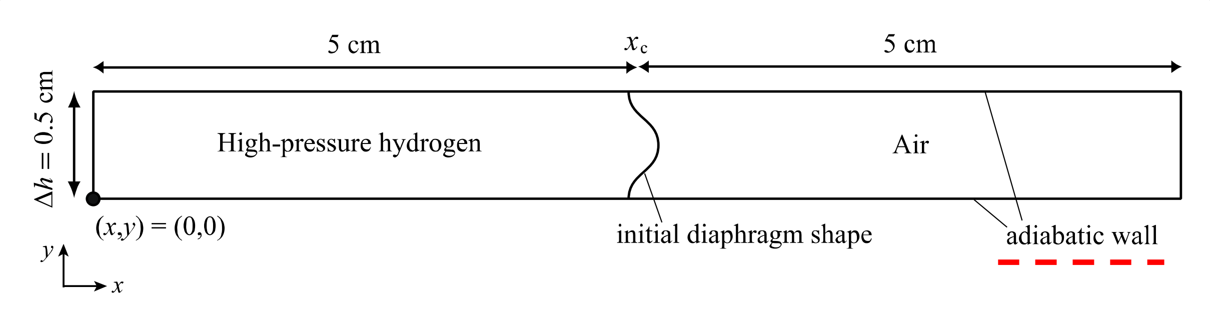
- CHEMKIN-II library used for thermodynamic and transport properties

☐ Chemical reaction

Dynamic multi-time scale (MTS, Gou et al. 2010) method for time integration
H_2 mechanism: UT-JAXA (Shimizu et al. 2011), 9 species and 34 reactions

Problem description

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



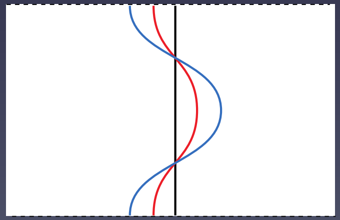
Schematic of computational domain

High-pressure H2	10 MPa, 300 K
Air	0.1 MPa, 300 K

- ☐ Effects of initial diaphragm shape on spontaneous ignition

$$x(y) = x_c - \delta \Delta h \cos(2\pi \frac{y}{\Delta h})$$

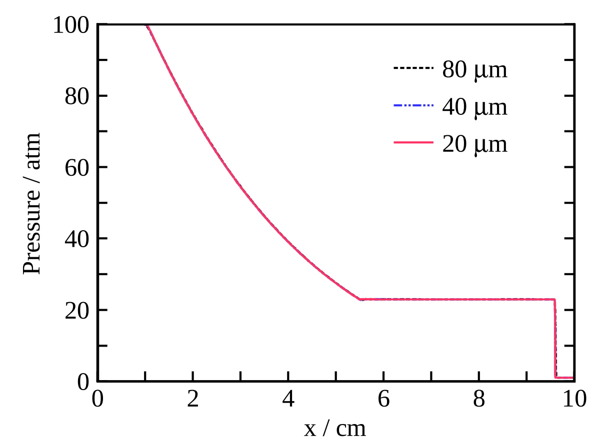
$$\delta = 0.0, 0.05, 0.1, -0.1$$



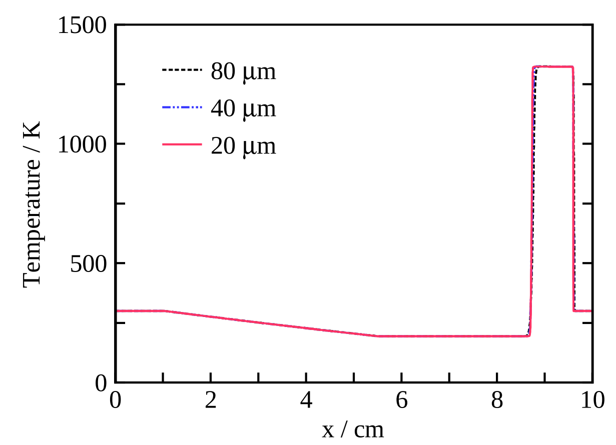
Deformations of initial diaphragm shap

Preliminary 0-D and 1-D studies

☐ 1-D shock tube problem



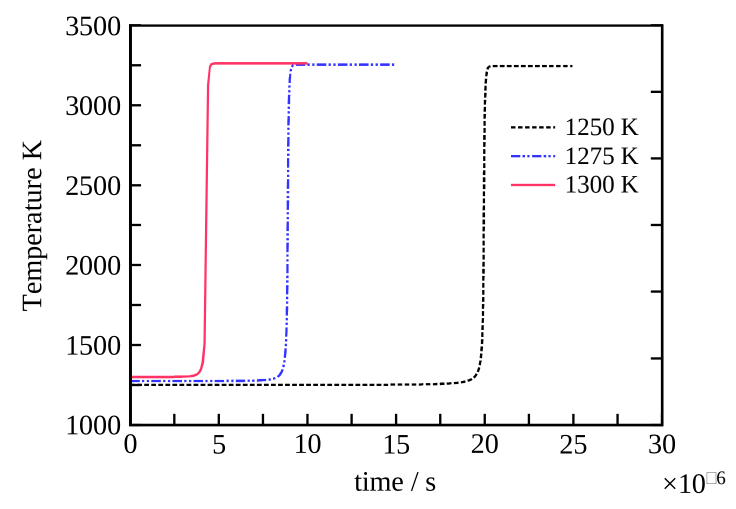
←2.3 MPa



←1320 K

Profiles at 30.0e-6 s

☐ Ignition delay using a 0-D computation

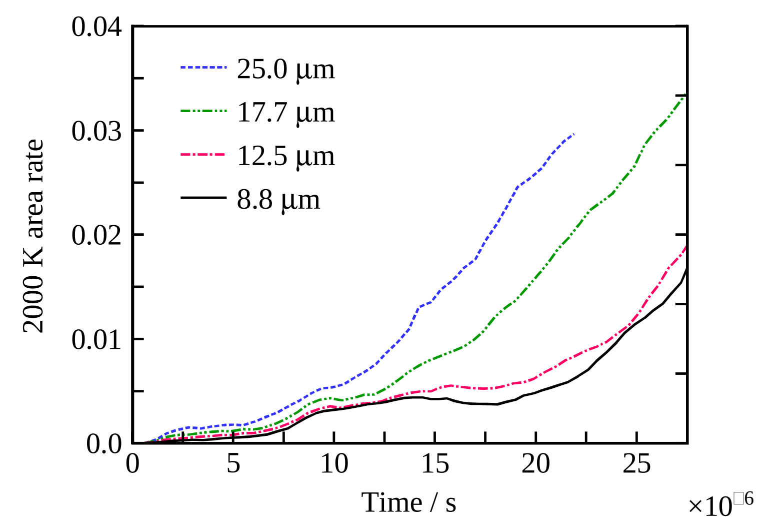


- $H_2/O_2/N_2=2/1/3.76$

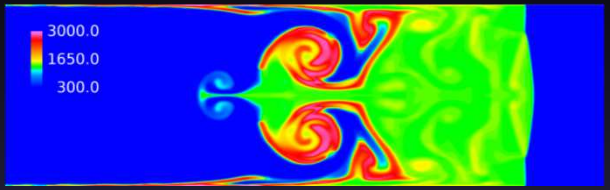
No ignition in 1-D

Grid convergence study in 2-D

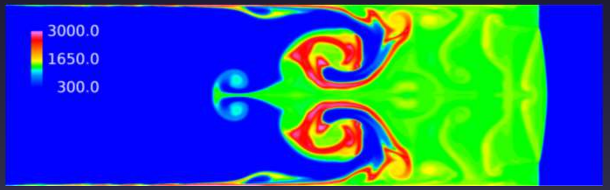
- Wen 2008, 2012, Yamada 2009, Lee 2009 $20-40\ \mu m$
- 2000 K area rate defined a $\bar{A}_{2K}(t) = \frac{1}{A_h}\sum_{j=1}\sum_{k=1} A_{j,k}^{T\geq 2000}$



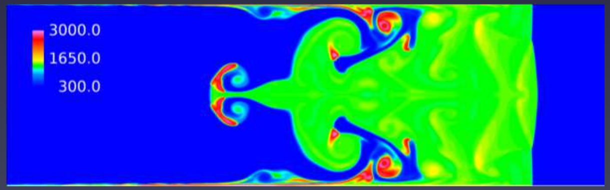
Time histories of 2000 K area rate



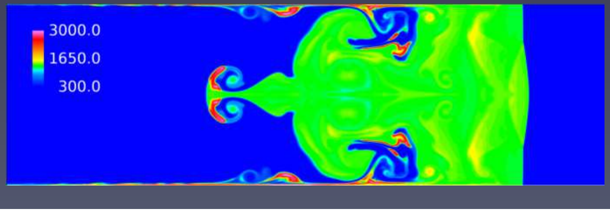
$25.0\ \mu m$



$17.7\ \mu m$



$12.5\ \mu m$



$8.8\ \mu m$

Straight diaphragm shape

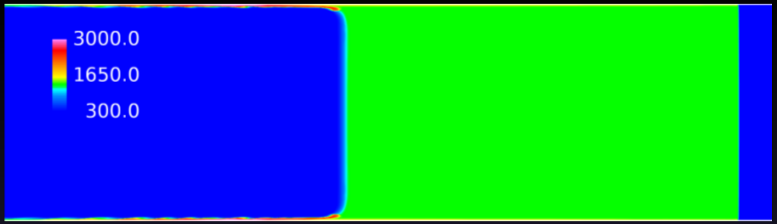
$\delta = 0.0$

- Temperature animation

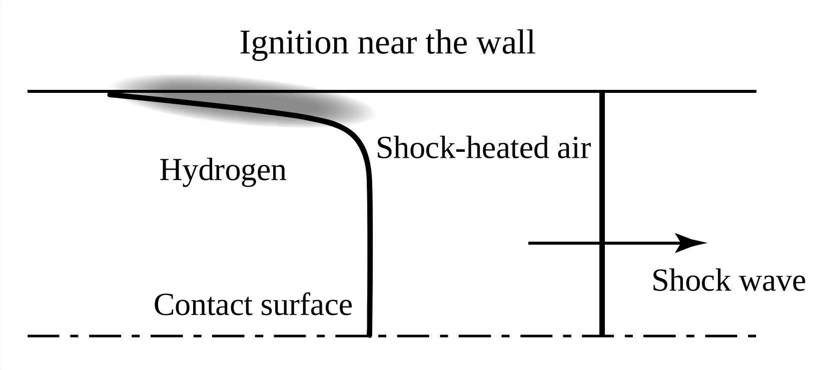
Straight diaphragm shape

$\delta = 0.0$

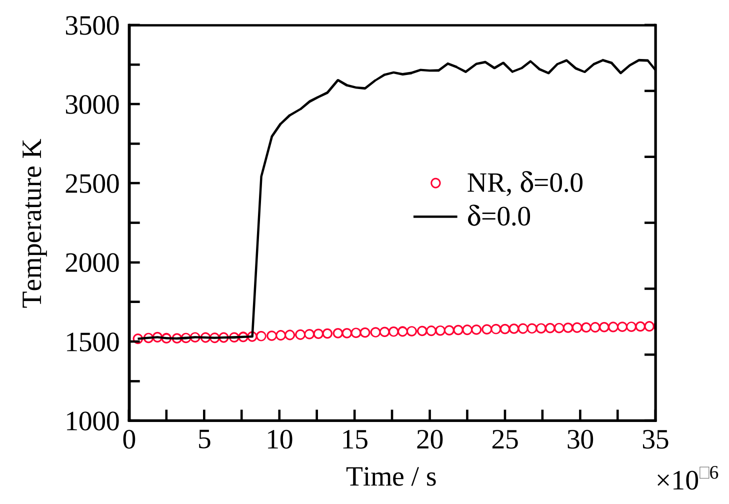
- ☐ Ignition near the wall due to adiabatic condition



Temperature distributions at $t = 32.1\ \mu$s



Schematic of the flow filed



Maximum temperature history

- Temperature near the wall (1500 K) > Temperature behind the shock (1300 K)

Largely deformed diaphragm shape

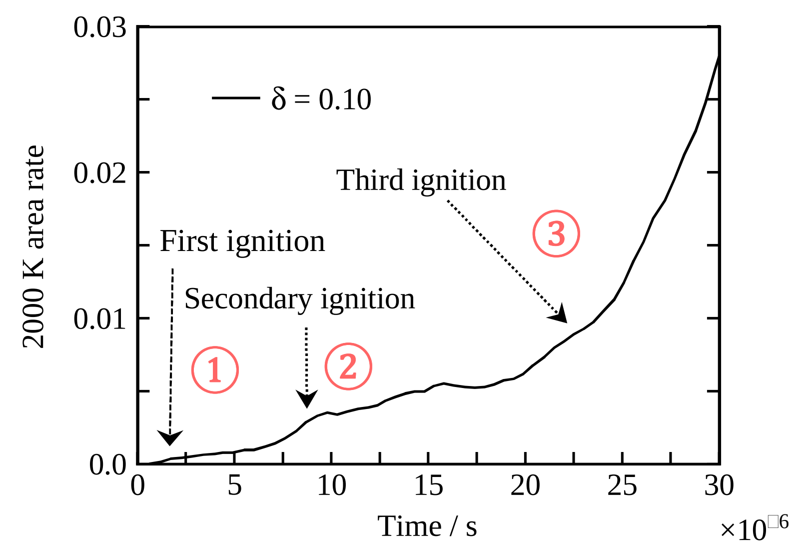
$\delta = 0.1$

- Temperature animation

Largely deformed diaphragm shape

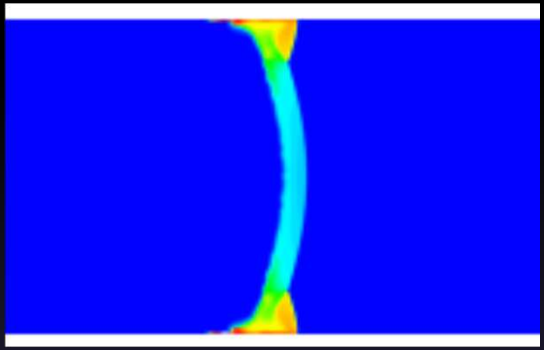
$\delta = 0.1$

- Three ignition events identified

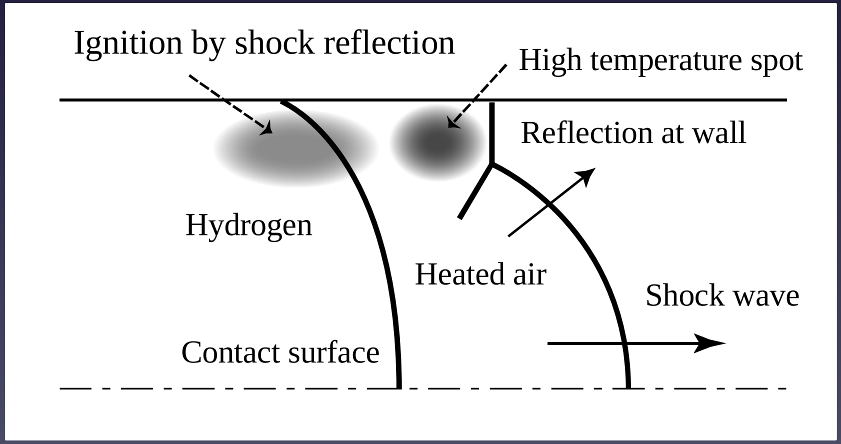


Time histories of 2000 K area rate

① First ignition



Temperature distributions at $t = 1.7\ \mu s$



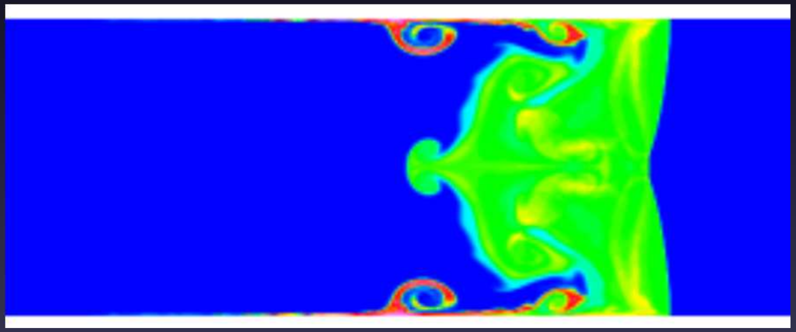
Schematic of the flow filed

Second ignition in largely deformed diaphragm shape

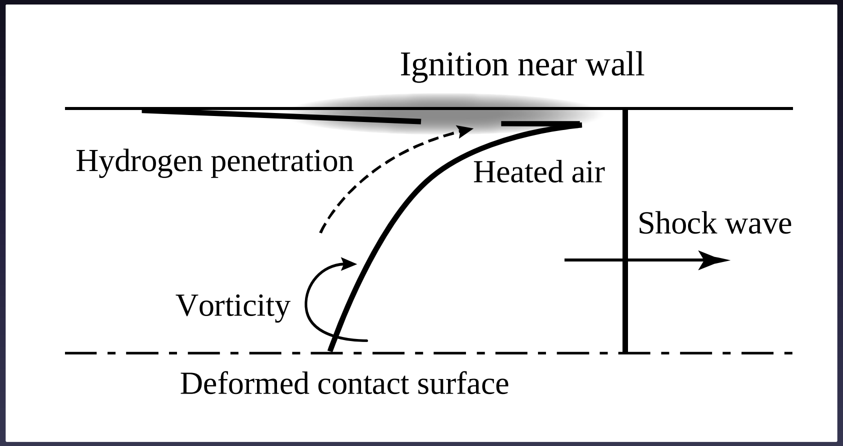
$\delta = 0.1$

② Second ignition

Whole view



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



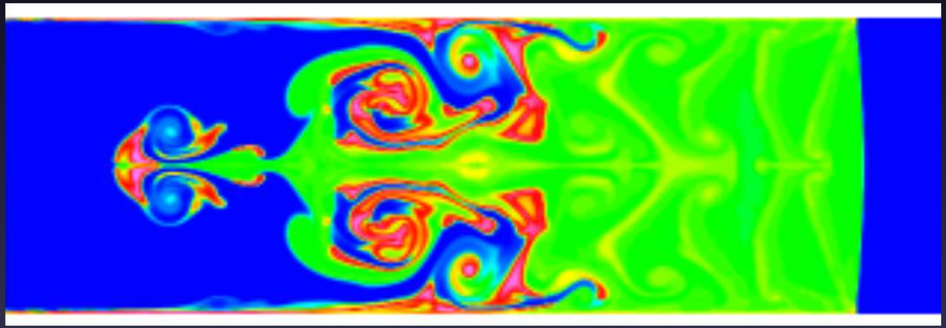
Schematic of the flow filed

Third ignition in largely deformed diaphragm shape

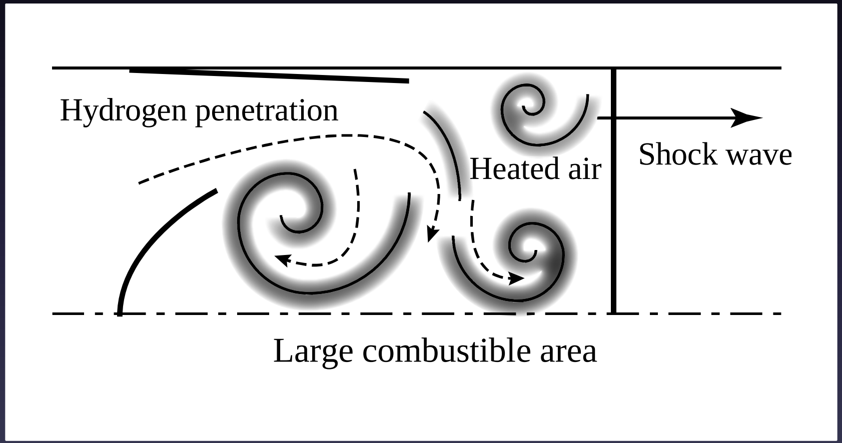
$\delta = 0.1$

③ Third ignition

Whole view



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



Schematic of the flow filed

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

$\delta = -0.1$

- Temperature animation

Mildly deformed diaphragm shape

$\delta = 0.05$

- Temperature animation