**Mechanism of Strong and Mild Ignition behind Reflected Shock Waves in Hydrogen Mixture**

<table>
<thead>
<tr>
<th>Makoto ASAHARA</th>
<th>Aoyama Gakuin University, JAPAN</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tsubasa KOYAMA</td>
<td>Aoyama Gakuin University, JAPAN</td>
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<tr>
<td>A. Koichi HAYASHI</td>
<td>Aoyama Gakuin University, JAPAN</td>
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<tr>
<td>Nobuyuki TSBOI</td>
<td>Kyusyu Institute of Technology, JAPAN</td>
</tr>
</tbody>
</table>
1. Backgrounds
   1.1 Motivation
   1.2 Previous Studies 1
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   1.4 Objective

2. Computational Approach
   2.1 Governing Equations
   2.2 Schemes
   2.3 Conditions

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   3.1 Comparison of ignition domain
   3.2 Comparison of ignition delay time

4. Results and Discussions
   4.1 Euler eq. vs. NS eq.
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   4.4 Induction delay time

5. Conclusions
Ignition behind the RS under
- constant pressure
- constant temperature
- “stationary medium ?!”

Measuring an ignition delay time have been conducted by the RS.

The medium behind the reflected shock wave is NOT stationary condition strictly.
Past study 1

Voevodsky and Soloukhin, 1958

To investigate an induction delay time

They said that the induction lags might be caused by boundary layer.

10000

1000

100

10

1

0.6 0.7 0.8 0.9 1 1.1 1.2 1.3

1000/T, K⁻¹

P₅=1.0 atm (theory)

Exp. By Voevodsky and Soloukhin
Past study 2

Meyer and Oppenheim, 1971

Classification of ignition type behind RS in a tube filled with H$_2$-O$_2$ as **strong ignition** and **mild ignition**.

**Strong Ignition**
- Instantaneous igniting
- on the end-wall
- Flat flame (reaction shock wave)
- High temperature

**Mild Ignition**
- Slow igniting
- Ignition caused by flame kernel near or away from the end-wall
- Complicated flame shape
Past study 2

Meyer and Oppenheim, 1971

- Strong Ignition
  - Instantaneously-ignition
  - Ignition on the end-wall
  - Flat flame
  - High temperature

- Mild Ignition
  - Reaction shock wave
  - Reaction shock wave
  - Flame kernel
  - Meyer and Oppenheim, 1971
  - To classify Ignition type behind RS in a tube filled with H₂-O₂ into strong ignition and mild ignition.

- Slowly-ignition
  - Ignition by build-up of flame kernel in an area slightly distant from the end-wall
  - Compressible flame shape

\[
\begin{array}{c|c|c|c|c|c|c|c}
\text{\(p_5\), atm} & \text{\(T_5\), K} & \text{\(T_5\), K} & \text{\(T_5\), K} & \text{\(T_5\), K} & \text{\(T_5\), K} & \text{\(T_5\), K} & \text{\(T_5\), K} \\
\hline
0,0 & 700 & 800 & 900 & 1000 & 1100 & 1200 & 1300 & 1400 \\
0,5 & 1,0 & 1,5 & 2,0 & 2,5 \\
\hline
\end{array}
\]
Past study 2

Meyer and Oppenheim, 1971

Strong Ignition
- Instantaneously-ignition
- Ignition on the end-wall
- Flat flame
- High temperature

Mild Ignition
- Reaction shock wave

To classify Ignition type behind RS in a tube filled with $H_2-O_2$ into
- Slowly-ignition
  - Ignition by build-up of flame kernel in an area slightly distant from the end-wall
  - Compressible flame shape

$p_s$, atm

$T_s$, K

0,0 0,5 1,0 1,5 2,0 2,5

0,0 0,5 1,0 1,5 2,0 2,5

no ignition mild ignition strong ignition

explosion limit

2,5 700 800 900 1000 1100 1200 1300 1400
it is not clear how much the hydrodynamic effect by boundary layer influences **strong ignition** and **mild ignition**.
Objective

To investigate the relationship between ignition and the flow induced by boundary layer.

Study Method

- Numerical Simulation
- Target for comparison is Meyer and Oppenheim’s experiment.
# Outline

1. Background
   - 1.1 Motivation
   - 1.2 Previous Studies 1
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2. Computational Approach
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   - 2.3 Conditions

3. Validation
   - 3.1 Comparison of ignition domain
   - 3.2 Comparison of ignition delay time

4. Results and Discussions
   - 4.1 Euler eq. vs. NS eq.
   - 4.2 Strong Ignition process
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5. Conclusions
**Governing equations**

2-D compressible Navier–Stokes equations

\[
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = \frac{\partial E_v}{\partial x} + \frac{\partial F_v}{\partial y} + S
\]

\[
Q = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho \end{pmatrix}, \quad E = \begin{pmatrix} \rho u \\ p + \rho u^2 \\ \rho uv \\ (e + p)v \\ \rho \end{pmatrix}, \quad F = \begin{pmatrix} \rho v \\ \rho vu \\ p + \rho v^2 \\ (e + p)v \\ \rho v \end{pmatrix}, \quad E_v = \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xu} + \tau_{yv} + q_x \\ \rho \end{pmatrix}, \quad F_v = \begin{pmatrix} 0 \\ \tau_{yy} \\ \tau_{yy} \\ \tau_{yu} + \tau_{yv} - q_y \\ \rho \end{pmatrix}, \quad S = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}
\]

**Detailed H₂/O₂ chemical kinetics model by Hong et al. (2011)**

**Induction delay time**

**Laminar flame speed**
Numerical methods

\[
\frac{\partial Q}{\partial t} + \frac{\partial E}{\partial x} + \frac{\partial F}{\partial y} = \frac{\partial E_y}{\partial x} + \frac{\partial F_x}{\partial y} + S
\]

**Time integration**  3step 3rd-order SSP Runge–Kutta method

**Convective fluxes**  AUSMDV scheme

**Viscous, thermal and mass diffusion fluxes**  2nd-order central difference scheme

**Source term**  Point implicit method
**Numerical conditions**

**Computational domain**

2-D shock tube: the same height as Mayer and Oppenheim

- Non-slip adiabatic wall
- Inflow
- Symmetry
- Non-slip adiabatic wall

Number of grid $I_{nx} \times j_{nx} = 901 \times 301$

**Boundary layer thickness at $p_1 = 0.03$ atm**

- $\Delta x_{\text{max}} = 290 \mu m$
- $\Delta y_{\text{max}} = 160 \mu m$
- $\Delta x_{\text{min}} = 25 \mu m$
- $\Delta y_{\text{min}} = 15 \mu m$
**Numerical conditions**

**Computational domain**

2-D shock tube: the same height as Mayer and Oppenheim

<table>
<thead>
<tr>
<th>Inflow</th>
<th>Symmetry</th>
<th>Non-slip adiabatic wall</th>
</tr>
</thead>
<tbody>
<tr>
<td>31.75mm</td>
<td></td>
<td>1000mm</td>
</tr>
</tbody>
</table>

**Initial conditions**

<table>
<thead>
<tr>
<th>High pressure region</th>
<th>Low pressure region</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{N}_2 )</td>
<td>( \text{H}_2\text{O}_2 ) ( ( \phi = 1.0 ) )</td>
</tr>
<tr>
<td>( p_4 )</td>
<td>( p_1 )</td>
</tr>
<tr>
<td>( 100p_1 \sim 300p_1 )</td>
<td>( 0.03 \text{ atm} )</td>
</tr>
<tr>
<td>( T_4 )</td>
<td>( T_1 )</td>
</tr>
<tr>
<td>( T_1 \sim 2.5T_1 )</td>
<td>( 0.04 \text{ atm} )</td>
</tr>
<tr>
<td></td>
<td>( 0.05 \text{ atm} )</td>
</tr>
<tr>
<td></td>
<td>( 0.10 \text{ atm} )</td>
</tr>
<tr>
<td></td>
<td>( 296 \text{ K} )</td>
</tr>
</tbody>
</table>
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5. Conclusions
Comparison between ignition regions (P-T diagram)

Mild Ignition (Exp. by Meyer & Oppenheim)

Strong Ignition (Exp. by Meyer & Oppenheim)
Comparison between ignition regions (P-T diagram)

- **Strong Ignition** (Exp. by Meyer & Oppenheim)
- **Mild Ignition** (Exp. by Meyer & Oppenheim)
- **Strong Ignition** (This study)
- **Mild Ignition** (This study)

- $p_1 = 0.10 \text{ atm}$
- $p_1 = 0.05 \text{ atm}$
- $p_1 = 0.04 \text{ atm}$
- $p_1 = 0.03 \text{ atm}$

![P-T diagram](image-url)
Comparison between induction delay times (Arrhenius plot)

- Mild Ignition (exp. by Meyer and Oppenheim)
- Strong Ignition (exp. by Meyer and Oppenheim)

The graph shows data points for different pressures (P_5) and temperatures (1000/T, K^{-1}) with lines representing the theory by Meyer and Oppenheim.
Comparison between induction delay times (Arrhenius plot)

- Mild Ignition (This study)
- Intermediate cases (This study)
- Strong Ignition (This study)
- Mild Ignition (calc. by Knisely et al.)
- Strong Ignition (calc. by Knisely et al.)
- Mild Ignition (exp. by Meyer and Oppenheim)
- Strong Ignition (exp. by Meyer and Oppenheim)
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5. Conclusions
Strong ignition

Density gradient, $\log|\nabla \rho|$

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<th>NS</th>
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Temperature, $T$

<table>
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<tr>
<th>1500 K</th>
<th>500 K</th>
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<tbody>
<tr>
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Mach number

<table>
<thead>
<tr>
<th>1.6</th>
<th>0</th>
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# Strong ignition

## Density gradient, \( \log|\nabla \rho| \)

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## Temperature, \( T \)

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<th>500 K</th>
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## Mild ignition

### Density gradient, $\log |\nabla \rho|$:

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### Temperature, $T$:

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Pressure profiles at the end-wall

Mild ignition process is different from strong ignition process.
⇒ Flame kernel is already generated before second pressure peak in mild ignition case.
Strong ignition

Density gradient, $\log|\nabla \rho|$

Temperature, $T$

Vorticity, $\omega$

Schlieren photograph of reflected shock by Meyer and Oppenheim, 1971
Influenced by multi-dimensional flow

$t = 27.0 \mu s$

$t = 28.6 \mu s$

$t = 30.2 \mu s$

$t = 32.8 \mu s$

Reaction shock wave

Local ignition

Density gradient, $\log|\nabla \rho|$

Vorticity, $\omega$

Vortex appears at the corner of the end-wall

ignition on the vortex

Strong ignition have little direct effect on hydrodynamics

ignition at whole surface of the end-wall

Propagation of reaction shock wave

Strong ignition (time history)
Mild ignition

Density gradient, $\log|\nabla \rho|$

Temperature, $T$

Reflected shock

Oblique shock

Separated vortex
Mild ignition (Time history 1)

- Vortex separation
- High temperature
- High temperature
- Vortex
Mild ignition (Time history 2)

- New vortex generation by separated vortices
- Local ignition at new vortex
- Reaction zone extension

- Influenced by multi-dimensional flow
- Mild ignition is influenced by hydrodynamics
Comparison between ignition delay times

- P$_5$=1.97 atm (theory)
- P$_5$=1.27 atm (theory)
- P$_5$=1.70 atm (theory)
- P$_5$=1.86 atm (theory)
- P$_5$=2.22 atm (theory)

**Ignition caused by chemical kinetics**

- M-S
- Mild
- Exp. By Voevodsky and Soloukhin

**Ignition caused by chemical kinetics and hydrodynamics (RSWBLI)**

Mild ignition estimates shorter ignition delay time because of flow induced by the reflected shock wave – boundary layer interaction.
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   4.4 Induction delay time

5. Conclusions
We obtained strong ignition and mild ignition using two-dimensional simulation with the detailed chemical kinetics model.

**Strong Ignition**
- Ignition at the vortex
- Ignition on the end-wall
- Propagation of reaction shock wave

**Mild Ignition**
- Vortex separation
- Ignition next to vortex
- Reaction zone extension

Strong ignition caused by chemical kinetics

Induction delay time for strong ignition with numerical calculation has good agreement with theoretical one. Induction delay time for mild ignition with numerical calculation is shorter than theoretical one.

Mild ignition estimates shorter ignition delay time because of flow induced by the reflected shock wave – boundary layer interaction.
Thank you for your kind attention !!
Appendix
**Backgrounds**

**Incident Shock Wave (IS)**

**Reflected Shock Wave (RS)**

Ignition behind RS under
- constant pressure
- constant temperature
- “stationary medium ?!”

Ignition delay time
The relationship between chemical kinetics and hydrodynamics (the complicated flows induced by RSWBLI) is unclear.
Shock Wave – Boundary Layer Interaction

Mark, 1958

Damazo, Odell and Shepherd, AIAA, 2012

Density distribution of reflected shock wave

Ziegler, 2012
Strong Ignition

Knisely, Austin Bacon, and Khokhlov, 2013
Mild Ignition

Meyer and Oppenheim, 1971
Mild ignition

Yamashita et al., 2011
Mild Ignition

Knisely, Austin Bacon, and Khokhlov, 2013
Incident Shock Wave Propagation

Theory

\[ \frac{p_2}{p_1} = 1 + \frac{2\gamma}{\gamma + 1} \left( M_{si}^2 - 1 \right) \]

\[ M_{si} = \sqrt{\frac{\gamma + 1}{2\gamma} \left( \frac{p_2}{p_1} - 1 \right) + 1} \]
Shock wave – boundary layer interaction

Before shock reflection

Temperature & velocity vector

Velocity boundary layer

After shock reflection

Reflected shock

Reflected shock

Oblique shock

BL
Strong Ignition (time history)

- Ignition around the corner at first
- Ignition on the end-wall
- Propagation of reaction shock wave

Influenced by multi-dimensional flow

Initiated by the IS (ignition delay time)

Flow behind the RS has a relatively small effect on the ignition delay time.
Numerical result of strong ignition

- Propagation of reaction shock
- Density gradient, $\log|\nabla \rho|$
- Strong Ignition
- Propagation of incident shock
- Propagation of reflected shock
- Shock reflection at the end-wall
- Propagation of reaction shock
## Viscosity effect (Euler Eqs. vs. NS Eqs.)

### Density gradient, $\log |\nabla \rho|$:

<table>
<thead>
<tr>
<th></th>
<th>Euler</th>
<th>NS</th>
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### Pressure, $p$:

<table>
<thead>
<tr>
<th></th>
<th>Euler</th>
<th>NS</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.00 atm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.05 atm</td>
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**Viscosity effect on strong ignition (Euler vs. NS)**

Density gradient, $\log |\nabla \rho|$:

| Density gradient, $\log |\nabla \rho|$ |
|-----------------|
| Euler           |
| NS              |

Temperature, $T$:

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<tbody>
<tr>
<td>1500 K</td>
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<tr>
<td>500 K</td>
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Vorticity, $\omega$:

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>$1.0 \times 10^6$</td>
</tr>
<tr>
<td>$-1.0 \times 10^6$</td>
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</table>

Ignition delay time of strong ignition with NS eq. is longer than that with Euler eq. It might effect in energy dissipation decrease due to viscosity.
Comparison between the results of NS eq. and Euler eq.

<table>
<thead>
<tr>
<th>NS equations</th>
<th>Euler equations</th>
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</table>
Comparison between the results of NS eq. and Euler eq.
P and T profiles of strong ignition at the end-wall

Euler equations

Pressure profile of strong ignition
(Meyer and Oppenheim)

NS equations

Pressure profile of strong ignition
(Meyer and Oppenheim)
The induction delay time with Euler eqs. is much the same time as one with NS equations.
Influenced by multi-dimensional flow

\[ t = 27.0 \mu s \]
\[ t = 28.6 \mu s \]
\[ t = 30.2 \mu s \]
\[ t = 32.8 \mu s \]

Reaction shock wave

Ignition on the vortex

Density gradient, \( \log |\nabla \rho| \)

Vorticity, \( \omega \)

Vortex appears at the corner of the end-wall

Strong ignition caused by chemical kinetics

Strong ignition caused by chemical kinetics

Reaction at whole surface of the end-wall

Propagation of reaction shock wave
Mild ignition

Density gradient, $\log|\nabla \rho|$ 

Temperature, $T$

Vorticity, $\omega$

Reflected shock

Oblique shock

Ignition
Mild ignition (Time history 1)

- $t = 21.0 \mu s$
- $t = 25.8 \mu s$
- $t = 30.4 \mu s$

$\ln |\nabla \rho|$

Temperature, K

Vorticity, 1/s

Vortex separation 1

Flame kernel
Mild ignition (Time history 2)

-3.0 \text{ ln}|\nabla \rho| 3.0
-4.0 \times 10^6 4.0 \times 10^6

800 1200

Exothermic region

Vortex separation 2
Comparison between ignition delay times

- **Mild Ignition** estimates shorter ignition delay time because of flow induced by the reflected shock wave – boundary layer interaction.

- Ignition caused by chemical kinetic and hydrodynamic (the RS – boundary layer interaction).

- Ignition caused by chemical kinetic.
* J. Damazo, J. Ziegler, J. Karnesky, and J. E. Shepherd, Proceedings of the 28th International Symposium on Shock Waves, University of Manchester, July 2011
Meyer and Oppenheim’s Theory (H₂-O₂)

\[ \ln \tau = A + \left( \frac{B}{T} \right) + C p^n \exp\left( \frac{D}{T} \right) - \ln\left( \frac{E p}{T} \right) \]

- \( A = -10.7 \)
- \( B = 9130 \)
- \( n = 2 \)
- \( C = 2 \times 10^{-9} \)
- \( D = 19000 \)
- \( E = 4.06 \)

\textit{p}: Pressure behind the RS
\textit{T}: Temperature behind the RS