Numerical Simulation on Dispersion Process of Unsteady Low Speed Hydrogen Jet Flow

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1. Background

Hydrogen jet problem

Fuel cell vehicles start to be sold since 2014.

- Increase to demand fuel cell vehicles
- Increase to install hydrogen stations

The hydrogen station, Kaminokura

Hydrogen is stored at 82MPa in a hydrogen reservoir.

If the hydrogen leaks and ignites, there are huge accidents.

We need to understand the dispersion behavior of hydrogen for risk assessment.

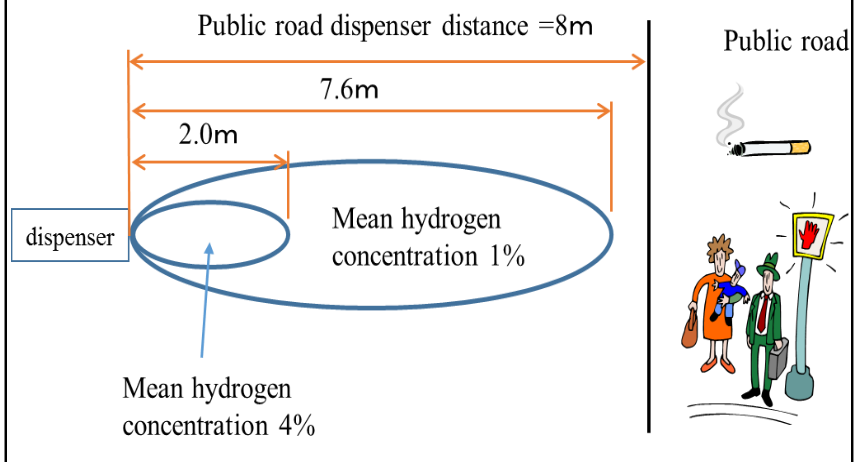
1. Background Unsteady hydrogen jet

The existing laws determines the safety distance by hydrogen concentration obtained by the steady jet.

➡ However, hydrogen jet is unsteady flow when high-pressure hydrogen leaks.

Hydrogen jet becomes unsteady low-speed flow far from the nozzle.

Safety distance by the existing lows in Japan



How to determine the safety distance in the existing laws

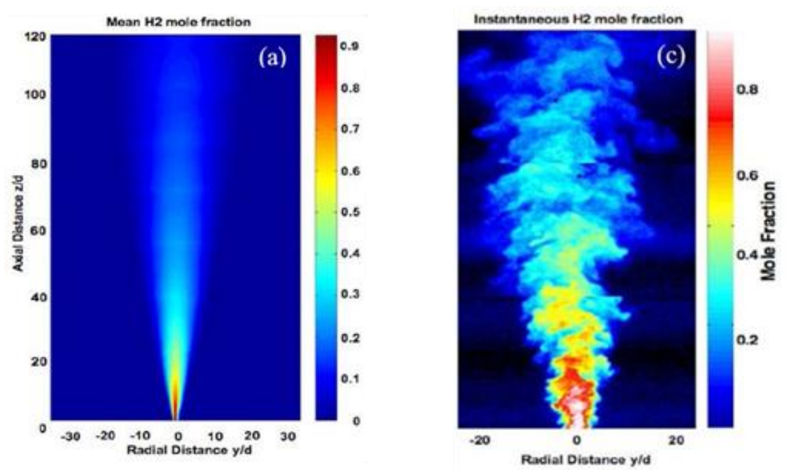
Previous study

Investigate dispersion behavior of low-speed hydrogen jet by experiment.

Schefer et al.*(2008)

➡ Ignition boundary does not coincide with the lower ignition limit of 4% of hydrogen.

It is necessary to understand **unsteady dispersion behavior** of hydrogen jet



Time mean field   Instantaneous field

The concentration distribution of the upward jet hydrogen ,Schefer et al,2011

*Schefer et al. ”Investigation of small-scale unintended releases of hydrogen: Buoyancy effects”, International Journal of Hydrogen Energy (2008)

)15)

1. Motivation　Preconditioning method

The stagnation pressure is approximately 82MPa in the hydrogen reservoir.

- ✓ High-pressure hydrogen jet becomes **compressible flow** near nozzle and becomes **incompressible flow** far from nozzle.
  → Solve the **compressible** and **incompressible** flow simultaneously in computational region.
- ✓ Multi-component gas: H_2, O_2, and N_2

Apply preconditioning method for solving compressible multi-component gas flow.

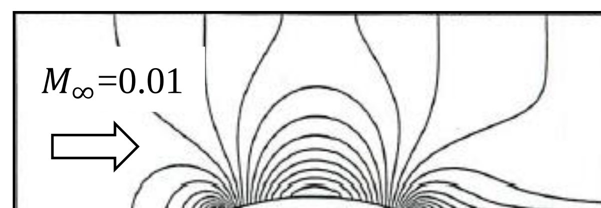
The previous study of preconditioning method

- ➢ Low speed flow over bump for M=0.01:

  Edwards et al.*(2000)

- ➢ Simulate all speed flow using compressible solver

without preconditioning method AUSM +



with Preconditioning method AUSM+(P)

Analysis of the flow in the flow channel that places the bump.　Edwards, 2000

＊Edwards et al. "Low-diffusion Flux splitting Methods for Real Fluid Flows with Phase Transitions", AIAA (2000)

2. Objective

Low-speed unsteady hydrogen jet is simulated to understand the dispersion behavior comparing with experiments of Schefer et al.

- ✓ Validate numerical results of unsteady dispersion jet calculated by preconditioning multi-component compressible viscous flow solver
- ✓ Understand dispersion behavior of unsteady low speed hydrogen jet

3. Analysis method

Numerical methods

- Governing equation : 3D preconditioning Compressible Navier-Stokes equation with nine species.
  ($H_2, O_2, H, O, OH, HO_2, H_2O_2, H_2O, N_2$)

$$\boxed{\frac{\partial Q}{\partial W_h}}\frac{\partial W_h}{\partial t}+\frac{\partial E}{\partial x}+\frac{\partial F}{\partial y}+\frac{\partial G}{\partial z}=\frac{\partial E_v}{\partial x}+\frac{\partial E_v}{\partial x}+\frac{\partial F_v}{\partial y}+\frac{\partial G_v}{\partial z}$$

Γ :Preconditioning matrix

Preservation variable

$$Q=[\rho,\rho u,\rho v,\rho w,e,\rho_i]^T$$

Primitive variable

$$W_h=[p,u,v,w,h,Y_i]^T$$

$$\Gamma=\frac{\partial Q}{\partial W_h}=\begin{bmatrix}\Theta & 0 & 0 & 0 & 0 & -\rho\Re_1 & \cdots & -\rho\Re_N \\ \Theta u & \rho & 0 & 0 & 0 & -\rho\Re_1 u & \cdots & -\rho\Re_N u \\ \Theta v & 0 & \rho & 0 & 0 & -\rho\Re_1 v & \cdots & -\rho\Re_N v \\ \Theta w & 0 & 0 & \rho & 0 & -\rho\Re_1 w & \cdots & -\rho\Re_N w \\ \Theta H-1 & \rho u & \rho v & \rho w & \rho & \rho H_1-\rho\Re_1 H & \cdots & \rho H_N-\rho\Re_N H \\ \Theta Y_1 & 0 & 0 & 0 & 0 & -\rho\Re_1 Y_1+\rho & \cdots & -\rho\Re_N Y_N \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \Theta Y_N & 0 & 0 & 0 & 0 & -\rho\Re_1 Y_N & \cdots & -\rho\Re_N Y_N+\rho\end{bmatrix}$$

$$\Re_i=\frac{R_i}{\sum_{i=1}^{N}Y_iR_i}\qquad H=\frac{\bar{h}+(u^2+v^2+w^2)}{2}\qquad \Theta=\frac{1}{U_r^2}-\frac{1}{c^2}$$

*Weiss et al,"Preconditioning Applied to Variable and Constant Density Flow", AIAA (1995)

3. Analysis method

Preconditioning method of Weiss et al*(1995)

1D basic equation

$$\frac{\partial \boxed{\mathbf{Q}}}{\partial t}+\frac{\partial \mathbf{E}}{\partial x}=\frac{\partial \mathbf{E}_v}{\partial x}$$

$\boldsymbol{\Gamma}$

Preconditioning matrix

Basic equation with preprocessing

$$\boxed{\frac{\partial \mathbf{Q}}{\partial \mathbf{W}}}\frac{\partial \boxed{\mathbf{W}}}{\partial t}+\frac{\partial \mathbf{E}}{\partial x}=\frac{\partial \mathbf{E}_v}{\partial x}$$

Convert conservation variables Q into primitive variables W.

Density base

$$\mathbf{Q}=\left[\rho,\rho u,e,\rho_i\right]^T$$

Pressure base

$$\mathbf{W}_h=\left[p,u,h,Y_i\right]^T$$

Eigenvalues without precondition: $\lambda=u,u+c,u-c$

Eigenvalues with precondition : $\lambda=u,u'+c',u'-c'$

$$u'=u(1-\alpha)$$

$$c'=\sqrt{\alpha^2u^2+U_r^2}$$

$$\alpha=\frac{1}{2}\left(1-\frac{U_r^2}{c^2}\right)$$

$$U_r^2=\begin{cases} K\left|V_\infty\right|^2 & \text{(Low speed)} \\ \left|V\right|^2 & \text{(Subsonic speed ,Transonic speed)} \\ c^2 & \text{(Supersonic)} \end{cases}$$

V_∞: Ambient flow velocity $K=0.25$

Preconditioning method for multi-component gas flow is important feature in this study.

3. Analysis method

Dual time-stepping technique

It is impossible to preserve time accuracy because preconditioning method changes eigenvalues artificially.

Dual time-stepping technique is required

The efficient unsteady flow using a pseudo time term

$$\boxed{\frac{\partial \boldsymbol{Q}}{\partial t}} + \boxed{\boldsymbol{\Gamma}\frac{\partial \boldsymbol{W}}{\partial \tau}} + \frac{\partial \boldsymbol{E}}{\partial x} = \frac{\partial \boldsymbol{E}_v}{\partial x}$$

t : Real time

τ : Pseudo time

Real time term

Pseudo time term

Shown in 2-order accurate 3-point backward difference.

$$\frac{3\boldsymbol{Q}^{s+1} - 4\boldsymbol{Q}^{n} + \boldsymbol{Q}^{n-1}}{2\Delta t} + \boldsymbol{\Gamma}\frac{\boldsymbol{W}^{s+1} - \boldsymbol{W}^{s}}{\Delta \tau} + \frac{\partial \boldsymbol{E}}{\partial x} = \frac{\partial \boldsymbol{E}_v}{\partial x}$$

s : Number of internal loop

If $\tau \rightarrow \infty$, pseudo-time term disappears. Then time accuracy is maintained.

Present simulation preserve time-accuracy as the inner loop is 10 times and residuals decreases three-order magnitude.

3. Analytical method Numerical method

Time integration	Preconditioned Euler explicit method
Convection term	Preconditioned AUSM-DV
Higher-order	2-order MUSCL (w/o limiter)
Viscous term	2-order central difference

3. Analysis method
Calculation conditions

To decide from experimental conditions of Schefer et al (2008)

<table>
<tr><th></th><th>Density [kg/m³]</th><th>Temperature [K]</th><th>Pressure [atm]</th><th>Velocity [m/s]</th><th>Mach [-]</th><th>Reynolds number [-]</th></tr>
<tr><td>Jet outlet</td><td>0.082</td><td rowspan="2">300</td><td rowspan="2">1</td><td>134</td><td>0.106</td><td>2384</td></tr>
<tr><td>Ambient</td><td>1.177</td><td>0</td><td>0</td><td>0</td></tr>
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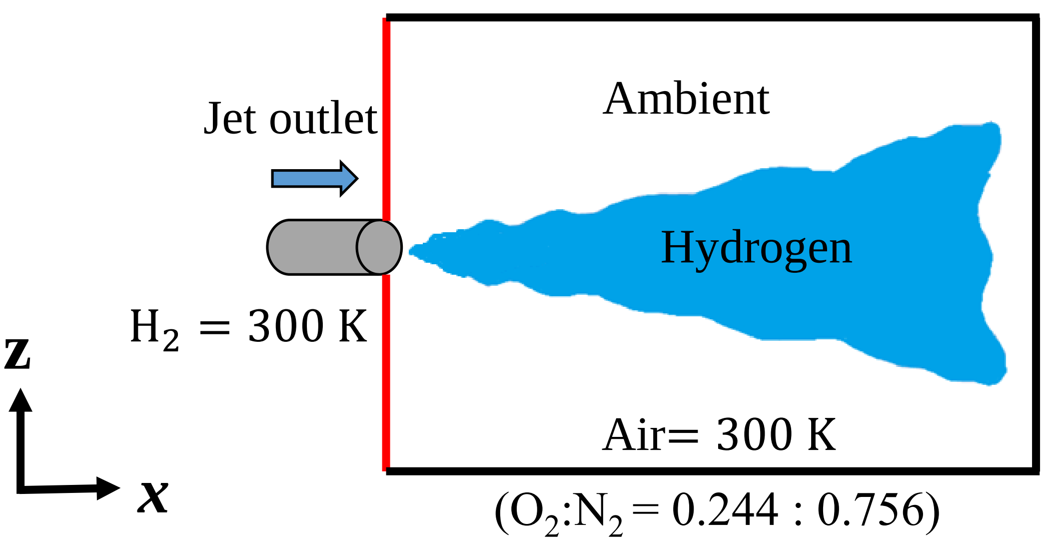


Jet gas. : Hydrogen

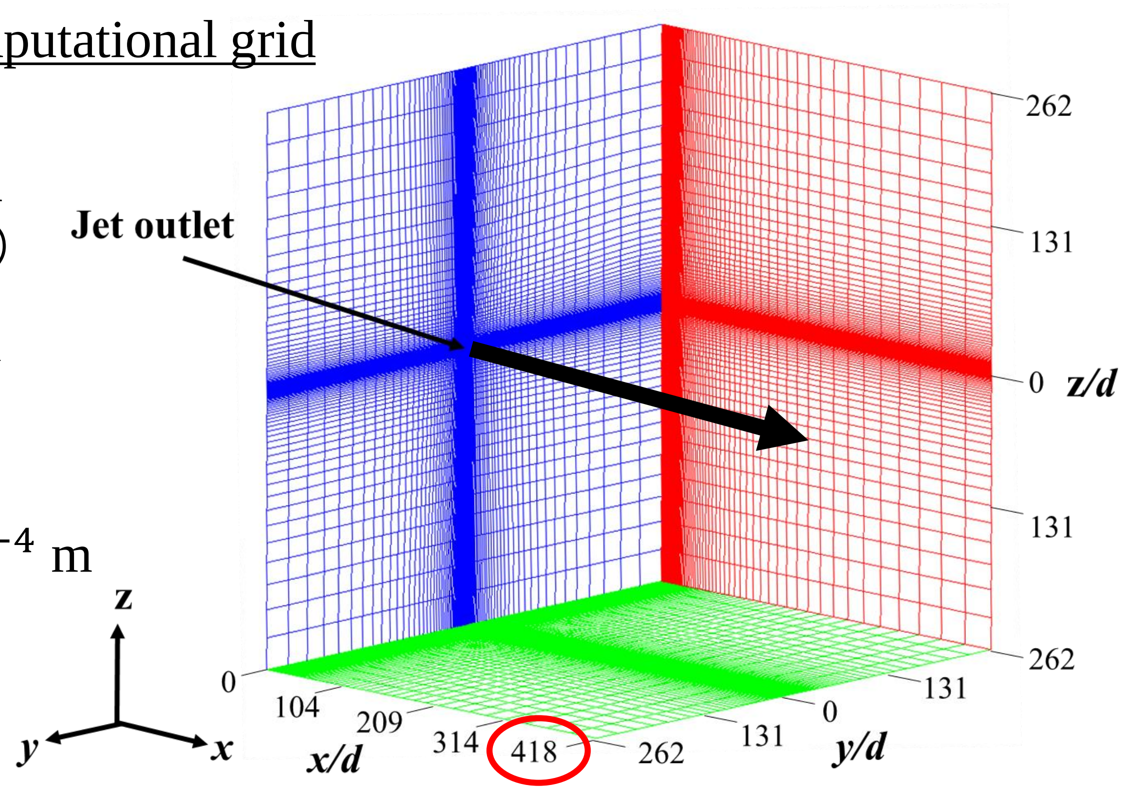
Ambient gas : Air

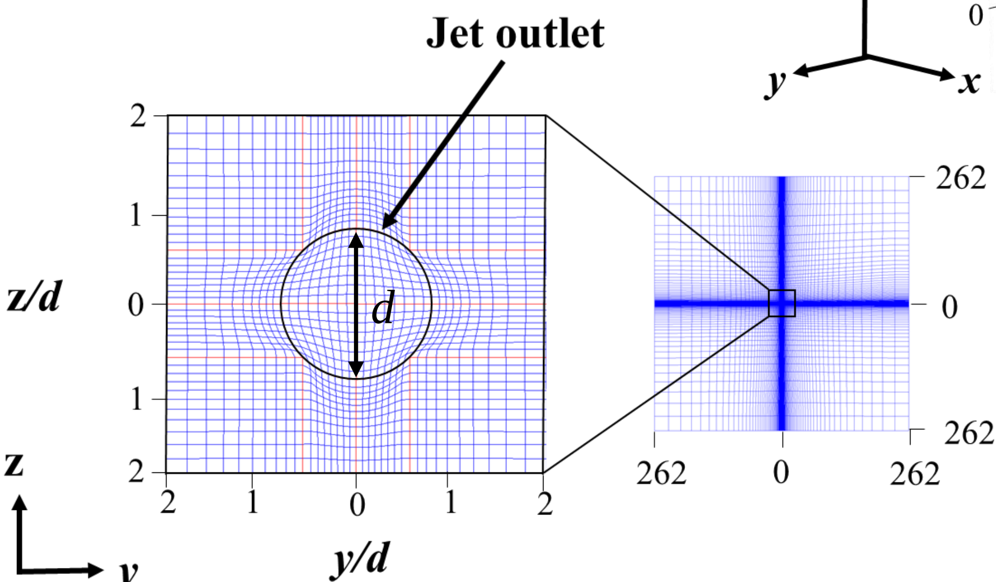
Jet diameter : φ1.91 mm

3. Analysis method

Computational grid

- Grid points：151 × 131 × 131
  （About 2.6 million points）
- Jet exit diameter： φ1.91 mm
- Minimum grid width：
  $\Delta x = \Delta y = \Delta z = 1.2 \times 10^{-4}$ m

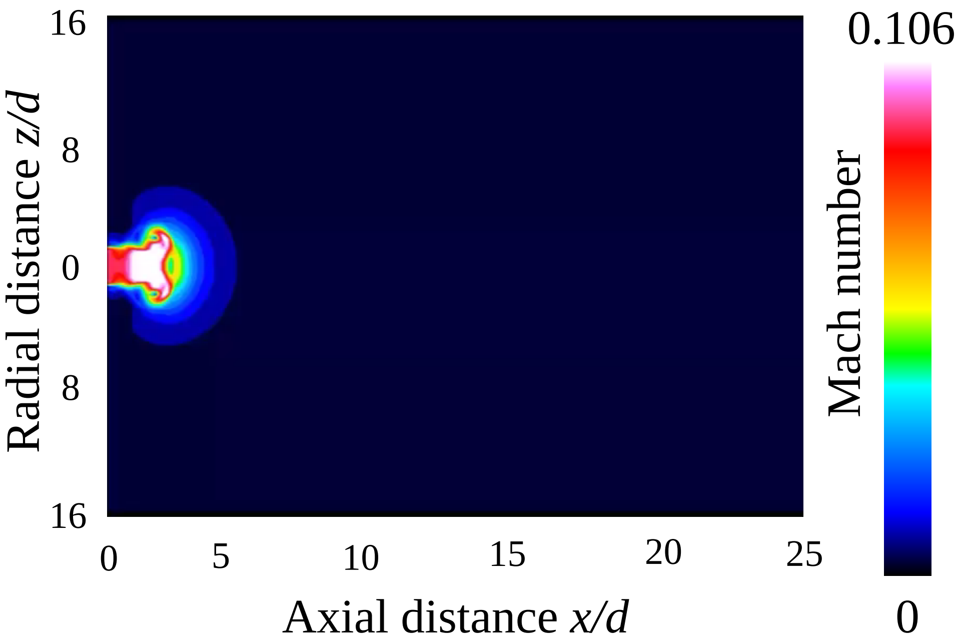




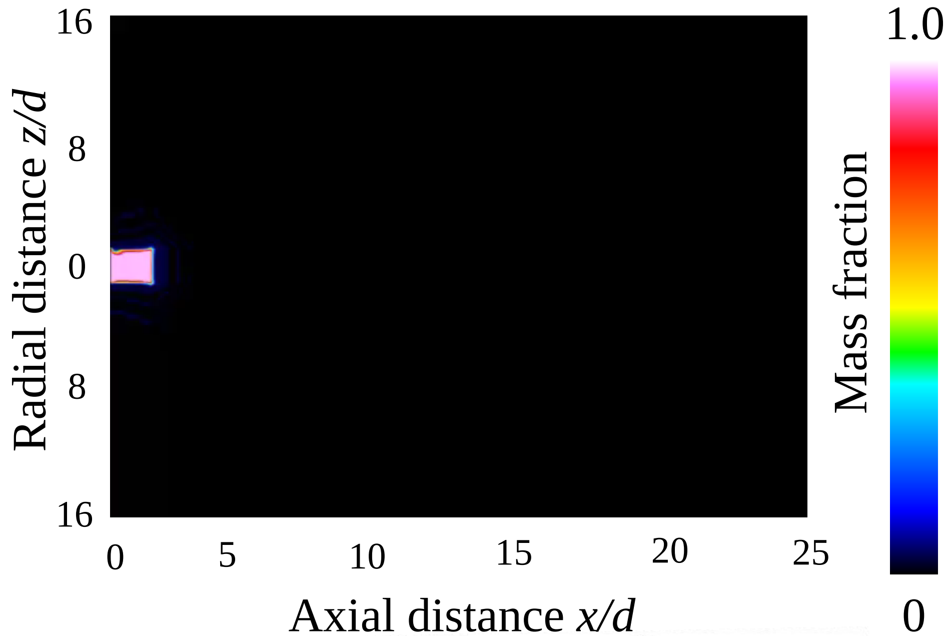
<u>4. Result</u>

<u>Unsteady dispersion jet</u>

Mach number distribution

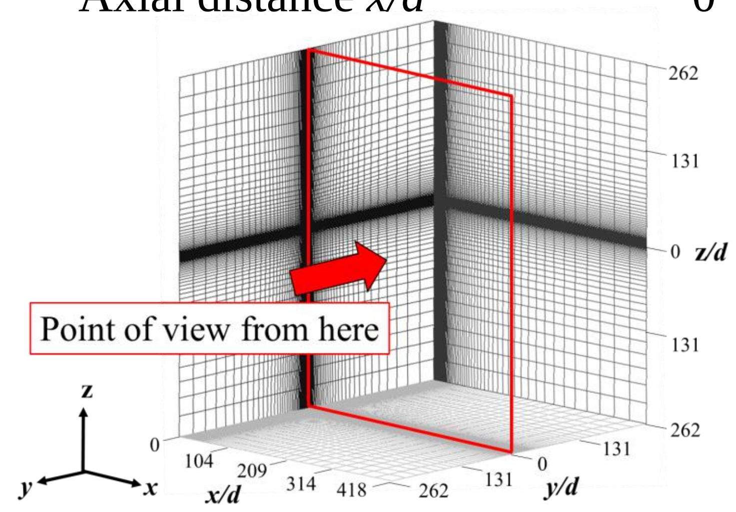


Mass fraction distribution



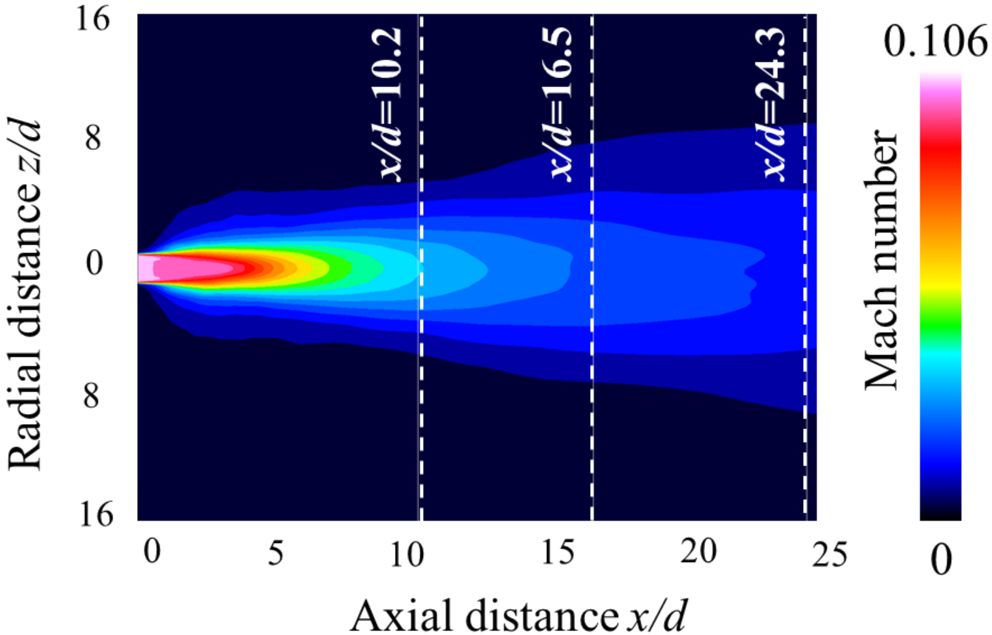
✓ Hydrogen is unsteadily dispersed from nozzle exit along the radial direction

➡ Capture dispersion behavior of unsteady low-speed hydrogen jet.

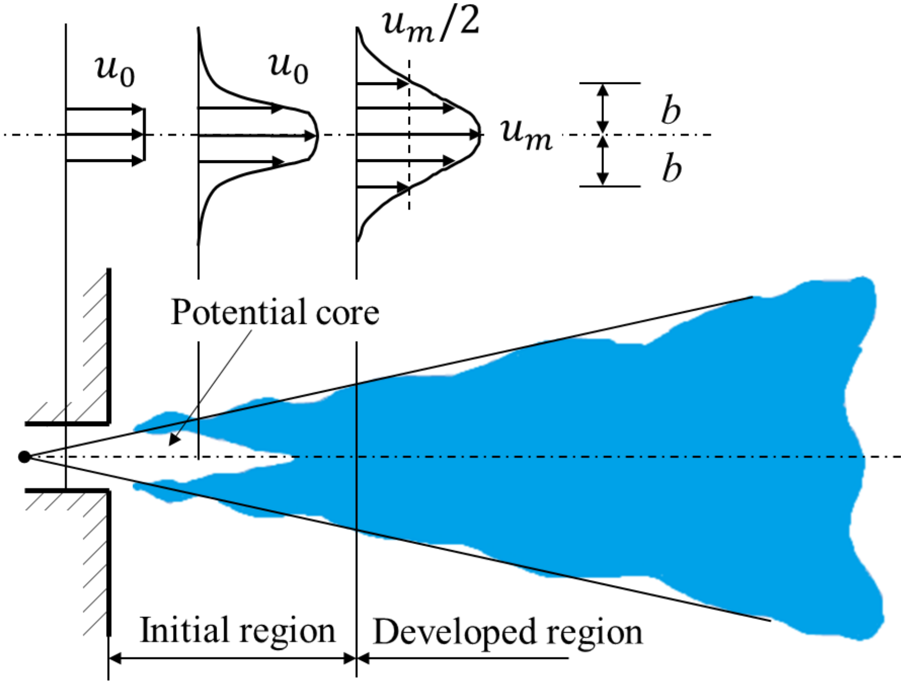


4. Result Validation of axisymmetric jet

Mean Mach number distribution



Axisymmetric jet flow configuration



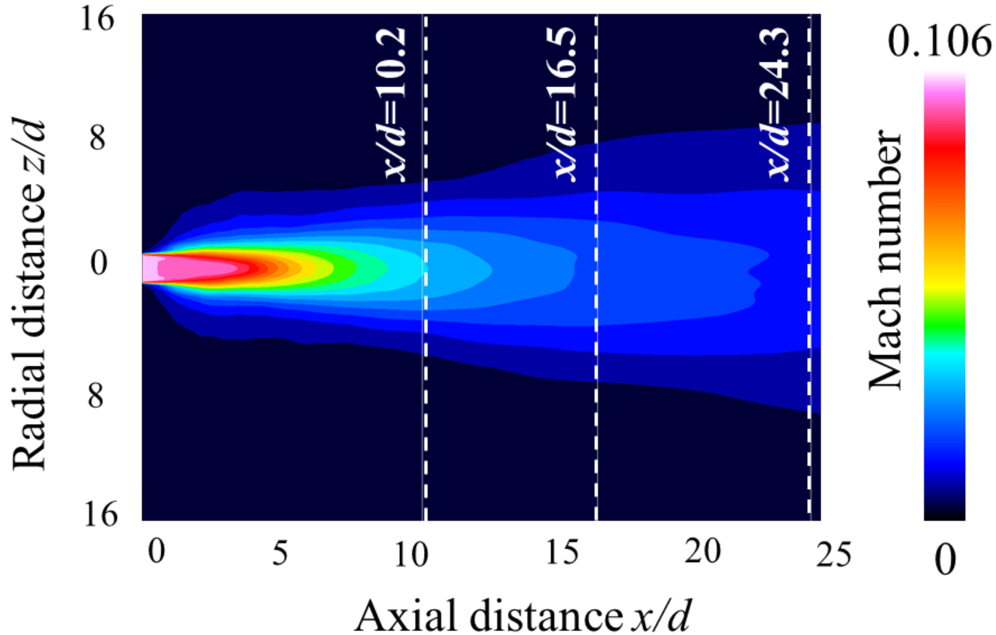
u_m : Speed on the central axis.
b : $u=u_m/2$ becomes radial direction position.

Averaged using a 1600 sheets instantaneous image of one per dimensionless time 0.04 interval.

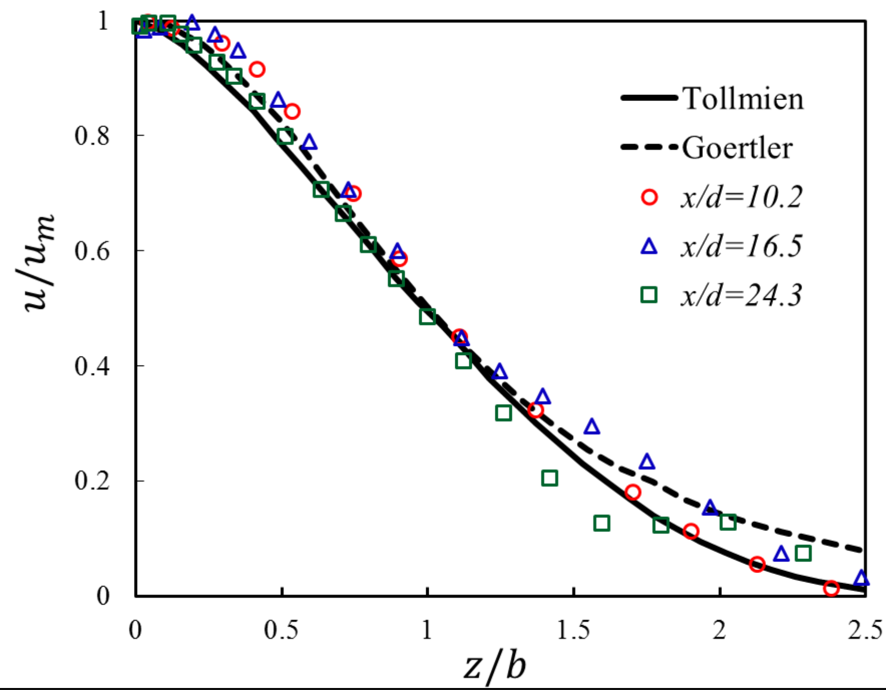
4. Result Validation of axisymmetric jet

*Foerthman,E.”Turbulent jet Expanision”, NACA, (1936)

Mean Mach number distribution



Radial profile of axial velocity



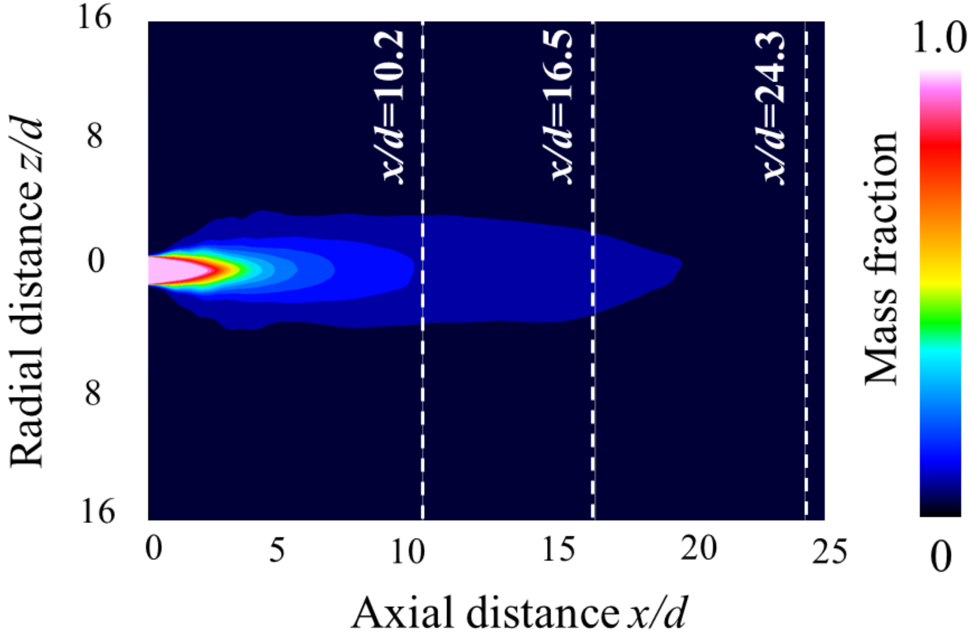
Tollmien, Goertler:The velocity distributions were theoretically determined.

- ✓ Agree well with theoretical profile of Goertler* near jet axis
- ✓ Agree well with theoretical solution of Tollmien* in external region

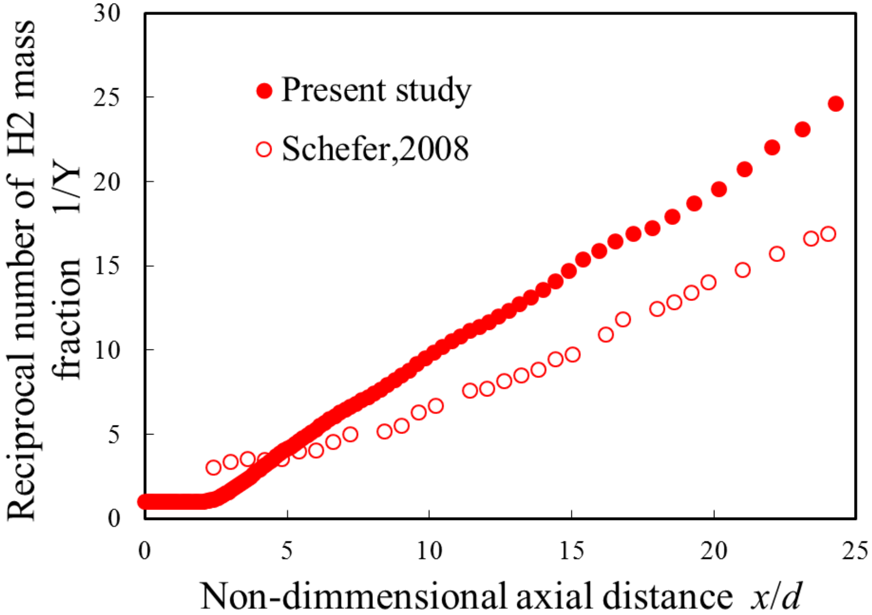
Present preconditioning method can simulate dispersion process of low-speed hydrogen jet.

4. Result Validation of axisymmetric jet

Mean mass fraction distribution

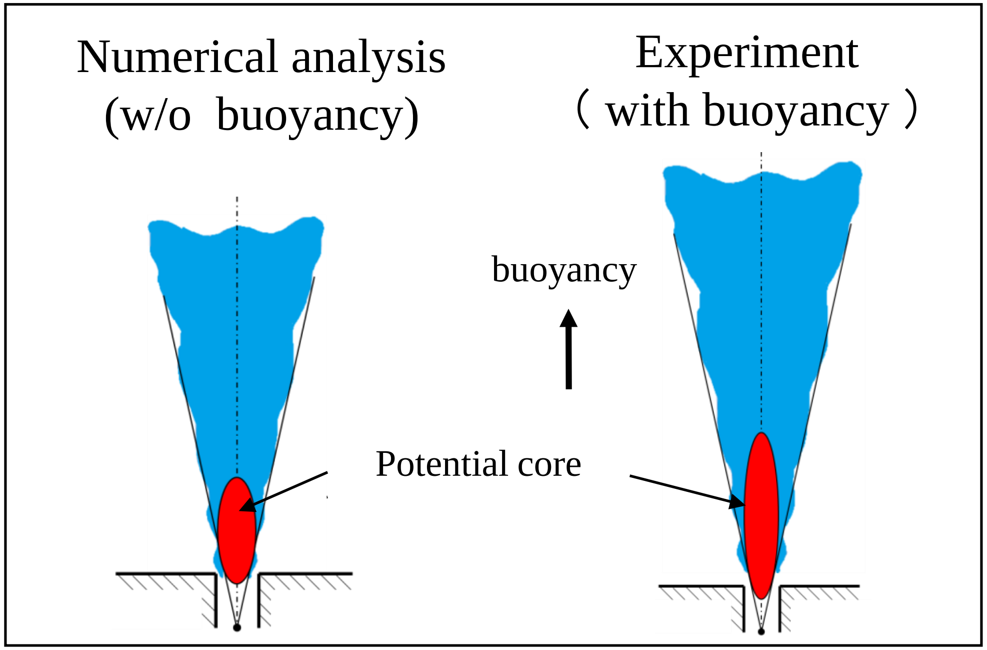


Mean mass fraction profile of jet axis

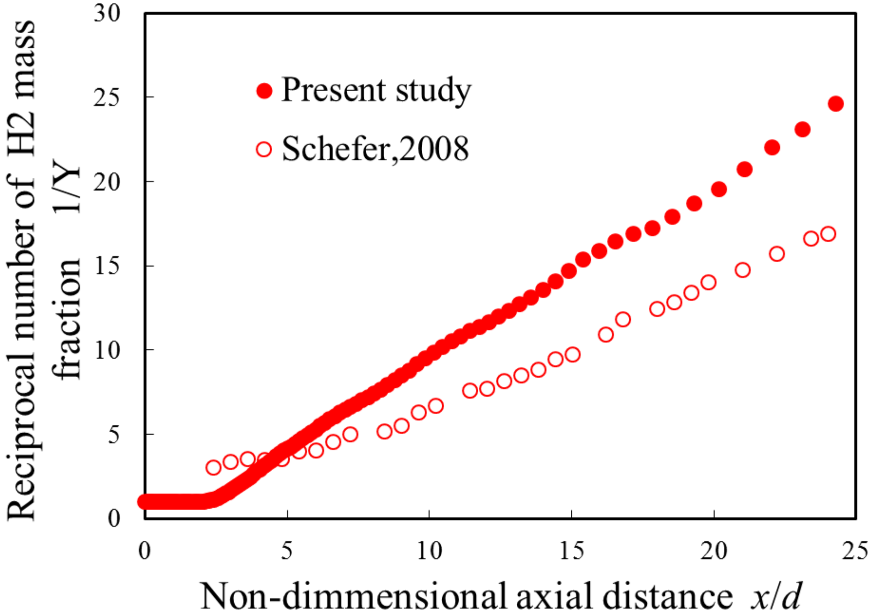


✓ The calculated hydrogen concentration becomes lower than the experimental values with the increasing distance from the nozzle exit.

4. Result Validation of axisymmetric jet



Mean mass fraction of the central axis



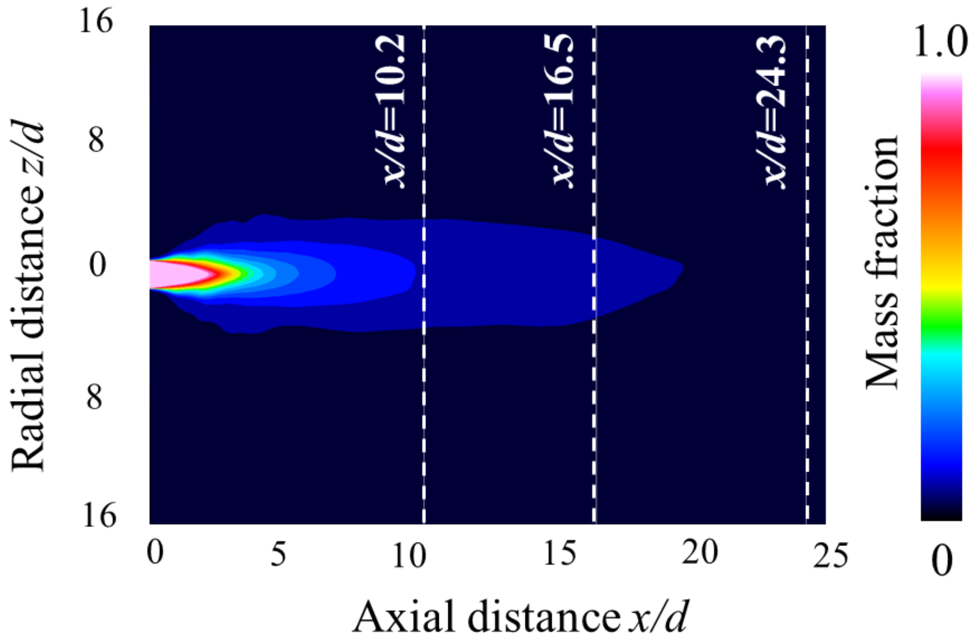
✓ The calculated hydrogen concentration becomes lower than the experimental values with the increasing distance from the nozzle exit.

➡ This is because jet and core in experiments elongate along jet axis due to buoyancy effects.

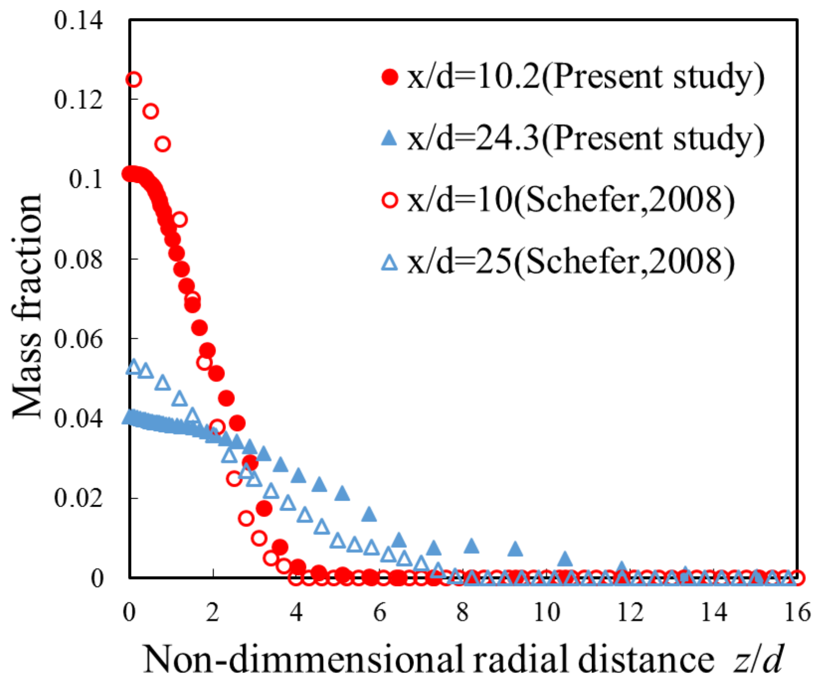
Because present study ignores buoyancy effects, discrepancy between simulations and experiments appears far from nozzle exit

4. Result Validation of axisymmetric jet

Mean mass fraction distribution



Mean mass fraction profile of the radial direction



- ✓ *x/d*=10.2 : good agreement
- ✓ *x/d*=24.3 : small discrepancy

The calculated hydrogen concentration in the radial direction agree well with experiments.

Present preconditioning method can simulate dispersion process of low-speed hydrogen jet.

5. Conclusion

Unsteady low-speed hydrogen jet flow was simulated by using unsteady preconditioning compressible full Navier-Stokes solver including multi-species mass conservation equations. The conclusions are as follows:

- ✓ It was possible to capture dispersion behavior of unsteady low-speed hydrogen jet.
- ✓ The calculated dimensionless velocity profiles along the radial direction show typical similarity and agree well with theoretical results.
- ✓ Comparing between present results and Schefer experiments, averaged mass fraction along jet axis appears influence of buoyancy. However, mean mass fraction along radial direction is in good agreement.

It was possible to obtain a reasonable calculation results of unsteady dispersion jet flow by using a preconditioning compressible full Navier-Stokes equations including multi-species mass conservation equations.

6. Future

- Influence of buoyancy
- Effects of inflow velocity distribution
- Grid resolution study
- Effects of preconditioning methods

Acknowledgments

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