



Numerical Investigation of Hydrogen Leakage from a High-Pressure Tank and Pipeline

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Utilization of hydrogen

Nowadays, utilization of hydrogen is rapidly expanding for energy source.
➡ It realizes conservation of global environment and sustainable society.

Production

plant



Transportation

high-pressure gas



Utilization

household fuel cell



renewable energy



pipeline



fuel cell vehicle

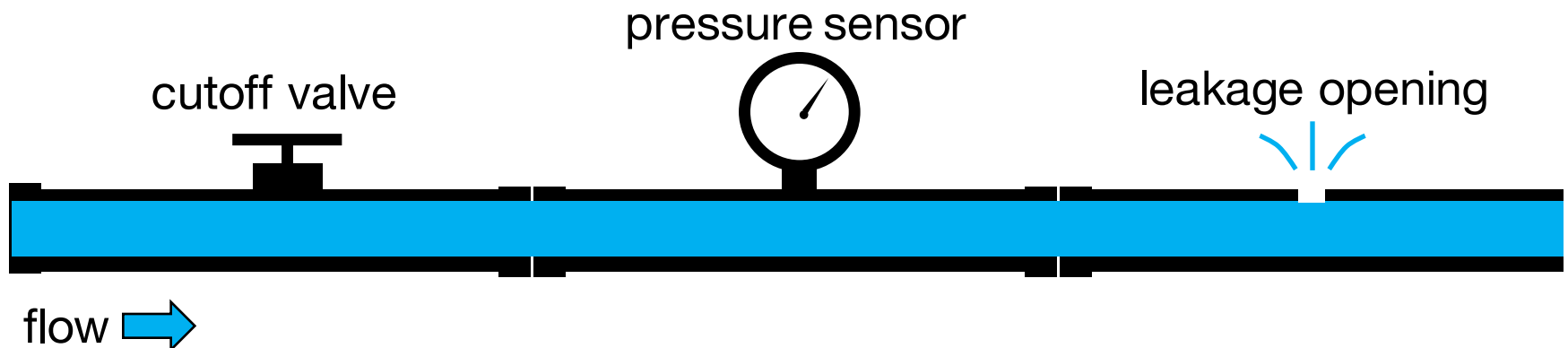


Introduction of hydrogen pipeline

We assume the practical application of the buried hydrogen pipeline for the introduction of hydrogen energy in the future.

- Hydrogen has **large flammability range**.
- **Minimum ignition energy** of hydrogen is so **small**.

➡ It is necessary to **clarify safety measures and standards** for hydrogen pipeline with leakage opening.



Objective

- Few studies focus on the flow field inside the hydrogen pipeline and outflow mass flow rate after leakage.
 - Experiments with many parameters such as pressure in the hydrogen pipeline or leakage opening area cannot be carried out many times because of high cost and risk of hydrogen.
- ➔ Using numerical analysis, it is required to quantify the pressure distribution, the outflow mass flow rate, and so on.

In this report

3D simulation is conducted to quantify

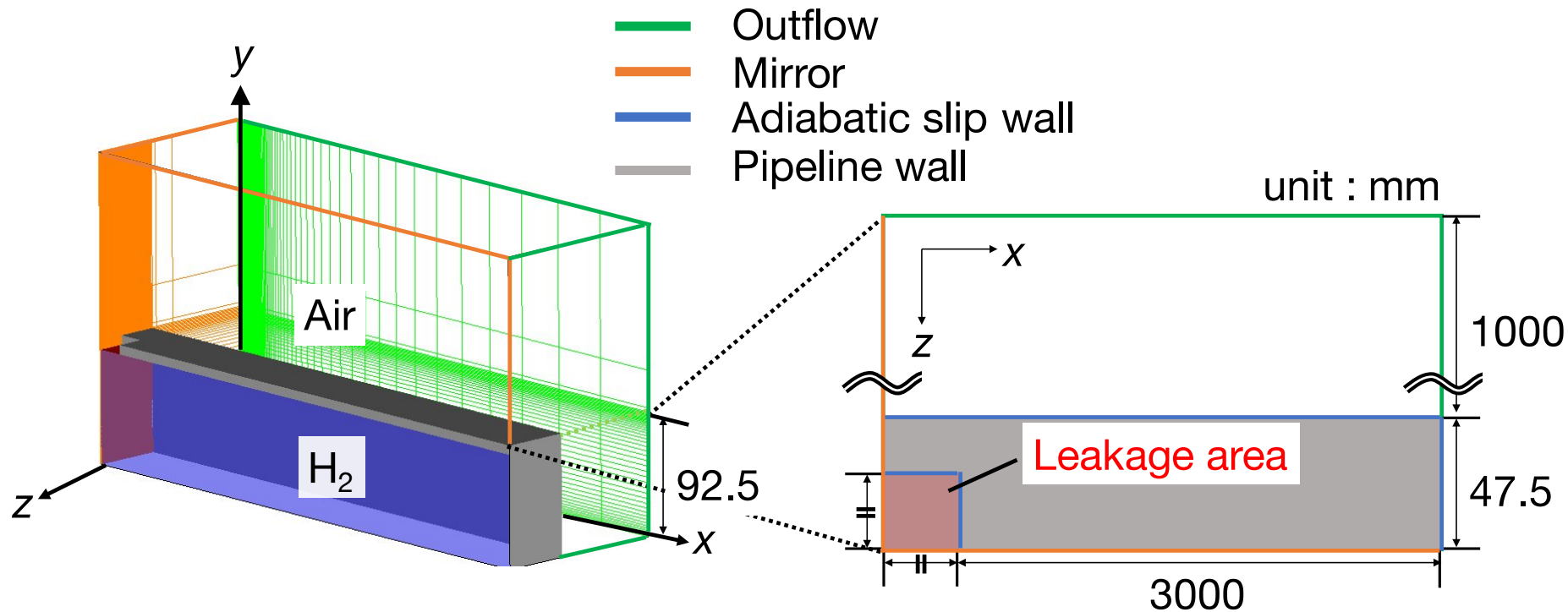
- **steady outflow mass flow rate**
- **pressure in the pipeline after leakage**

using the initial pressure and leakage opening area.

Numerical setup

- Governing equations
 - Three-dimensional compressible Euler equations
 - Conservation equations of chemical species (Air, H₂)
- Equation of state
 - Ideal gas equation of state
- The convective term
 - SHUS third-order by MUSCL
- Time integration method
 - Two stage Runge-Kutta method

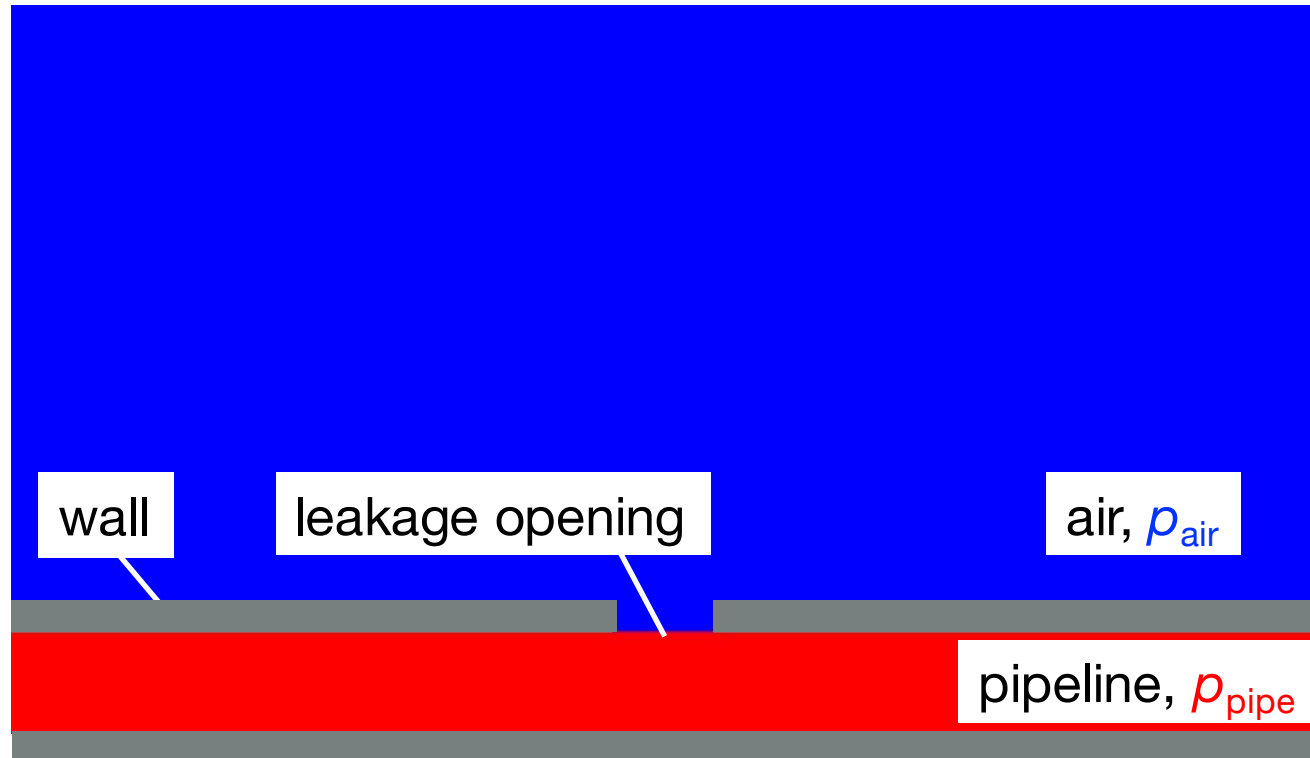
Computational target



- Leakage area 7.30, 20.3, 56.3 cm²
- In pipeline
 - Pressure 0.3, 0.5, 1.0 MPa
 - Temperature 293 K
 - Velocity 0 m/s
- In air
 - Pressure 0.101 MPa
 - Temperature 293 K

The flow field of the simulation results

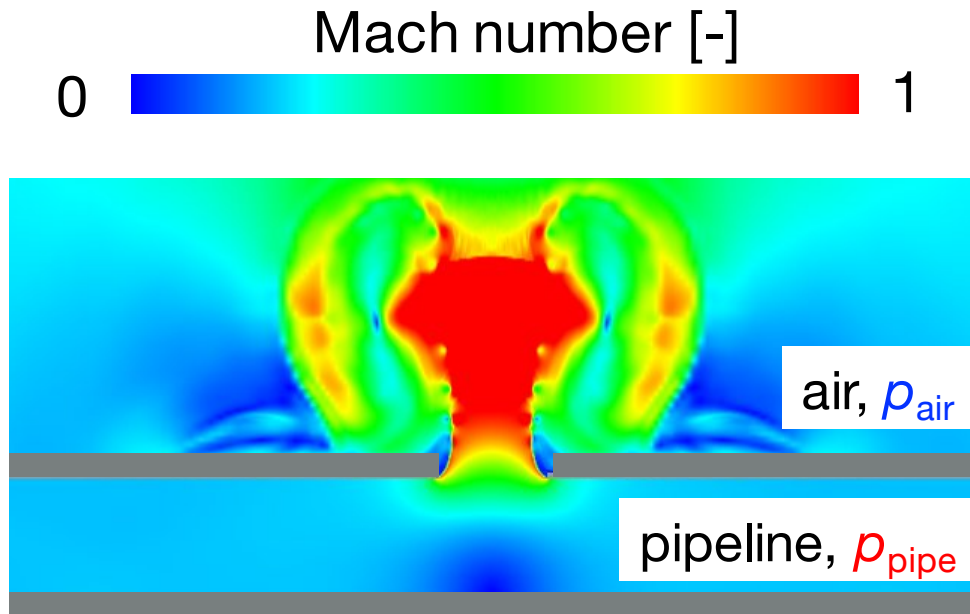
Flow field (2D sim.)



When the pressure ratio p_{air} / p_{pipe} is small enough,
Mach number is 1 and mass flow rate obtains maximum value.

➡ choked condition

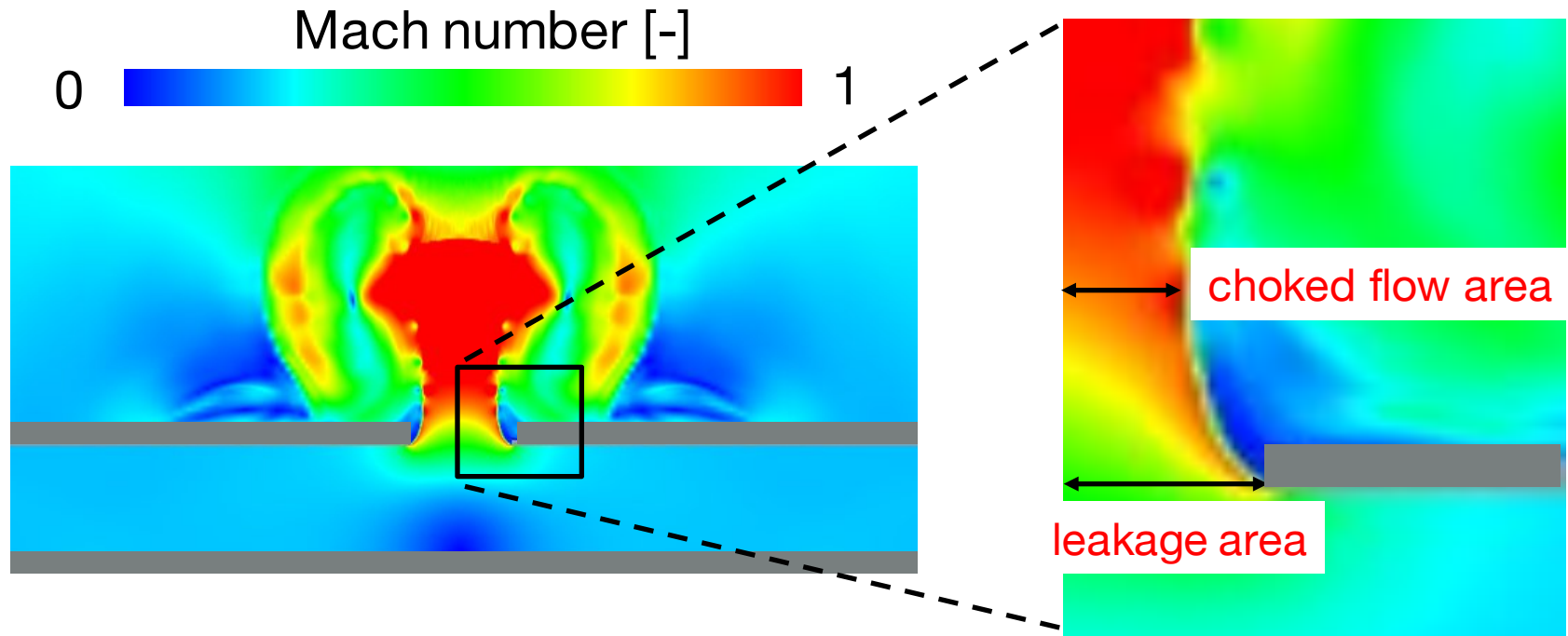
Contraction flow



When the pressure ratio $p_{\text{air}} / p_{\text{pipe}}$ is small enough,
Mach number is 1 and mass flow rate obtains maximum value.

➡ choked condition

Contraction flow

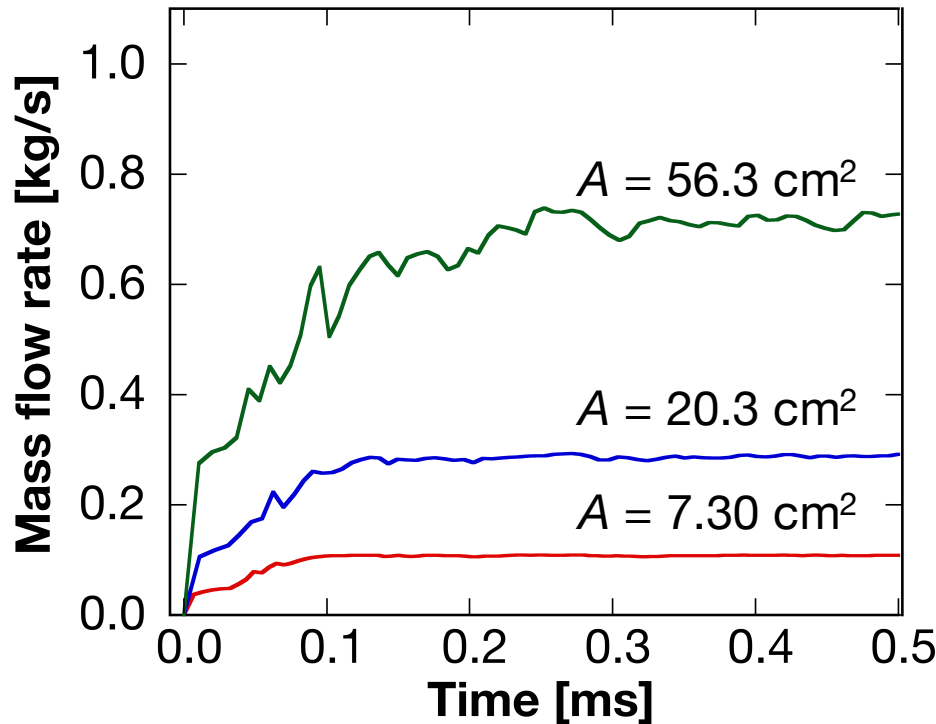


- As flow is shrink by the leakage opening, the position where flow is choked is upper from the opening.
- **Choked flow area** is smaller than leakage opening area.

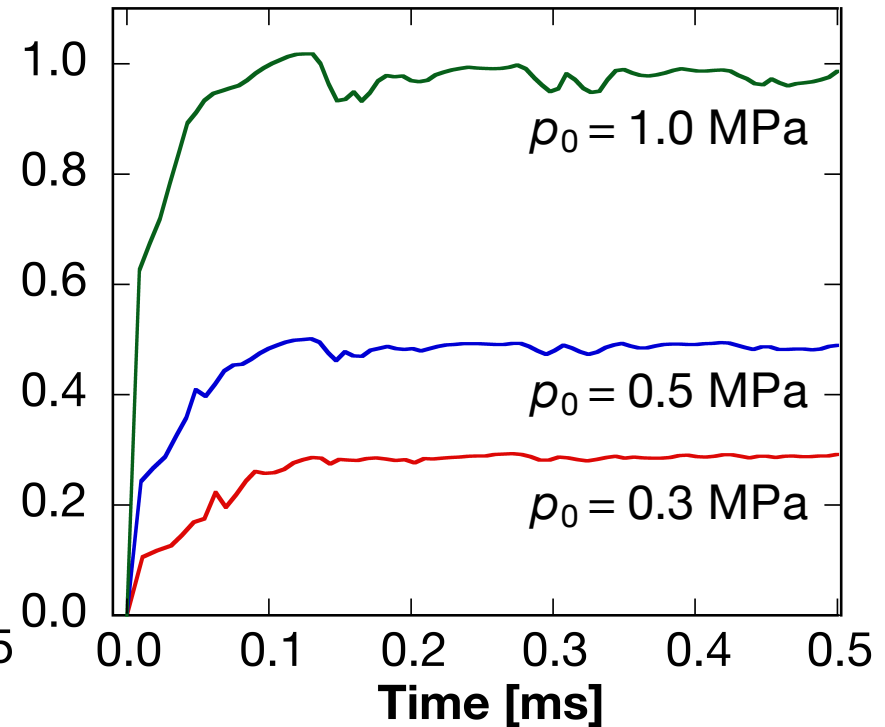
Mass flow rate history

A : Leakage opening area, p_0 : Initial pressure

$p_0 = 0.3 \text{ MPa}$

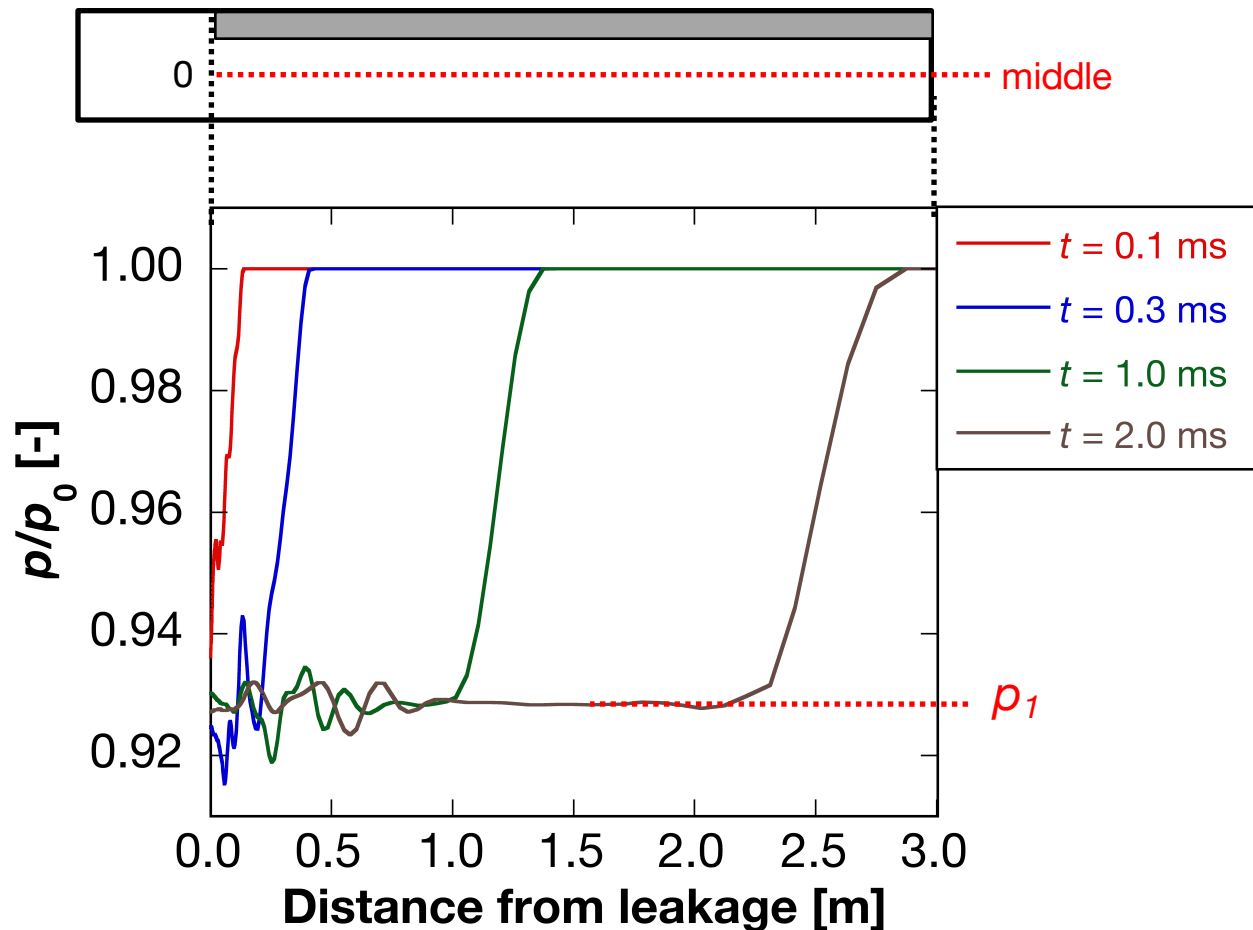


$A = 20.3 \text{ cm}^2$



- Mass flow rate converges to a constant value under any conditions because flow is choked around the leakage opening.
- Steady mass flow rate depends on both of initial pressure and leakage opening area.

Pressure distribution history ($p_0 = 0.3 \text{ MPa}$, $A = 20.3 \text{ cm}^2$)



- The pressure inside the pipeline is gradually decreasing as the expansion waves propagate.
- The pressure decrease is only approximately 10%.

Modeling the flow with leakage opening

- Theory of 1D model
- Comparison between 1D model with simulation results

The comparison with simple theory

Outflow mass flow rate is considered to be the maximum mass flow rate because flow is choked.

$$\dot{m}_{max} = \frac{A\sigma^*p_0}{\sqrt{RT_0}}$$

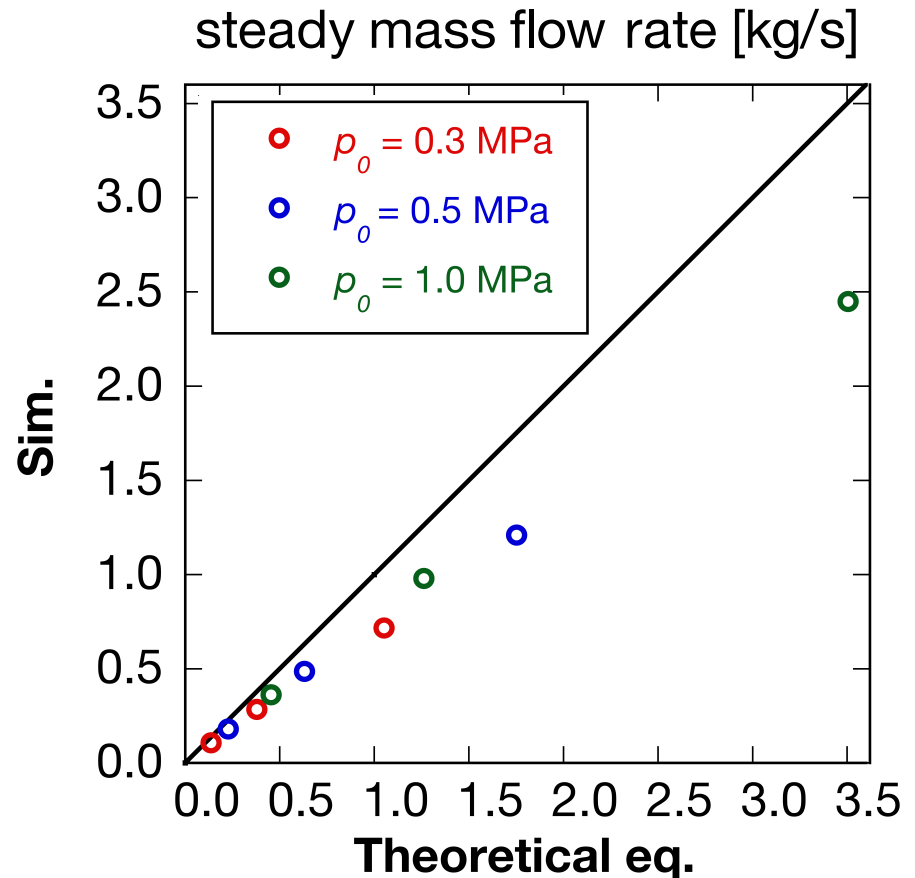
A : Leakage opening area

p_0 : Initial pressure

T_0 : Initial temperature

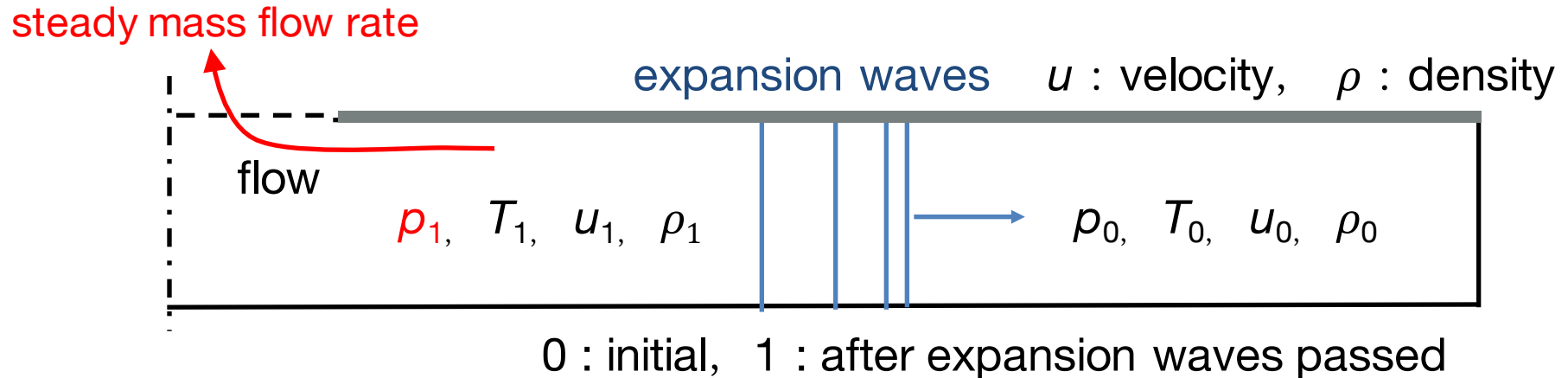
R : gas constant

σ^* : function of
the specific heat ratio



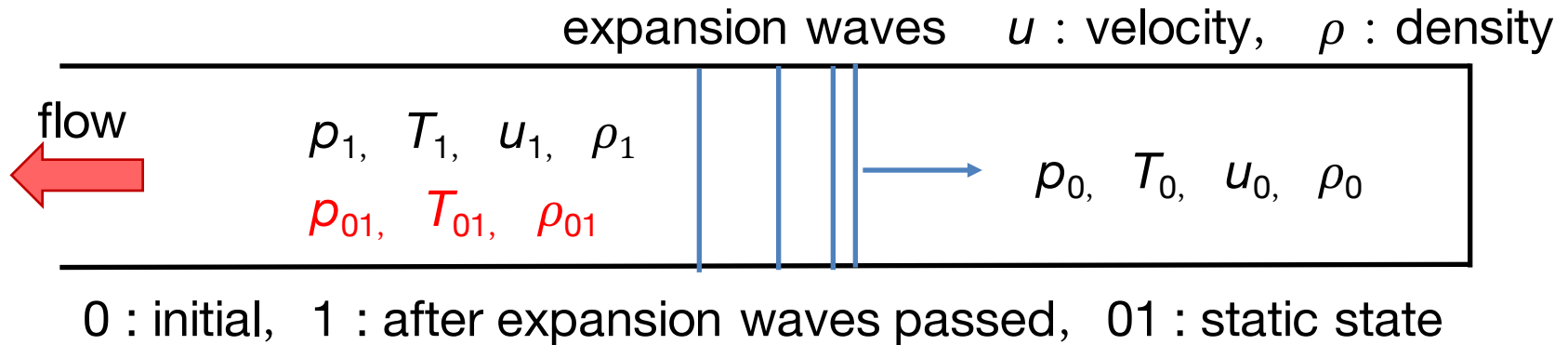
➡ 1D model needs to consider the effect of contraction flow to quantify steady mass flow rate in all cases.

The concept of 1D model



- In this calculation, **expansion waves propagate unsteadily** and **flow is accelerated by shrink of area after leakage**.
 - The object is to obtain both of **steady mass flow rate** and **pressure after expansion waves passed** by initial pressure and leakage opening area.
- ➡ In 1D model, flow is separated into unsteady expansion waves propagation phase and acceleration flow phase.

Unsteady expansion waves (1/2)



- After expansion waves passed, physical quantity changes in isentropic process.

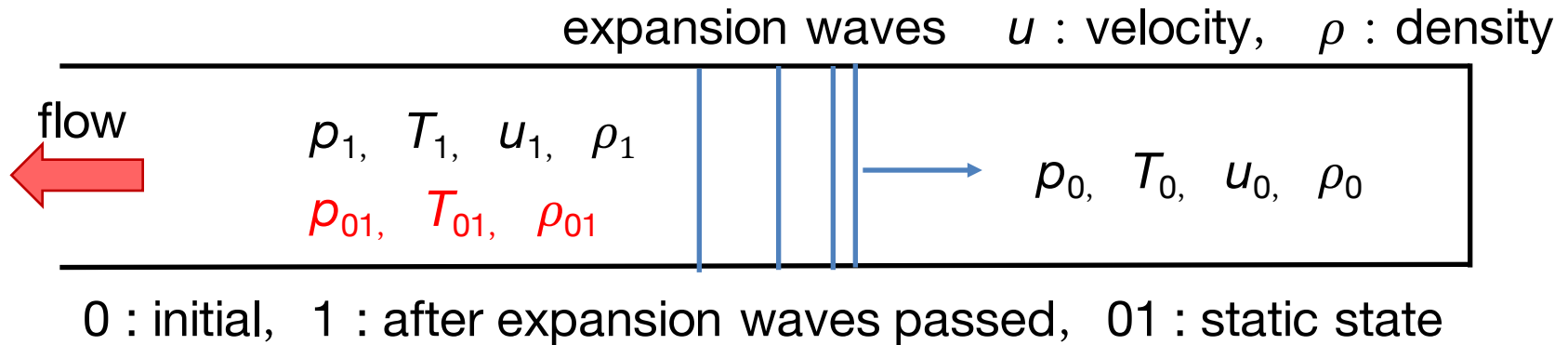
p_1 / p_0 is given,

$$\frac{p_1}{p_0} = \left(\frac{\rho_1}{\rho_0} \right)^\gamma = \left(\frac{T_1}{T_0} \right)^{\frac{\gamma}{\gamma-1}}$$

temperature after expansion waves passed is obtained.

- In unsteady expansion, total pressure and total temperature also change. ($p_0 \neq p_{01}$, $T_0 \neq T_{01}$, $\rho_0 \neq \rho_{01}$)

Unsteady expansion waves (2/2)



The Riemann invariant is constant after expansion waves passed.

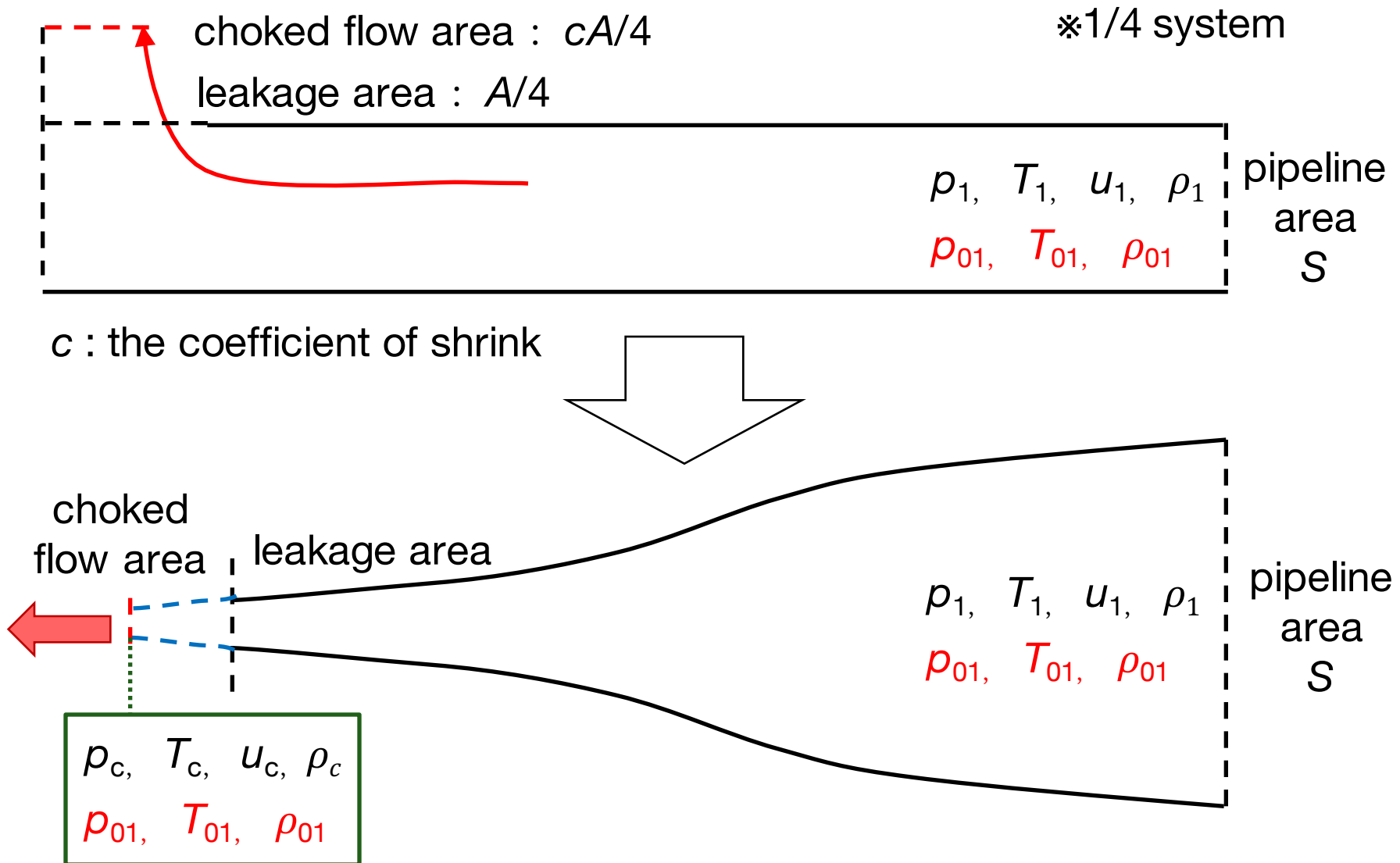
$$\frac{2a_0}{\gamma - 1} + u_0 = \frac{2a_1}{\gamma - 1} + u_1$$

M_1 can also be obtained from isentropic equation. (M : Mach number)

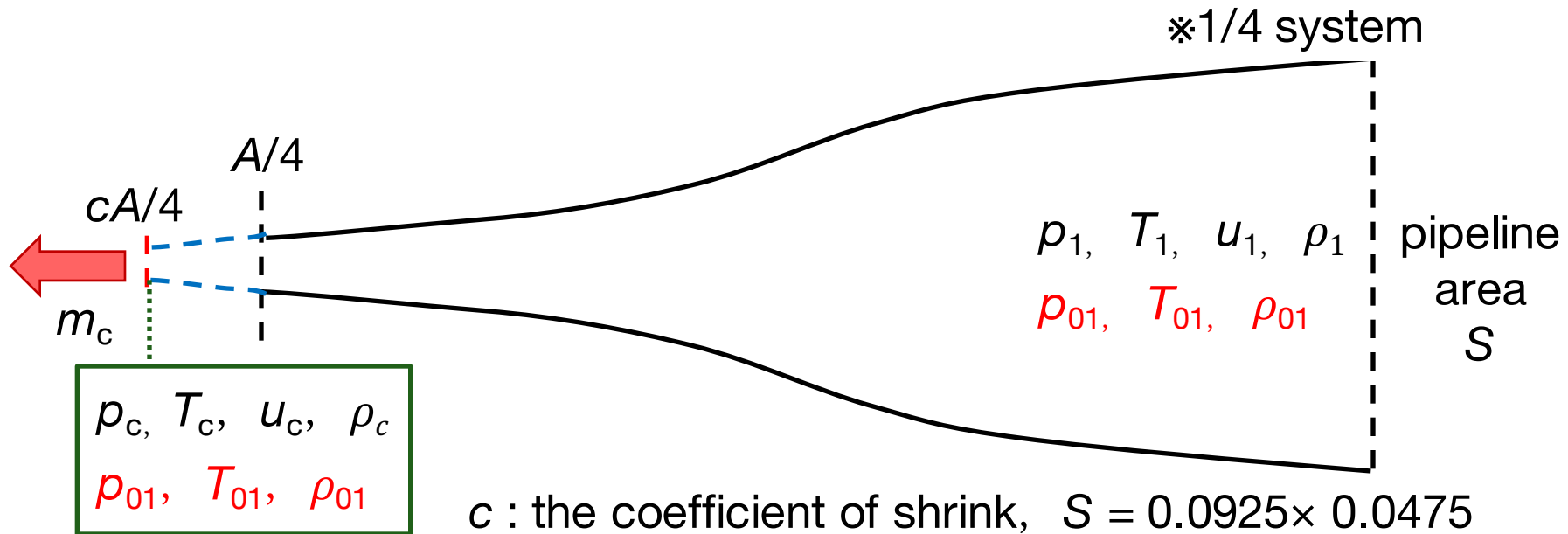
$$\frac{T_{01}}{T_0} = \left(1 + \frac{\gamma - 1}{2} M_1^2\right) \left(1 + \frac{\gamma - 1}{2} M_1\right)^{-2} = \left(\frac{p_{01}}{p_0}\right)^{\frac{\gamma - 1}{\gamma}}$$

Total temperature and pressure after expansion waves passed are obtained.

Acceleration by leakage opening (1/3)



Acceleration by leakage opening (2/3)

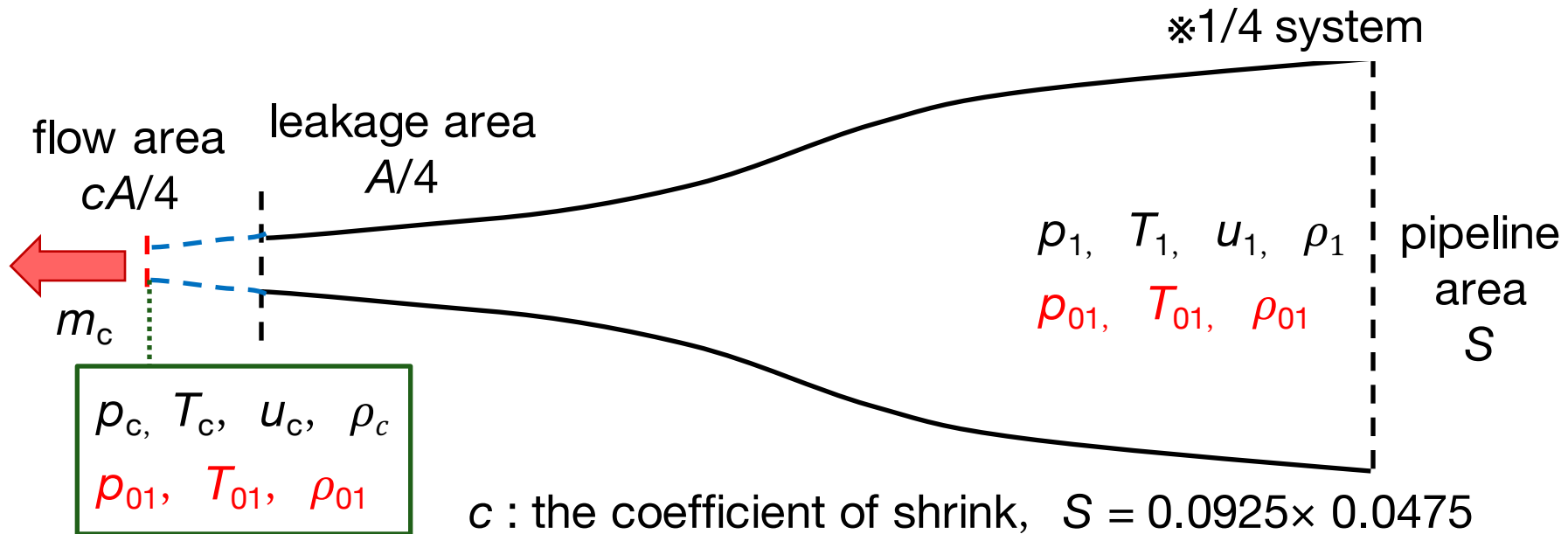


- Flow is accelerated by leakage opening and flow is shrink. Flow area is smaller than leakage opening area. ($A/4 \rightarrow cA/4$)
- Mach number at choked flow area is 1.

$$\frac{cA/4}{S} = M_1 \left[\frac{\gamma+1}{(\gamma-1)M_1^2+2} \right]^{\frac{\gamma+1}{2(\gamma-1)}}$$

A is obtained when c is set as appropriate value.

Acceleration by leakage opening (3/3)



Mass flow rate at flow area is equal to maximum mass flow rate.

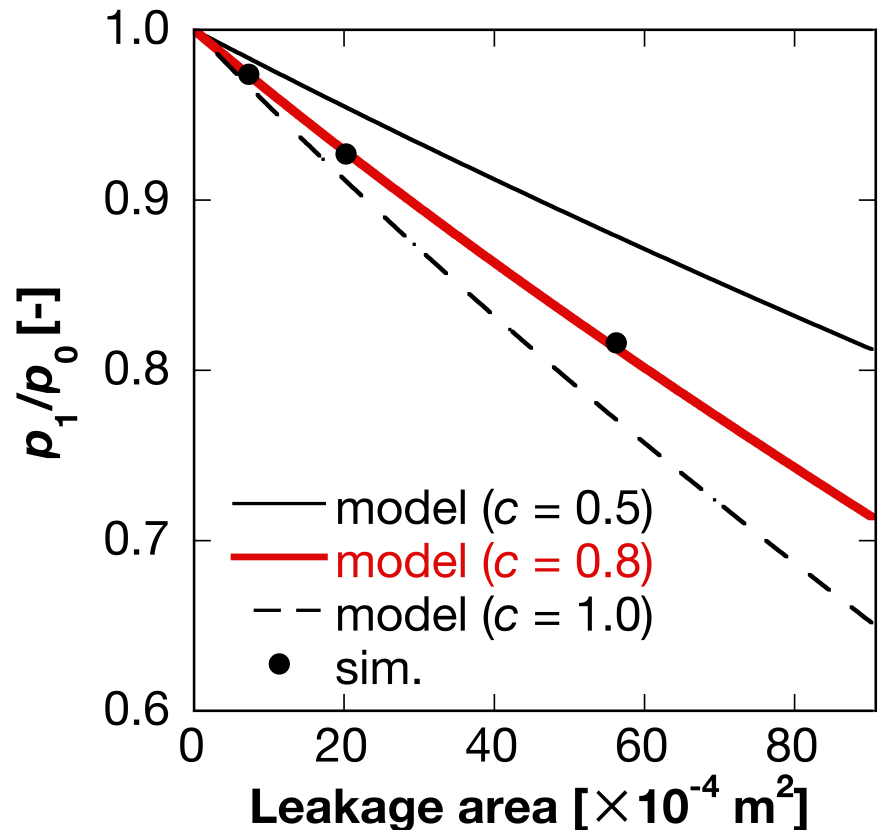
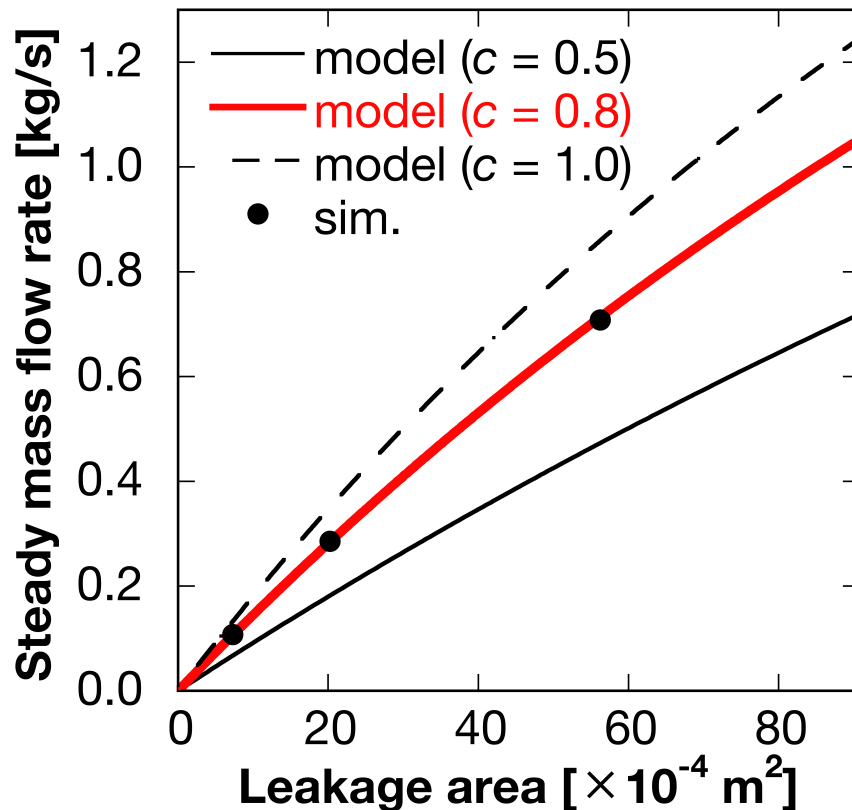
$$m_c = \sqrt{\gamma \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma+1}{\gamma-1}}} \cdot \frac{p_{01}}{\sqrt{RT_{01}}} \cdot \frac{cA}{4} \cdot 4$$

Outflow mass flow rate and leakage opening area are obtained from the pressure after expansion waves passed.

Modeling the flow with leakage opening

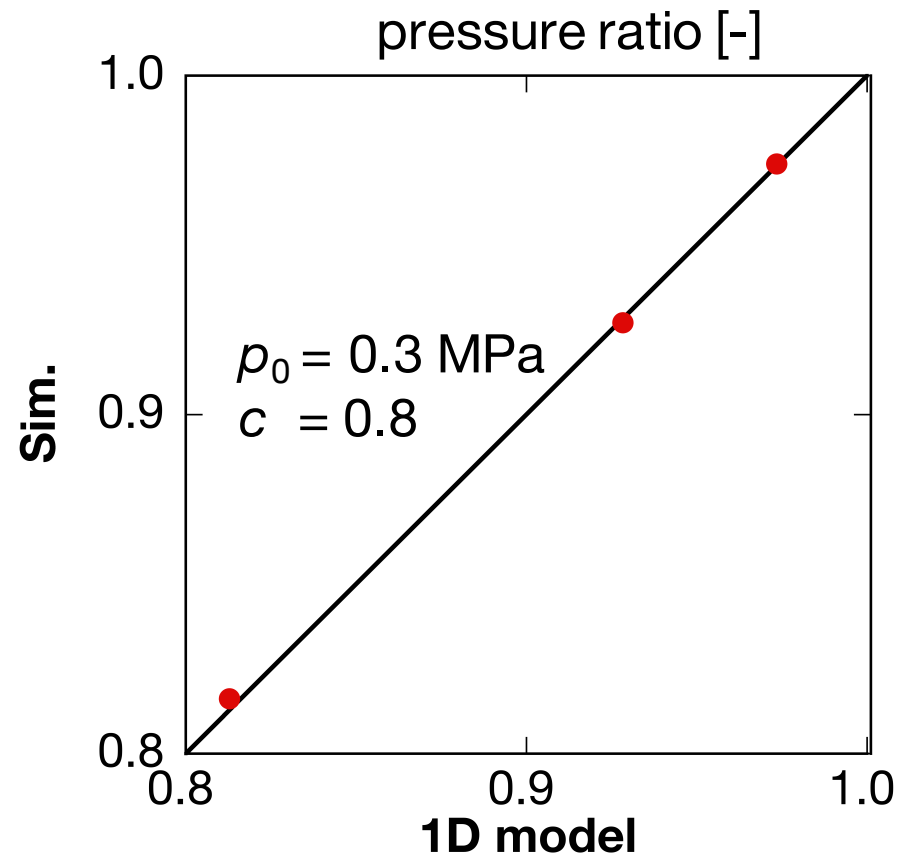
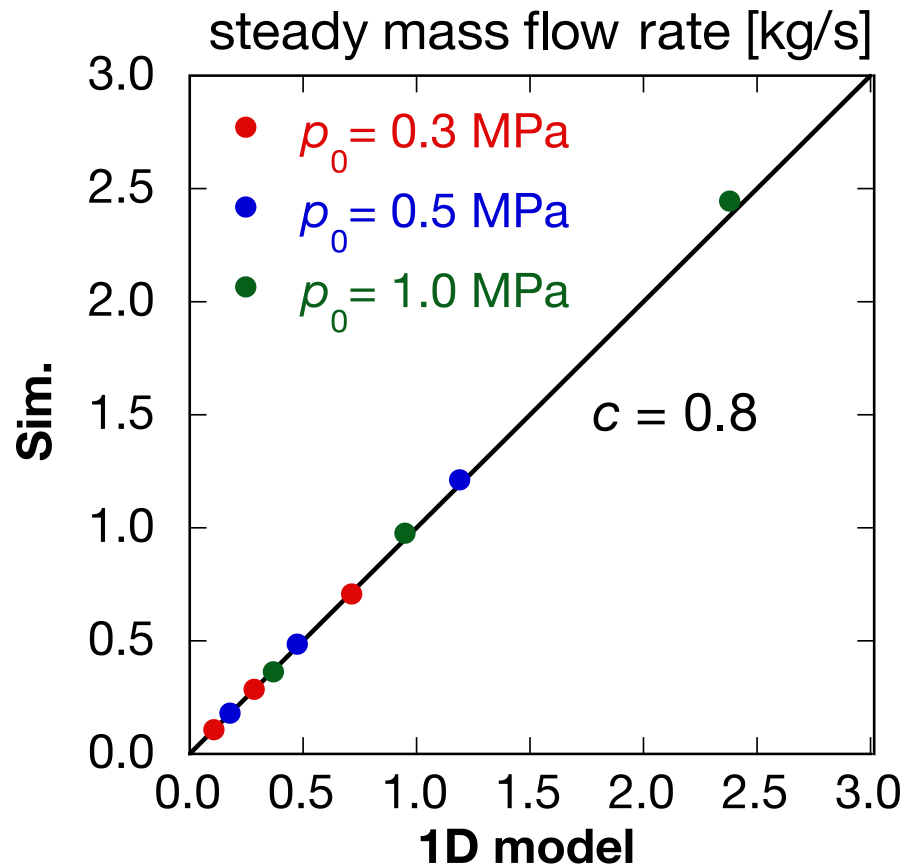
- Theory of 1D model
- Comparison between 1D model with simulation results

Comparison with 1D model ($p_0 = 0.3$ MPa)



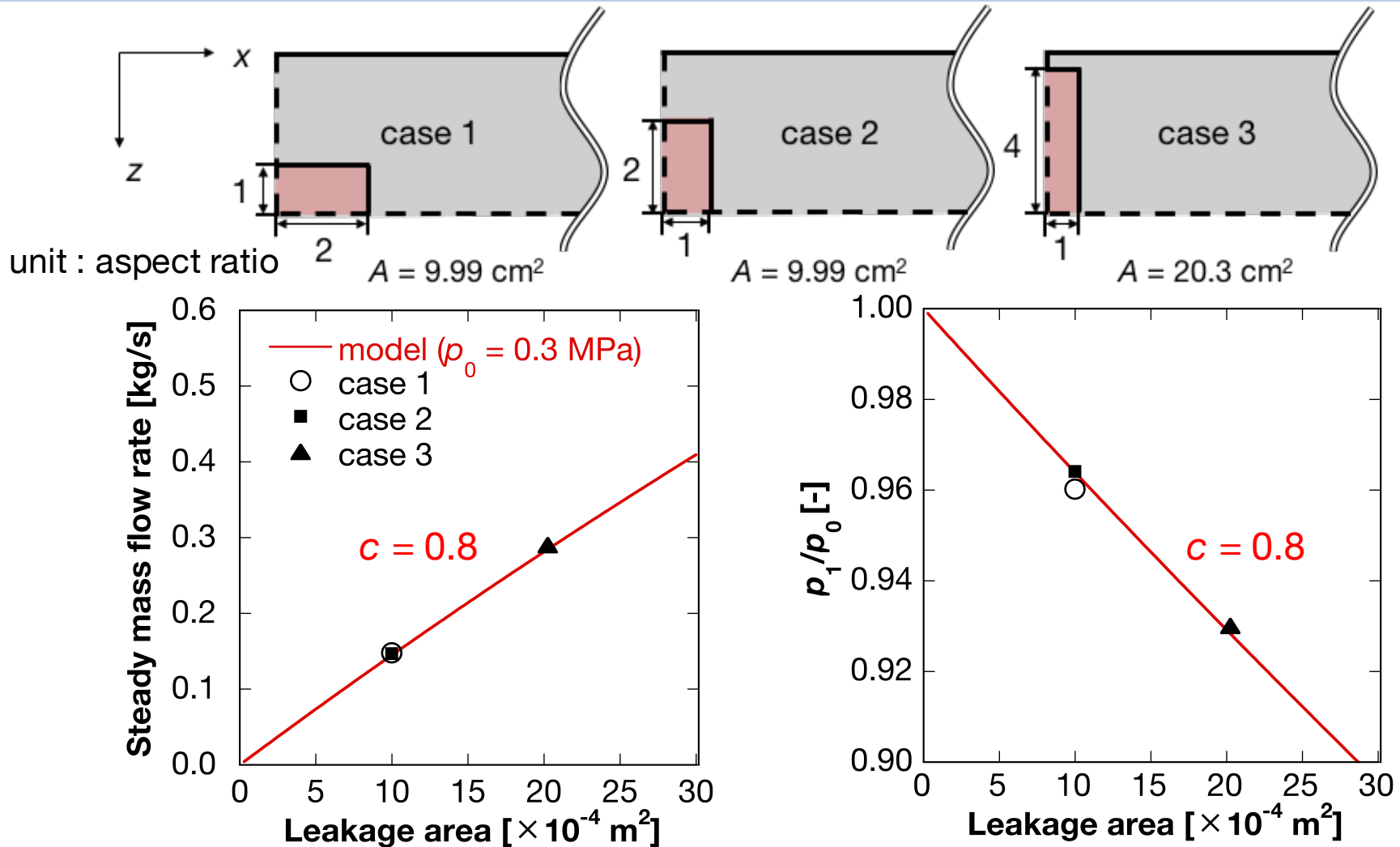
Simulation results are consistent with 1D model when c is set as 0.8.

Comparisons of all cases



Simulation results of steady outflow mass flow rate and pressure ratio are consistent with 1D model with $c = 0.8$ in all cases.

Rectangular opening cases



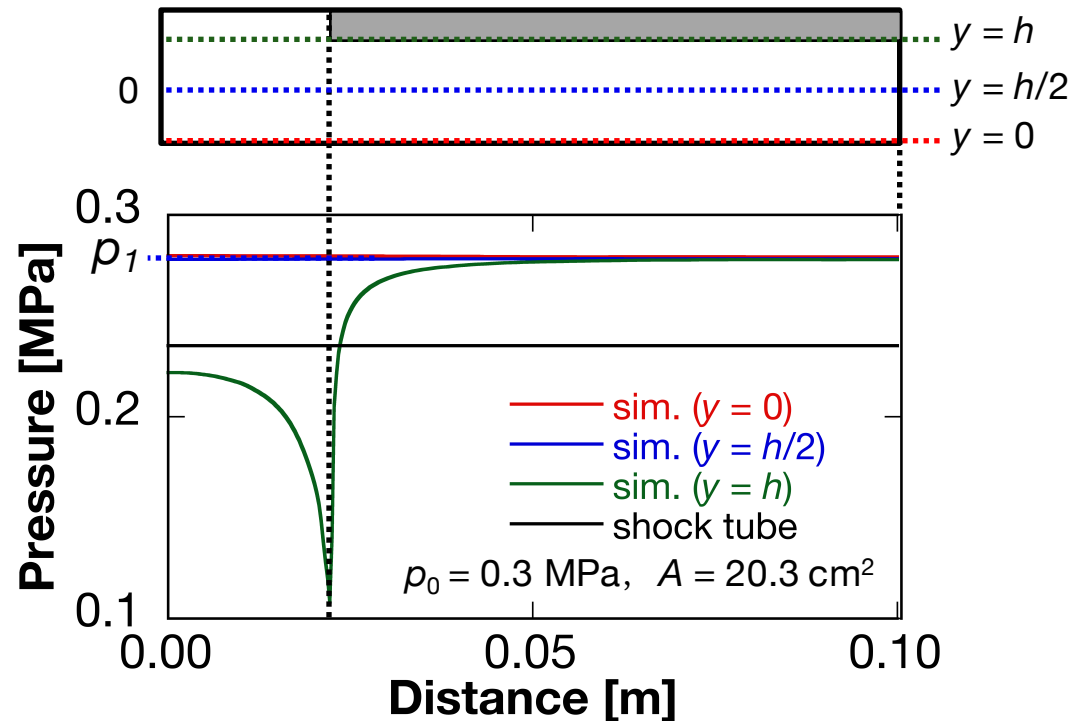
1D model can be also applied to the rectangular opening cases.

Conclusions

In this report, the modeling equation that expresses the pressure after leakage and outflow mass flow rate by leakage area and initial pressure is introduced.

- In 1D model, by dividing the flow into two phases of unsteady expansion waves propagation and acceleration, we can obtain the steady mass flow rate and pressure after leakage.
- In the case of a pipeline used in this analysis and the shape of leakage opening is square, the results show good agreement with 1D model when the shrink coefficient is 0.8.
- When the shape of leakage opening is rectangular, the results also show good agreement with 1D model. It suggests that they do not depend on the shape of the opening.

Pressure distribution in the pipeline



- The pressure at the bottom and the middle of the pipeline are same.
- Comparing the results of the shock tube model , the pressure is 16 % higher than that of shock tube model.

➡ The pressure in the pipeline after leakage cannot be simplified as shock tube model.

Governing equations

$$\frac{\partial \hat{\mathbf{Q}}}{\partial t} + \frac{\partial \hat{\mathbf{E}}}{\partial \xi} + \frac{\partial \hat{\mathbf{F}}}{\partial \eta} + \frac{\partial \hat{\mathbf{G}}}{\partial \zeta} = 0$$

$$\hat{\mathbf{Q}} = \frac{1}{J} \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ e \\ \rho_i \end{bmatrix}, \quad \hat{\mathbf{E}} = \frac{1}{J} \begin{bmatrix} \rho U \\ \rho u U + \xi_x p \\ \rho v U + \xi_y p \\ \rho w U + \xi_z p \\ (e + p)U \\ \rho_i U \end{bmatrix},$$

$$\hat{\mathbf{F}} = \frac{1}{J} \begin{bmatrix} \rho V \\ \rho u V + \eta_x p \\ \rho v V + \eta_y p \\ \rho w V + \eta_z p \\ (e + p)V \\ \rho_i V \end{bmatrix}, \quad \hat{\mathbf{G}} = \frac{1}{J} \begin{bmatrix} \rho W \\ \rho u W + \zeta_x p \\ \rho v W + \zeta_y p \\ \rho w W + \zeta_z p \\ (e + p)W \\ \rho_i W \end{bmatrix}$$

$$U = \xi_x u + \xi_y v + \xi_z w,$$

$$V = \eta_x u + \eta_y v + \eta_z w,$$

$$W = \zeta_x u + \zeta_y v + \zeta_z w$$

$$\rho = \sum_{i=1}^N \rho_i, \quad p = \sum_{i=1}^N \rho_i R_i T$$

Isentropic condition

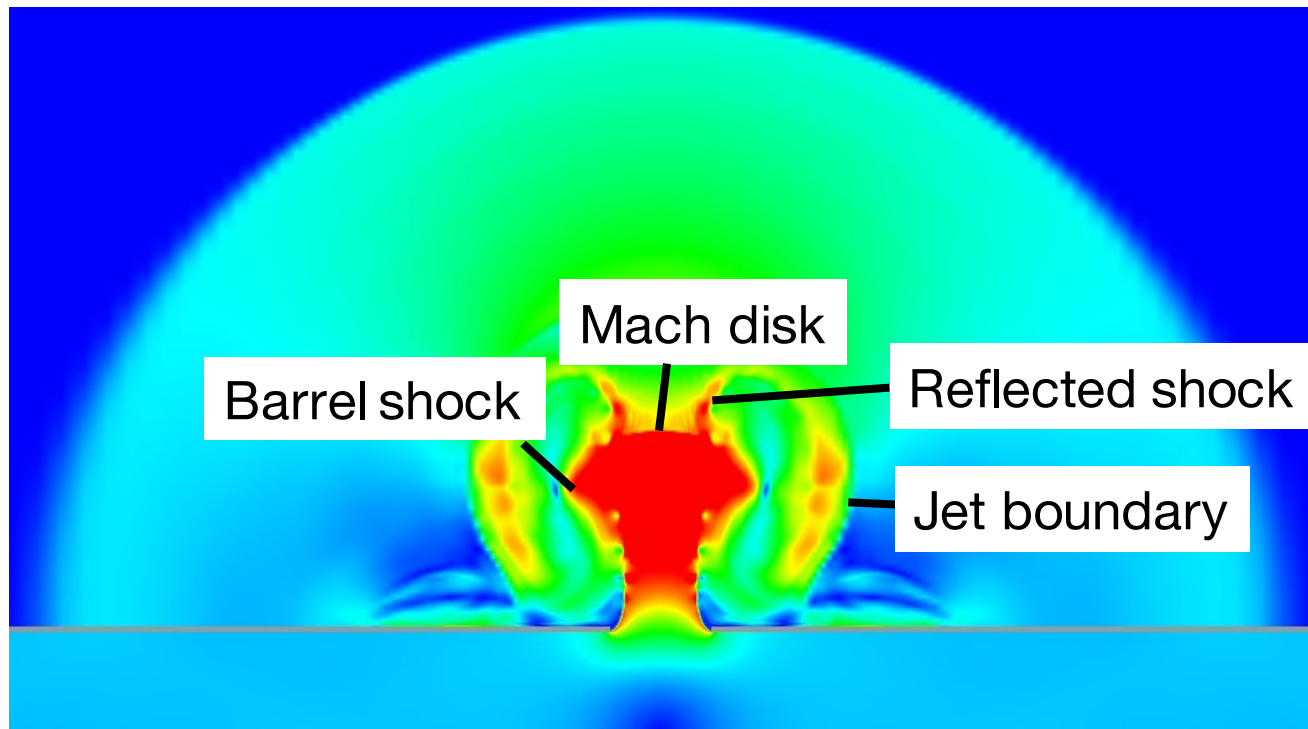
Isentropic process is **adiabatic** and **reversible** process.

- Increase of entropy by fluid viscosity and heat conductivity is proportional to the square of velocity and temperature gradient.
- As velocity and temperature gradient caused by the expansion waves is so small, the physical quantities variation can be regarded as isentropic change after expansion waves passed.

Jet composition

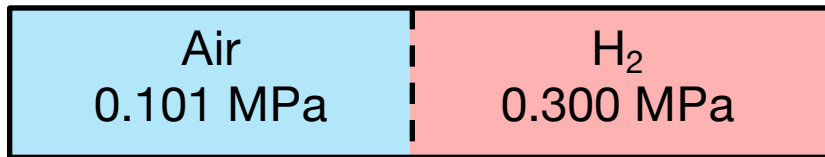
Mach number [-]

0 1

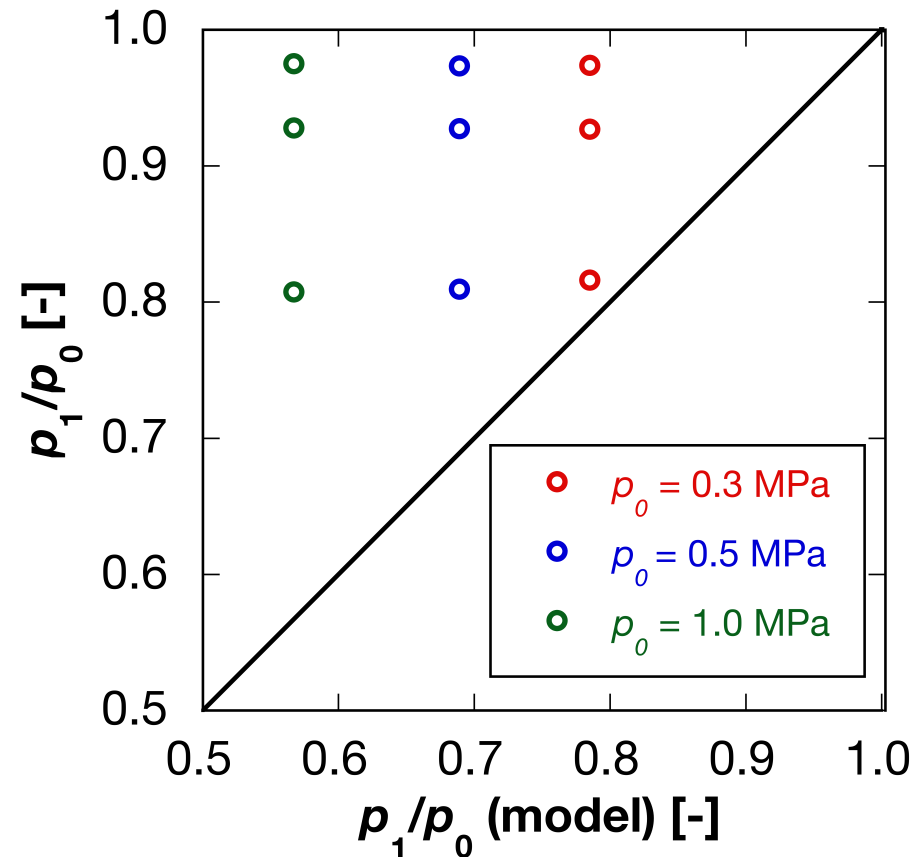


The comparison with shock tube model

shock tube model



- By using this model, the pressure after the expansion waves passed p_1 can be obtained.
- The values of p_1 at all conditions are higher than those of the shock tube model.



➡ The flow in the pipeline with leakage opening cannot be simplified as **the shock tube model**.