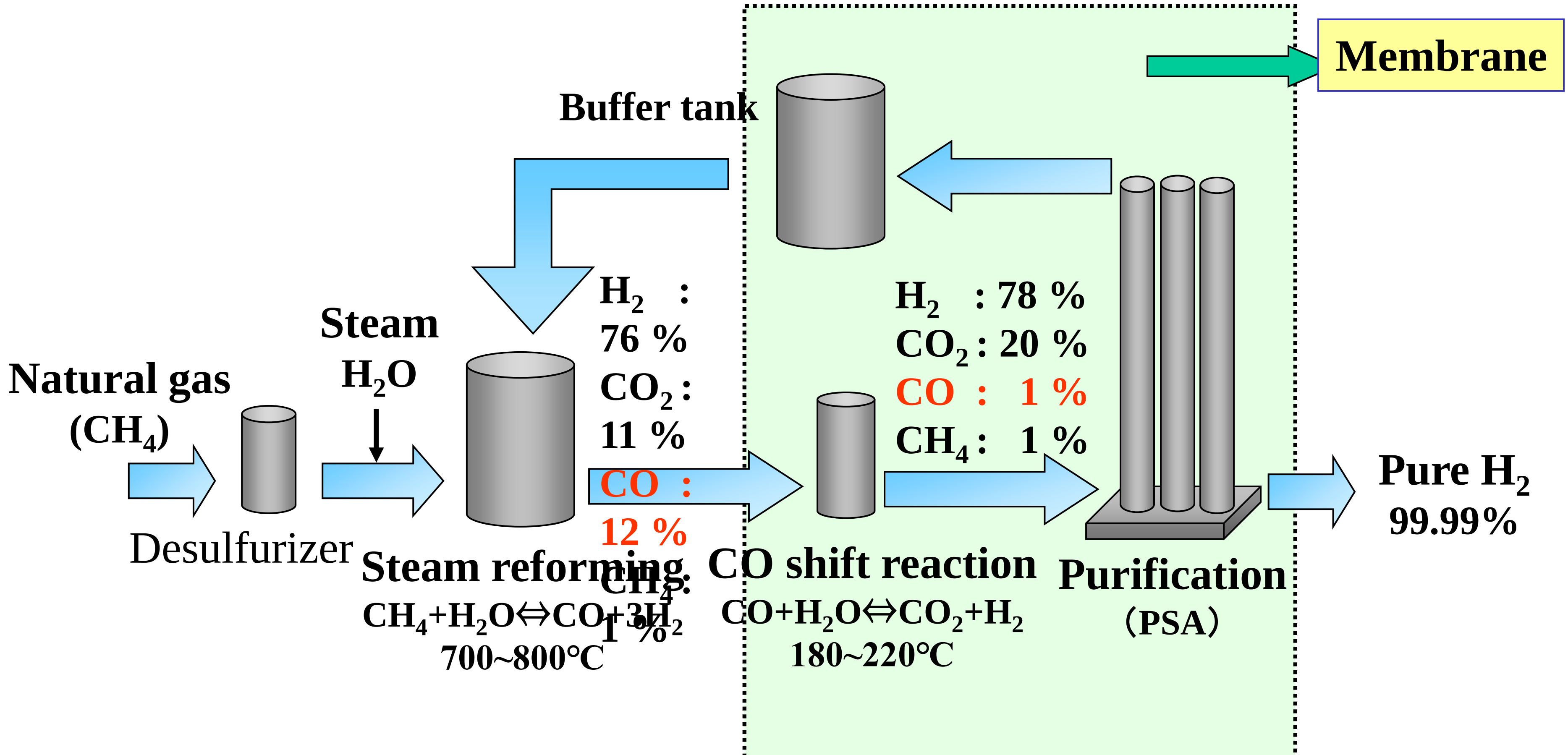
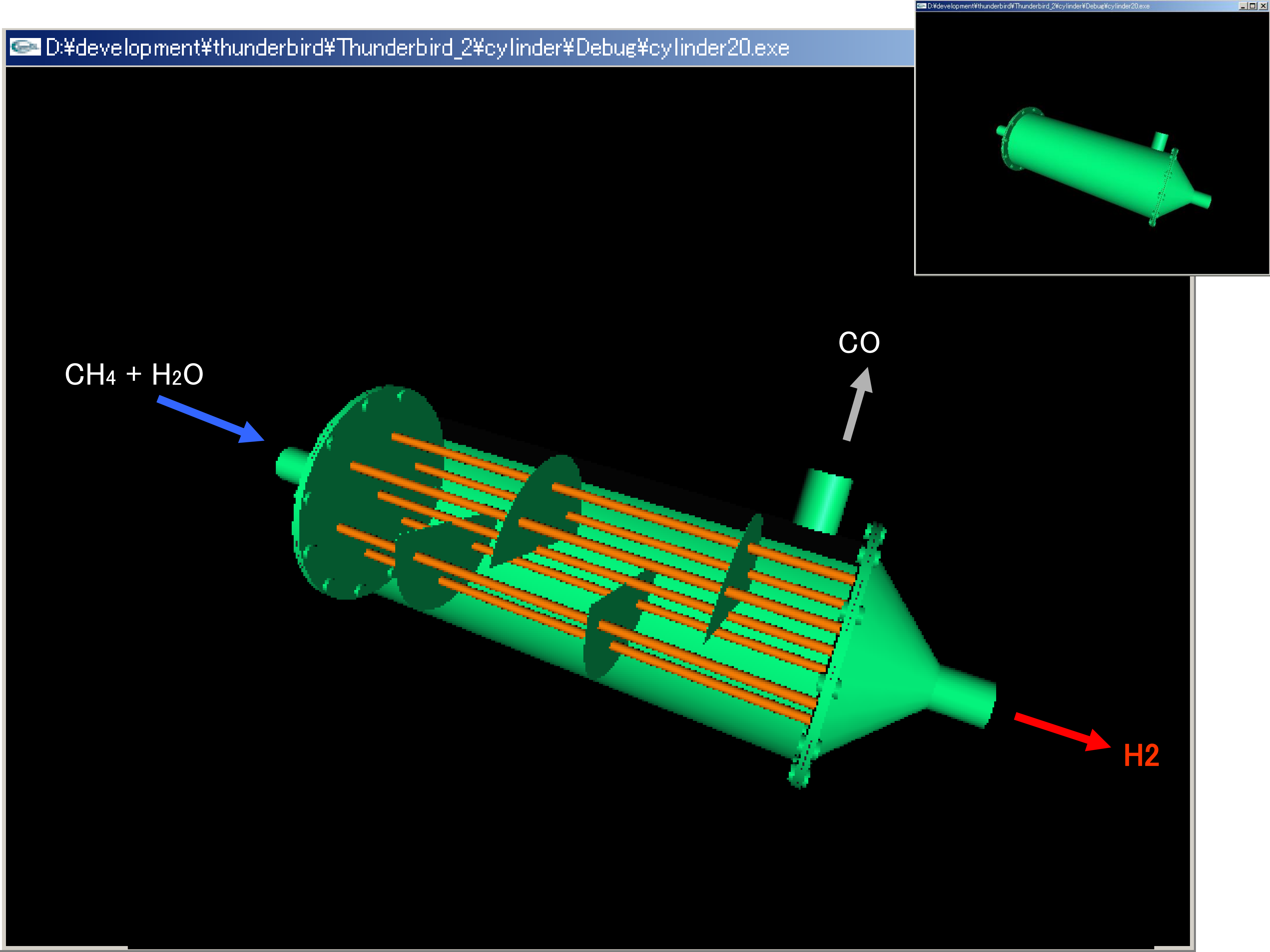
「気体分離膜の流体力学計算」

東京大学大学院工学系研究科　高羽洋充

takaba@chemsys.t.u-tokyo.ac.jp

H_2 Production by Steam Reforming



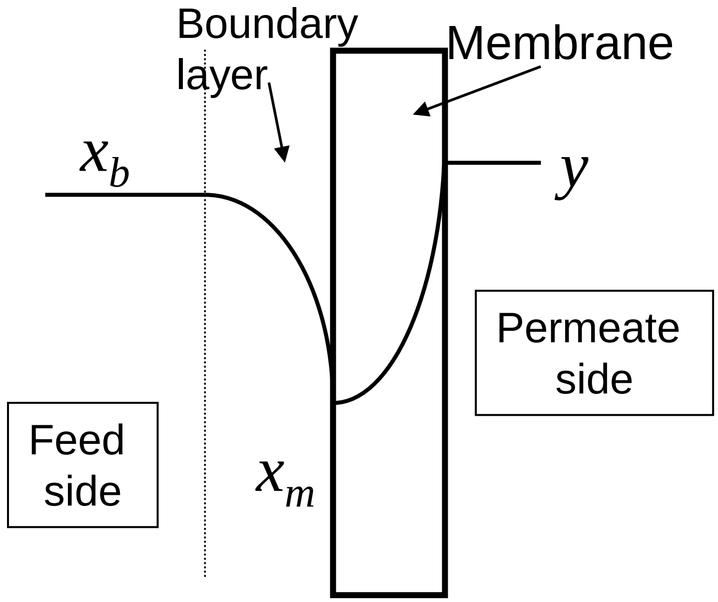

D:¥development¥thunderbird¥Thunderbird_2¥cylinder¥Debug¥cylinder20.exe
CH4 + H2O
CO
H2

Concentration Polarization

$$J_{H2} = A\phi_{H2}(Ph_{H2} - Pl_{H2})$$

$$J_{CO} = A\phi_{CO}(Ph_{CO} - Pl_{CO})$$

$$\alpha = \frac{J_{H2}}{J_{CO}}$$



Concentration Polarization

↓

Flux and Selectivity *DOWN!*

Objective

<u>Development of CFD simulator to design a gas separation module and check the validity for concentration polarization prediction</u>

<u>Outline</u>

1. **Introduction of theory**
2. **Comparison with the ideal flow calculation result (plug flow model) to test the validation of CFD**
3. **Comparison with experimental result to investigate the concentration polarization effect**

Theory in CFD Simulator

Basic Differential Equation for Fluid

$$\frac{\partial \rho}{\partial t} + div(\rho \nabla \vec{u}) = 0$$

$$\frac{\partial}{\partial t}(\rho u) + \rho(\vec{u} \cdot \nabla)\vec{u} = -\nabla P + \mu \nabla^2 \vec{u}$$

Finite Volume Method

isothermal operation

Mass Transfer Through Membrane

Differential Equation for Component

$$\rho = \frac{P}{RT} M \qquad M = 1/\sum\left(\frac{Y_i}{m_i}\right)$$

$$\frac{\partial}{\partial t}(\rho Y_i) + div(\rho \vec{u} Y_i - \rho D_i grad(Y_i)) = \nabla(J_i A/V)$$

$$P_i = P_{TOTAL} \frac{Y_i M}{m_i}$$

$$J_i = A\phi_i (P_i^1 - P_i^2)$$

Solved variables:

Y_i(weight fraction), P(pressure drop), u(velocity)

Calculation condition

MODEL → H_2 separation from H_2/CO gas mixture

Feed

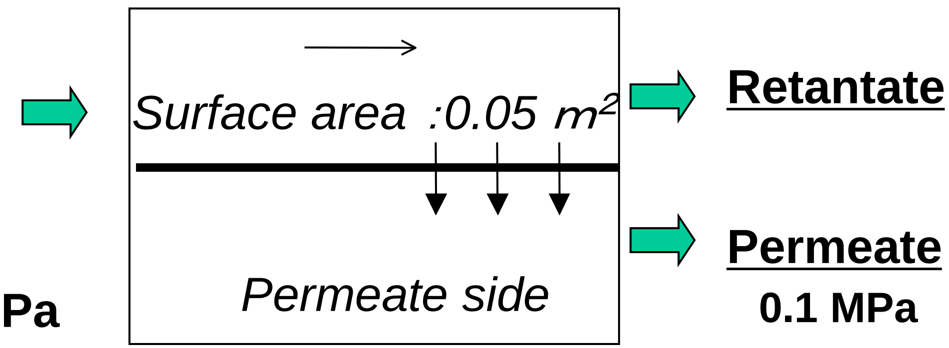
H_2:CO = 0.75 : 0.25

773 K

0.8 MPa

α(H_2/CO) = 1000

***D* (cm²/s) = 1.46 at 0.8 MPa**

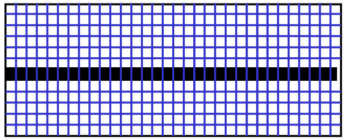


CFD Model
(*non-ideal flow*)

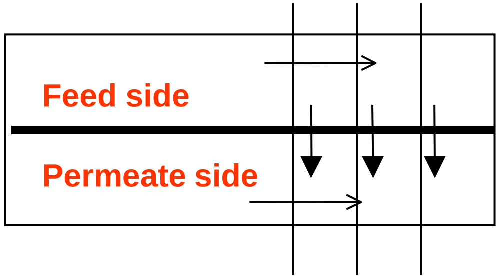
CFD cell size : *0.5 m × 0.1 m × 0.05 m*

Mesh : 40x1x20

D : *f(T,P)*



Parallel Plug Flow Model
(PFM, *ideal flow*)



Θ (non-dimensional parameter)

(Membrane Performance)

= f (*surface area(S)*, permeance (P_{H2}), ΔP, flow volume(F), height of module(d))

$$\Theta = \frac{P_{H2} \cdot S \cdot \Delta P}{F}$$

S : 0.05 m^2
d : 0.01m
ΔP : 7 x10^5 Pa

⇨ *Constant!* ⇨ P_{H2} *and u are changed.*

Plug flow model →

Separation factor and flux are as a function of only Θ!

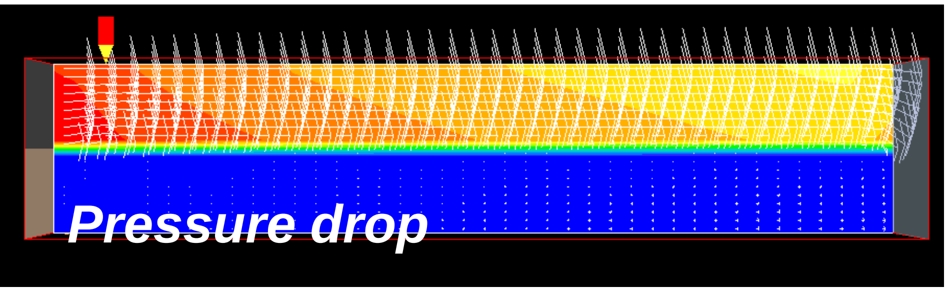
Calculation condition: F [m^3/s]

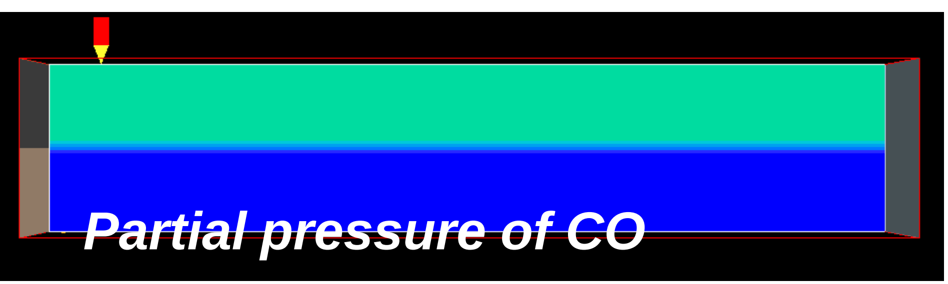
K_{H2}	Θ=2.0	Θ=1.0	Θ=0.1	Θ=0.01	Θ=0.001	Θ=0.0001
10^{-5}	$1.406x10^{-3}$	$2.812x10^{-3}$	$2.812x10^{-2}$	$2.812x10^{-1}$	$2.812x10^{0}$	$2.812x10^{1}$
10^{-6}	$1.406x10^{-4}$	$2.812x10^{-4}$	$2.812x10^{-3}$	$2.812x10^{-2}$	$2.812x10^{-1}$	$2.812x10^{0}$
$5x10^{-7}$	$7.03x10^{-5}$	$1.406x10^{-4}$	$1.406x10^{-3}$	$1.406x10^{-2}$	$1.406x10^{-1}$	$1.406x10^{0}$
10^{-7}	$1.406x10^{-5}$	$2.812x10^{-5}$	$2.812x10^{-4}$	$2.812x10^{-3}$	$2.812x10^{-2}$	$2.812x10^{-1}$
10^{-8}	$1.406x10^{-6}$	$2.812x10^{-6}$	$2.812x10^{-5}$	$2.812x10^{-4}$	$2.812x10^{-3}$	$2.812x10^{-2}$
10^{-9}	$1.406x10^{-7}$	$2.812x10^{-7}$	$2.812x10^{-6}$	$2.812x10^{-5}$	$2.812x10^{-4}$	$2.812x10^{-3}$

$\alpha(K_{H2}/K_{CO})$ ＝1000

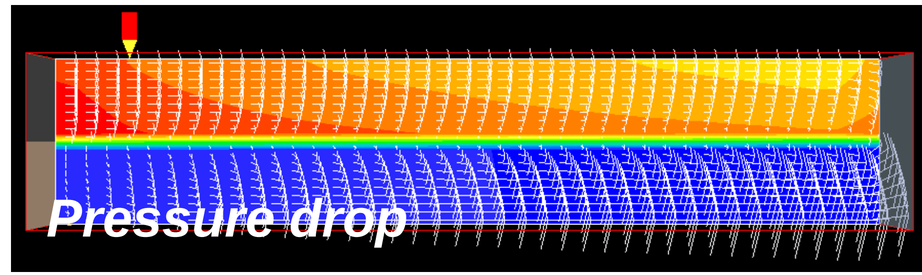
CFD Result（flow volume; $F = 2.812 \times 10^{-8}$ m^3/s)

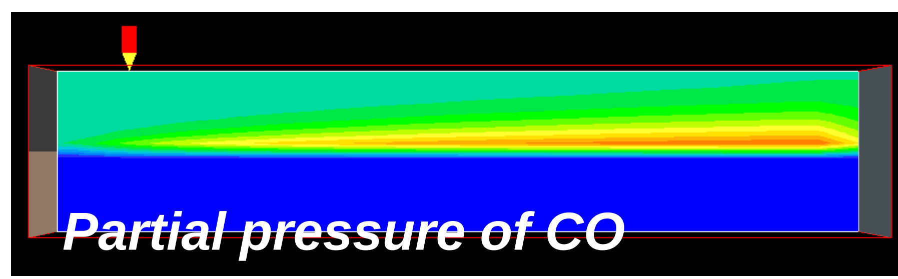
$KH_2 = 1.0 \times 10^{-8}$



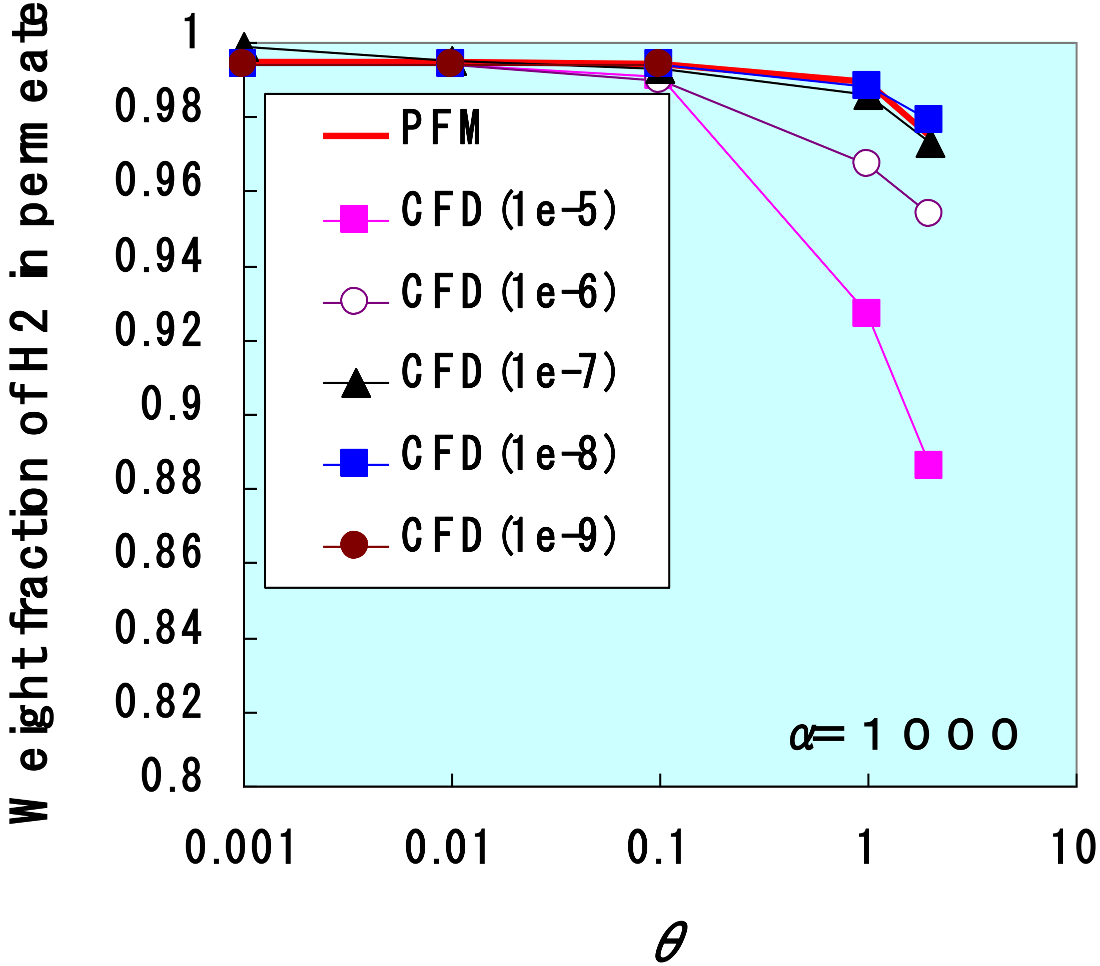


$KH_2 = 1.0 \times 10^{-6}$



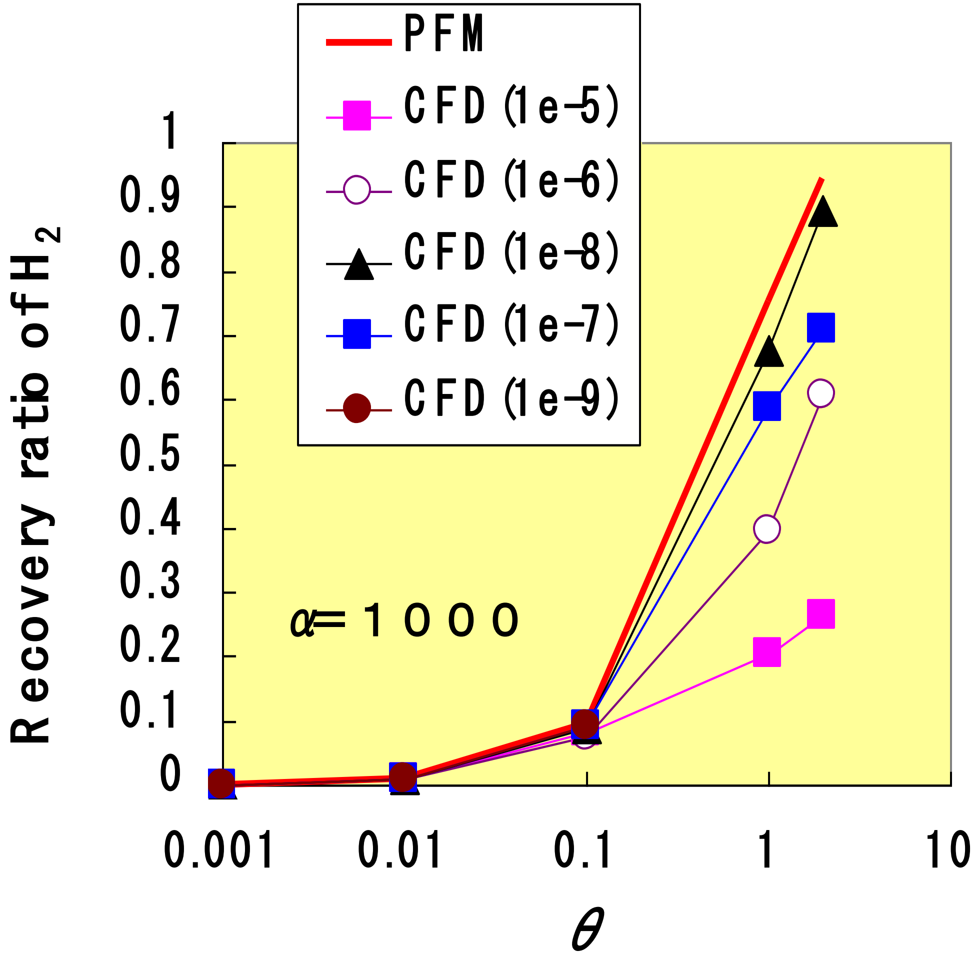


CFD vs PFM -y_{H2}-



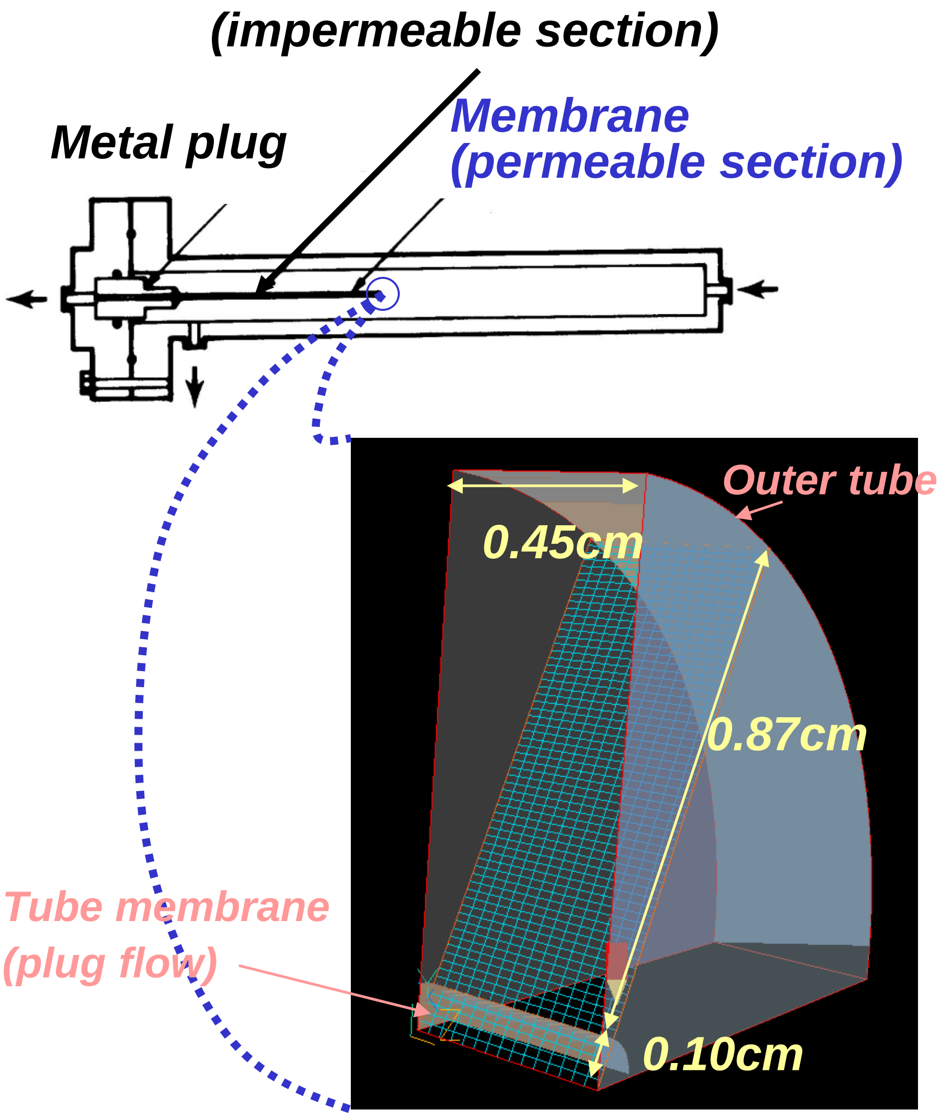
When permeance of H_2 is smaller than $1x10^{-6}$ mol/m^2sPa, CFD agrees with PFM.

CFD vs PFM -R_{H2}-



When permeance of H_2 is smaller than $1x10^{-6}$ mol/m^2sPa, CFD agrees well with PFM.

CFD Model for Polarization



K. Haraya et al., *Sep. Sci. Tech.*, *22 (1987) 1425.*

Hydrogen and carbon monoxide mixture gas

K_{H_2} (mol/s m^2 Pa) = 2.67×10^{-6}

K_{H_2}/K_{CO} = 3.74

P_h (MPa) = 1.1

P_l (MPa) = 0.5-0.6

D (cm^2/s) = 1.06 at 1.1 MPa

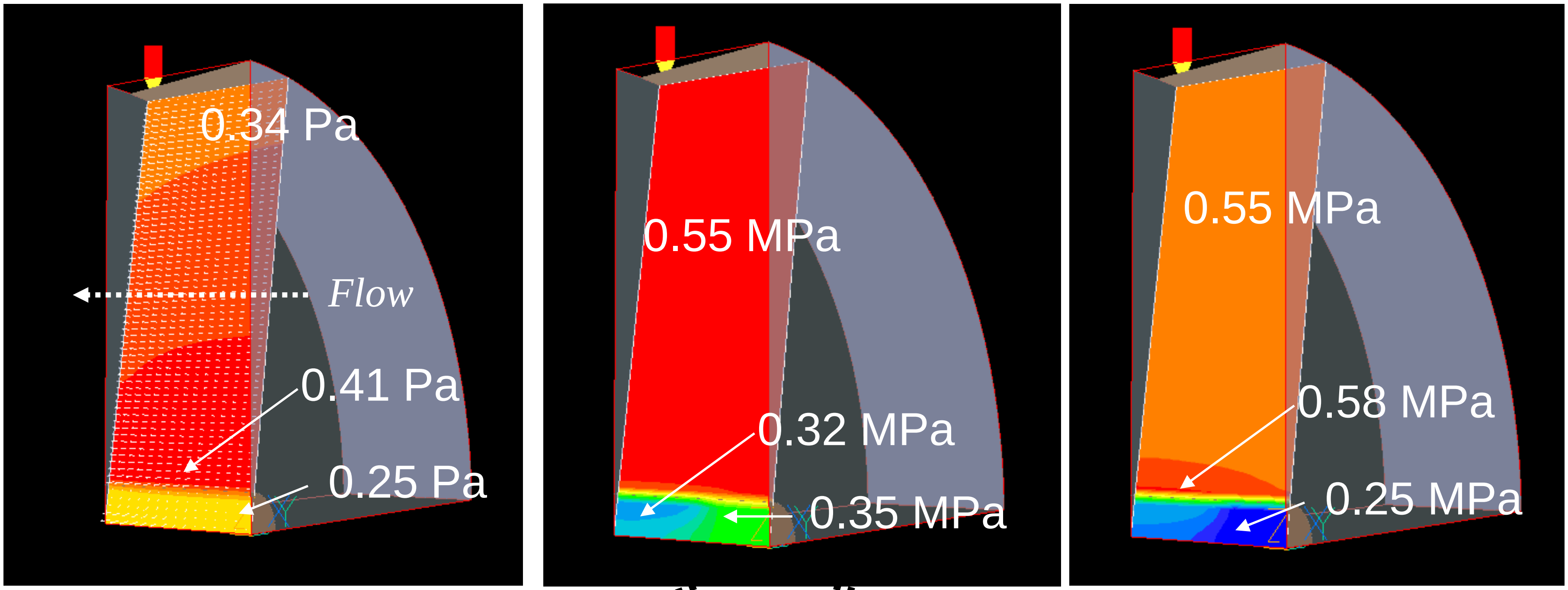
Sc = 0.24

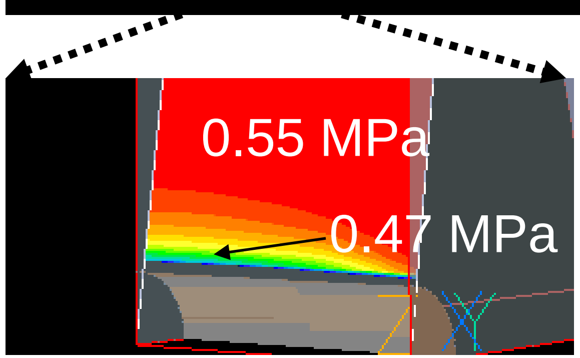
Feed (cm/s) = 2.5, 3.75, 5.0

Jv (cm/s) = 0.4

Partial Pressure Distribution

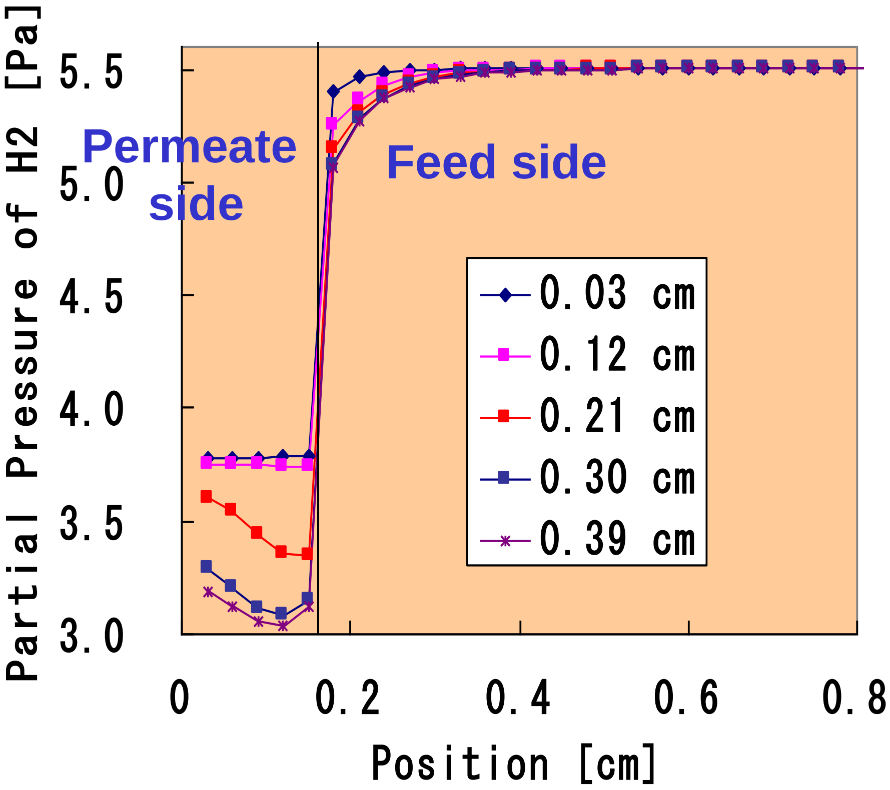
Δp | P of H_2 | P of CO



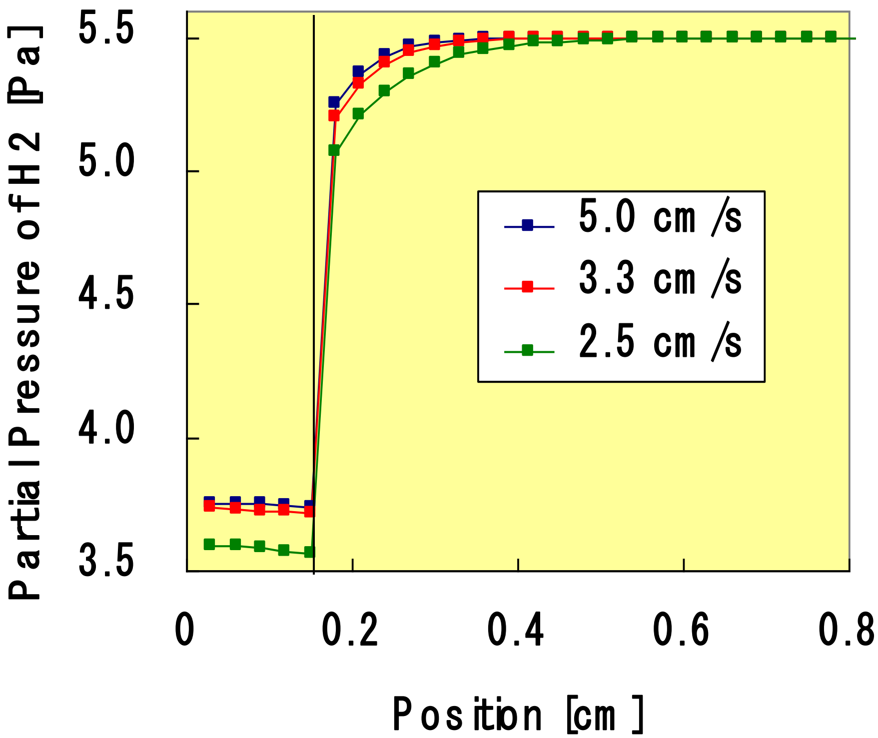


Feed velocity = 5 cm/s

Partial Pressure Distribution

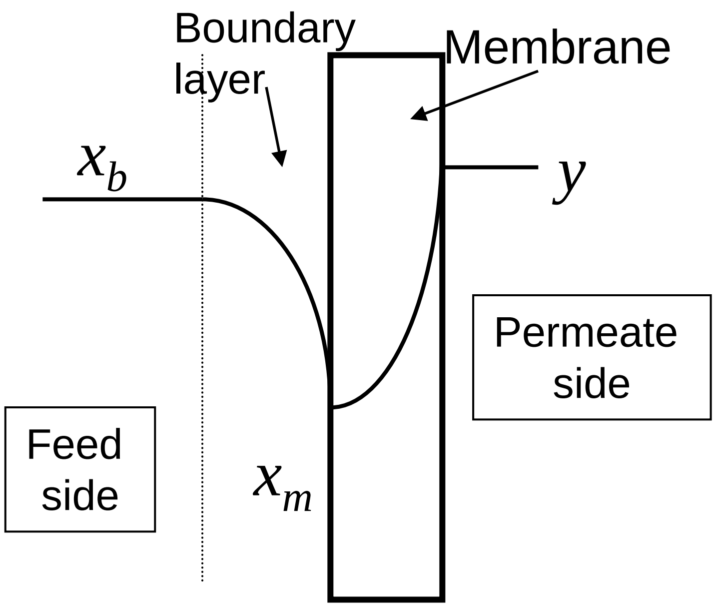


P(H_2) along flow direction
Feed velocity is 5 cm/s.



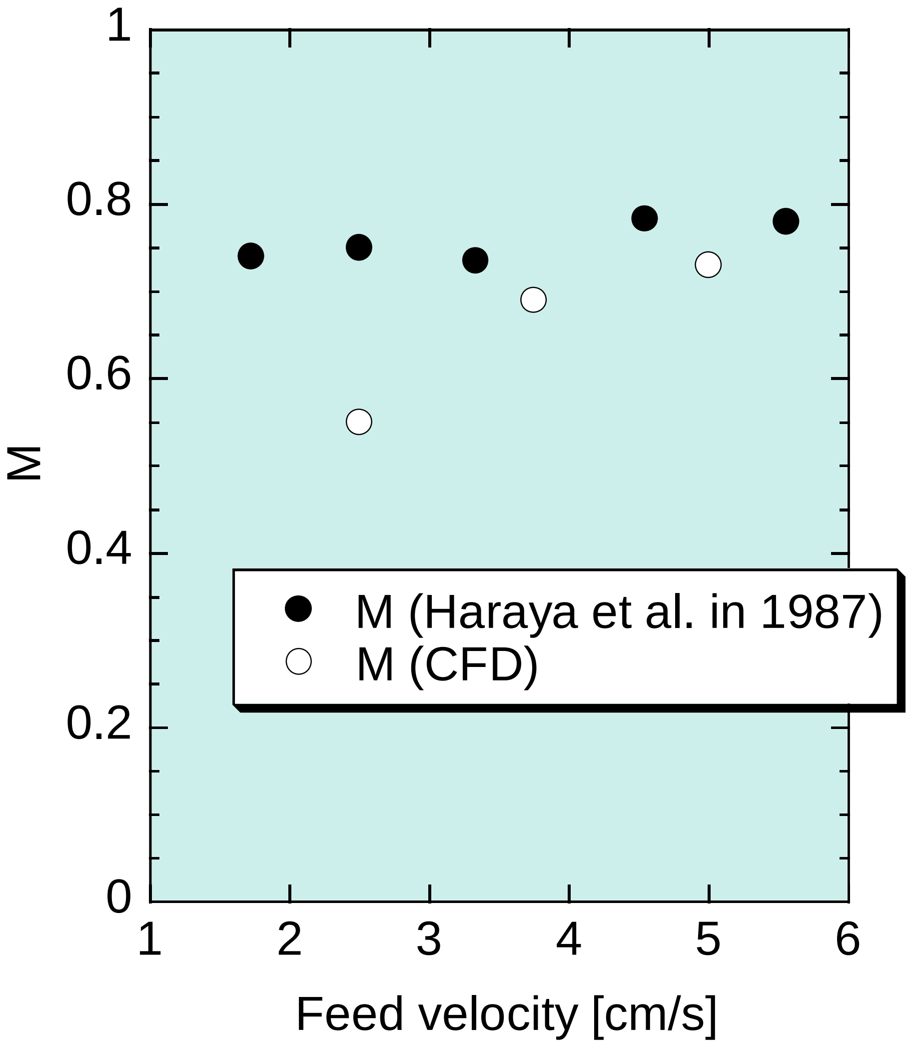
Change of *P*(H_2) for different feed Velocity. Position of flow direction Is 0.12 cm.

Comparison with experiment



M is the modulus of concentration polarization

$$M = \frac{y - x_b}{y - x_m}$$



Conclusion

CFD simulator was developed and tested using a model based on the separation process of a hydrogen/carbon monoxide gas mixture in the steam reforming process.

1. CFD results agree with the PFM results when the permeance of H_2 becomes smaller than 1×10^{-7} mol/m^2sPa.

2. When the permeance of H_2 is larger than 1×10^{-6} mol/m^2sPa, the volume flux and selectivity decreases.

3. The concentration polarization observed in the CFD simulation results compared well with the experimental results.

Acknowledgement

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