

Simulation of Low-Density Gas Flows

정찬홍 교수

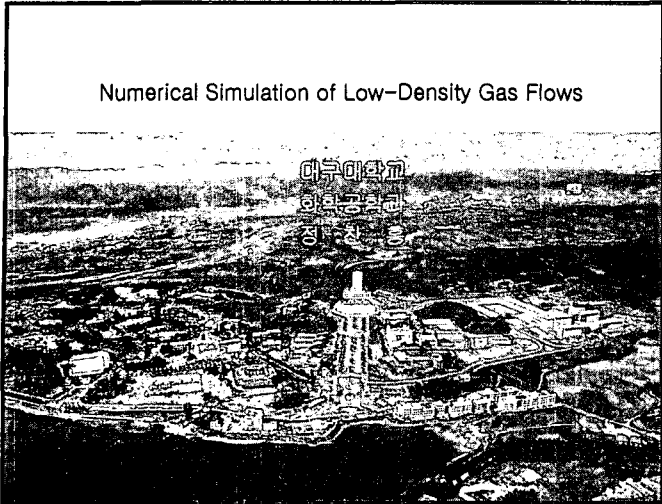
대구대학교 화학공학과

유동장의 특성을 구분할 수 있는 척도는 평균자유행로와 특성거리의 비인 누셀수이다. 누셀수에 따라서 유장은 연속체영역, 미끄럼영역, 천이영역, 및 자유분자영역으로 나누어진다. 고고도에서 비행체 주위의 유동장, 진공에서의 유동장 등이 비연속체영역 즉 저밀도유동장에 해당 된다. 비연속체영역에 해당되는 또 다른 중요한 분야는 미세 유동장이다. 최근에 관심이 대두되고 있는 미세항공기(MAV)와 실리콘혁명 이래 유망한 미래기술중의 하나인 MEMS 장치 주위의 유동장 등이 바로 미세 유동장이다. 비연속체영역에서 유체의 이동 및 전달현상을 기술하기 위하여는 Boltzmann 방정식을 해석하여야한다. Navier-Stokes 방정식을 이용한 기존의 CFD 기법이 적용되지 않는 새로운 유동영역이기 때문이다.

본 발표에서는 Boltzmann 방정식의 유력한 해법인 직접모사(Direct Simulation Monte Carlo)법을 이용한 저밀도 유동장 해석이 소개될 것이다. 또한 직접모사법이 이용되기 어려운 다양한 저속 유동장에 대한 해석결과도 소개될 것이다.

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목 차

- Flow Regimes of Gas Dynamics
- Boltzmann Equation
- 직접모사법(Direct Simulation Monte-Carlo Method)
Low Thrust Nozzle, Hypersonic Scramjet Inlet
- Finite-Difference Method Coupled with Discrete Ordinate Method
Microchannel flow, Micro Plate, NACA 0012 airfoil

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Flow Regimes of Gas Dynamics

Kn	0.0	0.01	0.1	10.0
Flow Regimes	Continuum	Slip	Transition	Free Molecular
Molecular Approach	Boltzmann Equation			
Continuum Approach	Navier-Stokes			
$L_c = 1\text{ m}$	0.0	80 km	100 km	130 km
at 1 atm	$5\ \mu\text{m}$	$0.5\ \mu\text{m}$	$0.005\ \mu\text{m}$	

Knudsen number

$$Kn = \lambda/L$$

λ : mean free path
 L : characteristic length

Local Knudsen number

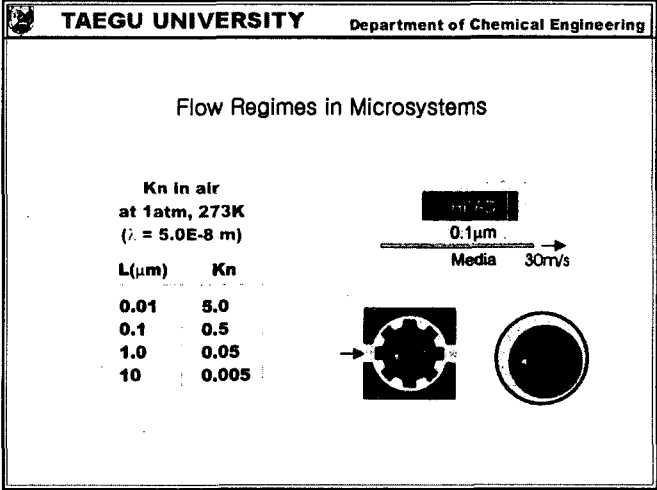
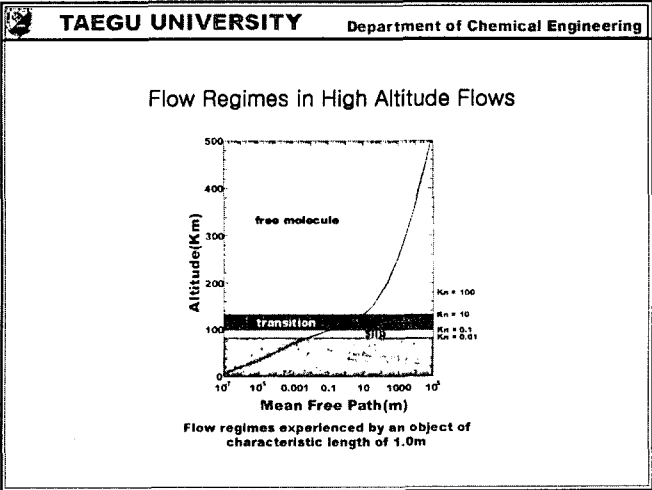
$$L = \frac{\rho}{d_p/dx}$$

L : scale length of the macroscopic gradients

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Fields of Application

	High Altitude Flow	spacecraft, satellite, plume/low-thrust nozzle, spacecraft contamination/charging
Rarefied Gas Dynamics	Vacuum	vacuum pump, etching, coating, chemical vapor deposition
	Others	Microelectromechanical systems(MEMS), gas bearing, computer flying head



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Boltzmann's Integro-Differential Equation

$$\frac{\partial f}{\partial t} + \vec{c} \cdot \frac{\partial f}{\partial \vec{r}} + F \cdot \frac{\partial f}{\partial \vec{c}} = \int \int_{-\infty}^{+\infty} (f'' f_1'' - f f_1) c_1 \sigma d\Omega d\vec{c}_1$$

$f = f(t, \vec{r}, \vec{c})$: Particle Distribution Function (number of molecules with velocity \vec{c} at position \vec{r} at time t .)

Macroscopic Flow Variables

$$n(t, \vec{r}) = \int f d\vec{c}, \quad n\vec{U}(t, \vec{r}) = \int \vec{c} f d\vec{c}, \quad \frac{3}{2} nkT(t, \vec{r}) = \int \frac{1}{2} m(\vec{c} - \vec{U})^2 f d\vec{c}$$

Chapman-Enskog Expansion

$$f = f_0 [1 + \Phi_1(Kn) + \Phi_2(Kn^2) + \dots]$$

0th order: Euler equation
 1st order: Navier-Stokes equations
 2nd order: Burnett equations

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Direct Simulation Monte Carlo Method

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Direct Simulation Monte-Carlo(DSMC) Method

A computer technique to solve the Boltzmann equation by concurrently following the motion and intermolecular collisions of representative molecules

molecular movement
 $\vec{x}_j = \vec{x}_j + \vec{c}_j \Delta t$

- into or out of the simulation domain
- interaction with solid surface

molecular collision

- translational energy exchange
- internal energy exchange

chemical reaction

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EXAMPLE FLOW PROBLEMS

- Low Thrust Nozzle
- Hypersonic Scramjet Inlet

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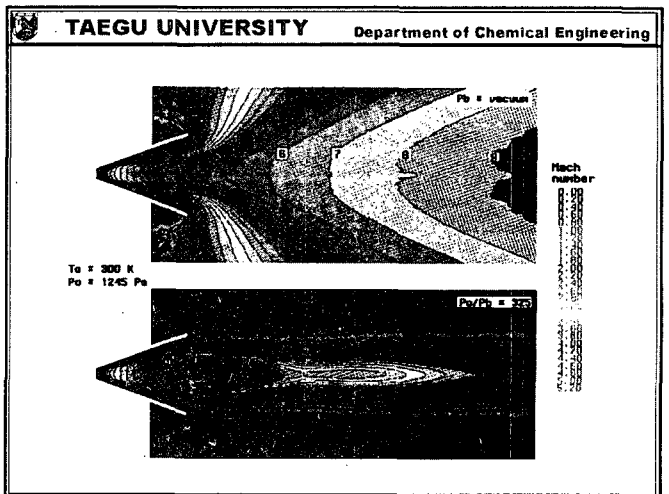
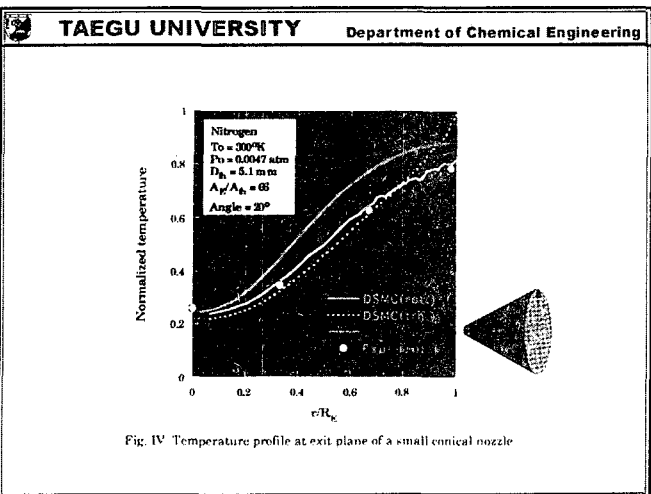
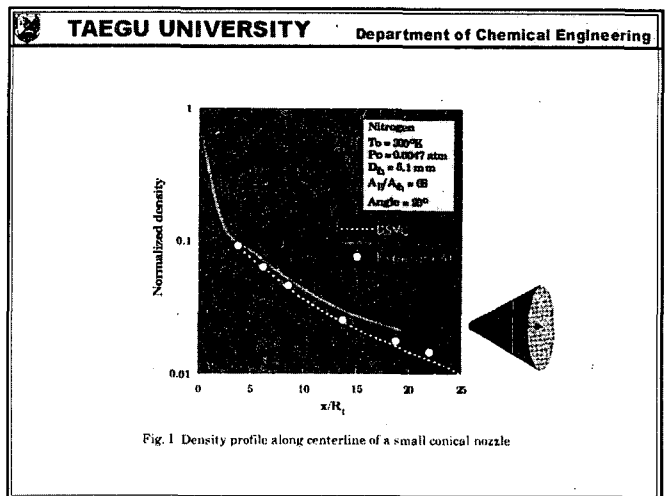
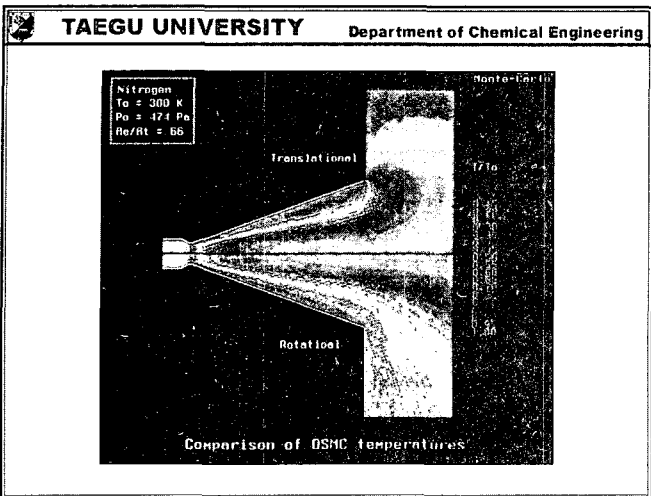
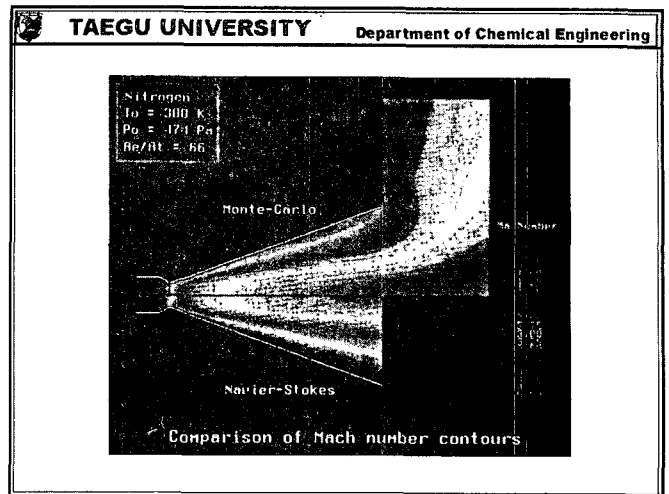
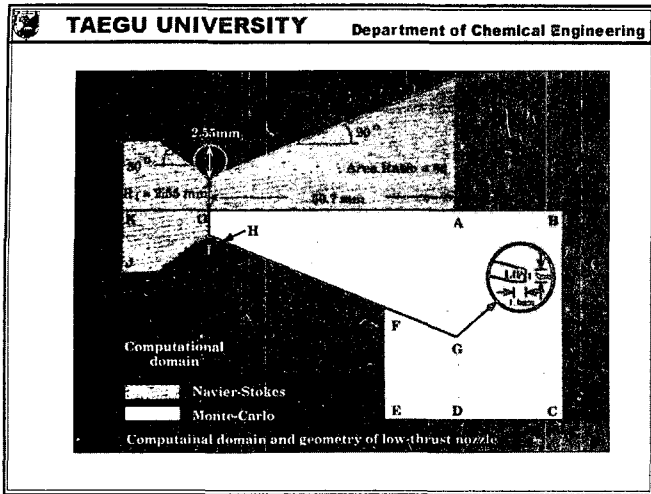
LOW THRUST NOZZLE FLOW

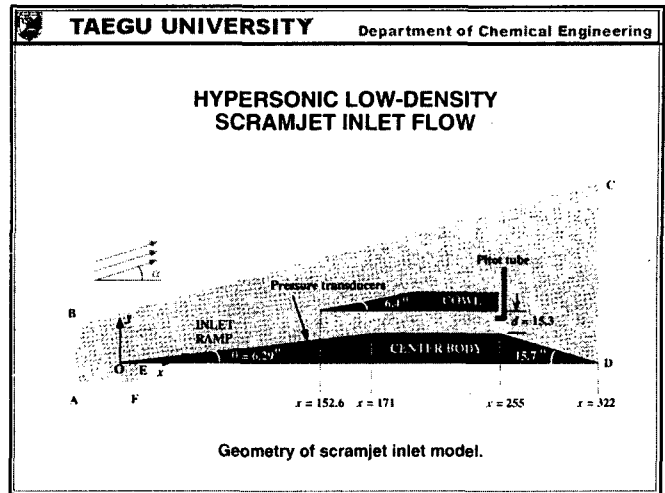
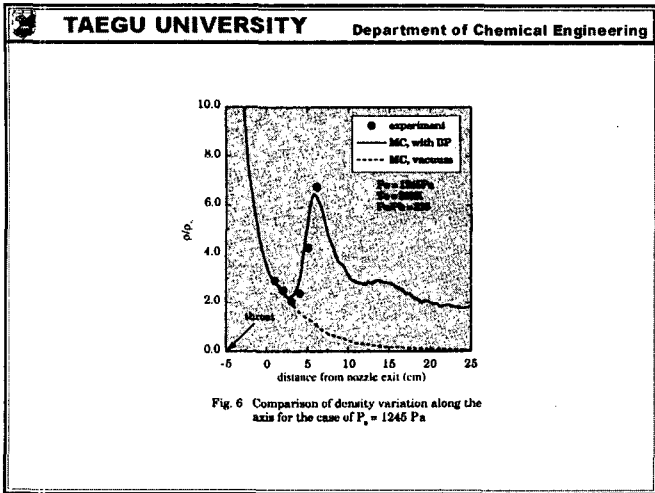
Fig. 1 Geometry of low-thrust graphite nozzle (Expt. by Rothe, Cornell Lab., 1971)

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Table 1 Flow conditions

	Case I	Case II
Test gas	N ₂	N ₂
Stagnation temperature, T ₀	300 K	300 K
Stagnation pressure, P ₀	474 Pa	1245 Pa
Ambient pressure, P _b	1.5 Pa	3.8 Pa
Wall temperature, T _w	300 K	300 K
Reynolds number, Re _w	270	709
Knudsen number, Kn	2.3 × 10 ⁻³	8.8 × 10 ⁻⁴





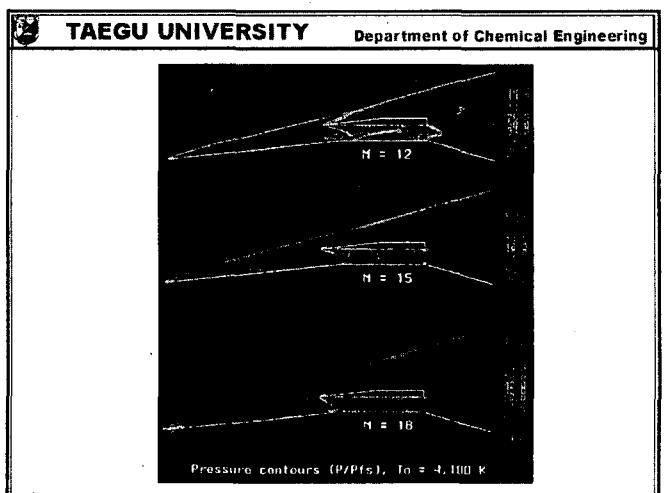
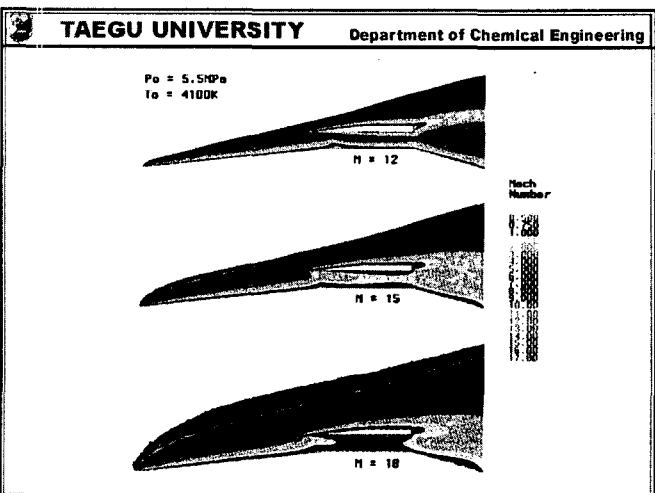
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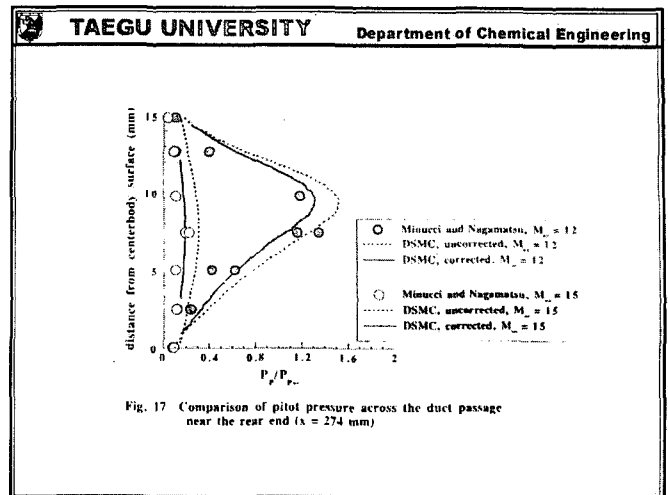
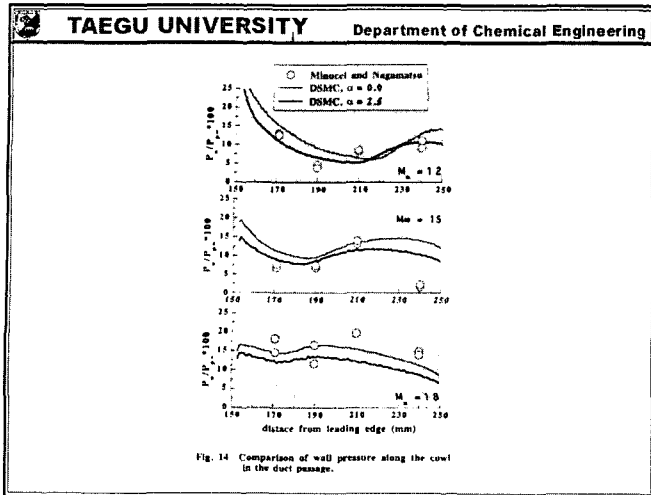
FREE STREAM FLOW CONDITIONS

- Dry air
- $T_0 = 4,100$ K

	M_∞	T_∞ (K)	P_∞ (Pa)	Kn (λ_∞/d)	Re_∞ (m^{-1})
Case I	12.0	208.0	11.0	0.02	46,000
Case II	15.0	135.0	2.4	0.06	23,000
Case III	18.0	94.3	0.68	0.12	14,000

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- ### CHARACTERISTICS OF THE FLOW
- Shock/boundary layer interaction
 - Shock impingement and shock induced separation
 - Thick viscous layer due to low-density fluid
 - Thermal nonequilibrium and velocity slip





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모델 볼츠만방정식을 이용한
Finite-Difference Method Coupled
with Discrete Ordinate Method

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저속 유동장 해석 시 직접모사법의 문제점

DSMC Cell

$$C_j = U + C_{i,j}$$

$$U_c = \frac{1}{N} \sum_{j=1}^N C_j = U + \frac{1}{N} \sum_{i=1}^N C_{i,j}$$

$$U_c = U + u'$$

Air at 298K
 u' - fluctuations in macroscopic flow velocity (m/s)

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Finite-Difference Method
Coupled with Discrete Ordinate Method

Boltzmann Equation with BGK model

$$V_x \frac{\partial f}{\partial x} + V_y \frac{\partial f}{\partial y} = A_c (F - f) \quad (1)$$

A_c : collision frequency

$$F = n(2\pi RT)^{-3/2} \exp[-(V-U)^2 / 2RT] \quad (2)$$

$$n = \int f dV$$

$$nU = \int V f dV \quad (3)$$

$$3nRT = \int (V-U)^2 f dV$$

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Discrete Ordinate Method

$$n = \int f dV \quad \hat{n} = \sum_{\delta} \sum_{\sigma} P_{\delta} P_{\sigma} \hat{g}_{\delta\sigma} \quad (10-a)$$

$$nU = \int V f dV \quad \hat{n}\hat{U}_x = \sum_{\delta} \sum_{\sigma} P_{\delta} P_{\sigma} V_{\delta} \sin \phi_{\sigma} \hat{g}_{\delta\sigma} \quad (10-b)$$

$$\hat{n}\hat{U}_y = \sum_{\delta} \sum_{\sigma} P_{\delta} P_{\sigma} V_{\delta} \cos \phi_{\sigma} \hat{g}_{\delta\sigma} \quad (10-c)$$

$$3nRT = \int (V-U)^2 f dV \quad 3\hat{n}\hat{T} / 2 = \sum_{\delta} \sum_{\sigma} P_{\delta} P_{\sigma} (h_{\delta\sigma} + V_{\delta}^2 \hat{g}_{\delta\sigma}) - \hat{n}(\hat{U}_x^2 + \hat{U}_y^2) \quad (10-d)$$

V_{δ} discrete speed
 ϕ_{σ} discrete velocity angle
 $\hat{h}_{\delta\sigma}(\xi, \eta, V_{\delta}, \phi_{\sigma})$ discrete distribution functions
 $\hat{g}_{\delta\sigma}(\xi, \eta, V_{\delta}, \phi_{\sigma})$

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마이크로채널 유동해석

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MICROCHANNEL

- MEMS 장치를 구성하는 가장 기본적이고 단순한 형상
- 지금까지의 대부분 연구 결과가 매우 짧은 microchannel 또는 고속 유동장으로 한정

(Not to scale)
Microchannel geometry.

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Micro channel flow with small L/h ratio

Gas	N_2
Channel Length	$15 \mu m$
Channel Height	$0.50 \mu m$
L/h ratio	30
Upstream Chamber Pressure	2.5 bar
Downstream Chamber Pressure	1.0 bar
$T_{IN}, T_{OUT}, T_{WALL}$	300 K
Mean Knudsen Number	0.06
Computational Grid (Cell)	80×50 (81×51)

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$Kn = 0.06$
 $h = 0.50 \mu m, L = 15 \mu m$
 $L/h = 30$

Density contours

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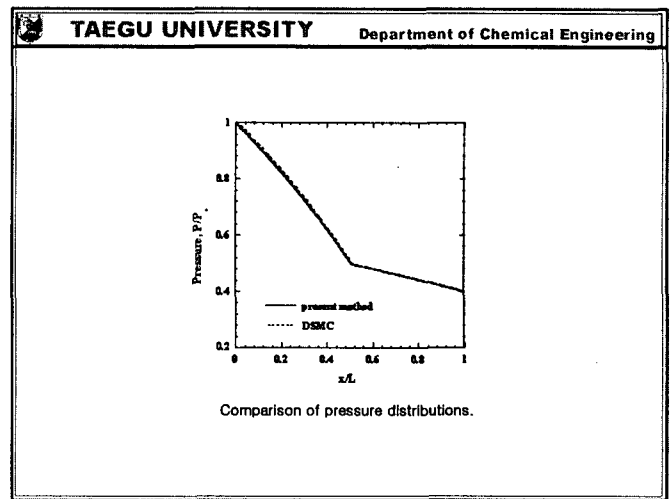
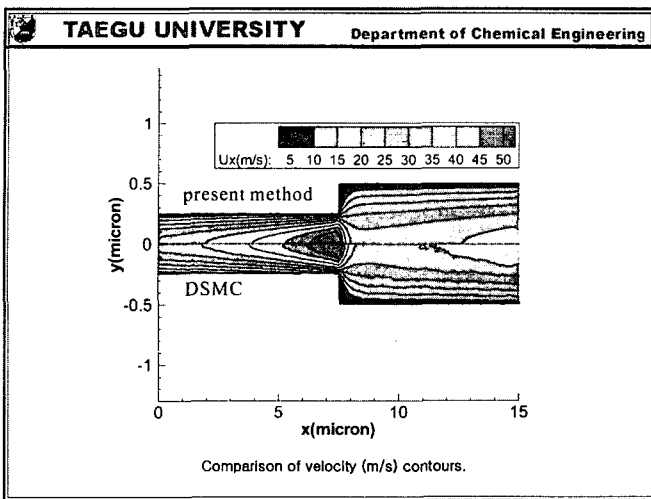
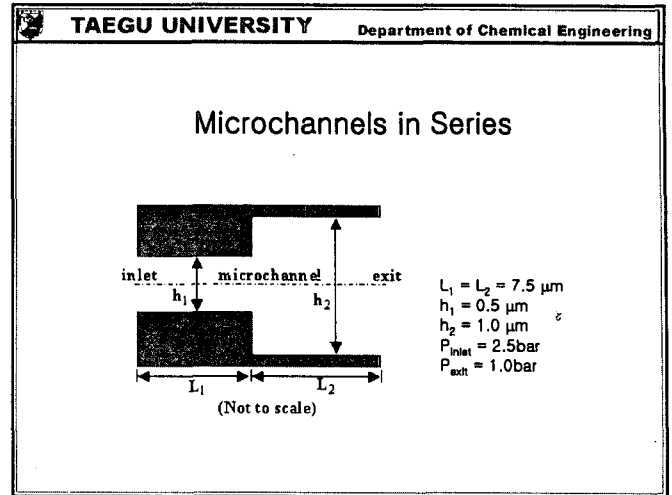
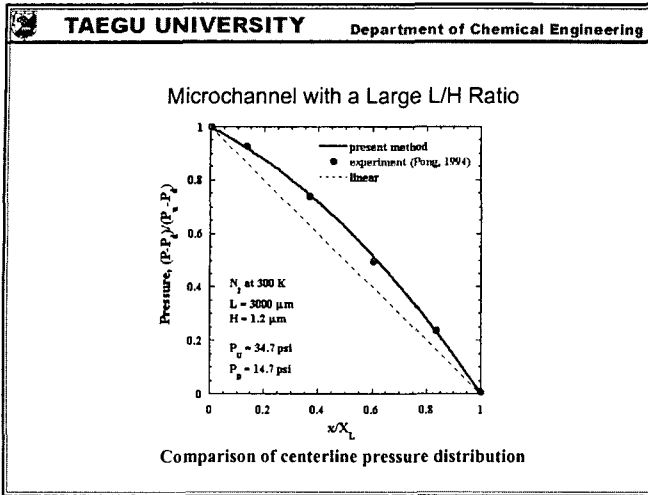
$Kn = 0.06$
 $h = 0.53 \mu m, L = 15 \mu m$
 $L/h = 30$

X-velocity contours

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$h = 0.50 \mu m$
 $L = 15.0 \mu m$
 $P_{in} = 2.5 \text{ bar}$
 $P_{out} = 1.0 \text{ bar}$
 $Kn = 0.06$

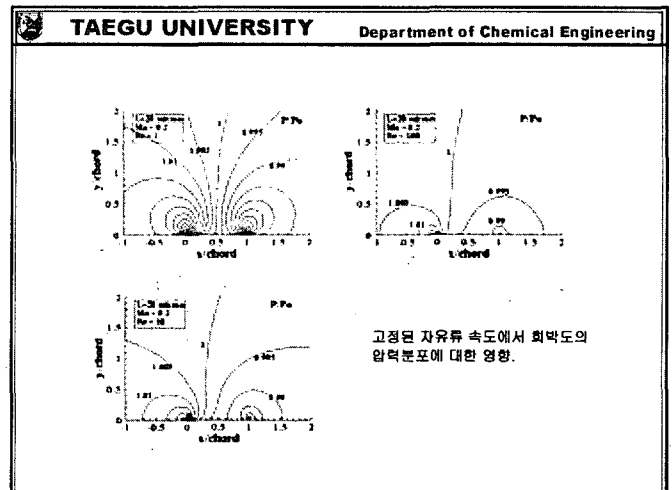
Comparison of x-velocity contours(m/s): color contours, present method, dot-dashed lines, DSMC method, dashed lines, Navier-Stokes with slip.

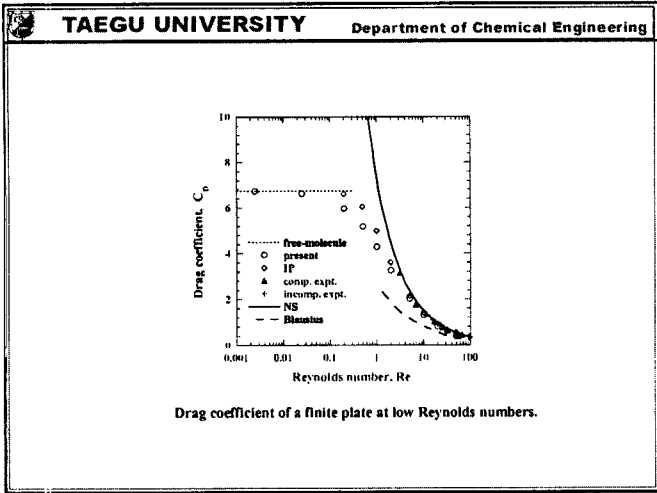


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두께가 없는 2차원 평판 주위의 저속 희박류

Gas	air
Plate Length	20 μm
Plate thickness	0 μm
Free stream velocity	69 m/s
Free stream Mach number	0.2
Free stream temperature	295 K
Knudsen Number	0.03
Computational Grid	241x161

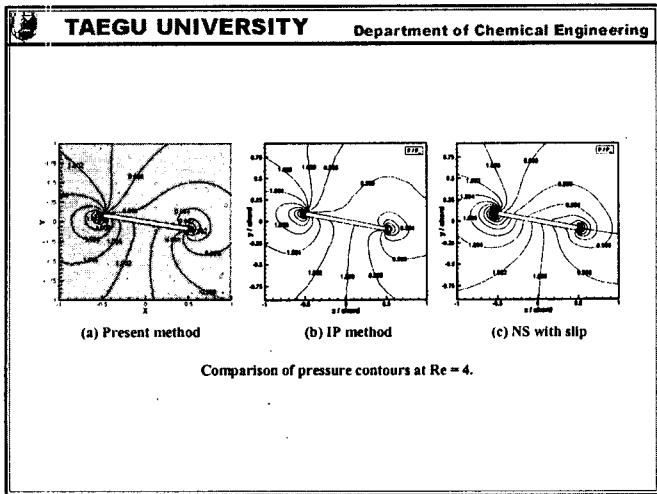




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5% 평판 주위의 저속 희박류

Gas	air
Plate Length	20 μm
Plate thickness	1 μm
Free stream velocity	30 m/s
Free stream Mach number	0.087
Free stream temperature	295 K
Knudsen Number	0.03
Computational Grid	231x169

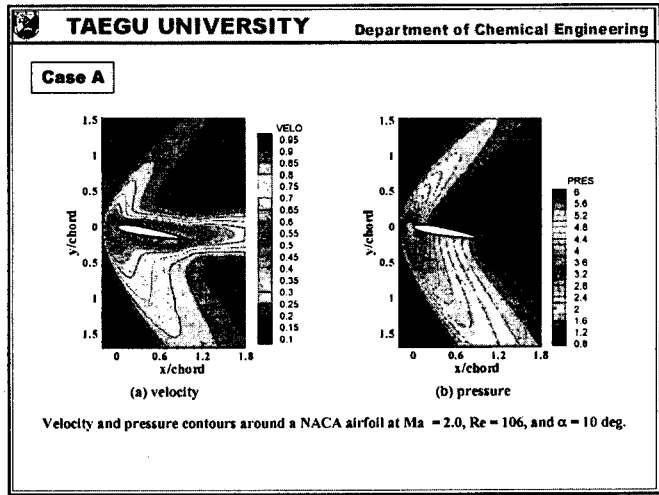
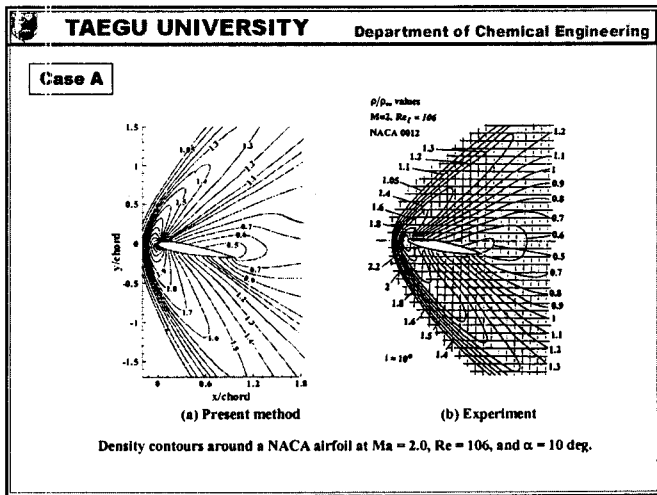


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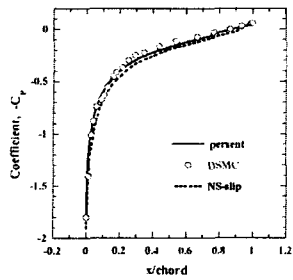
NACA 0012 익형 주위의 저속 희박류

Case	Ma	Re	α (deg)	P_o ($\times 10^{-5}\text{atm}$)	T_o (K)	U_o (m/s)
A	2.0	106	10	2.759	161	509
B	2.0	106	0	2.759	161	509

$L_c = 0.04\text{m}$



Case B



Comparison of pressure coefficients at $Ma = 2.0$ and $Re = 106$, and $\alpha = 0$ deg.

CONCLUSIONS

1. Two different methods to analyze rarefied gas flows, the DSMC and the FDDO methods, have been introduced.
2. The validity of the methods is demonstrated by comparing the results with those from experiment and other methods.
3. It is shown that the DSMC method is an accurate tool for high speed rarefied flows.
4. For low speed rarefied flows, the DSMC method suffers from statistical scattering. New tools such as the FDDO method are required for low speed rarefied flows