저압 장비 열유동 해석

㈜경원이앤씨

Content

- CFD-ACE+ 소개
- Semiconductor 해석에 필요한 모델 소개
  - Low pressure simulation
  - Convection : Forced vs Natural
  - Effect of Rotating Solids
  - Radiation Effect
  - Chemistry Mixing & reaction
  - Plasma

경원이앤씨 Engineering & Communication

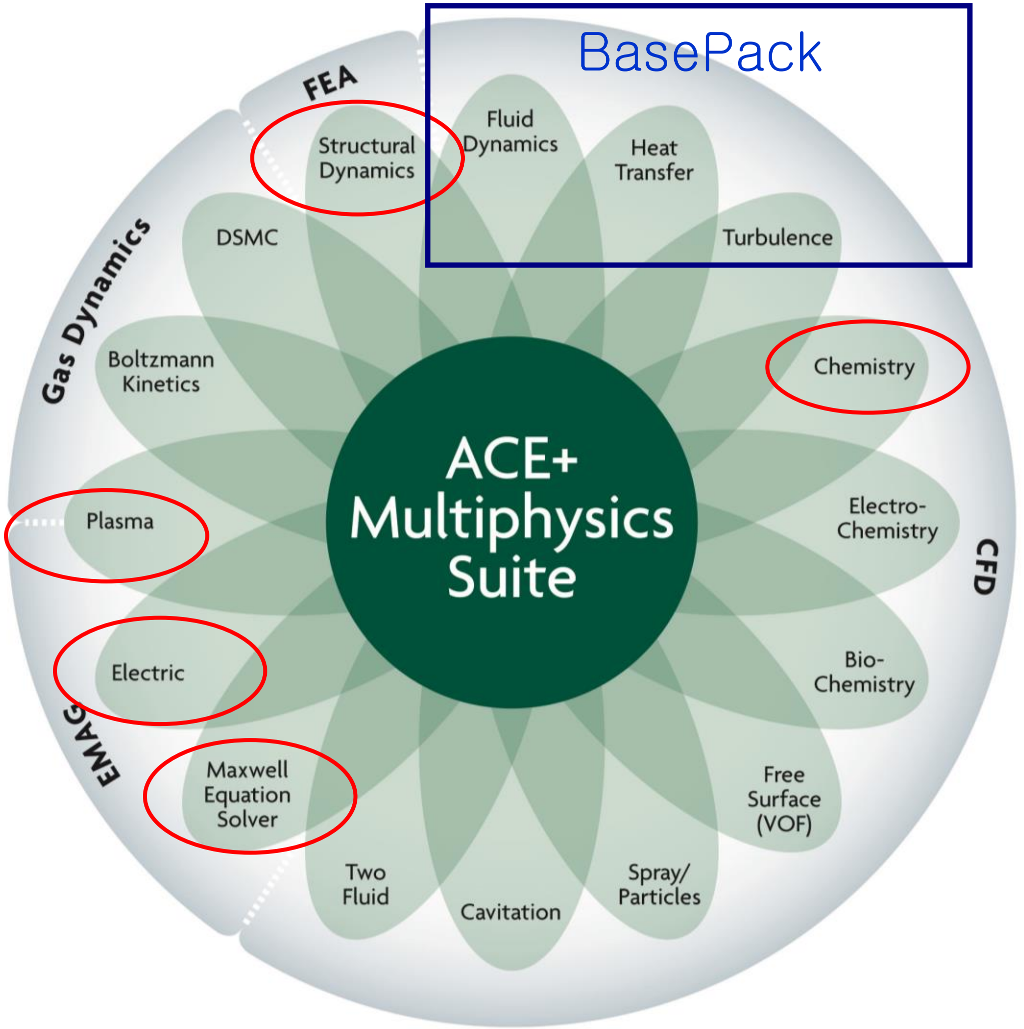
Advanced CFD and Multiphysics Software

Understanding, Implementation and Analysis of Multiphysics simulations :

Excellent Engineers in KWEnC

Customers in various industry :

Has many Industrial Partners !!



CFD-ACE+ Product Overview

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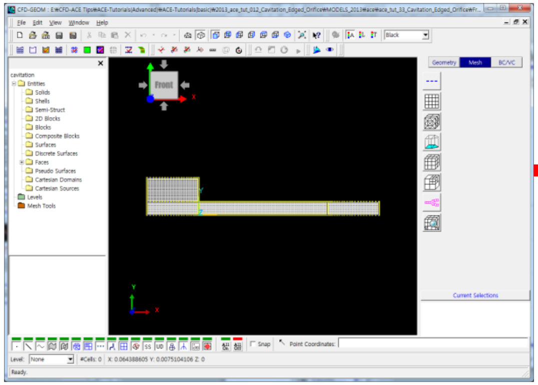
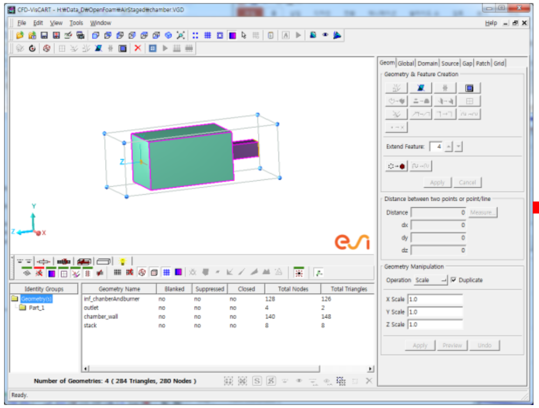
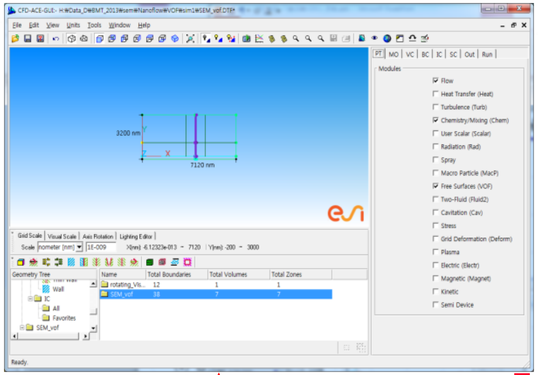
CFD-GEOM (*.GGD)
CFD-VisCART(*.VGD)

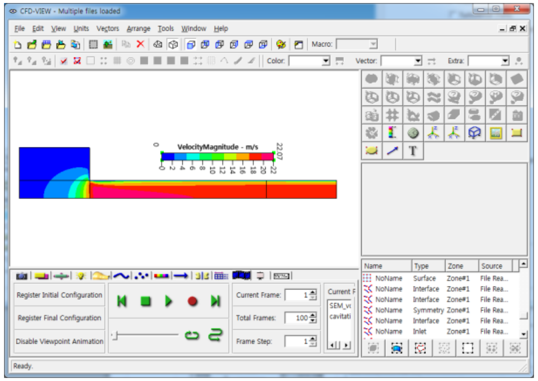




CFD-ACE-GUI (*.DTF)



CFD-VIEW



Computational Grid and BC / VC Locations

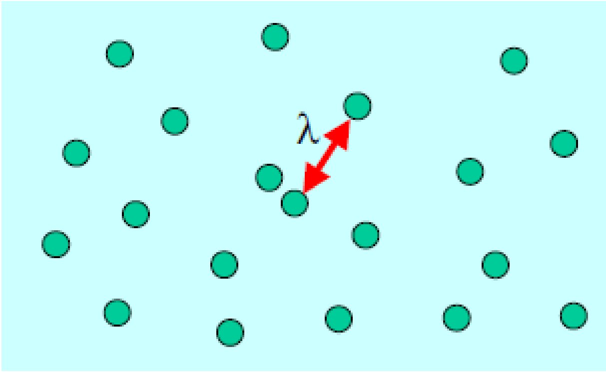
Input Files

Graphical Results

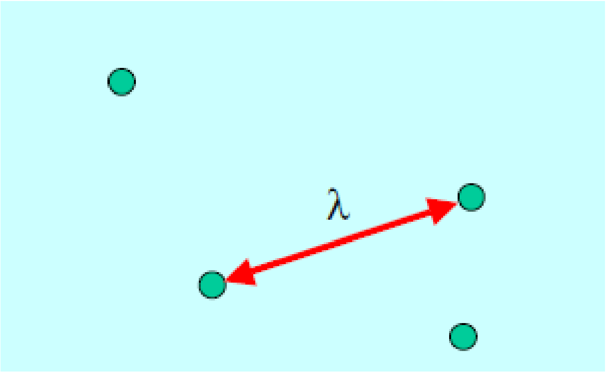
Batch Solver
CFD-ACE-SOLVER

Text Results

- **Implications of Mean Free Path**



$p = p_0$



$p = p_0/5$

High collision probability with each other
Low collision probability with boundary

Low collision probability with each other
High collision probability with boundary

Diffusive Transport

Ballistic Transport

Equilibrium

Non-Equilibrium

Low Pressure Simulation

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- **Applicability of N-S equation**
  - *Kn* = Mean Free Path / Characteristic length = l/L

$Kn < 0.01$: Continuum

NS equation with conventional no-slip condition

$0.01 < Kn < 0.1$: Slip Flow Regime

NS with slip-velocity BC

CFD-ACE+ 적용 가능

$0.1 < Kn < 3$: Transitional Regime

Continuum assumption breaks down

Discontinuum 영역

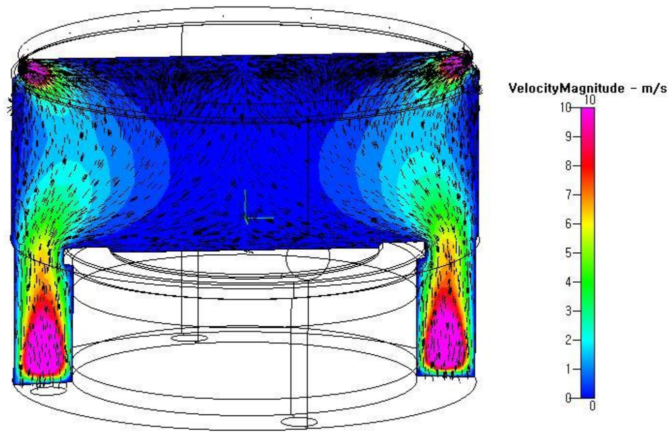
$3 < Kn$: Continuum assumption approach breaks down completely

Free Molecular Regime

※ CFD-ACE+의 진공 해석 가능 압력은 1mTorr 이상 영역에서 적용가능

Low Pressure Simulation

- Example(Low pressure reactor)



➤ Conditions
- Gas = Argon
- Pressure = 45 mTorr

➤ Boundary condition
- Wall = "No slip condition " & "Isothermal = 300 K"
- Inlet= "Fix Mass.(Normal) : Argon 200 SCCM"
- Outlet = "Fixed Pressure"

Gas	σ_c(m)
Air	3.66×10^{-10}
Ar	3.58×10^{-10}
CO_2	4.53×10^{-10}
H_2	2.71×10^{-10}
He	2.15×10^{-10}
Kr	4.08×10^{-10}
N_2	3.70×10^{-10}
NH_3	4.32×10^{-10}
Ne	2.54×10^{-10}
O_2	3.55×10^{-10}
Xe	4.78×10^{-10}

From CRC handbook

Mean free path : $\lambda = \dfrac{RT}{\sqrt{2}\pi\sigma^2 P N_{av}} = \dfrac{kT}{\sqrt{2}\pi\sigma^2 P}$

σ: collision diameter of molecule

N_{av}: avogardro's number

P : local pressure

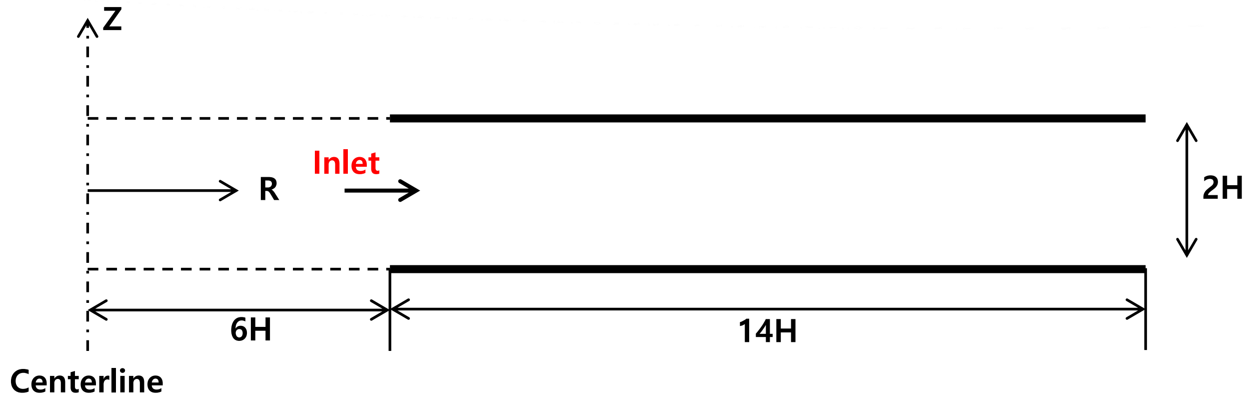
k : Boltzmann constant $(1.380622 \pm 0.00043) \times 10^{-23}$ J/K

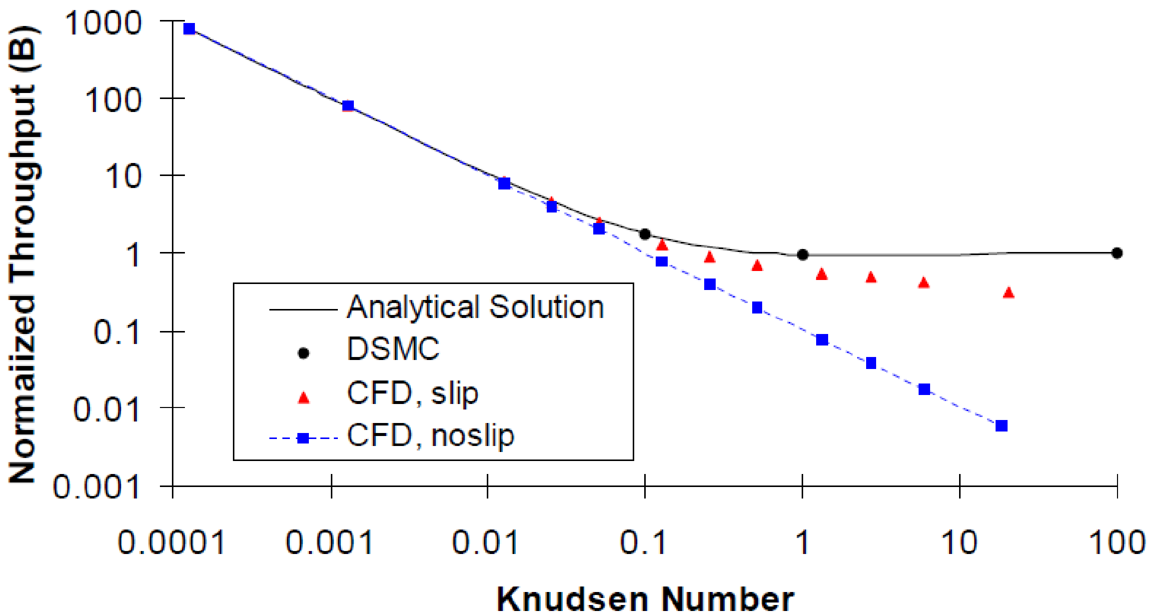
258mm 장치 직경, 진공상태에서(충돌직경 약 3.58×10^{-10}m)의

$$\lambda = \frac{1.38 \times 10^{-23} \times 298}{\sqrt{2} \times 3.14 \times (3.58 \times 10^{-10})^2 \times 6} = 1.152 \times 10^{-3} m$$

$$Kn = \frac{\lambda}{L} = \frac{1.152 \times 10^{-3} m}{0.258 m} = 4.465 \times 10^{-3}$$ → Continuum regime

- Validation Study (Performed by Novellus)

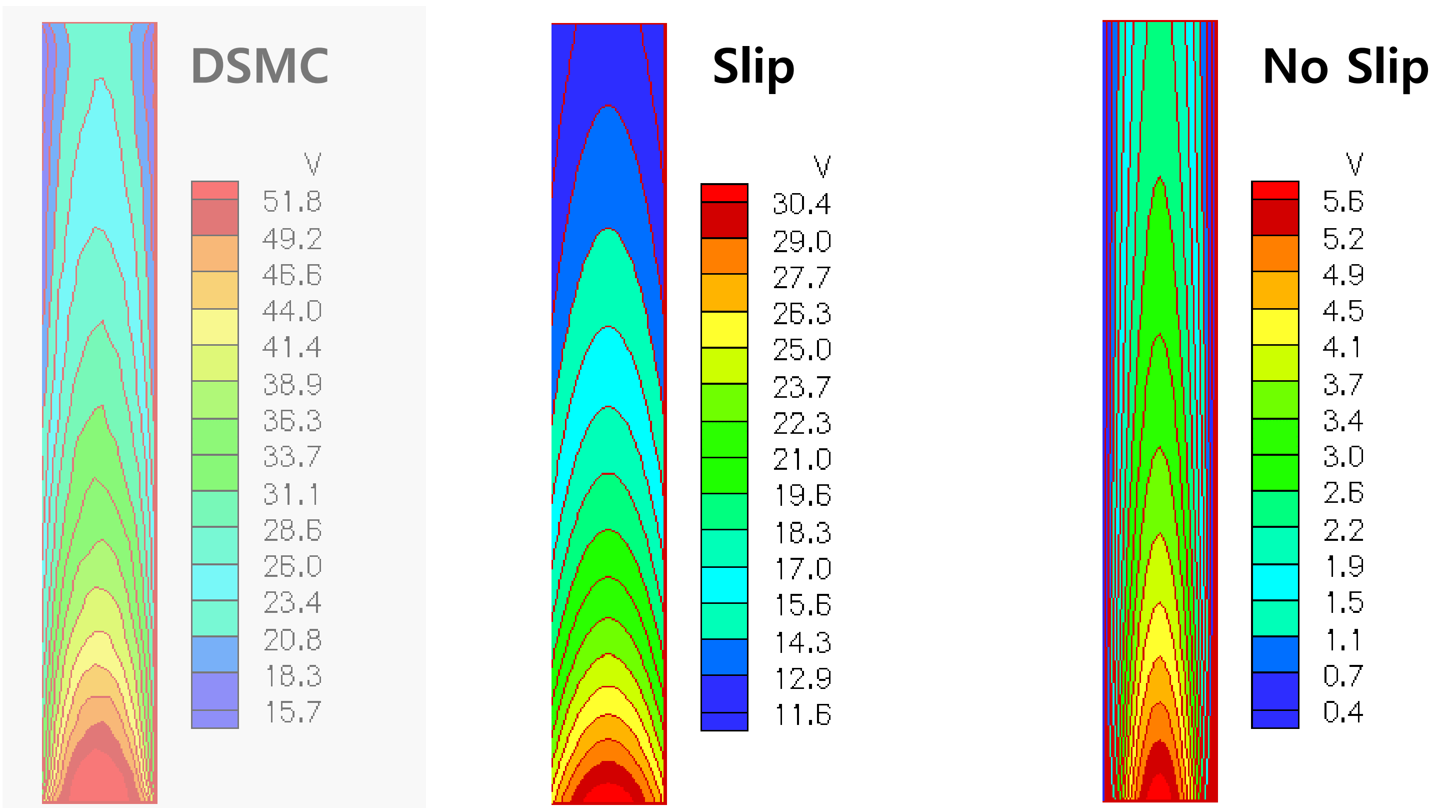




Low Pressure Simulation

- **Validation Study (Performed by Novellus)**

Velocity contours for Kn = 1.0



현재 CFD-ACE+는 Slip 영역까지 해석 가능

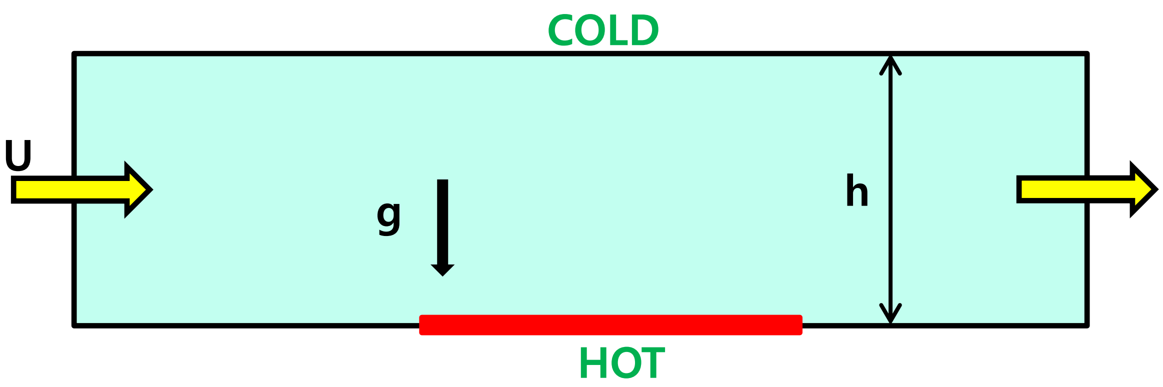
Convection : Forced vs Natural

- **Richardson Number**
  - For a given reactor geometry, the Richardson number indicates if natural convection is going to be influential or not !!!
  - Non-dimensional Numbers

$$\mathrm{Ri} = \frac{\text{Buoyancy Force}}{\text{Inertia Force}} = \frac{Gr}{\mathrm{Re}^2}$$

$$\mathrm{Re} = \frac{\text{Inertia Force}}{\text{Viscous Force}} = \frac{\rho U D_h}{\mu}$$

$$\mathrm{Gr} = \frac{\text{Buoyancy Force}}{\text{Viscous Force}} = \frac{g \beta \Delta T h^3 \rho^2}{\mu^2}$$



h = 10 cm, U = 0.1 m/s, g = 9.8 m/s^2, m = 10^{-5}kg/m/s, Mol. Wt. = 29 kg/kmol

- **Baseline Case**

$$\mathrm{Re} = \frac{\rho U D_h}{\mu}; \quad \rho = \frac{pM}{RT}; \quad D_h = 2h$$

$$p = 1.1325E+5, \ M = 29, \ R = 8314, \ T = 300, \ \mu = 10^{-5}, \ U = 0.1, \ h = 0.1$$

$$D_h = 2h = 0.2, \ \rho = 1.178$$

$$\mathrm{Re} = 1178$$

$$\mathrm{Gr} = \frac{g\beta\Delta T h^3 \rho^2}{\mu^2}; \ \beta \approx \frac{1}{(T_H + T_C)/2}; \ \Delta T = T_H - T_C$$

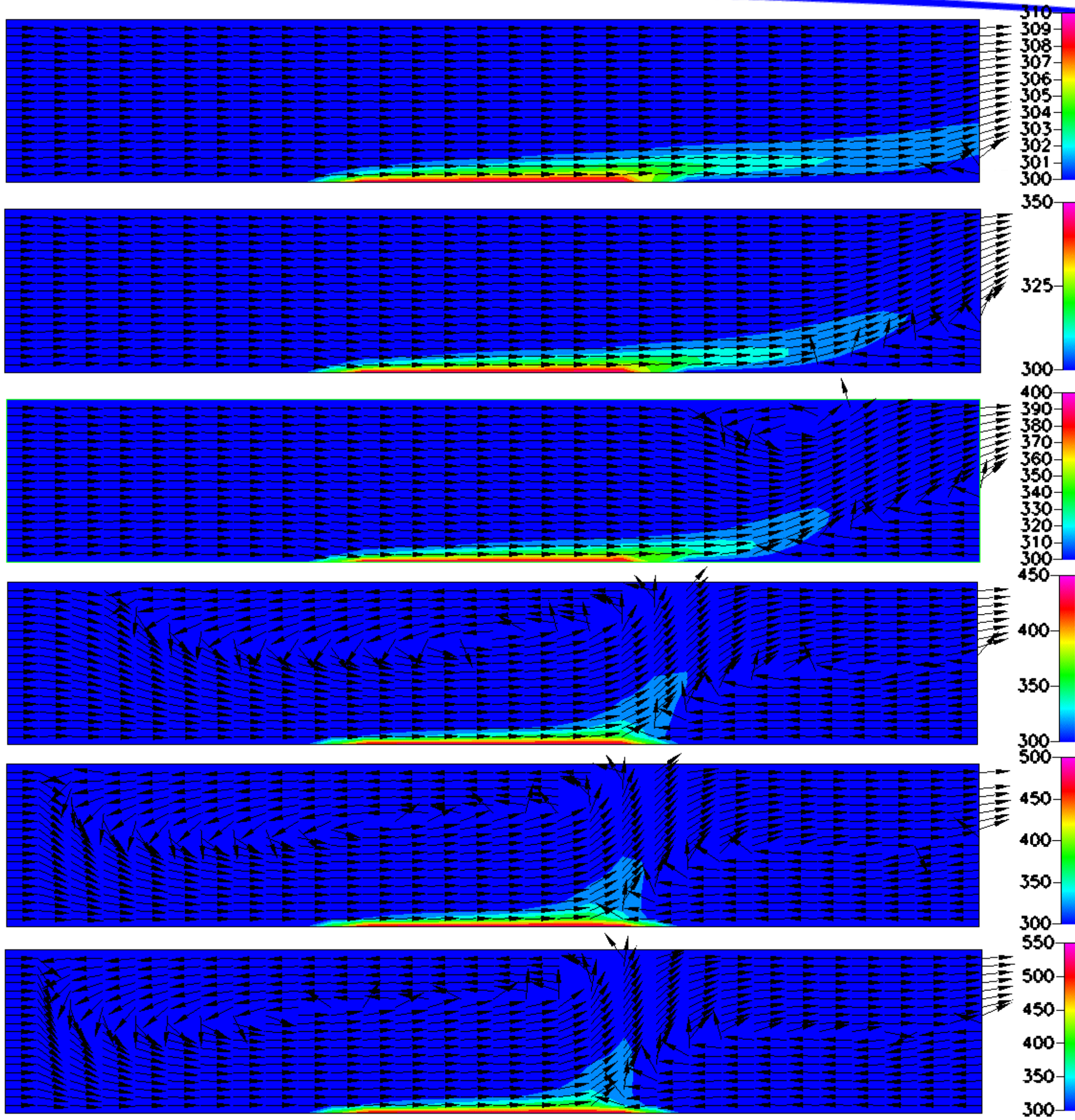
$$T_H = 310, \ T_C = 300$$

$$\Rightarrow \Delta T = 10, \ Gr = 446337$$

$$Ri = \frac{Gr}{\mathrm{Re}^2} = 3.2$$

T_H	$\triangle T$	$Ri=Gr/Re^2$
310	10	3.2
350	50	15.1
400	100	28
450	150	39.2
500	200	49.1
550	250	57.7

Convection : Forced vs Natural



Ri = 3

Ri = 15

Ri = 28

Ri = 39

Ri = 49

Ri = 57

Conclusion: If Ri > 10, Natural Convection will be important

Convection : Forced vs Natural

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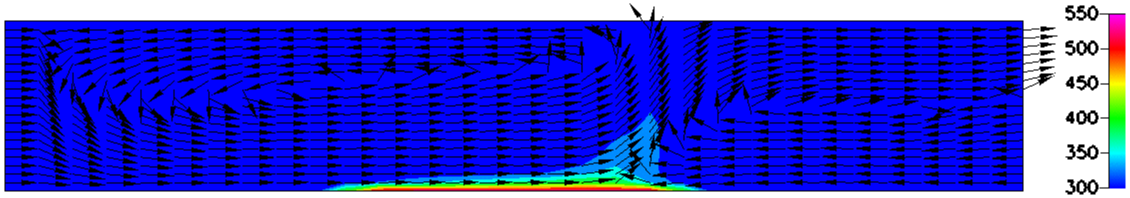
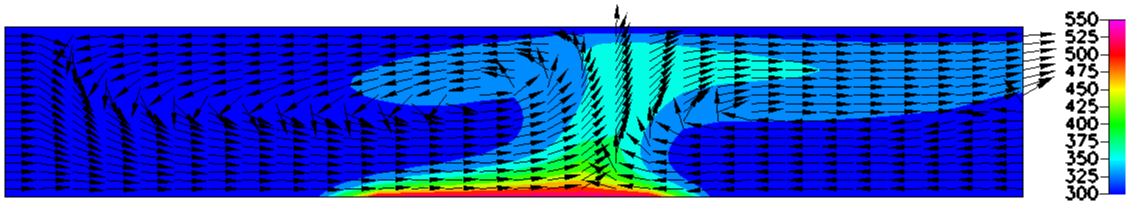
- Effect of Pressure

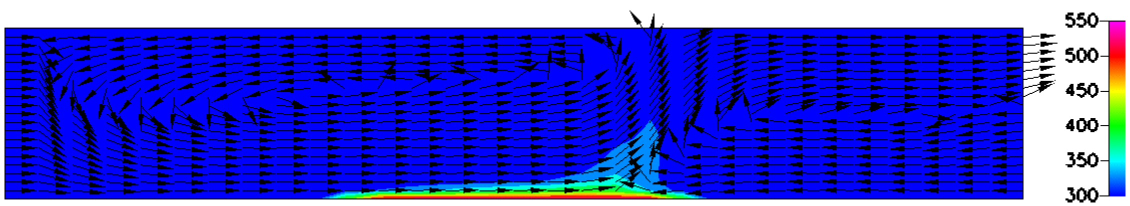


1bar
Ri = 57



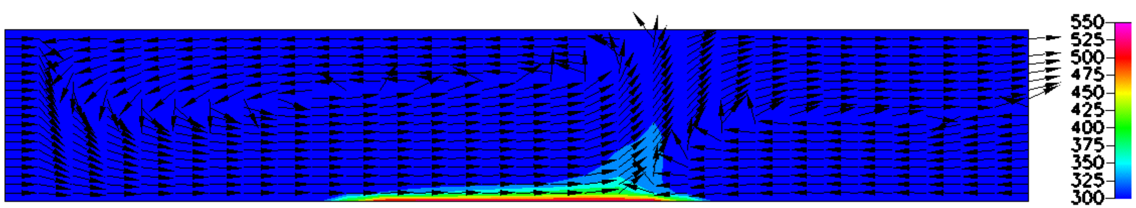
0.1bar
Ri = 57

- Significance of non-dimensional parameters



p = 1
m = 10^{-5}
k = 0.0236

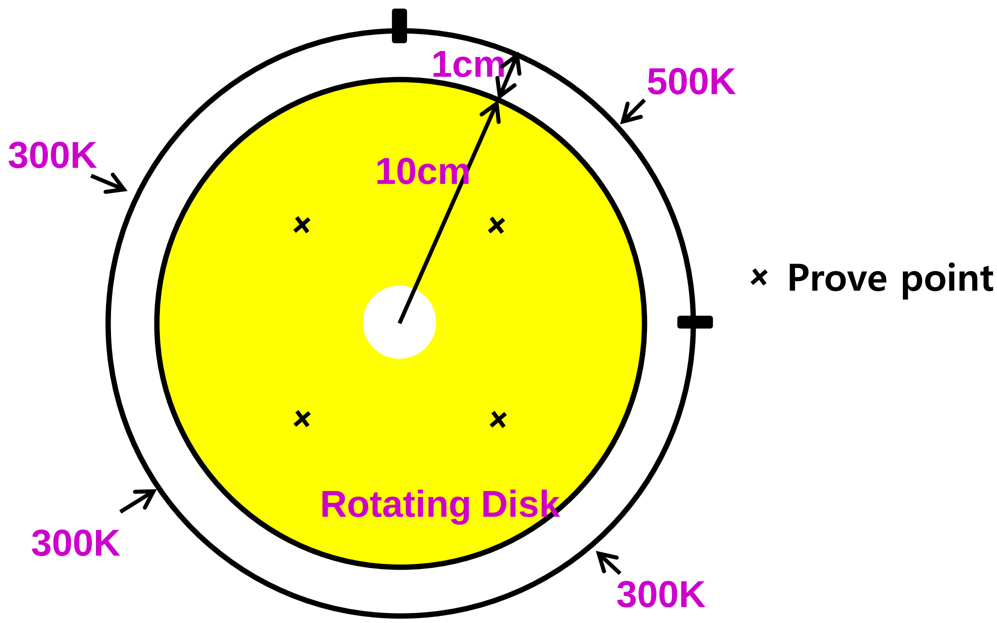
Ri = 57   Pr = 0.5   Re = 1178



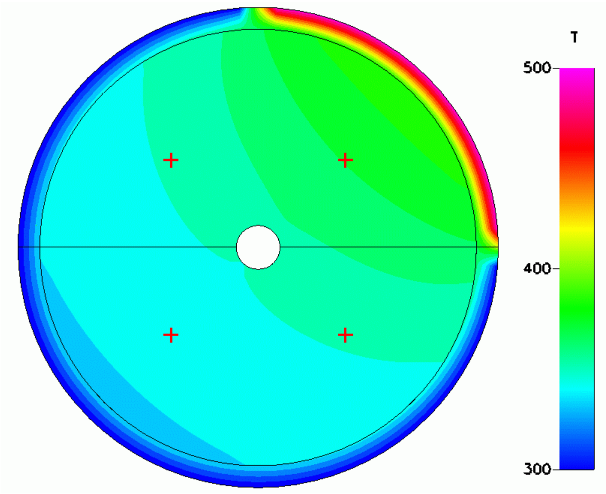
p = 0.1
m = 10^{-6}
k = 0.00236

Effect of Rotating

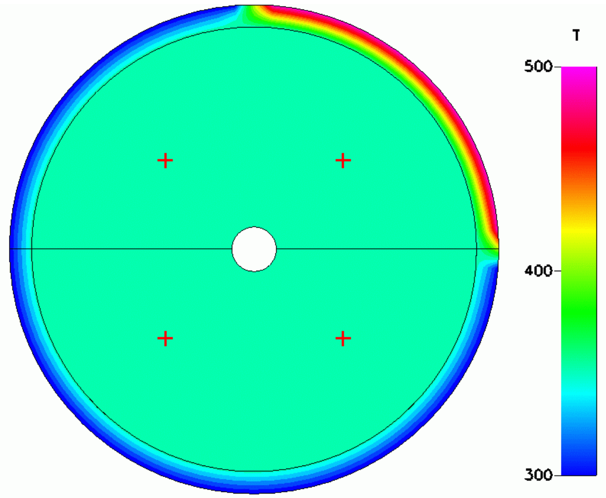
- **Validation Study : rotating solids**



No Rotation



Rotation, 1RPM

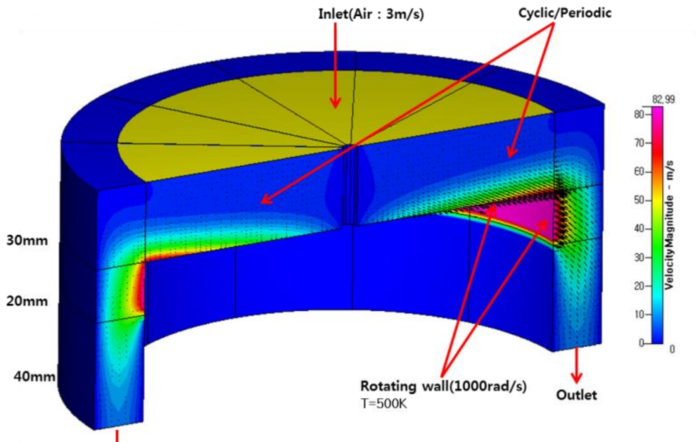


Effect of Rotating

- CFD-ACE+에서 적용 가능한 회전체
  - Rotating wall : wall boundary에 rotating 경계조건 적용
  - Solid moving : Conjugate해석과 rotating 해석을 동시에 진행 할 경우 적용
  - MRF : 회전체 정상상태 해석 → Fan, blade 해석에 적합
  - Arbitrary interface : 회전체 비정상상태 해석

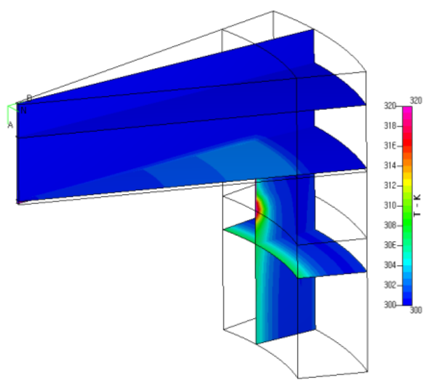
Effect of Rotating

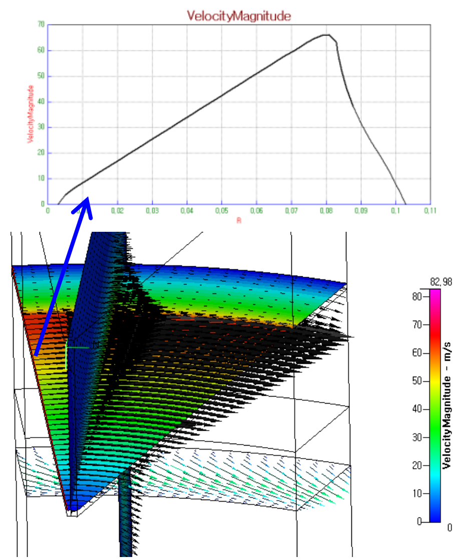
Rotating wall



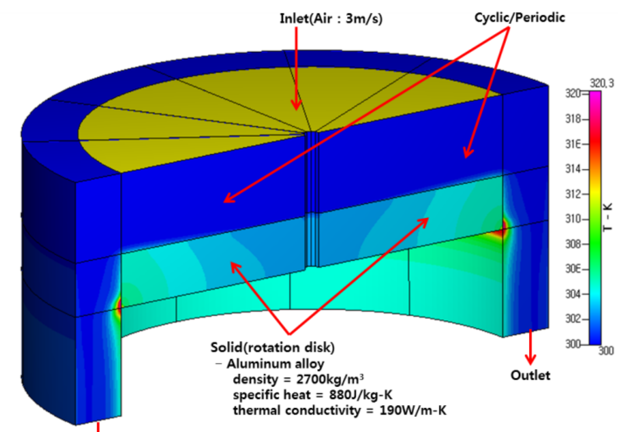
Ro=103mm
Ri=83mm

작동유체 : water
- density : 997kg/m³
- viscosity(kinematic) : 0.01589m²/s ← 실제 점성X1000
- specific heat : 4179J/kg-K
- thermal conductivity : 0.613W/m-K





Moving solid



작동유체 : water
- density : 997kg/m³
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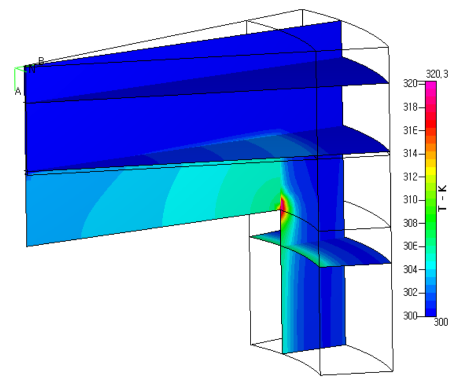
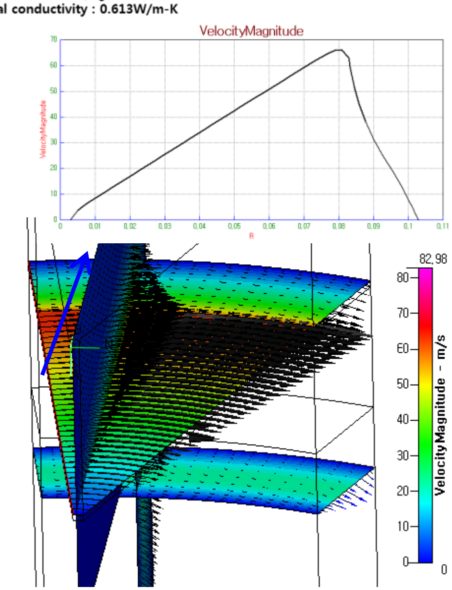
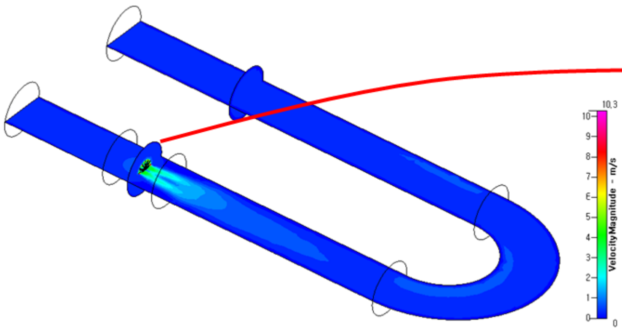
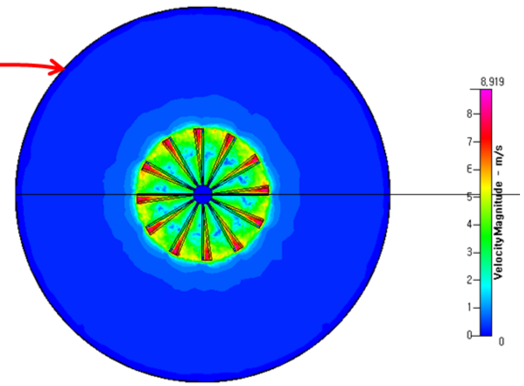


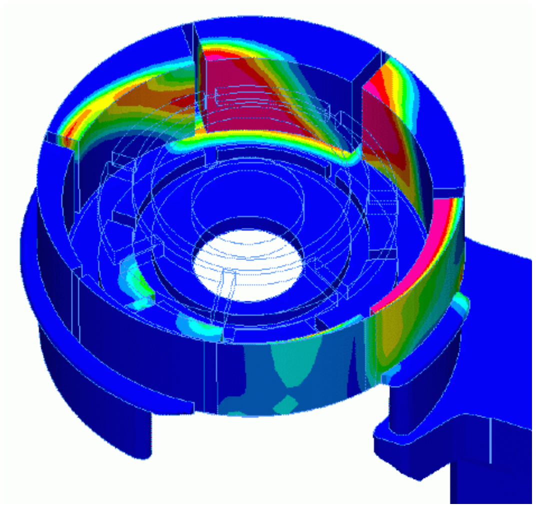


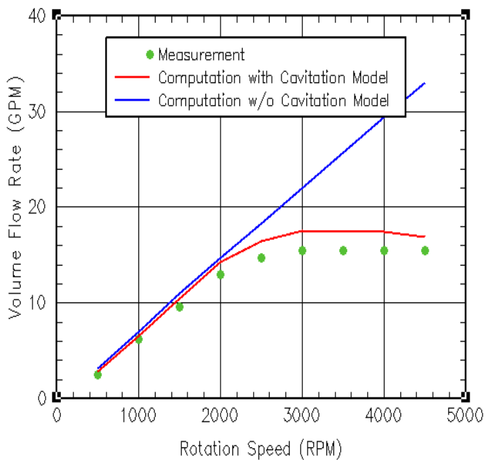
- MRF(Multiple Reference Frame) : 정상상태 해석





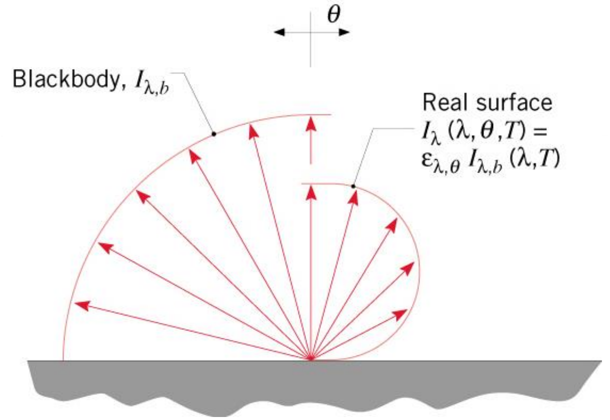
- Arbitrary interface : 비정상상태 해석



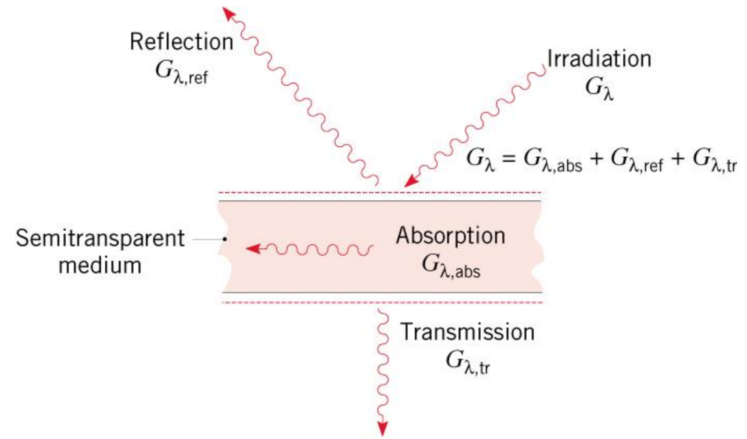


Radiation Effect

- Surface Emissivity
  - 물질의 고유 특성 Hand book 참조



- Response to Surface Irradiation: Absorption, Reflection and Transmission



  - Reflection from the medium $\left(G_{\lambda,ref}\right)$.
  - Absorption within the medium $\left(G_{\lambda,abs}\right)$.
  - Transmission through the medium $\left(G_{\lambda,tr}\right)$.

Radiation balance ⟶

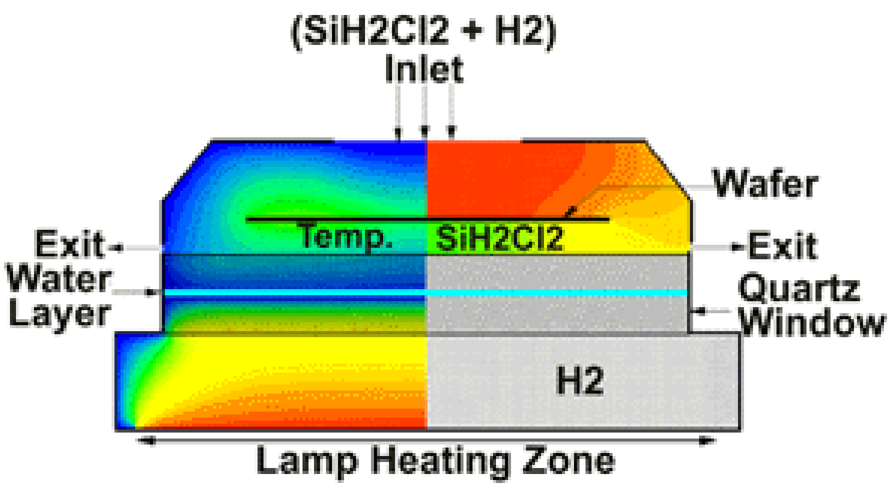
$$G_\lambda = G_{\lambda,ref} + G_{\lambda,abs} + G_{\lambda,tr}$$

- In contrast to the foregoing volumetric effects, the response of an opaque material to irradiation is governed by surface phenomena and $G_{\lambda,tr} = 0$.

$$G_\lambda = G_{\lambda,ref} + G_{\lambda,tr}$$

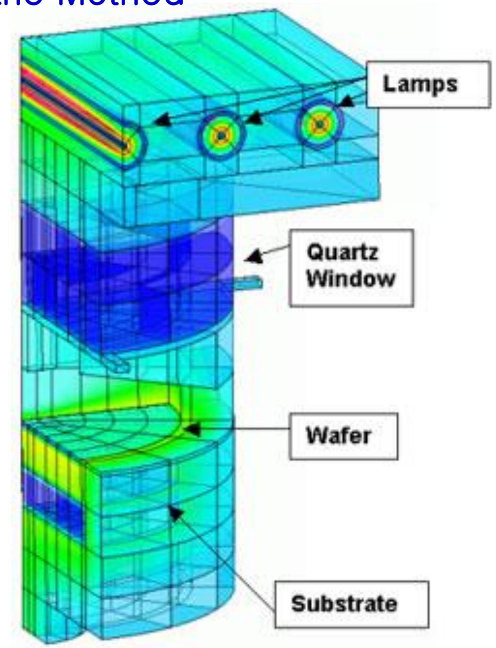
Radiation Effect

Discrete Ordinate Method (DOM)



CFD-ACE+ Simulation of SEMATECH Benchmark Case with Radiative heating of a wafer via a quartz window with water cooling

Monte Carlo Method



CFD-ACE+ : Simulation of an RTP Reactor using the Monte Carlo Radiation model

Radiation model은 DOM, Monte Carlo Moethod, STS(surface to surface), P1 모델 등이 있으며 일반적으로 DOM model을 주로 사용함
물성 : 기본물성인 density, specific heat, thermal conductivity 이외에 Absorption coefficient, Emissivity등의 물성이 요구 됨.

Radiation Effect

- **Effect of Specular Reflection (vs Diffuse)**

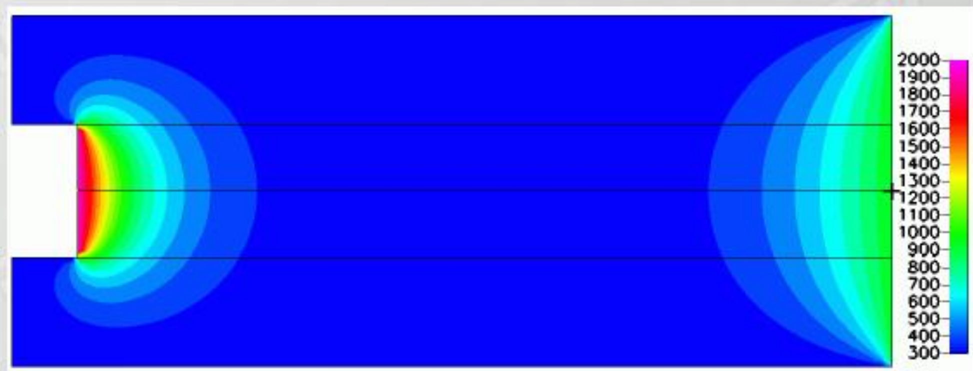
No Radiation: 300.03 K

DOM, Diffuse: 993.5 K

MC, Diffuse: 1115.5 K

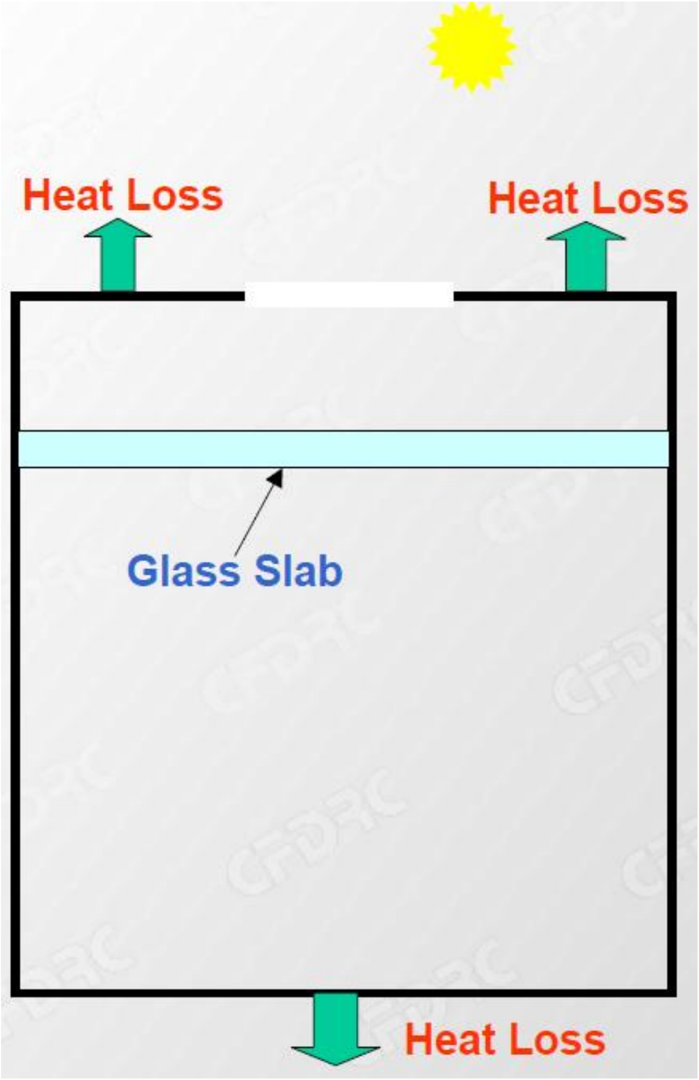
MC, partial specular (0.5): 1127.2 K

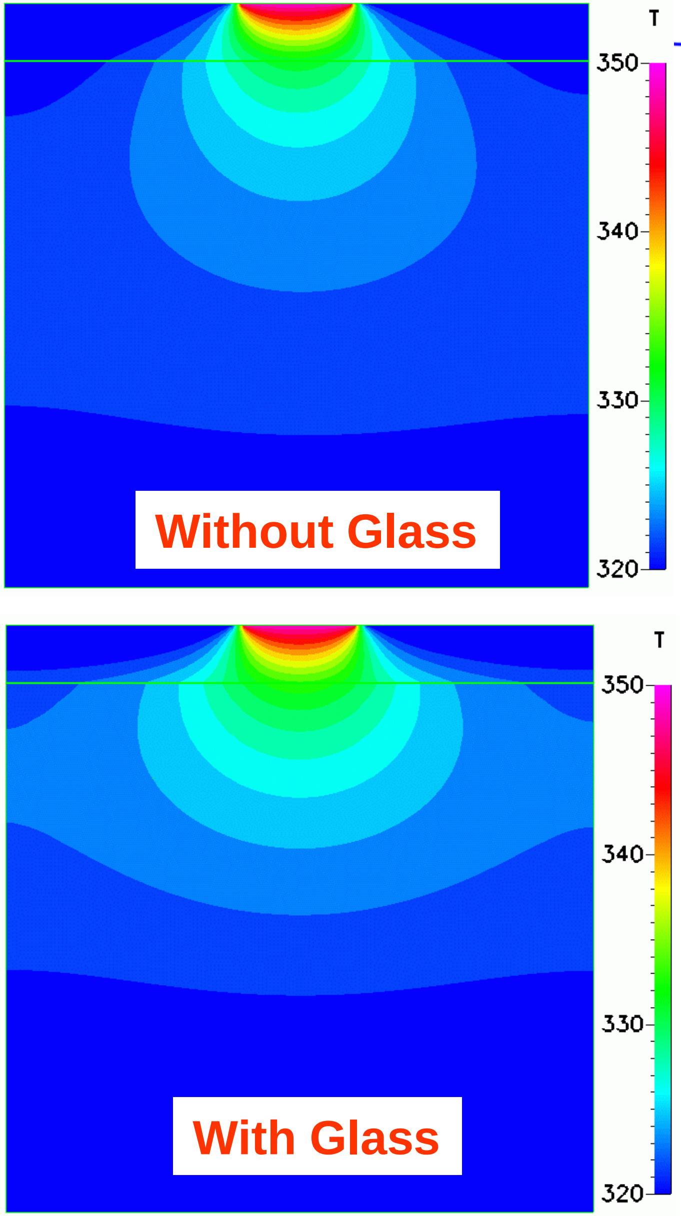
MC, specular: 1259.9 K



Radiation Effect

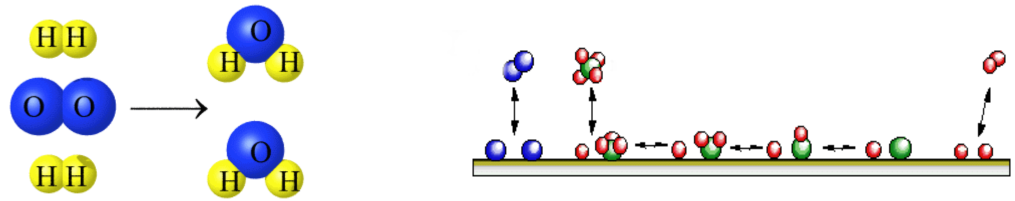
- **Non-Gray Effects**



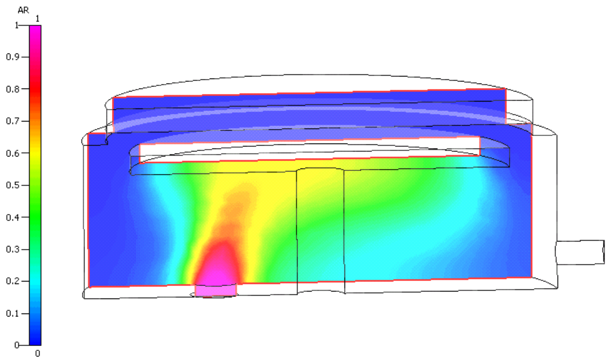


Chemistry Mixing & reaction

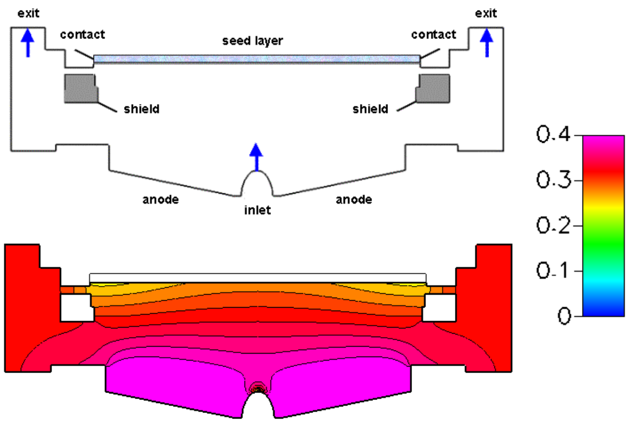
- **단순 혼합 or 화학 반응**
  - Mixing
  - Gas phase reaction(homogeneous)
  - Surface reaction(heterogeneous)



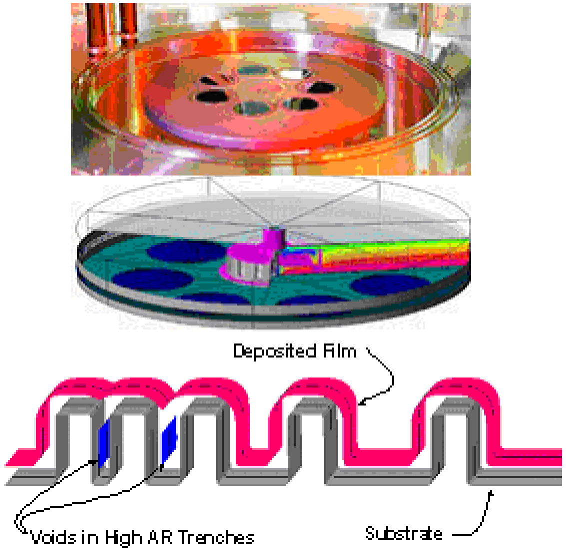
Homogeneous **Heterogeneous**



CVD chamber – chemistry mixing



Electroplating



반도체 제조 공정 해석

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- **Species Continuity (or Transport) Equation**

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot \rho U Y_i = \nabla \Big| \cdot J_i + \dot{\omega}_i$$

$\dot{\omega}_i$ is the rate of production of the i-th species due to chemical reaction in the bulk

J_i is the diffusion flux of the i-th species

$$\mathrm{J}_\mathrm{i} = J_i^C + J_i^T + J_i^P$$

$$J_i^C = \rho D_i \nabla Y_i$$ Fick's Law

$$J_i^T = \rho D_i^T \frac{\nabla T}{T}$$ Soret diffustion

$$J_i^P = \rho D_i^P \frac{\nabla P}{P}$$ Pressure diffusion, usually neglected

Chemistry Mixing & reaction

- Species Diffusion Coefficient
  - The rate of diffusion of each specie depends on the background species
  - The overall diffusion coefficient of a specie in a given mixture is some combination of the diffusion rates of that specie in each specie of the mixture

- Diffusion Coefficient Calculations
  - Method 1 : Schmidt Number
  - Method 2 : Multi-Component Diffusion 사용

1Torr 초과

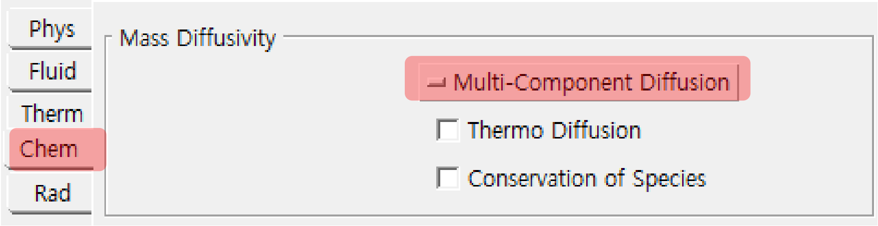
Schmidt Number 사용

$$Sc = \frac{\text{Momentum Diffusivity}}{\text{Mass Diffusivity}} = \frac{\nu}{D}$$

$$\Rightarrow D = \frac{\nu}{Sc}$$

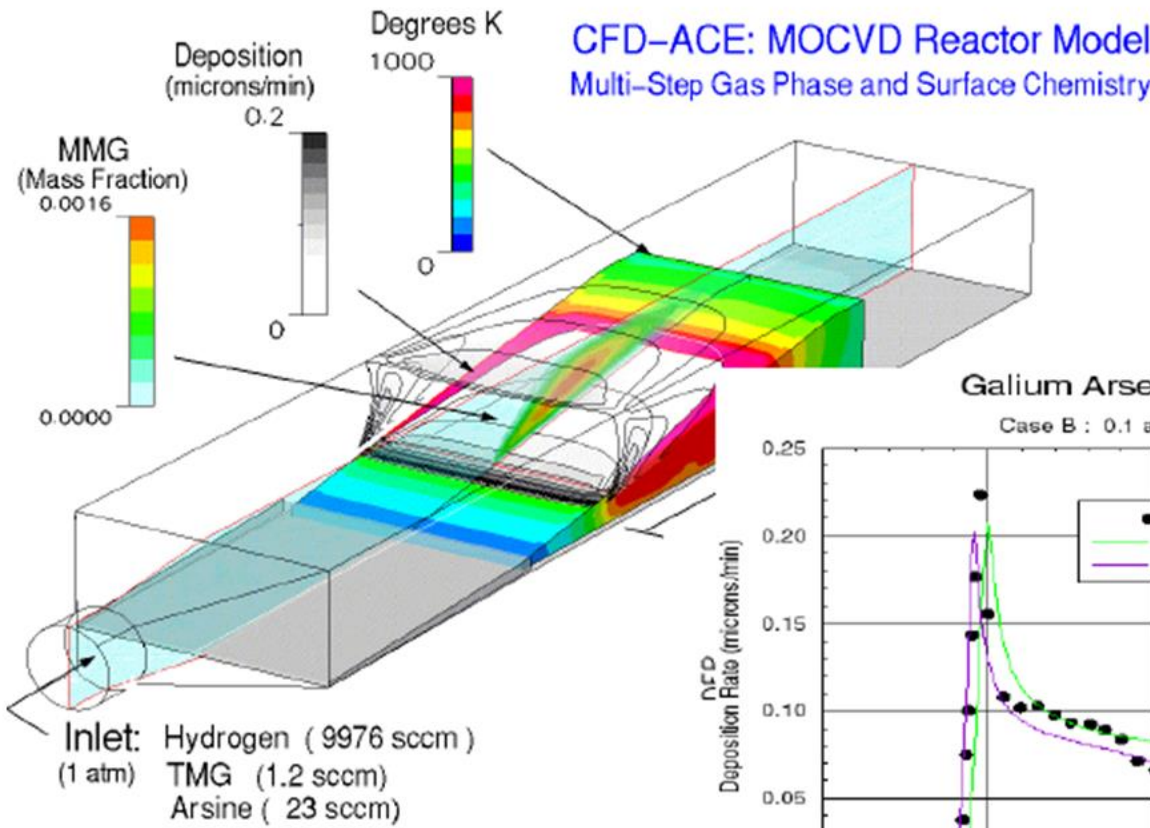
1Torr 이하

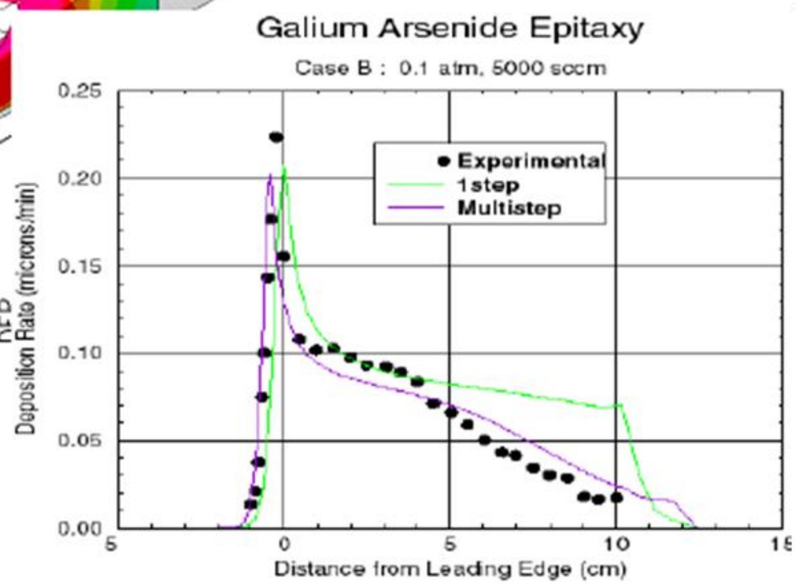
Multi-Component Diffusion 사용



Chemistry Mixing & reaction

- Applications(Gas & surface reaction)





Plasma

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- Plasma Applications

플라즈마

선택적 조절 능력

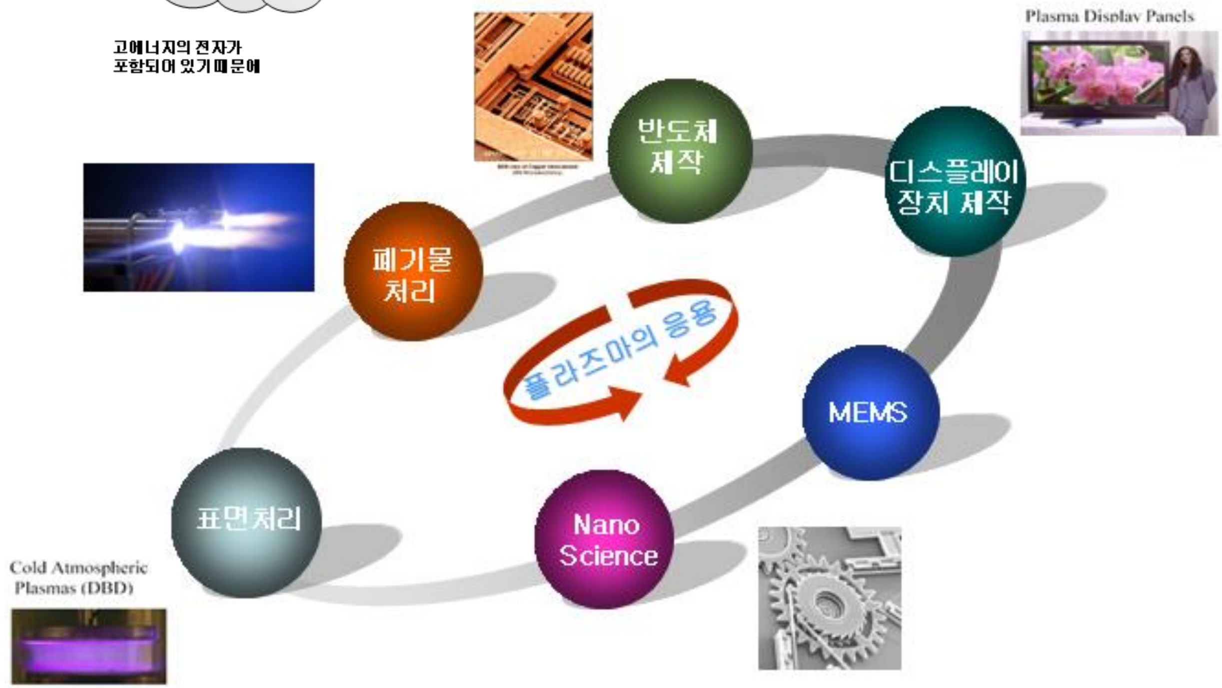
하전입자들을 전기장 이나 자기장으로 쉽게 제어할 수 있기 때문에

매우 높은 반응성

고에너지 입자들로 이루어져 있기 때문에

매우 높은 활성화 능력

고에너지의 전자가 포함되어 있기 때문에



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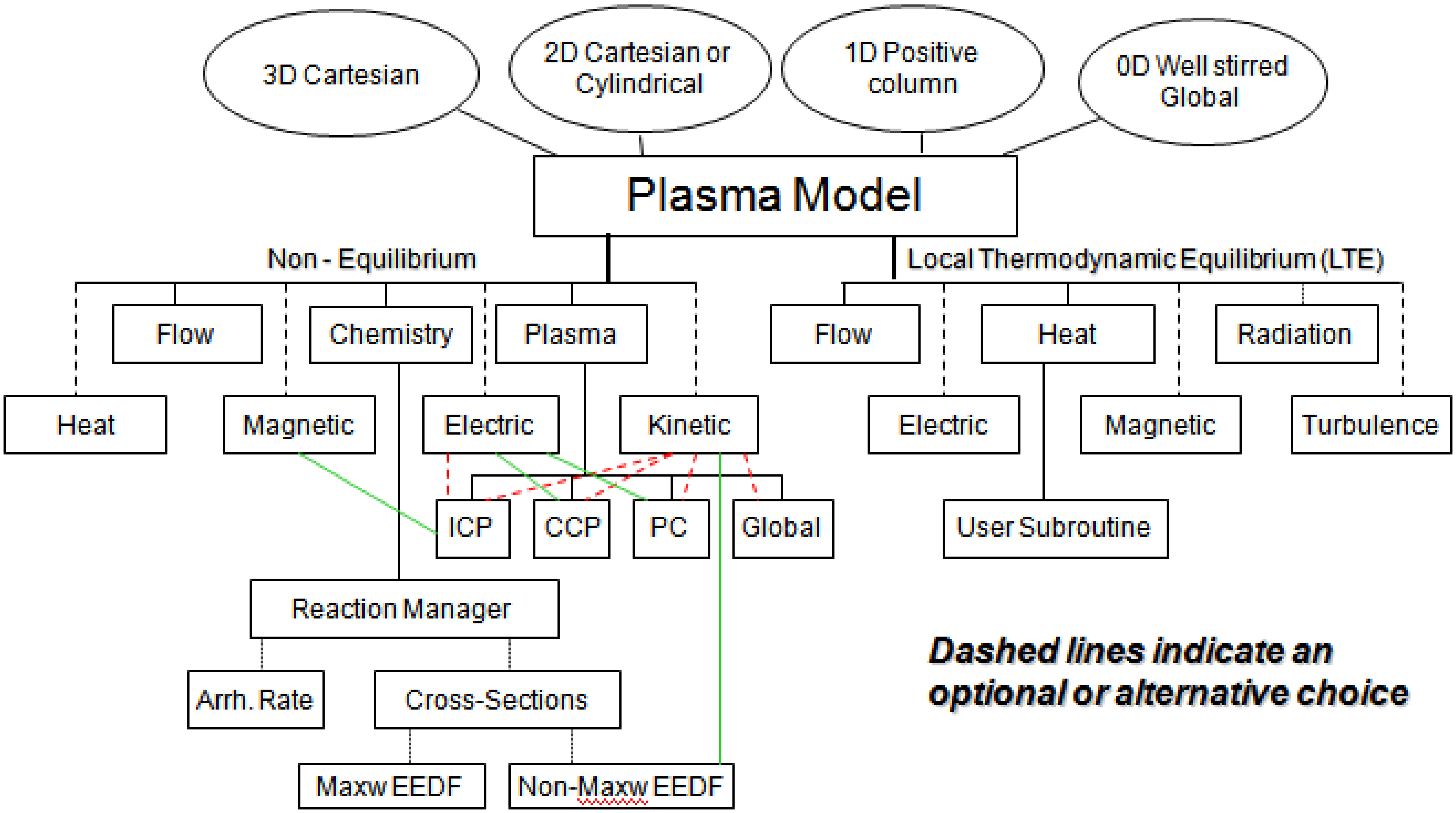
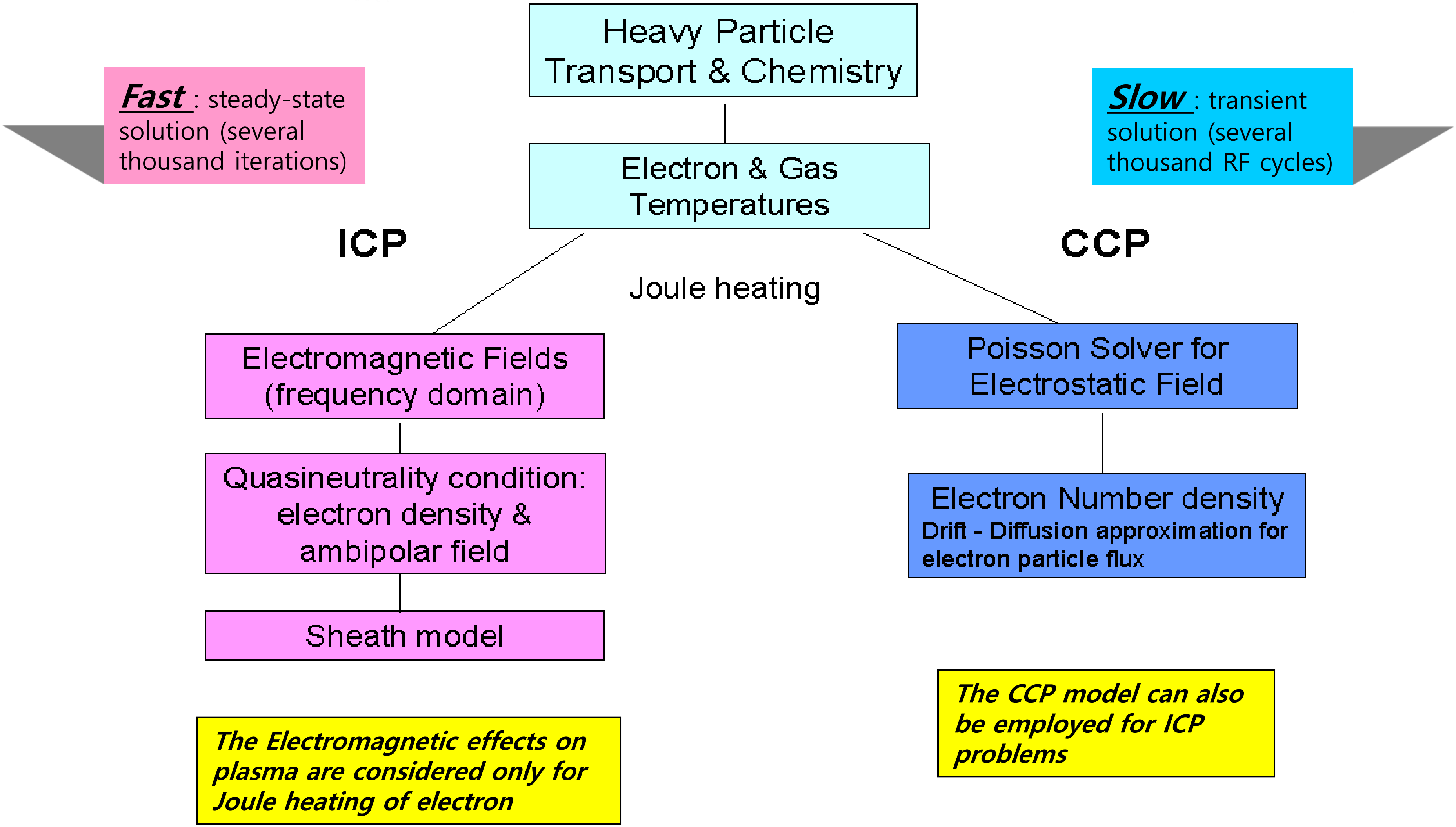
- Plasma Simulation Logic.



CFD-ACE+ Plasma Model



Plasma

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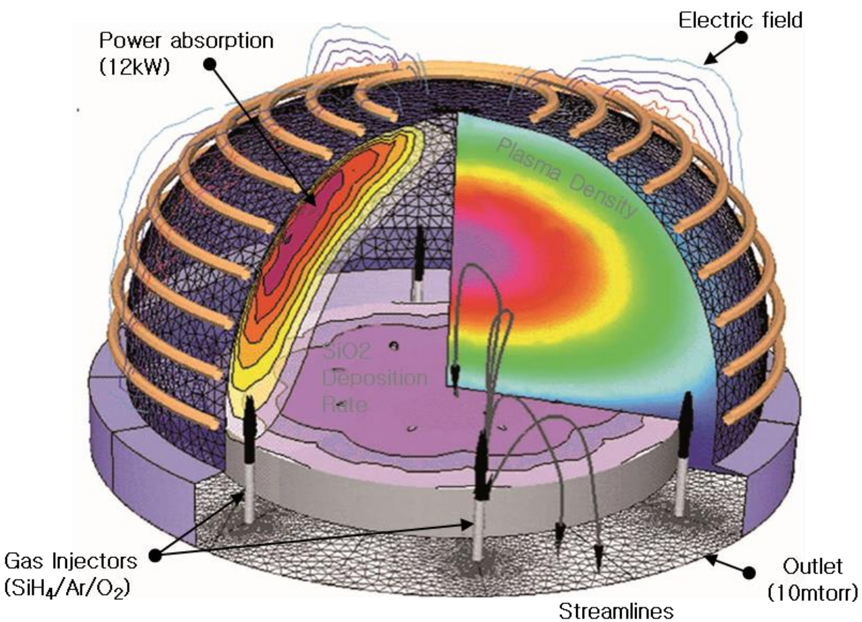
Inductively Coupled Plasma (ICP)

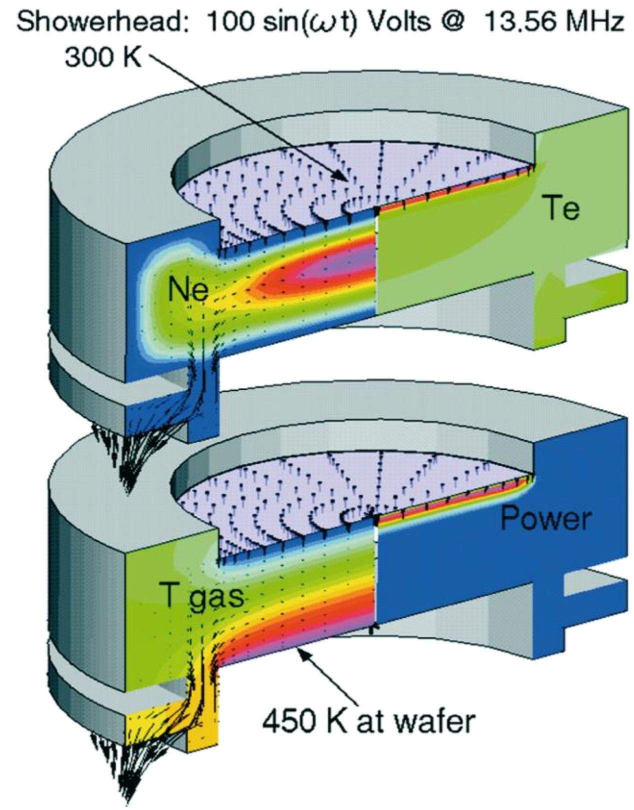
CFD-ACE+ - Simulation of SiO2 deposition in an Inductively Coupled Plasma (ICP) reactor



Inductively Coupled Plasma(ICP) Reactor

Capacitively Coupled Plasma (CCP)

CFD-ACE+ 3D - Simulation of Capacitively Coupled Plasma (CCP) for Oxygen at 400 millitorr



Capacitively Coupled Plasma(CCP) Reactor