アテナシス
（Athenasys Co., Ltd）の
ご紹介

会社紹介

https://athenasys.co.jp/

設立：2008年 10月 1日

事業内容：ライセンス販売・サポート，コンサルティング

取り扱っている製品とパートナー会社

Bosprom：プラズマシミュレーションで必要となる
輸送係数・反応レートの計算ツール（自社製品）

CFD-ACE+：マルチフィジックスソフトウェア

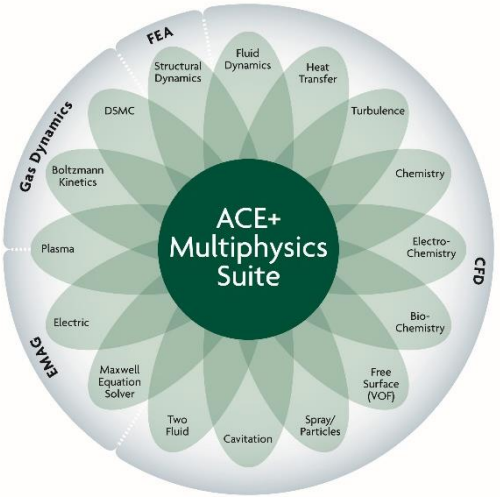
CFD-TOPO：形状シミュレーター

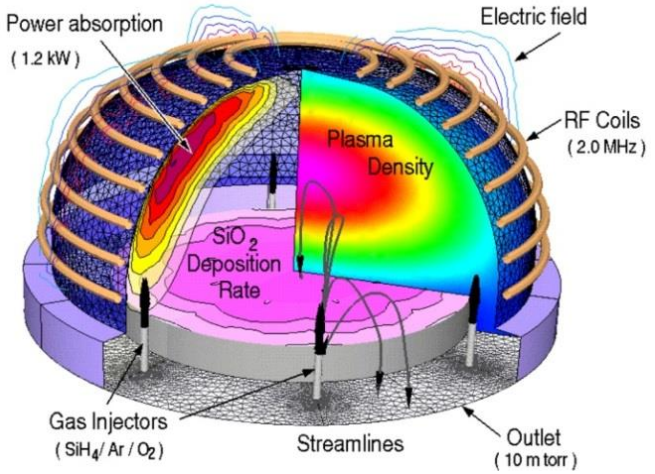
＊ 日本ESI（販売元）のエージェント

QEC：分子に対する電子衝突断面積の計算ツール

QDB：プラズマシミュレーションで必要となる反応データベース

＊ Quantemol（開発元）の国内代理店





重点分野：

熱放射を含む熱流体解析全般

半導体製造装置のプロセスシミュレーション

主要なお客様：

半導体製造装置メーカー，デバイスメーカー

自動車メーカー

担当者はアネルバ（現キヤノンアネルバ）で半導体製造装置の研究開発に長年従事

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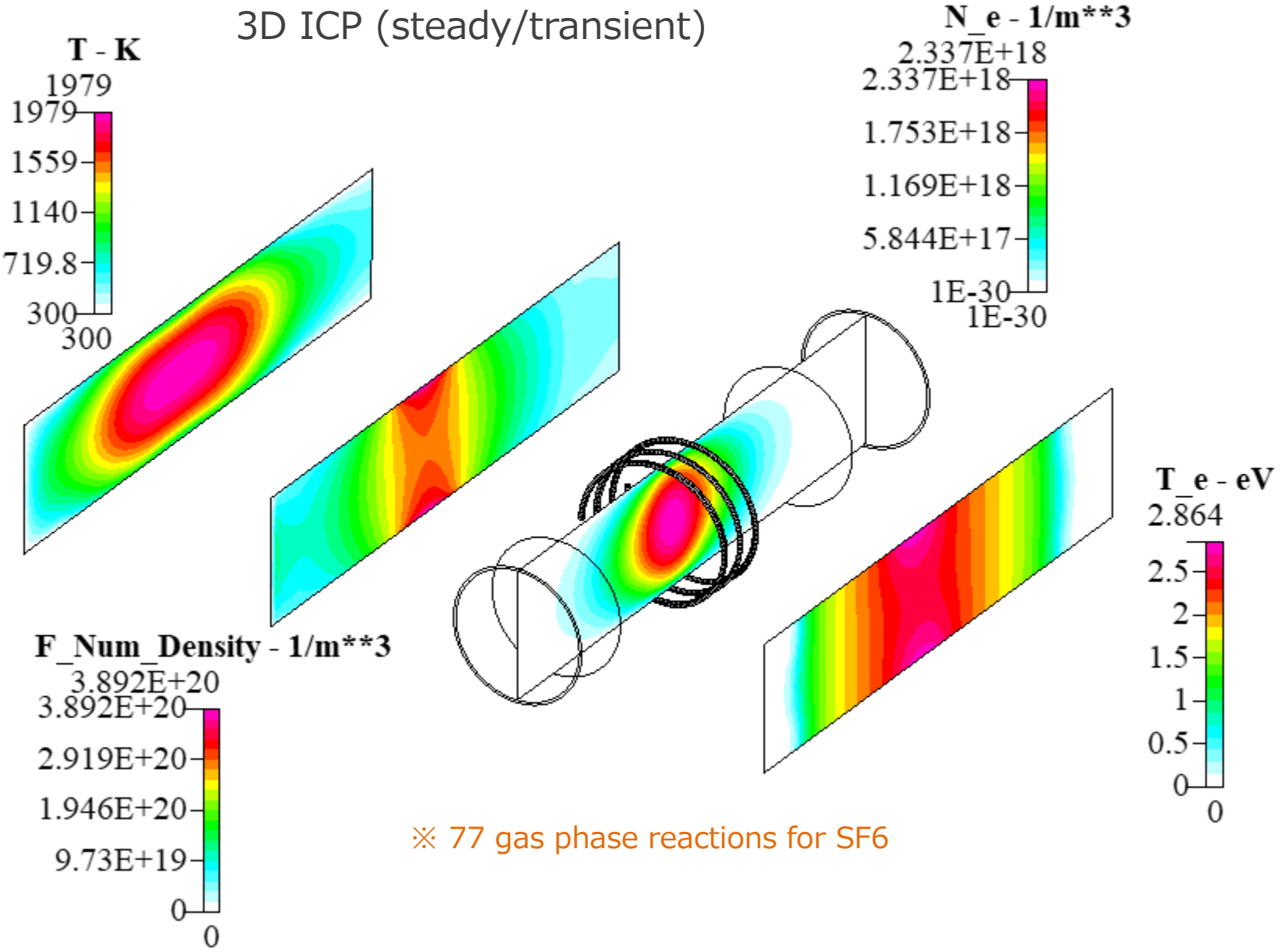
マルチフィジックス ソフトウェア

CFD-ACE+ Suite

Application examples

✓ *Low pressure*

3D ICP (steady/transient)



※ 77 gas phase reactions for SF6

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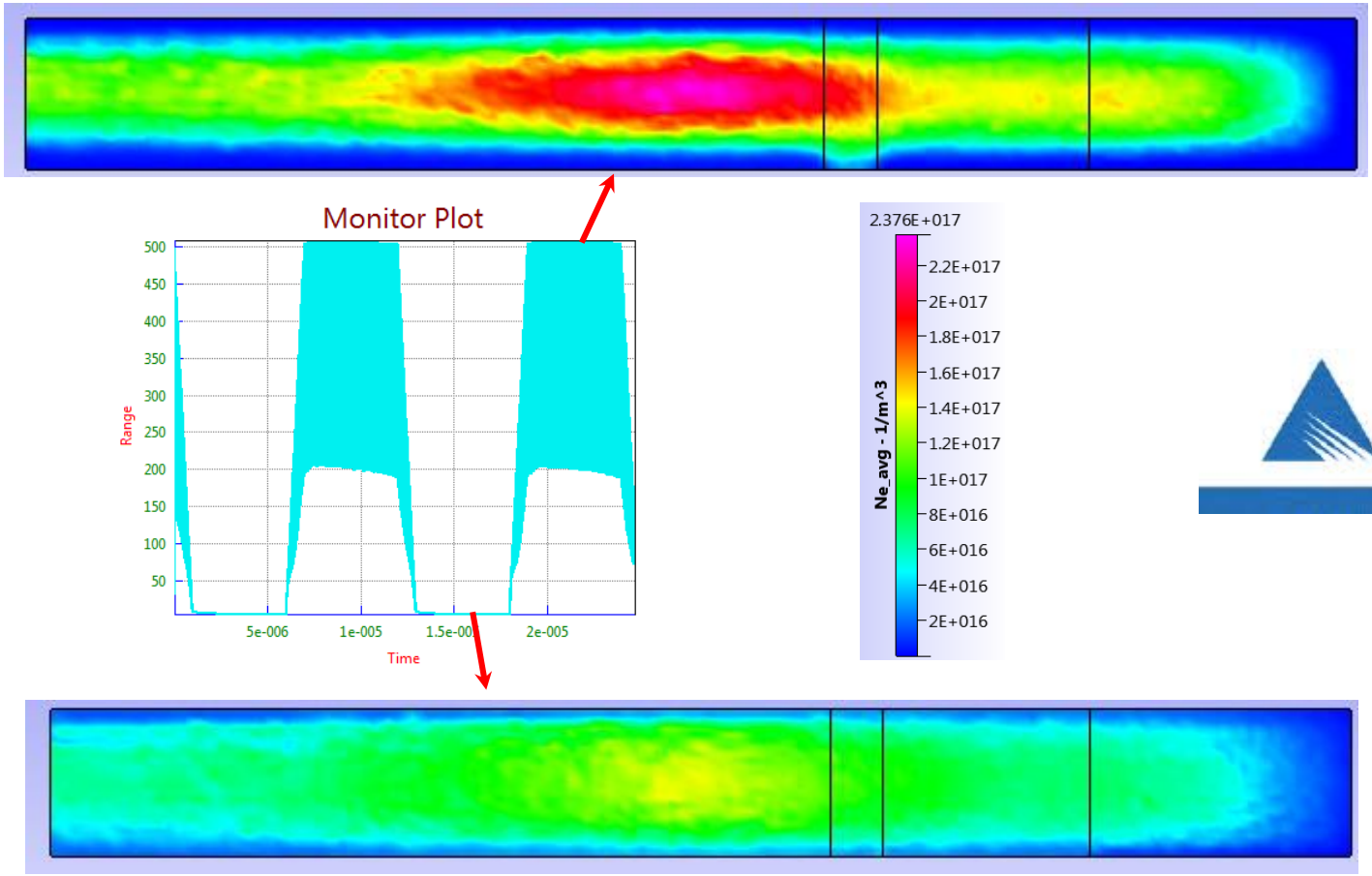
Application examples (cont.)

✓ ***Pulsed CCP***



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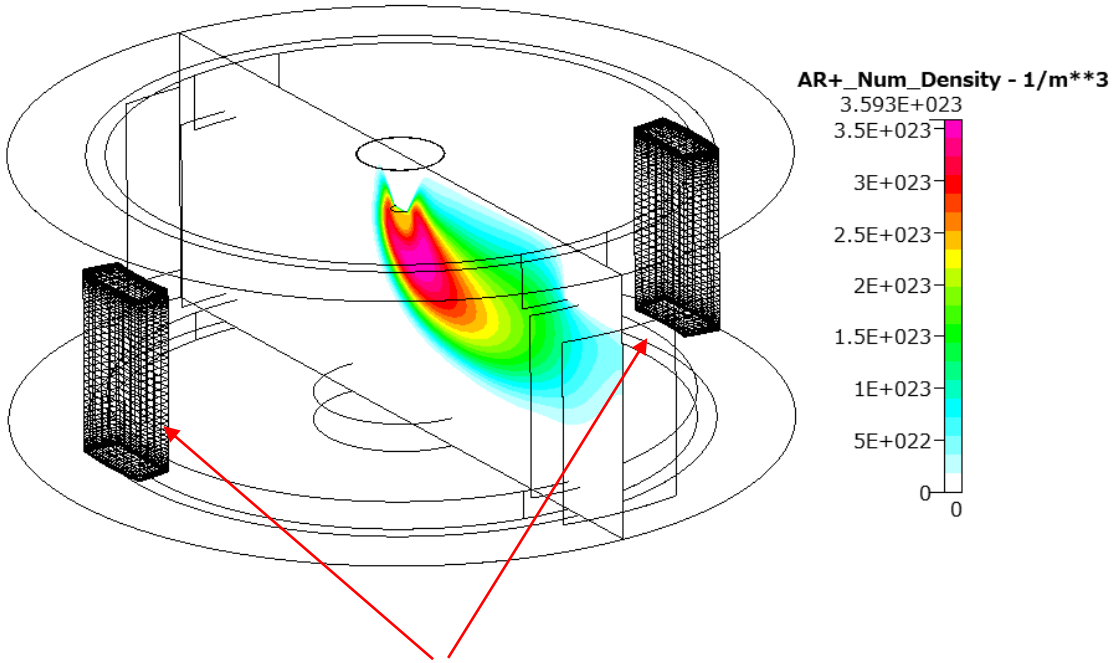
Application examples (cont.)

DC Arc (with Lorentz force)



✓ *Atmospheric pressure (and higher pressure)*

Dielectric Barrier Discharge

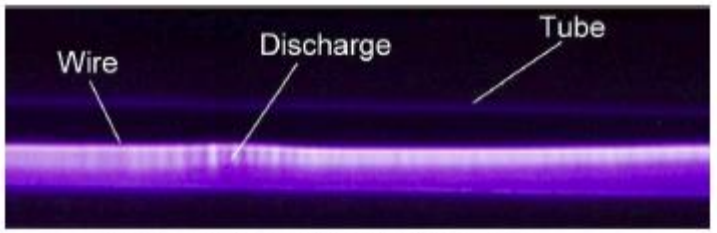


Fig. 2 Side view of the DBD in the tube

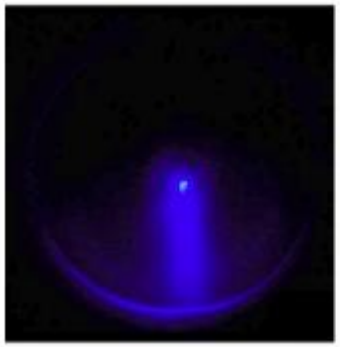


Fig.3 Spectrum photograph through band-pass filter of 450 nm (half-width: 10 nm)

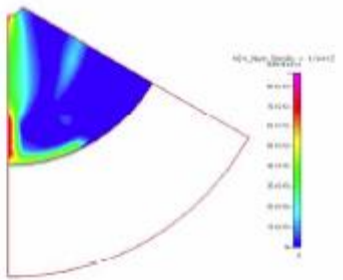


Fig. 4 Distribution of number density of the N_2^+.

Takehiko Sato, Osamu Furuya, Kei Ikeda and Tatsuyuki Nakatani
1st International Conference on Plasma Medicine (ICPM-1), Corpus Christi, Texas, (2007) pp. 48-50

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Application examples (cont.)

✓ *3-D (with filament model)*

真空, 50 (2007) p. 424

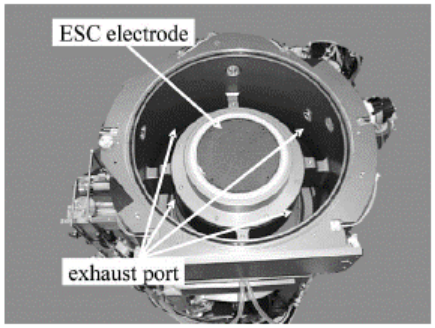


Fig. 4 Top view of the reactor

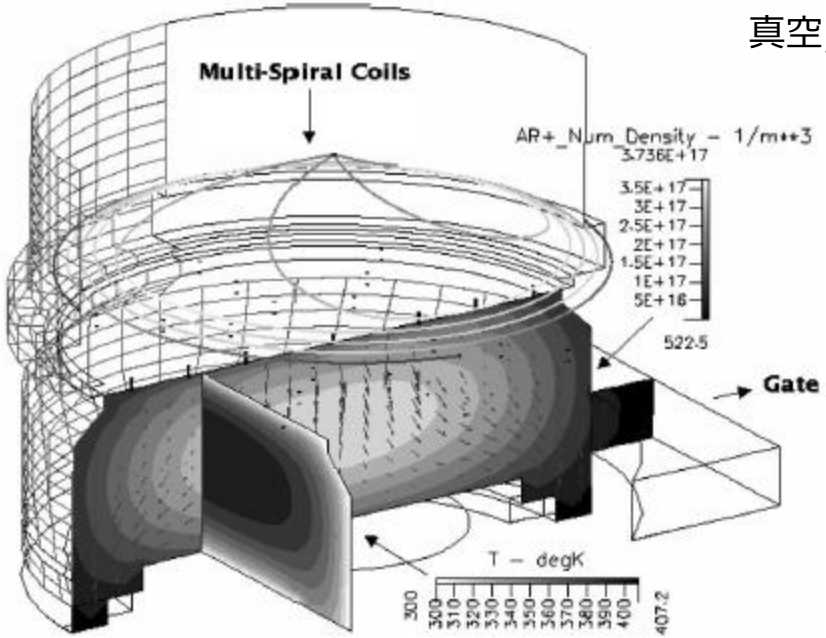
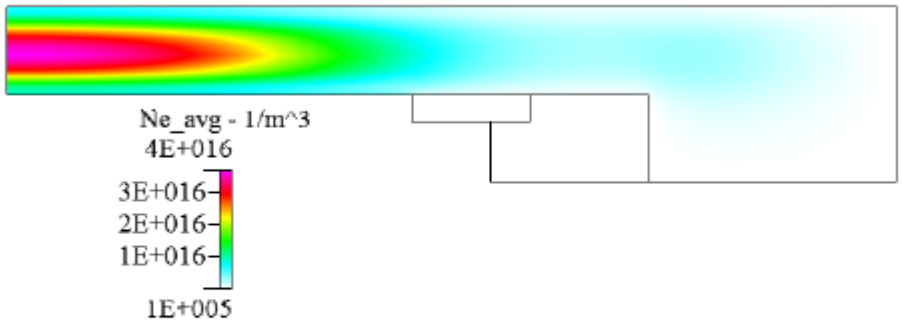


Fig. 6 Ar^+ density and gas temperature distribution (computational grid on the reactor wall and RF antenna in this model are also shown)

✓ *Magnetized Plasma*

JIEED Japan Vol.57 No.3 (2014) p.27
(放電学会シンポジウム)



(b) 150 G

Fig. 3. Cycle-averaged electron number density.

Application examples for plasma (cont.)

Self-consistent kinetic model coupling the Boltzmann and Poisson equations

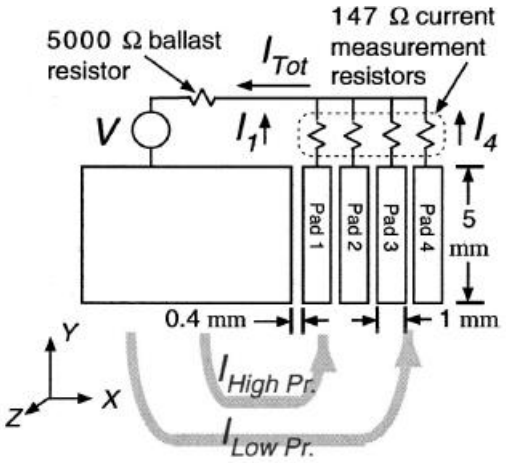


FIG. 1. Planar Ti electrode configuration, patterned on glass to measure cathode current density. Cathode is split into separate paths, where the current is independently measured. Polarity can be reversed to measure anode current density.

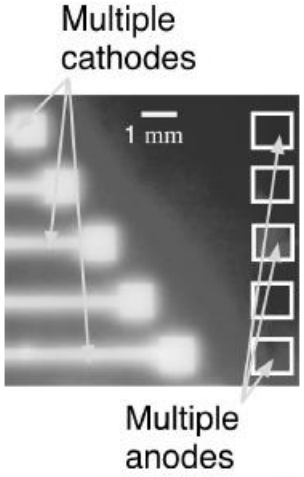
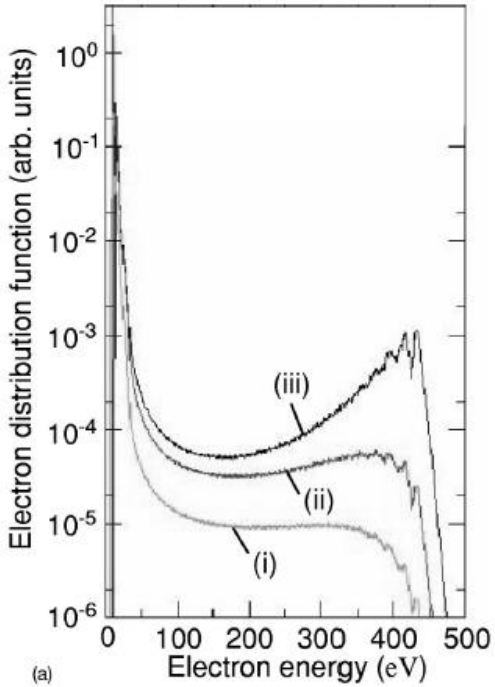


FIG. 4. Microplasmas generated at 2 Torr, in air, at 423 V. The microplasma glow region is confined over the cathode, and is independent of the anode–cathode spacing.



Profiling and modeling of dc nitrogen microplasmas
Wilson et al. J. Appl. Phys., 94 (2003) 2845

※ Kinetic solver :

Four dimensional Fokker–Planck solver for electron kinetics in collisional gas discharge plasmas
V. Kolobov, R. Arslanbekov / Computer Physics Communications 164 (2004) 195–201

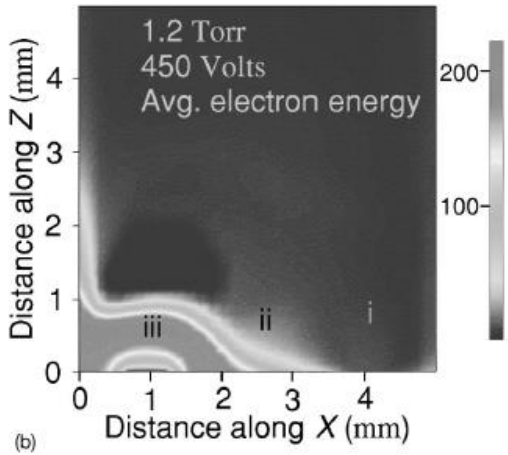
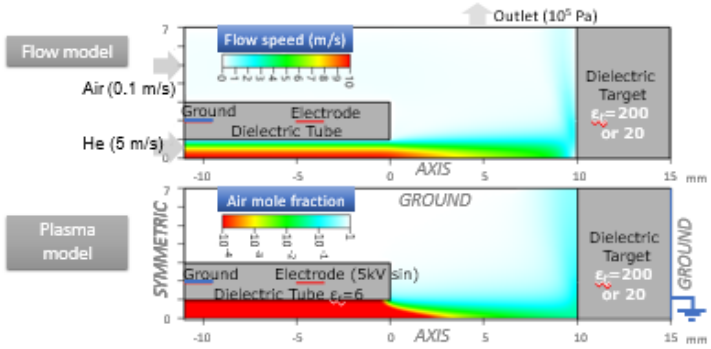


FIG. 13. Modeled electron energy distribution function has bimodal nature near the cathode.

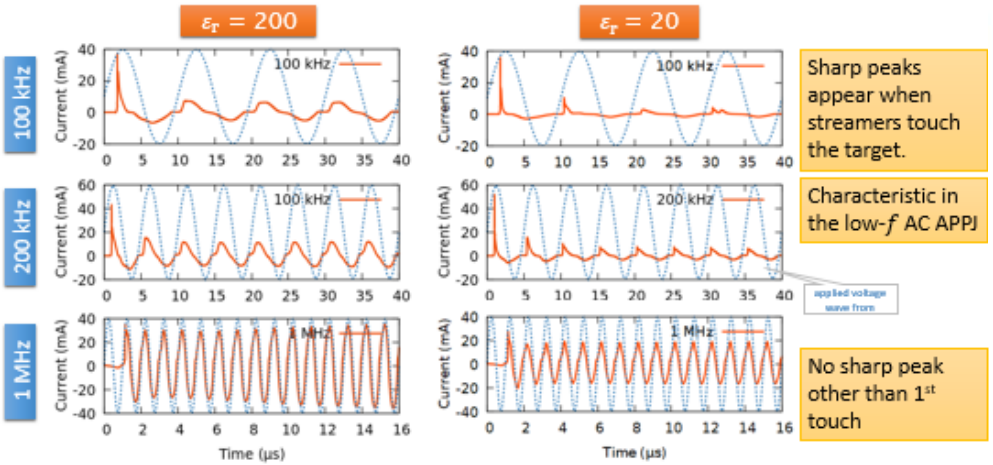
Application examples for plasma (cont.)

Modeling study on AC atmospheric pressure He plasma jets interacting with a dielectric target

DPS 2019 (by Kobayashi)



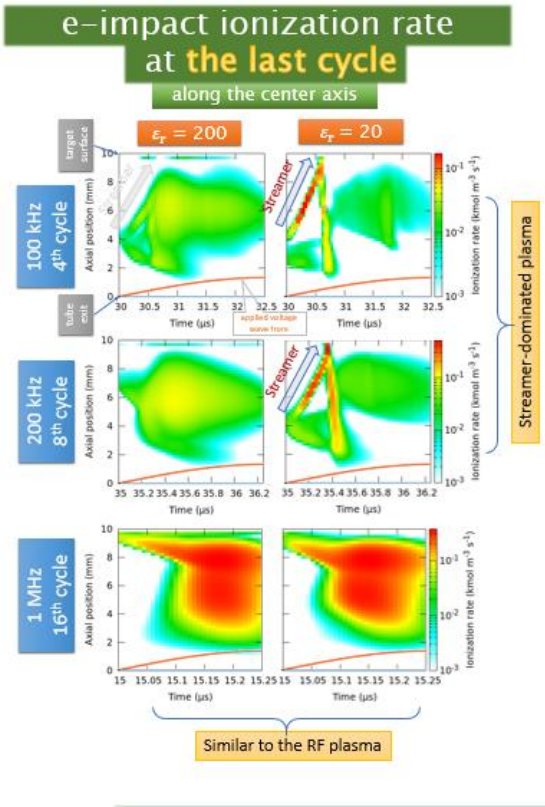
- Sequence: Gas flow model → Plasma model with fixing the gas flow
- Chemistry: 20 species and 80 reactions
- EEDF: Maxwellian
- Surface O destruction $\gamma = 0.02$, SEEC $\gamma = 0.1$
- Seed electrons ~ 2×10^{13} m^{-3} (instead of photoionization)
- Gas temperature = 300 K (const.)
- Electrode voltage: 5 kV sinusoidal AC at f = 100 kHz, 200 kHz, 1MHz
- Time integration: up to 4 cycles (100 kHz), 8 cycles (200 kHz), 16 cycles (1 MHz)
- Time step: 20 ps

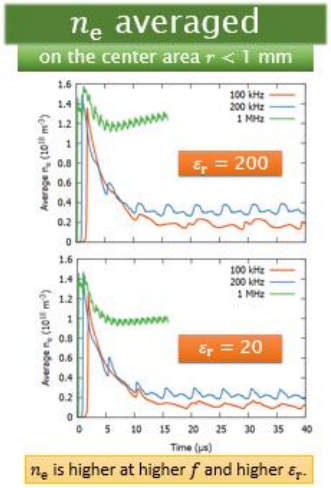


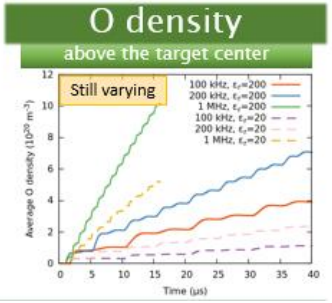
Sharp peaks appear when streamers touch the target.

Characteristic in the low-f AC APPJ

No sharp peak other than 1st touch







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Application examples for plasma (cont.)

PECVD for Silicon Nitride

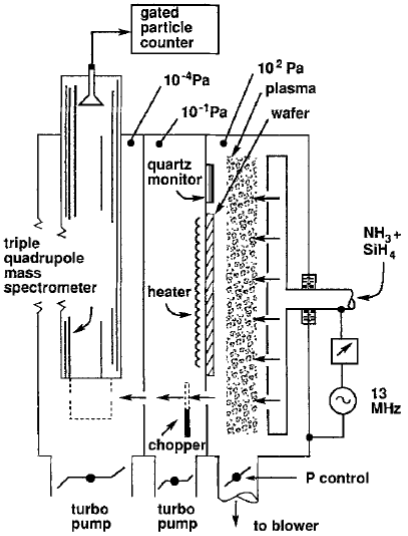
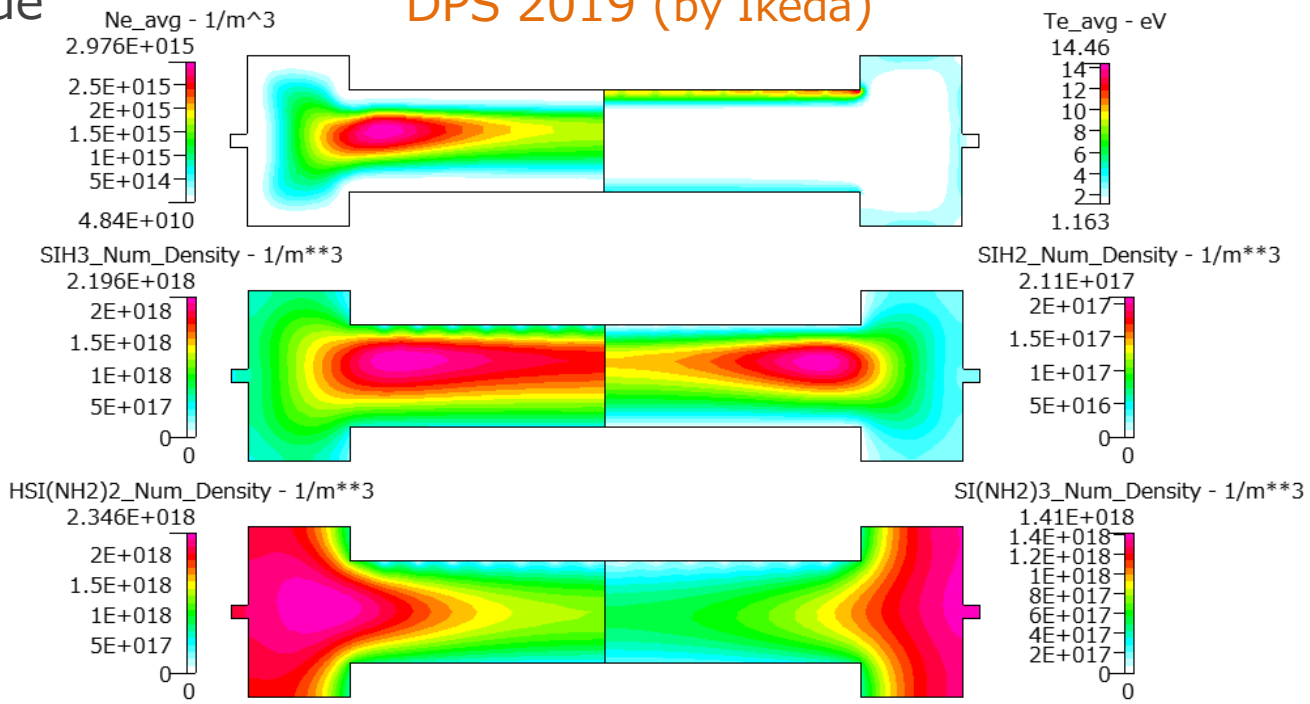
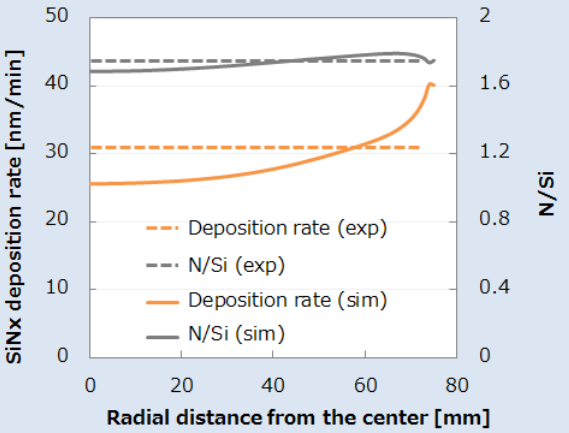
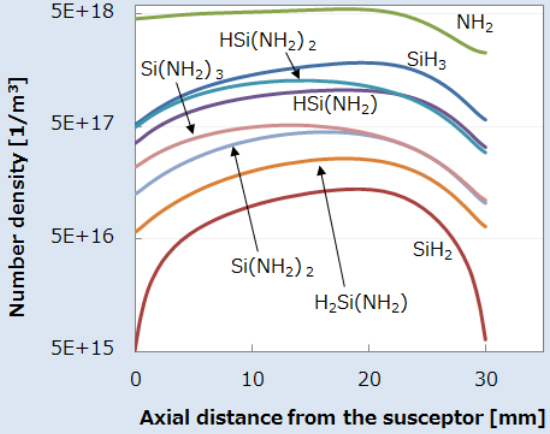


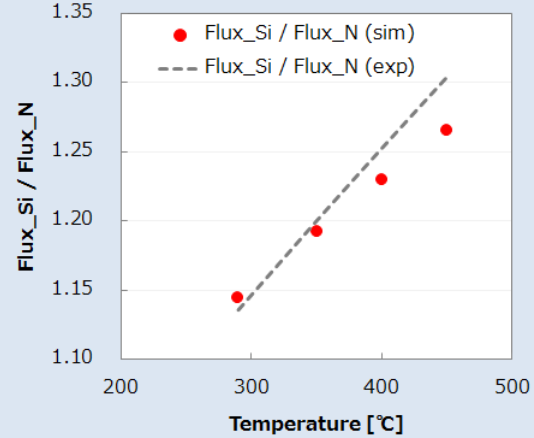
Fig. 1. Plasma reactor and analytical equipment, including quartz deposition monitor in wafer plane and line-of-sight mass spectrometric sampling.

DPS 2019 (by Ikeda)









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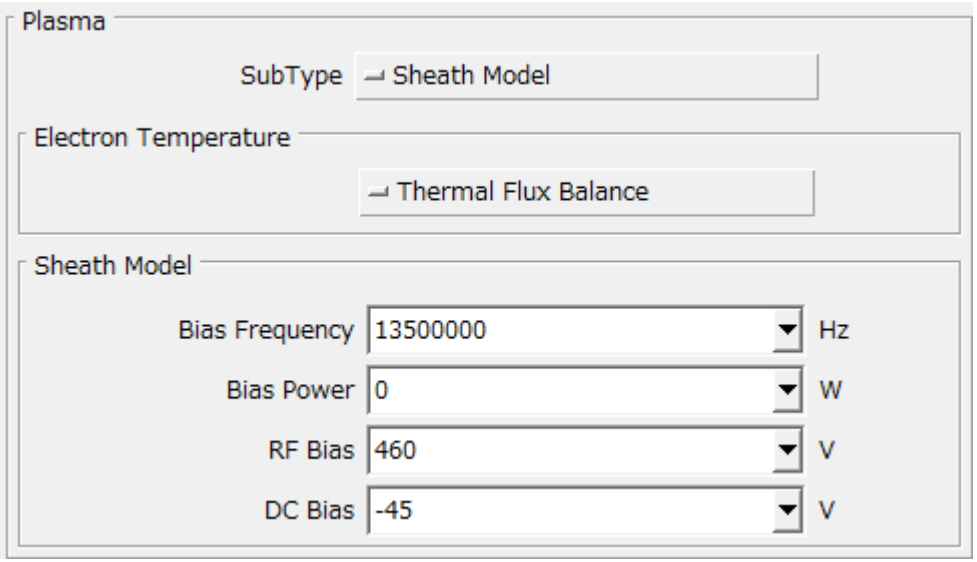
Sheath model (Boundary condition)

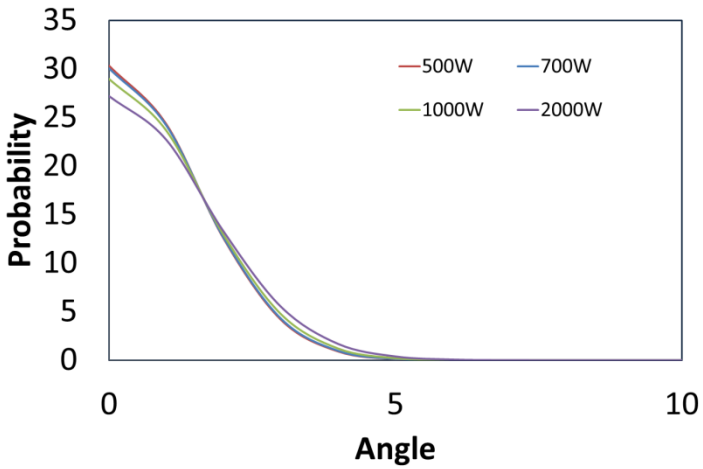
Ion energy dependency for the reaction rate and yield can be set when ICP (w/o CCP option) is chosen.

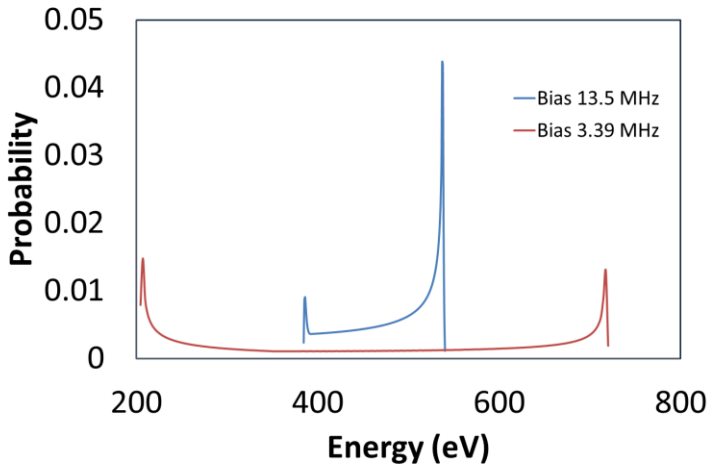
The sheath is not mesh resolved.

Semi-analytic sheath model is used to compute the IEADs at wafer.

The bias needs to be specified: V_{rf} , V_{dc} and Frequency.







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Monte Carlo to compute IEADFs

Characterization of an asymmetric parallel plate radio-frequency discharge using a retarding field energy analyzer

Plasma Sources Sci. Technol. 21 (2012) 015002

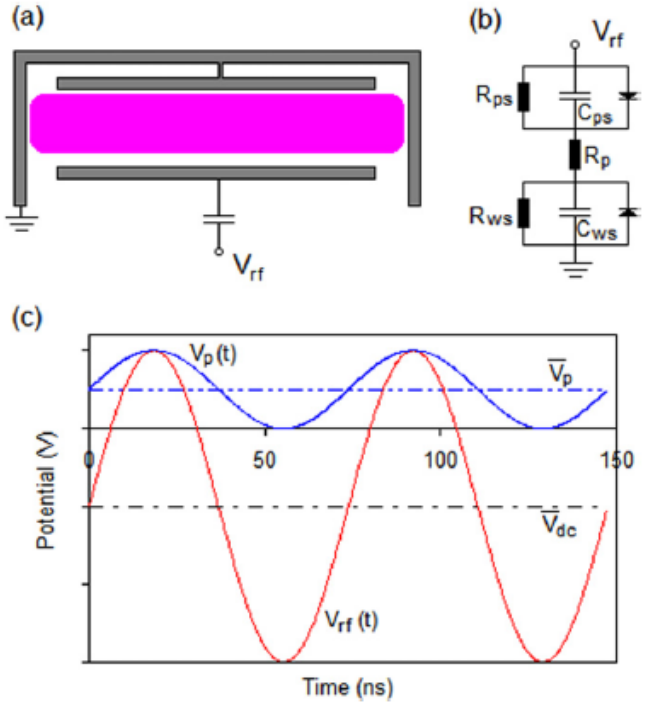
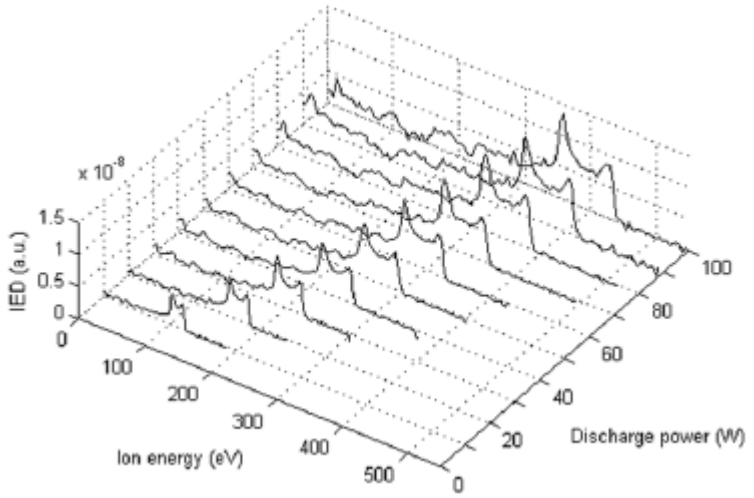


Figure 3. (*a*) Schematic of capacitively coupled asymmetric rf discharge, (*b*) equivalent circuit where R_{ps} and C_{ps} are the powered sheath resistance and capacitance, respectively, and R_{ws} and C_{ws} are the wall/ground sheath resistance and capacitance, respectively. R_p is the bulk plasma resistance, (*c*) illustrative discharge potentials where $V_{rf}(t)$ and $\overline{V}_{dc}$ are the excitation potential and dc self-bias, respectively, and $V_p(t)$ and $\overline{V}_p$ are the time-varying and time-averaged components of the plasma potential, respectively.



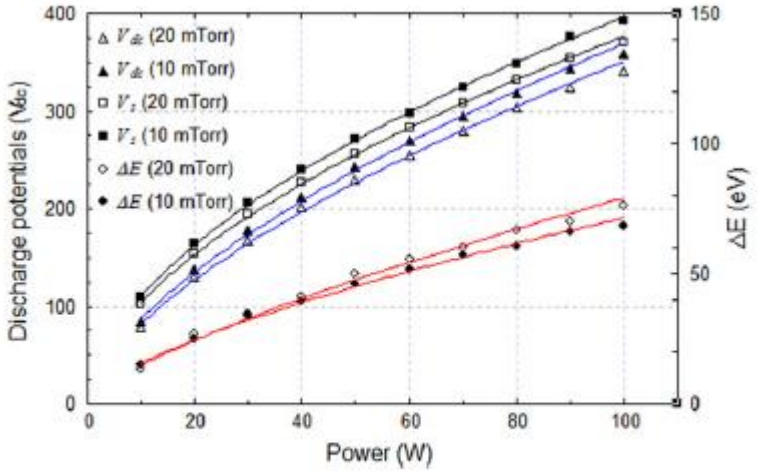
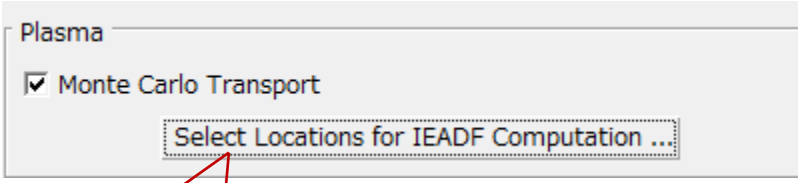


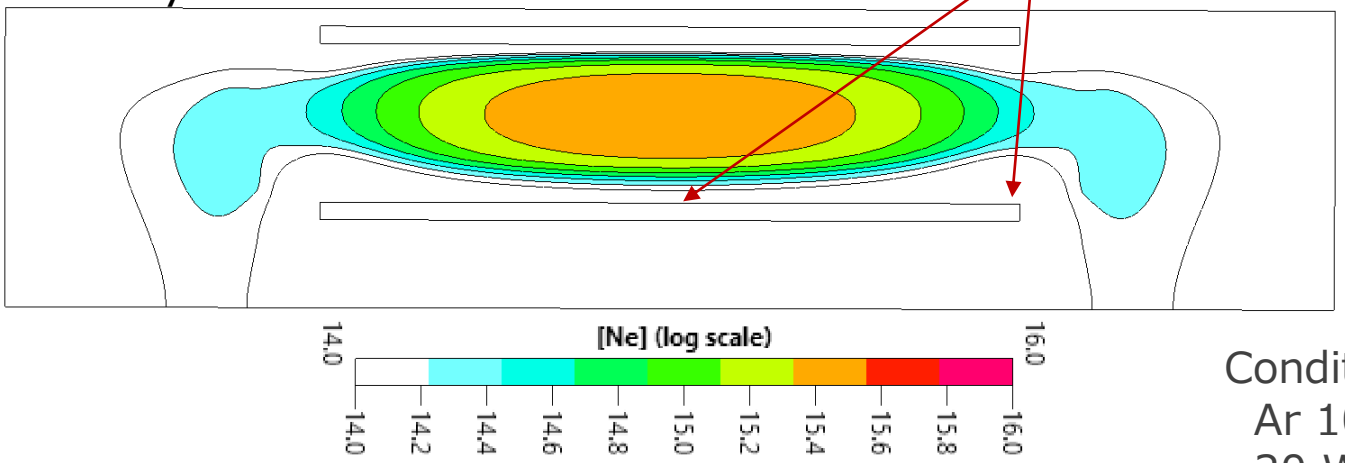
Figure 6. Self-bias voltage (measured directly), time-averaged sheath potential and collisionless ion peak separation (calculated from the IED measurements) as a function of power and pressure.

Monte Carlo to compute IEADFs (2)

Specify positions to compute IEADF

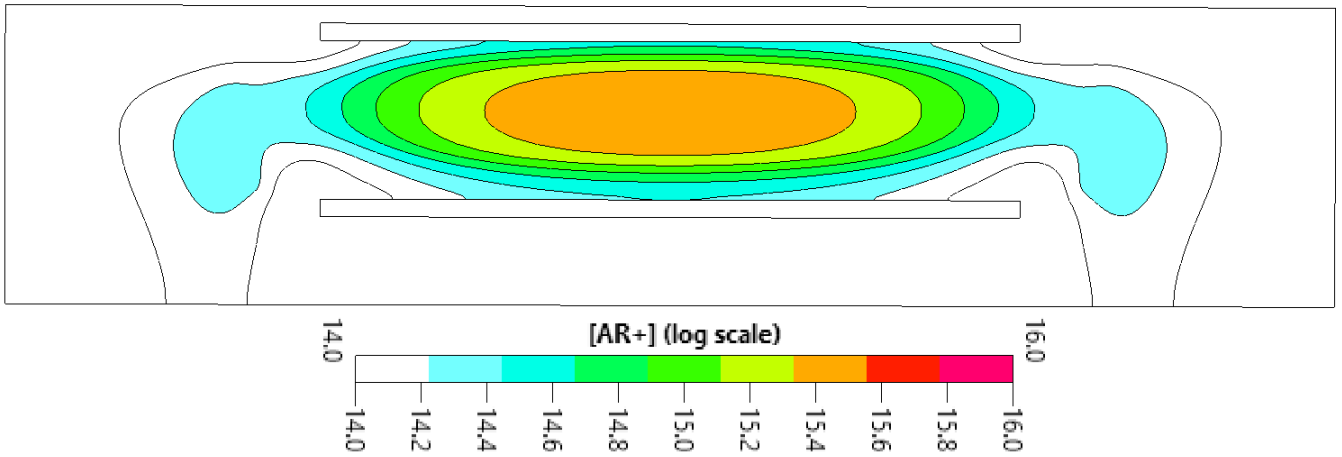


Electron Density



Conditions:
Ar 10 mTorr
20 W, 13MHz

Ar+ Density



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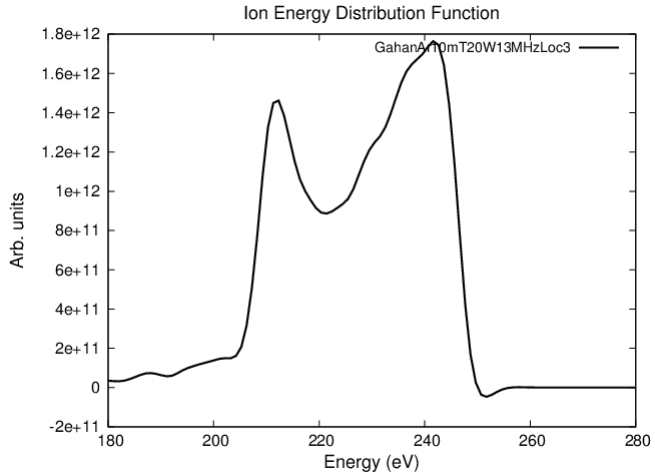
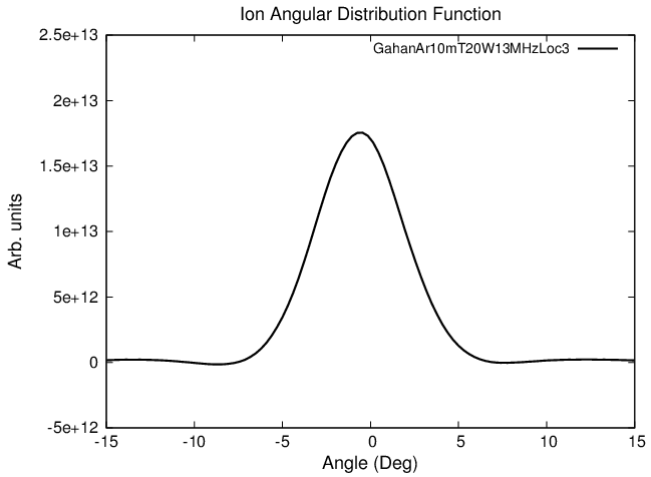
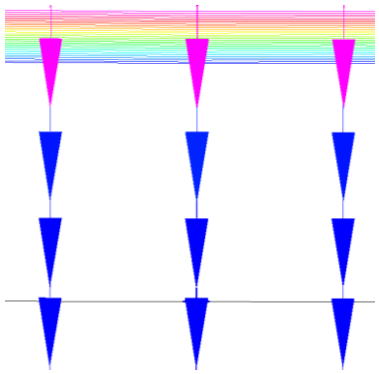
Monte Carlo to compute IEADFs (3)

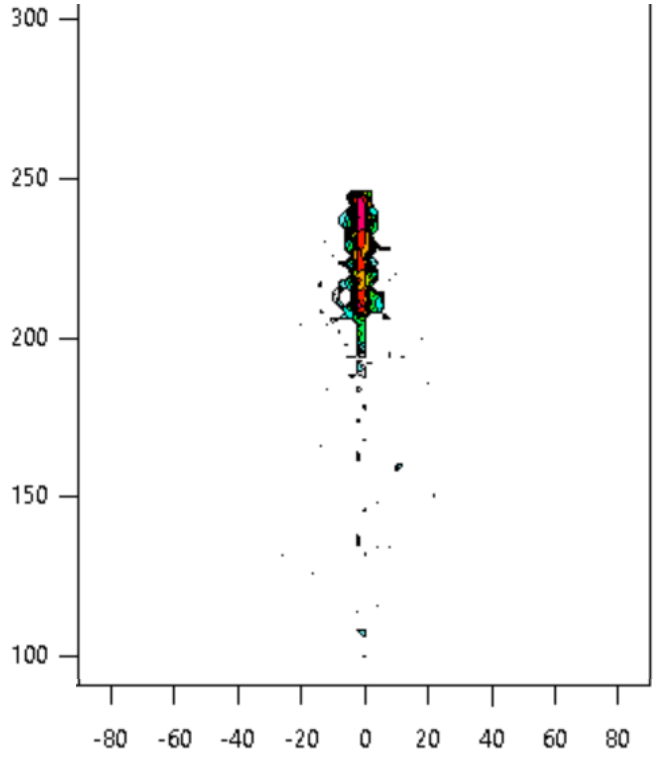
Position : Wafer center





Ion Flux





Estimated	Elow	206 eV
(compare to MC)	Ehigh	231 eV

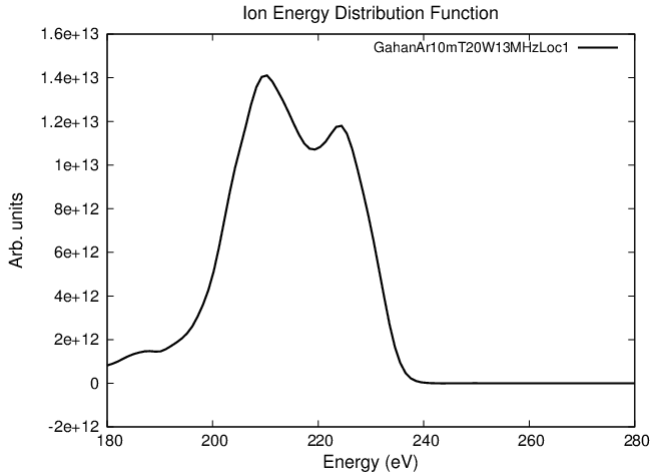
Monte Carlo Computation:

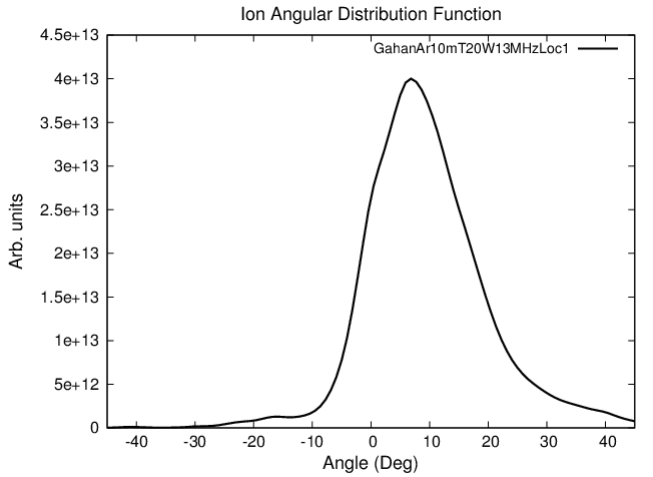
E_{low} ~ 210 eV

E_{high} ~ 242 eV

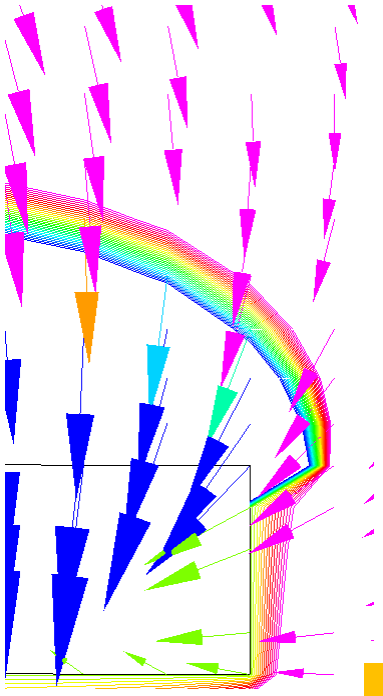
Monte Carlo to compute IEADFs (4)

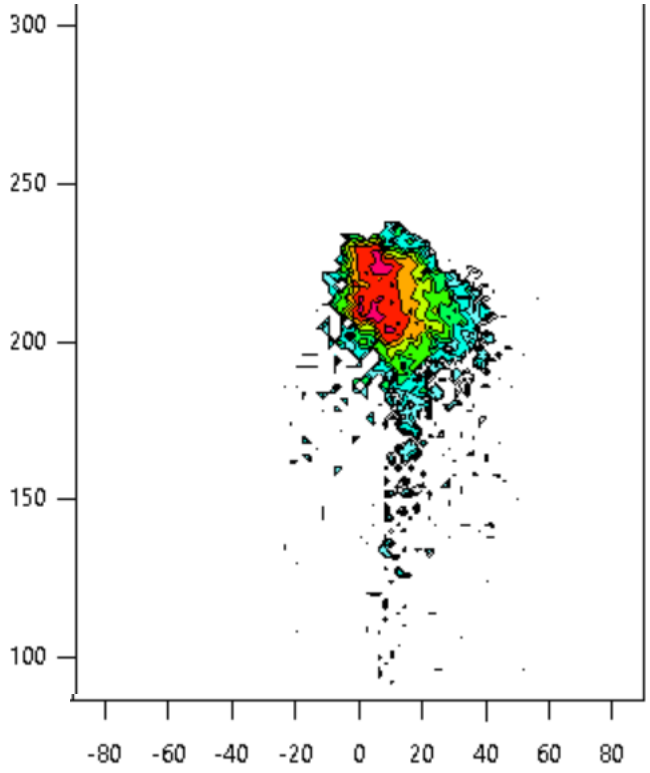
Position : Wafer edge





Ion Flux





Estimated (compare to MC)	Elow	214 eV
	Ehigh	223 eV

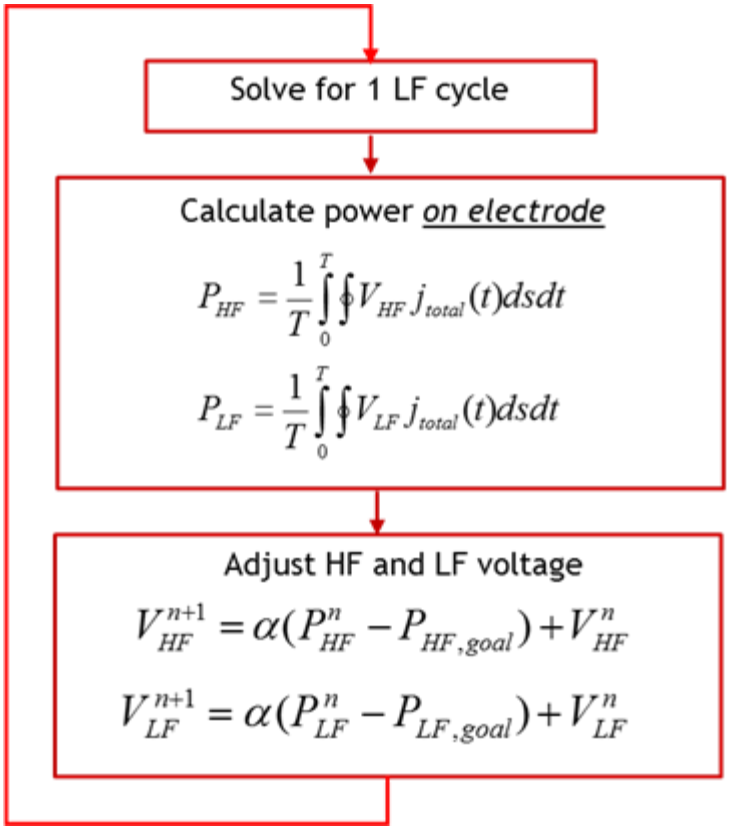
Monte Carlo Computation:

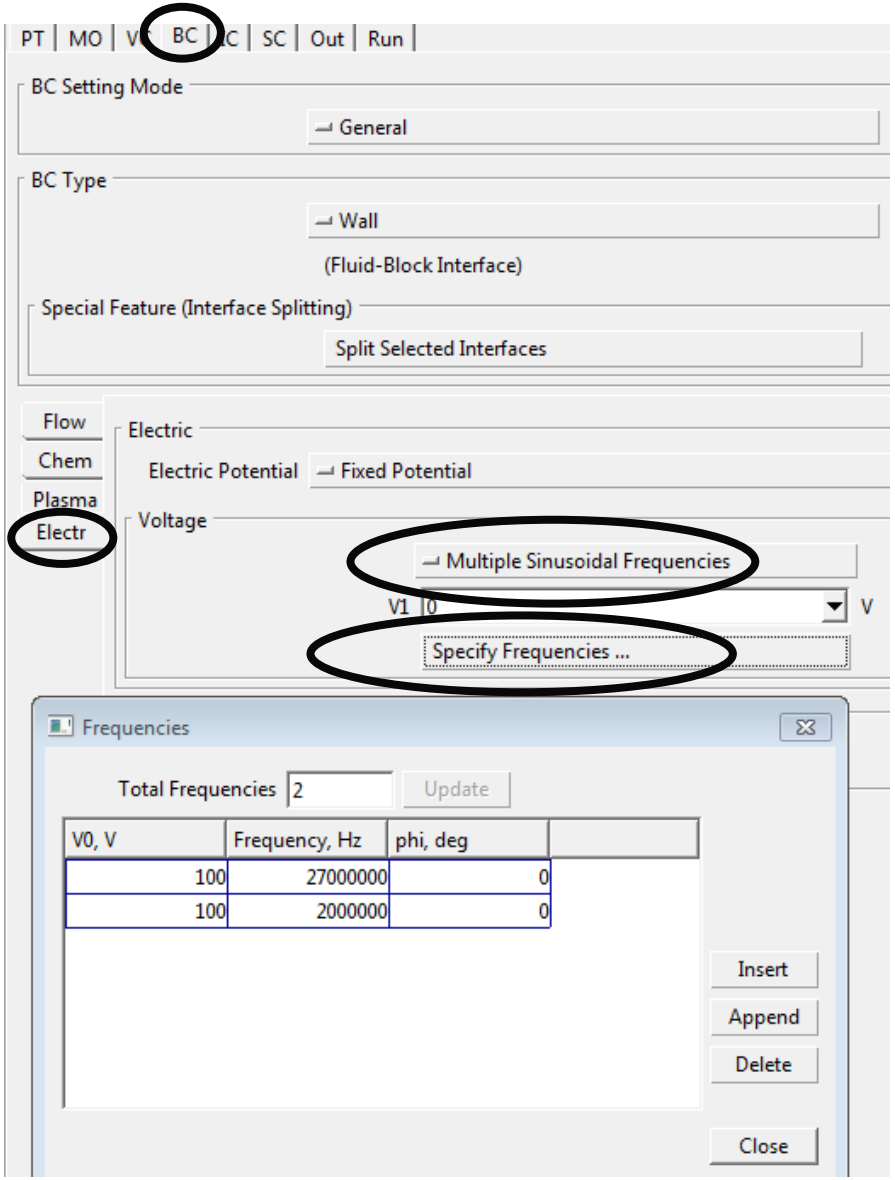
E_{low} ~ 210 eV

E_{high} ~ 226 eV

Multi-frequency CCP

Dual frequency on one electrode can be set easily





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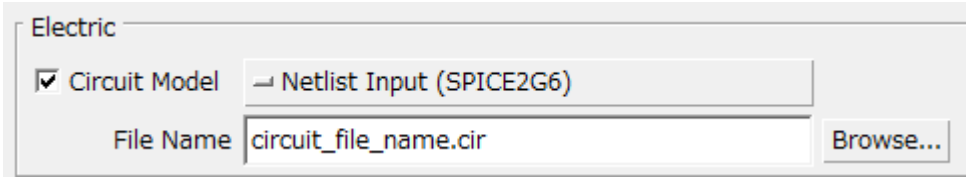
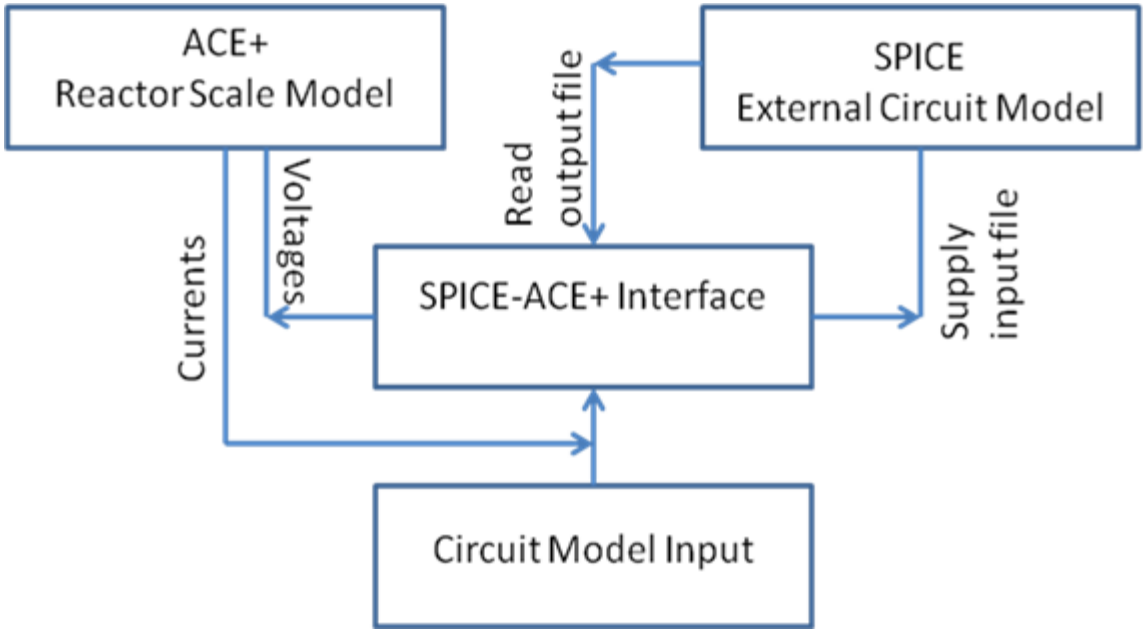
Spice coupling

CFD-ACE+ Plasma solver accounts for **external circuit** interactions to a greater degree of generality. Proposed external circuit coupling to **SPICE** will enable generic circuit representations at several reactor surfaces.





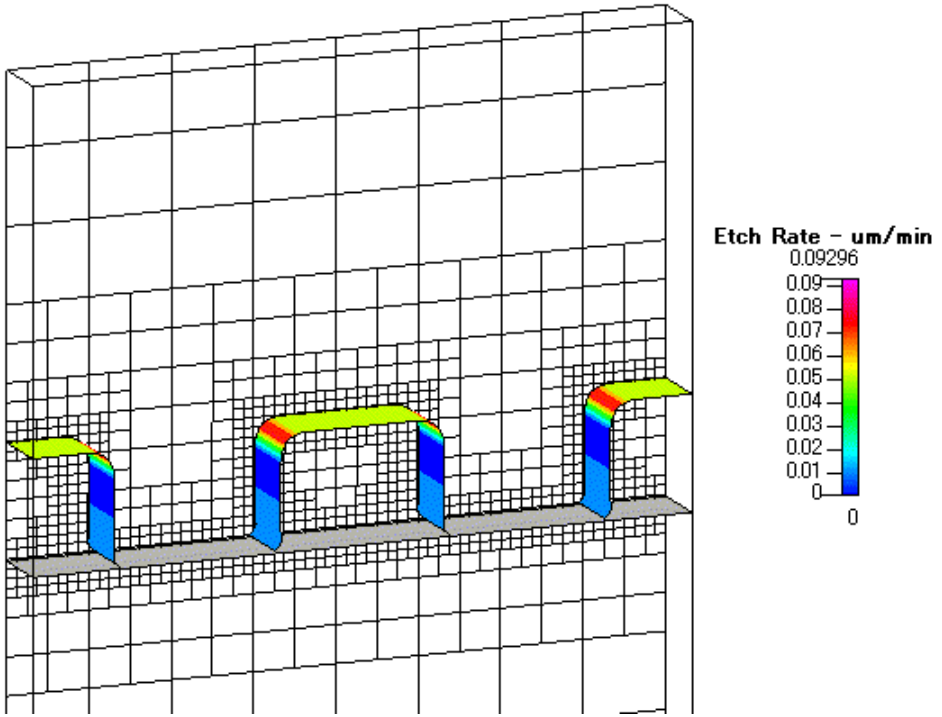
形状シミュレータ

CFD-TOPO

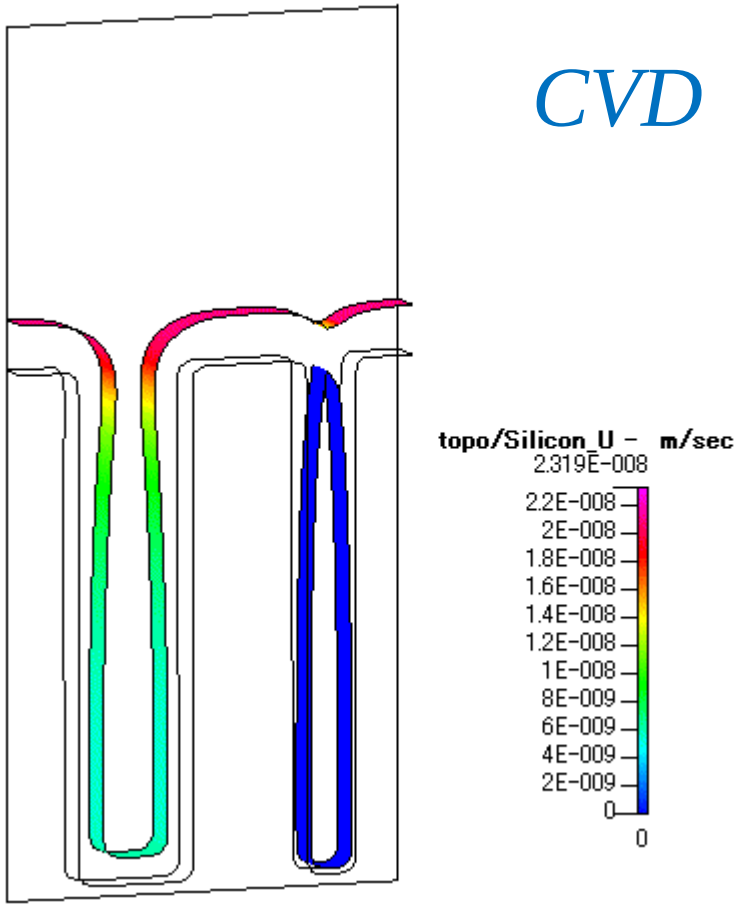
Topology simulation by CFD-TOPO

※ Input file can be obtained by CFD-ACE+

Etching



CVD



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Swarm パラメータ，反応レートの Lookup Table 作成ツール

Bosprom

プロパゲータ法 (分布関数 $f(\vec{v})$ 計算法の一種)

流体モデル

$n_e(\vec{r},t)$
$T_e(\vec{r},t)$

CFD-ACE+など

近似：Maxwell分布

Boltzmann eq. $f(\vec{r},\vec{v},t)$

近似：位置空間一様

簡略化Boltzmann eq.

$$\frac{\partial}{\partial t}f(v,\theta,t)=\left[-a\frac{\partial}{\partial v_x}+\left(\frac{\partial}{\partial t}\right)_{\text{coll}}\right]f(v,\theta,t)$$

近似： $f \propto F_0(\varepsilon)+F_1(\varepsilon)\cos\theta$

二項近似

BOLSIG+, CFD-ACEなど

確率的解法

Monte-Carlo法

MagBoltzなど

直接解法

プロパゲータ法

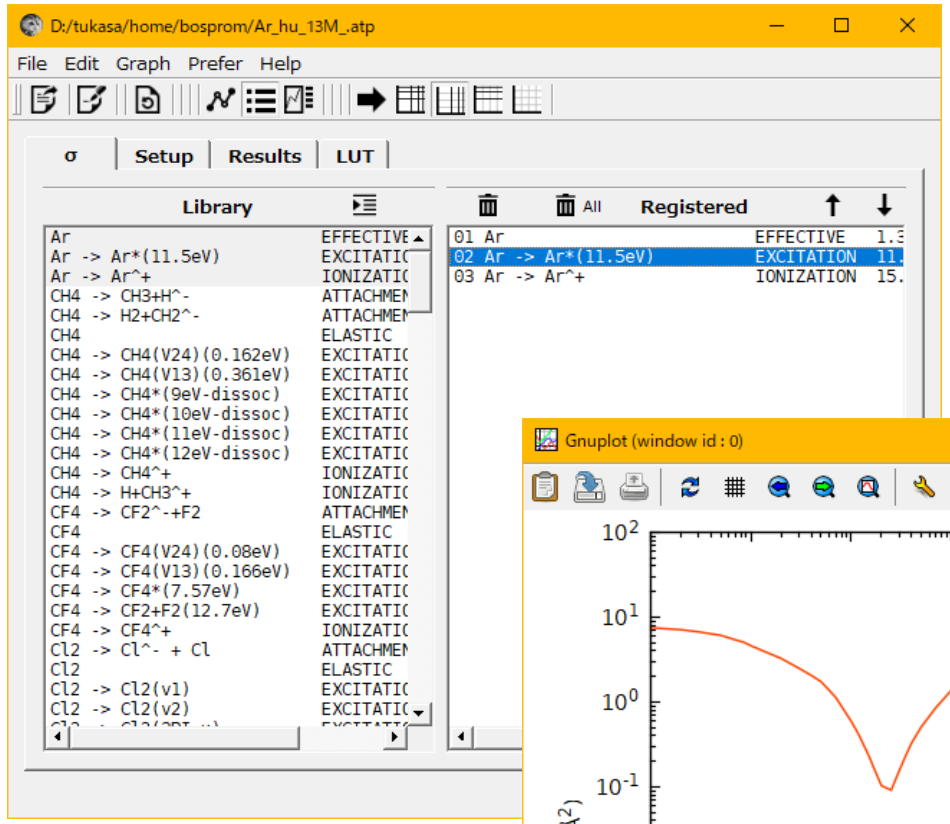
Bosprom

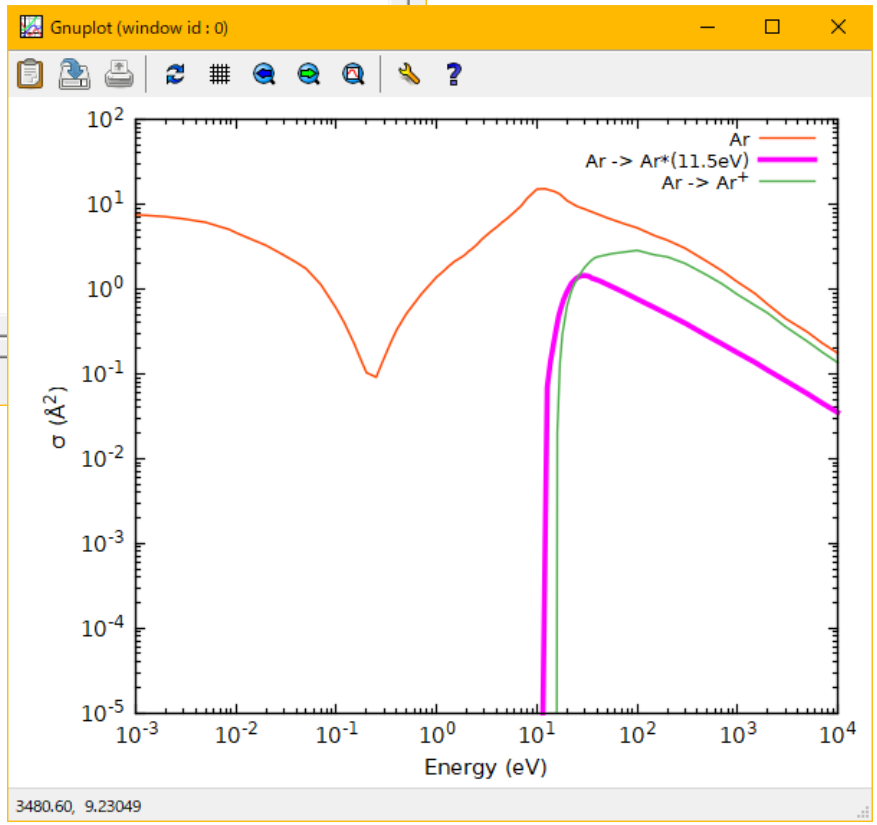
(**Bo**ltzmann **S**olver by **Pro**pagator **M**ethod)

衝突断面積 → 分布関数 f → 反応レート定数, 輸送係数(移動度, 拡散係数)

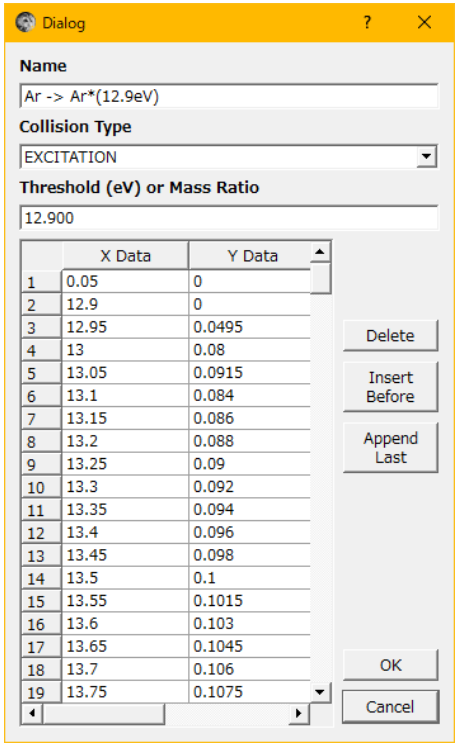
Swarm parameters

Bosprom:衝突断面積データ選択・編集画面





- 断面積データの編集が可能



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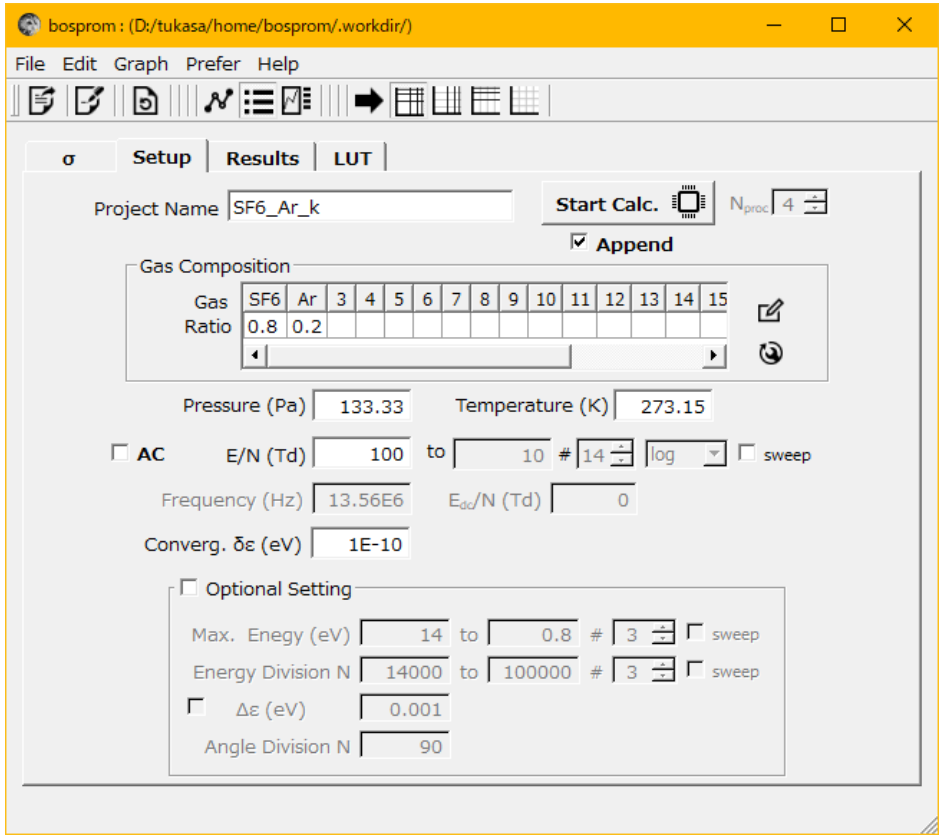
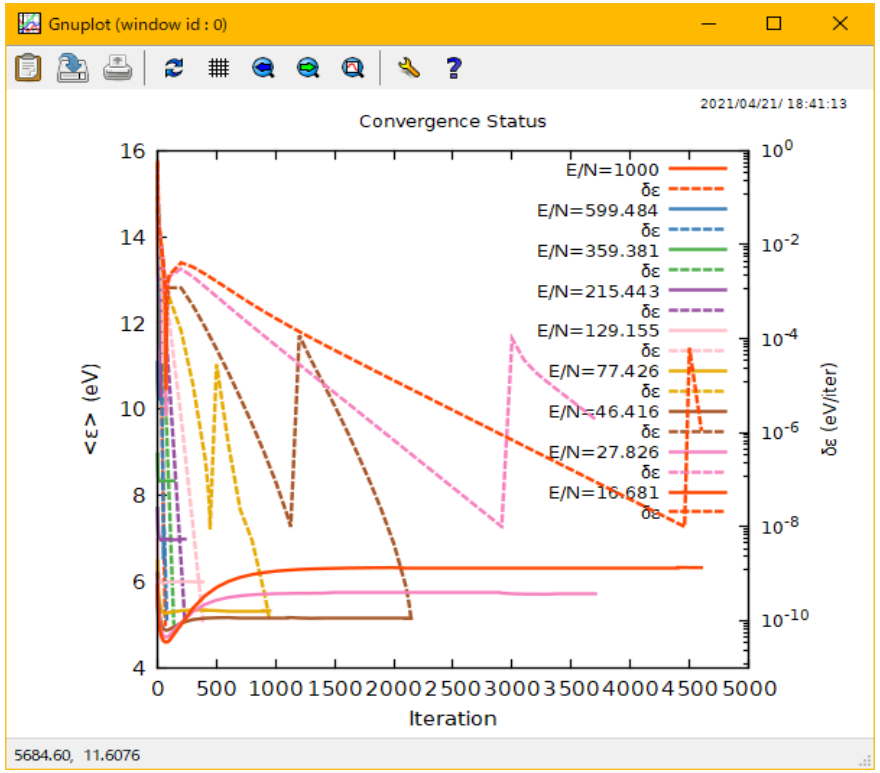
Bosprom:計算条件設定画面・収束状況表示





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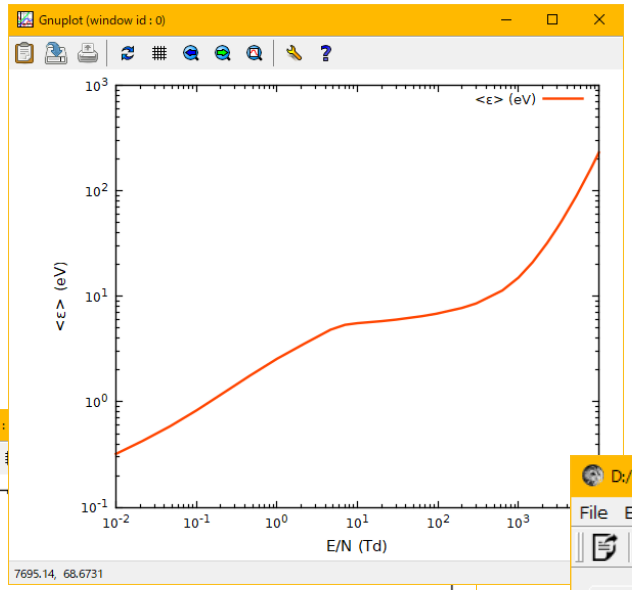
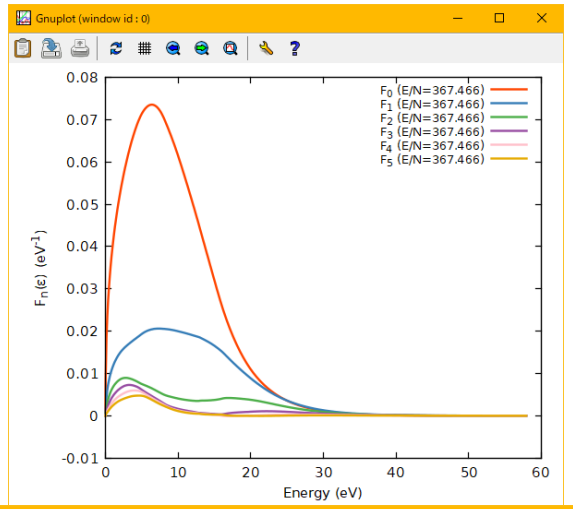
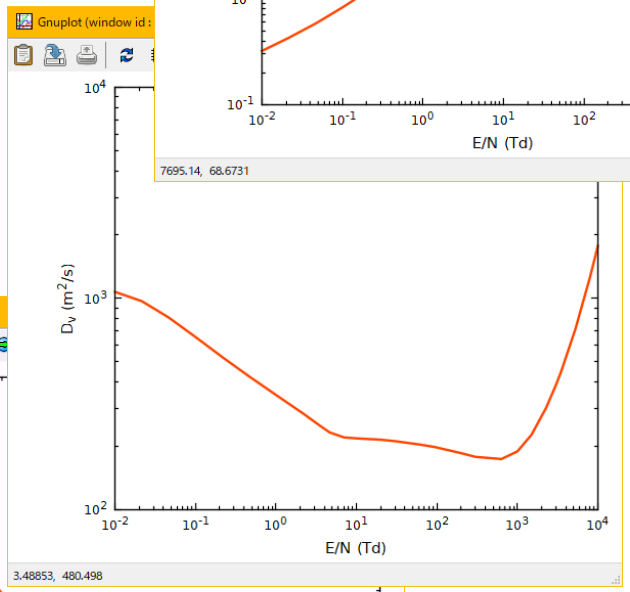
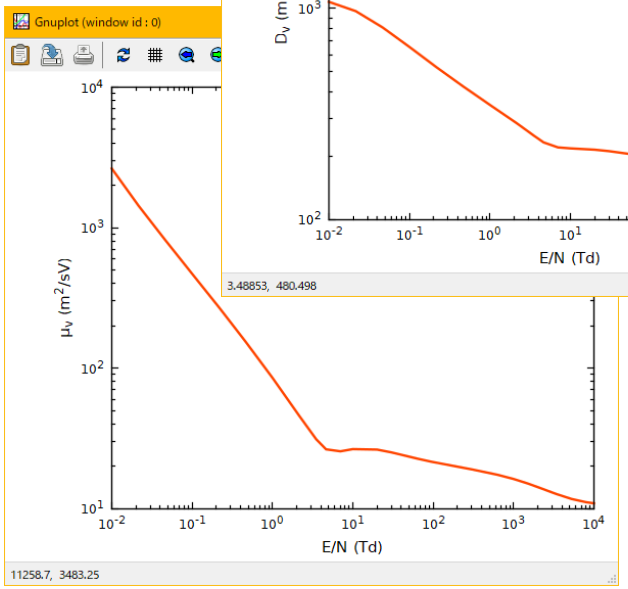
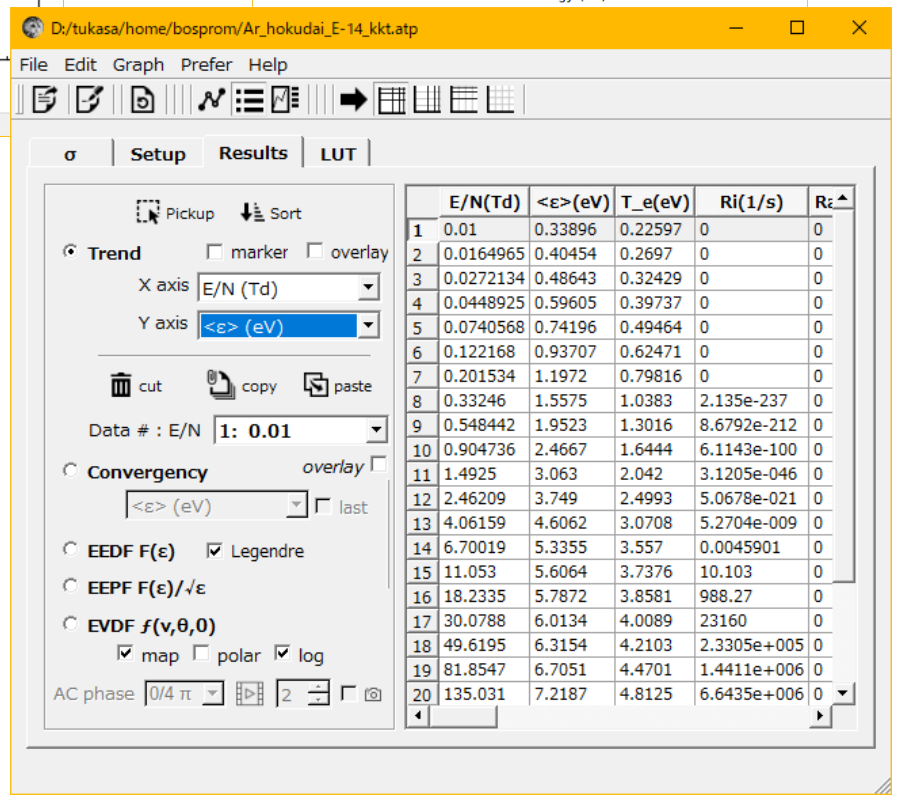
Bosprom:結果表示画面











	E/N(Td)	<ε>(eV)	T_e(eV)	Ri(1/s)	Ra
1	0.01	0.33896	0.22597	0	0
2	0.0164965	0.40454	0.2697	0	0
3	0.0272134	0.48643	0.32429	0	0
4	0.0448925	0.59605	0.39737	0	0
5	0.0740568	0.74196	0.49464	0	0
6	0.122168	0.93707	0.62471	0	0
7	0.201534	1.1972	0.79816	0	0
8	0.33246	1.5575	1.0383	2.135e-237	0
9	0.548442	1.9523	1.3016	8.6792e-212	0
10	0.904736	2.4667	1.6444	6.1143e-100	0
11	1.4925	3.063	2.042	3.1205e-046	0
12	2.46209	3.749	2.4993	5.0678e-021	0
13	4.06159	4.6062	3.0708	5.2704e-009	0
14	6.70019	5.3355	3.557	0.0045901	0
15	11.053	5.6064	3.7376	10.103	0
16	18.2335	5.7872	3.8581	988.27	0
17	30.0788	6.0134	4.0089	23160	0
18	49.6195	6.3154	4.2103	2.3305e+005	0
19	81.8547	6.7051	4.4701	1.4411e+006	0
20	135.031	7.2187	4.8125	6.6435e+006	0

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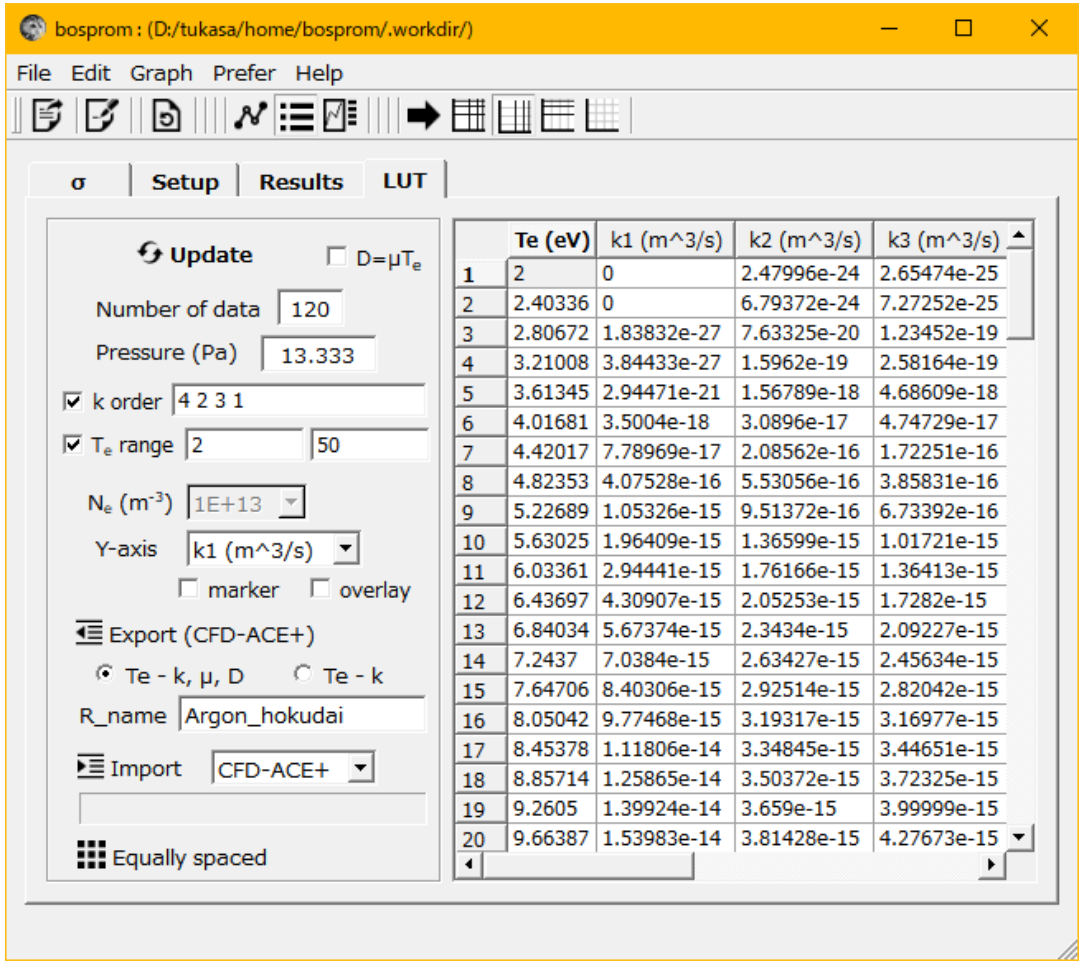
Bosprom:プラズマ計算用 lookup-table 作成画面



	Te (eV)	k1 (m^3/s)	k2 (m^3/s)	k3 (m^3/s)
1	2	0	2.47996e-24	2.65474e-25
2	2.40336	0	6.79372e-24	7.27252e-25
3	2.80672	1.83832e-27	7.63325e-20	1.23452e-19
4	3.21008	3.84433e-27	1.5962e-19	2.58164e-19
5	3.61345	2.94471e-21	1.56789e-18	4.68609e-18
6	4.01681	3.5004e-18	3.0896e-17	4.74729e-17
7	4.42017	7.78969e-17	2.08562e-16	1.72251e-16
8	4.82353	4.07528e-16	5.53056e-16	3.85831e-16
9	5.22689	1.05326e-15	9.51372e-16	6.73392e-16
10	5.63025	1.96409e-15	1.36599e-15	1.01721e-15
11	6.03361	2.94441e-15	1.76166e-15	1.36413e-15
12	6.43697	4.30907e-15	2.05253e-15	1.7282e-15
13	6.84034	5.67374e-15	2.3434e-15	2.09227e-15
14	7.2437	7.0384e-15	2.63427e-15	2.45634e-15
15	7.64706	8.40306e-15	2.92514e-15	2.82042e-15
16	8.05042	9.77468e-15	3.19317e-15	3.16977e-15
17	8.45378	1.11806e-14	3.34845e-15	3.44651e-15
18	8.85714	1.25865e-14	3.50372e-15	3.72325e-15
19	9.2605	1.39924e-14	3.659e-15	3.99999e-15
20	9.66387	1.53983e-14	3.81428e-15	4.27673e-15

- 計算結果から T_e ベースの LUT (lookup-table) を作成
- CFD-ACE+ や BOLSIG+のファイルを import してグラフ表示・編集も可能

Lennard-Jones
パラメータ推算ツール

分子の加算因子・沸点から Lennard-Jones パラメータを推算

熱流体・プラズマのシミュレーションで必要となる species data を準備

表２－１　Lyndersenの臨界定数の加算因子

	個数
非環状加算因子	
-CH3	1
-CH2-	0
>CH-	0
>C<	0
=CH2	0
=CH-	0
=C<	0
=C=	0
#CH	0
#C-	0
環状加算因子	
-CH2-(R)	0
>CH-(R)	0
>C<(R)	0
=CH-(R)	6
=C<(R)	0
=C=(R)	0

	個数
ハロゲン加算因子	
-F	5
-Cl	0
-Br	0
-I	0
酸素加算因子	
-OH(Alcohol)	0
-OH(Phenol)	0
-O-	0
-O-(R)	0
>C=O	0
>C=O(R)	0
O=HC-(Aldehyde)	0
-COOH(Acid)	0
-COO-(Ester)	0
=O	0

	個数
窒素加算因子	
-NH2	0
>NH	0
>NH(R)	0
>N-	0
>N-(R)	0
-CN	0
-NO2	0
イオウ加算因子	
-SH	0
-S-	0
-S-(R)	0
=S	0
その他	0
>Si<	0
>B-	0

Lyndersenの方法		
標準沸点Tb(K):	390.65	(Input)
分子量（M）:	182.10	(Input)
偏心因子ω	0.51	
Tc	548.65	
Pc	26.71	
Vc	401.00	
Lennard-Jones		
σ	6.33	
ε/k	481.79	(K)

電子衝突断面積の推算ツール

QEC

反応モデルのデータベース

QDB

Quantemol
Plasma Chemistry Experts

Quantemol Ltd was founded in 2004 as a spin-out of University College London's Physics Department. We develop software tools based on highly sophisticated research codes and provide unique data for plasma modelling

We can offer as consultancy:

QEC electron collisions

- ✓ Elastic collisions and momentum transfer
- ✓ Electron and rotational excitation
- ✓ Super-elastic cross-sections
- ✓ Quenching cross-sections
- ✓ Dissociative electron attachment
- ✓ Electron impact ionisation

… and more!

- Electron collision cross-section calculations
- Calculations for new type of molecules (such as precursors for deposition)
- Photoionization calculations
- Cross-sections for molecules containing heavy atoms (Ti, In, I, Ga …)
- Electron impact dissociation
- Electron impact ionisation

… and more!

QDB plasma chemistry

- ✓ > 40 pre-assembled self-consistent chemistry sets
- ✓ Download formats for plasma modelling software: QVT, CHEMKIN, Comsol, **CFD-ACE+**, VizGlow...
- ✓ Dynamic Chemistry for fast chemistry assembling
- ✓ Data comparison between individual reactions
- ✓ User-friendly interface

- Assemble a chemistry set for your gas mixture
- Optimise it for your pressure conditions reducing from hundreds to dozens of reactions without loosing key reactions
- Estimate or calculate missing reactions
- Create a surface chemistry mechanisms set & calibrate it with your experiment
- Run multiple calculations & conduct a sensitivity analysis for explored contributing factors

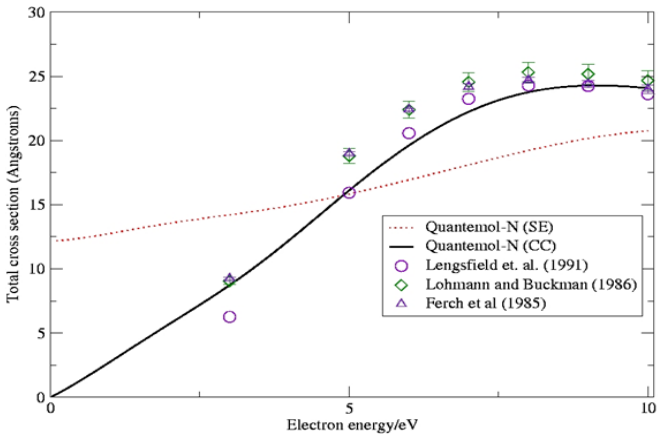
Based in London, we work with academic and industrial partners around the globe, including customers in:

Cross sections validation by QEC

Input: ONLY geometry!

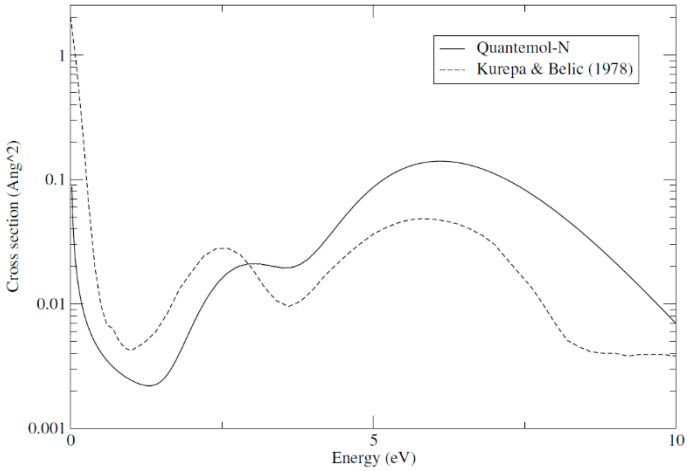
Output: cross sections, Reaction rates

Total cross sections for e-CH_4



"Methane/hydrogen plasmas have been reported to be sources both for a-C:H film deposition and for compound semiconductor etching." – Duan 2011¥

Dissociative attachment to Cl_2



"Atomic chlorine and its ions are a very common in silicon etching… and thus data regarding the chlorine molecule's dissociation are needed. The chlorine gas is highly toxic and therefore measurements of this substance are dangerous" – Hamilton 2017

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Dynamic Chemistry App

Feed gases

- Choose your chemistry among the species available in QDB

Species

- The app will scan the database and find all possible species related to your chemistry. Choose the ones you want to be included in your set

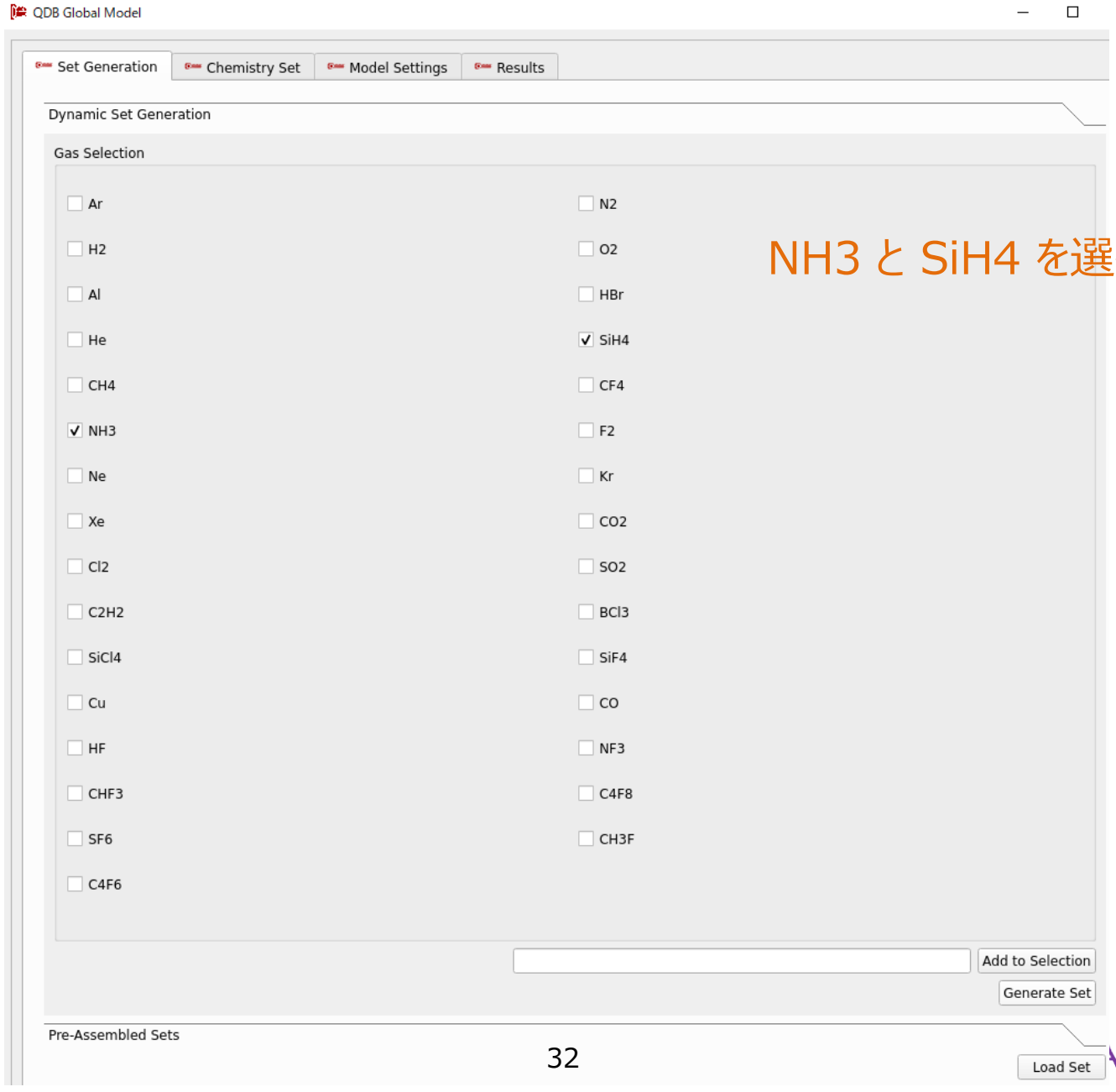
Reactions

- The app will search for all reactions with the species you chose. You can select ones you want to include

Gold users: Download data in formats compatible with: HPEM, **CFD-ACE+** (CHEMKIN), COMSOL, VisGlow

Set Generation

※ Dynamic Chemistry App の例



NH3 と SiH4 を選択した例

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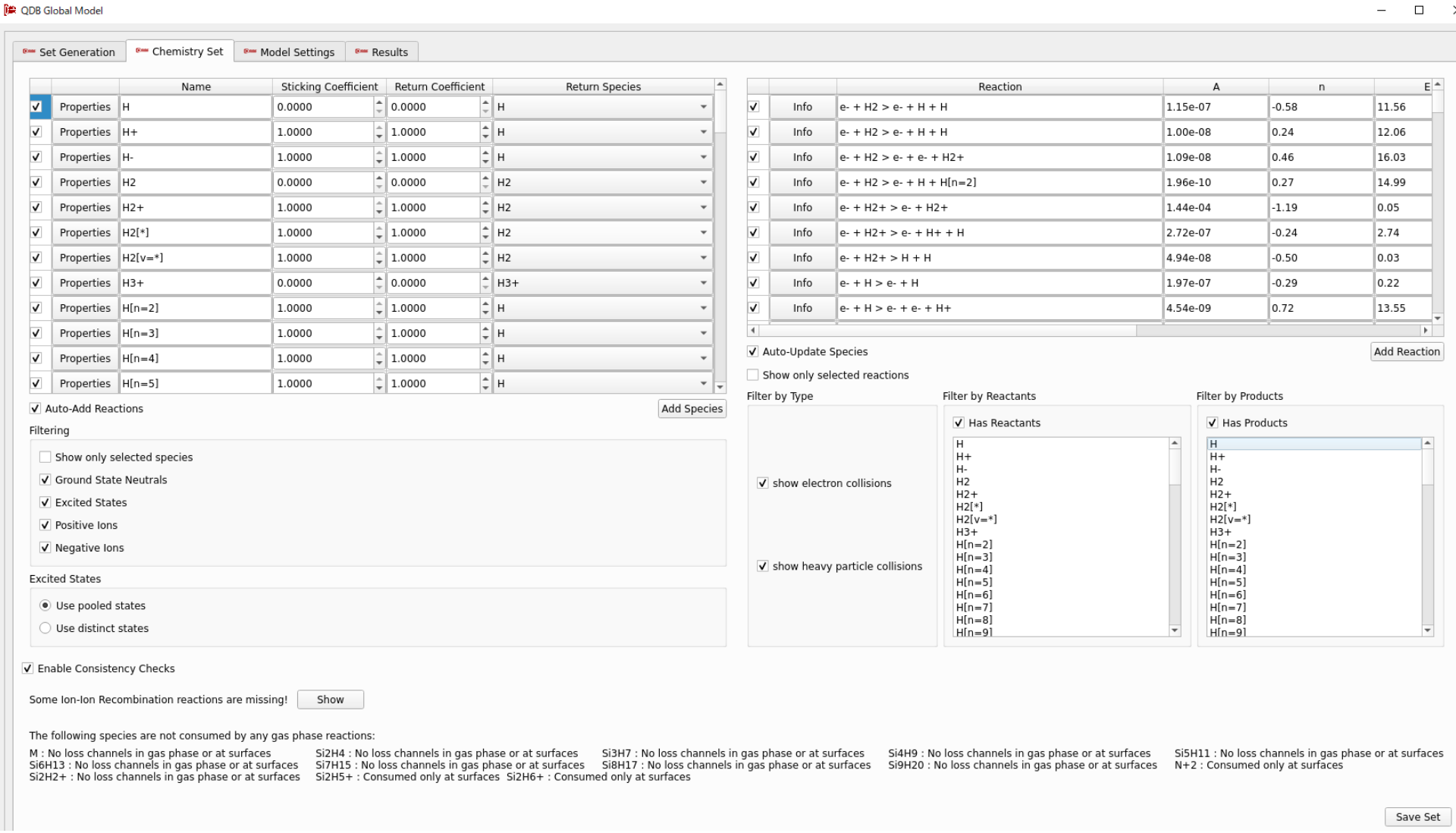
Chemistry Set

Species と reaction steps の確認



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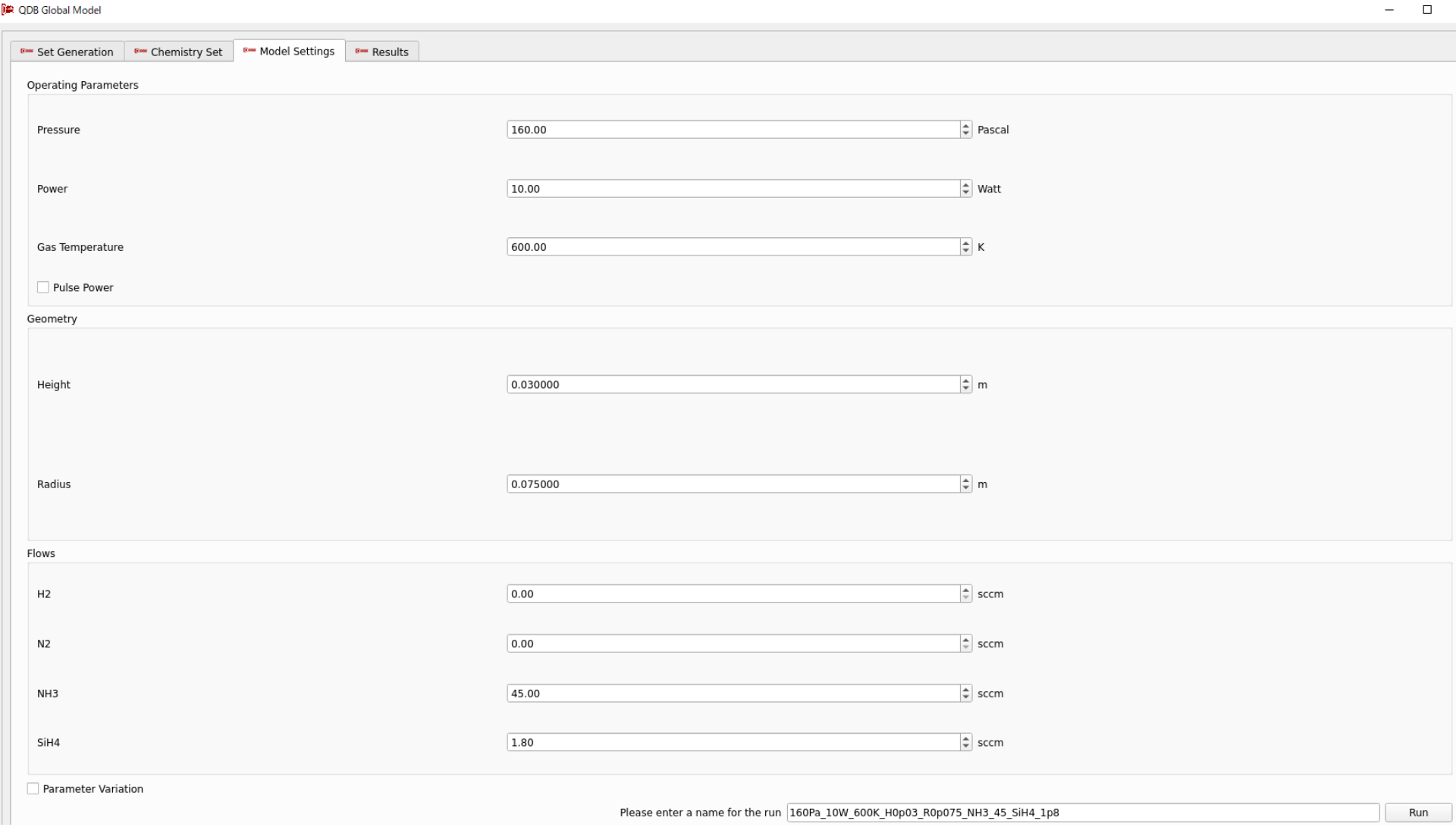
Model Settings 装置の寸法やプロセス条件の設定



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Results

計算終了後の結果

QDB Global Model

Set Generation | Chemistry Set | Model Settings | Results

Single Runs

Time-Dependent Results

Hold CTRL and click to select multiple runs

160Pa_10W_600K_H0p03_R0p075_NH3_45_SiH4_1p8

Simulation Parameters

Power: 10.00 W
Pressure: 160.00 Pa
Radius: 7.50e-02 m
Height: 3.00e-02 m
Flows: 45.00\1.80 sccm NH3\SiH4

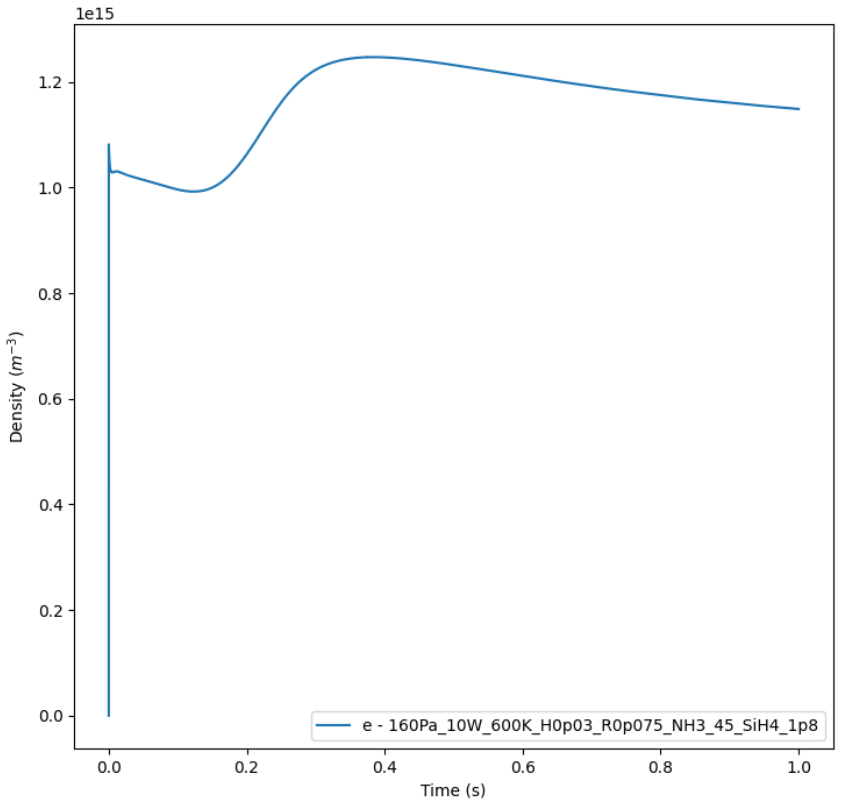
Hold CTRL and click to select multiple parameters

e
Te
H
H2
N
N2
N2H
N2H2
N2H3
N2H4
NH
NH2
NH3
Si
Si2H4
Si2H5
Si2H6
Si3H7
Si3H8

Plot all neutrals | Plot all positive ions | Plot all negative ions

Include excited states

Export | Save | Load



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Results (Final neutral species) 中性粒子の数密度の結果

QDB Global Model

Set Generation | Chemistry Set | Model Settings | Results

Single Runs | Final Results

Hold CTRL and click to select multiple runs

160Pa_10W_600K_H0p03_R0p075_NH3_45_SiH4_1p8

Simulation Parameters

Power: 10.00 W
Pressure: 160.00 Pa
Radius: 7.50e-02 m
Height: 3.00e-02 m
Flows: 45.00\1.80 sccm NH3\SiH4

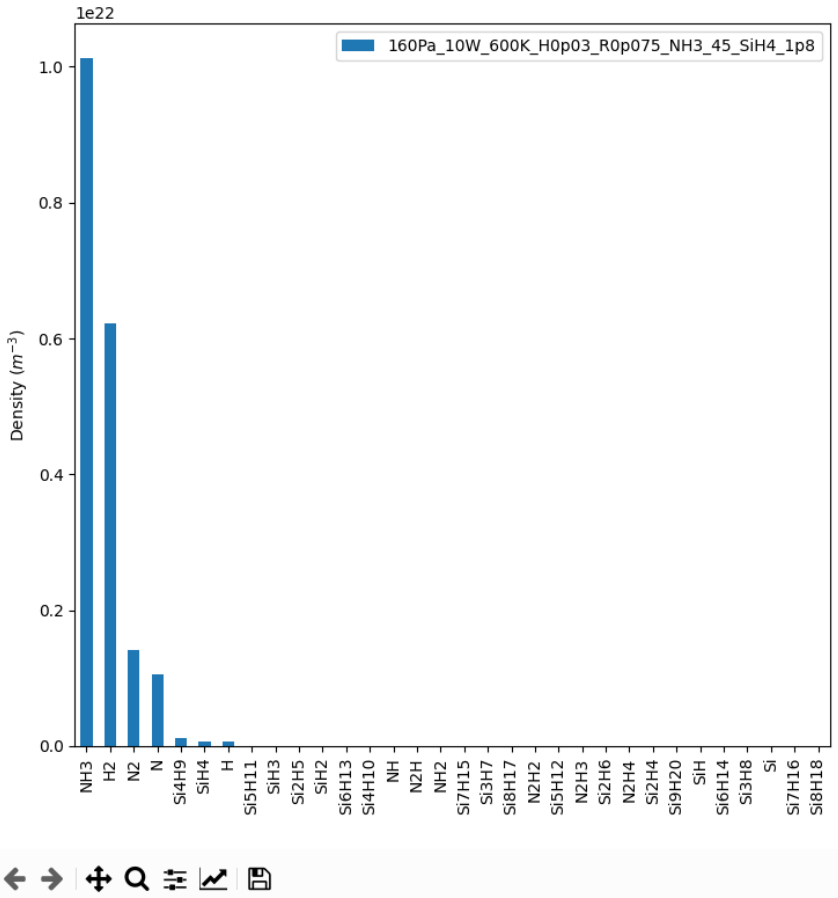
Hold CTRL and click to select multiple parameters

e
Te
H
H2
N
N2
N2H
N2H2
N2H3
N2H4
NH
NH2
NH3
Si
Si2H4
Si2H5
Si2H6
Si3H7
Si3H8

Plot all neutrals | Plot all positive ions | Plot all negative ions

Include excited states

Export | Save | Load



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