Usage of cross sections in plasma simulations

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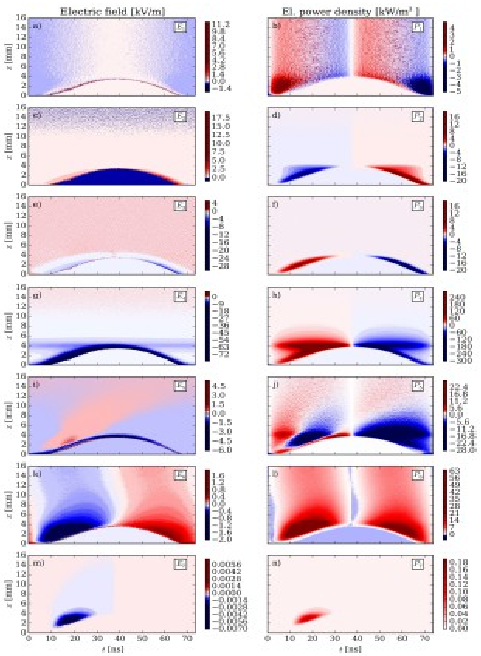
Quantemol

Why do simulations?

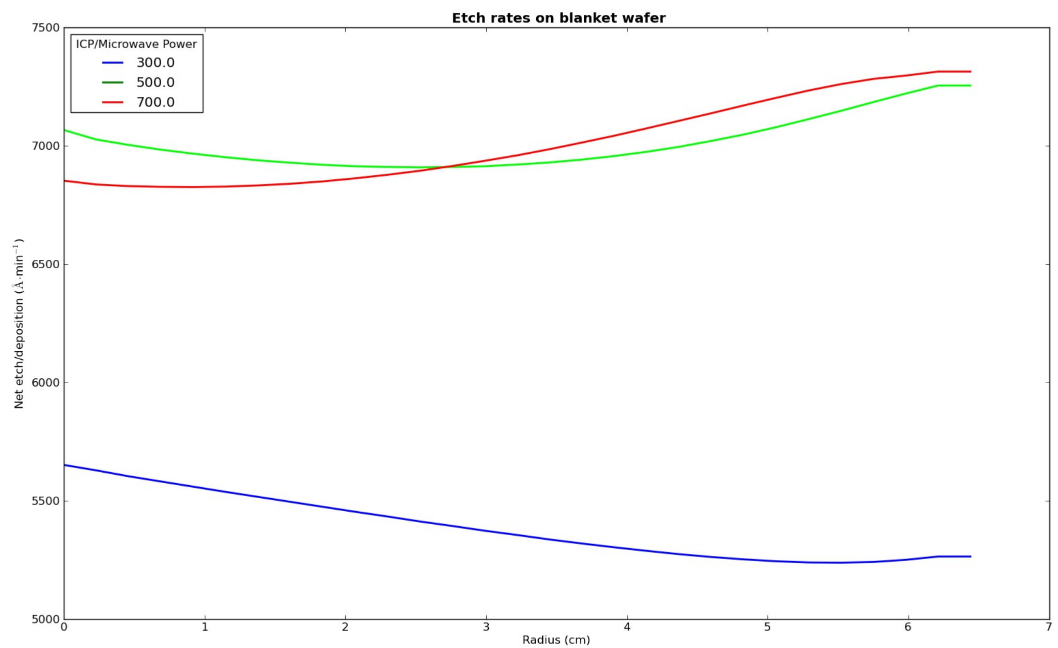


Simulations can provide insights into fundamental plasma physics which cannot be experimentally obtained easily.

J Schulze et al *Plasma Sources Sci. Technol.* **27** (2018) 055010

In industrial settings, simulations can be used to find process parameters which give the desired results.

Shown are the etch rates of silicon in a fictional SF_6/O_2 ICP. The etch rates do not increase above powers of 500 W, so there is no need to use higher powers.



Overview of a plasma simulation

- Physical model: describes particle transport, electromagnetic fields, particle distribution functions. Advances mostly driven by numerical/computational advances
- Chemical model: describes reactions between particles via cross sections, rate coefficients, reaction probabilities as input for physical model. Advances mostly data-driven.

Continuity equation in fluid model:

$$\frac{\partial n}{\partial t} = -\nabla \Gamma + S$$

Source term S contains rate coefficients derived from cross sections

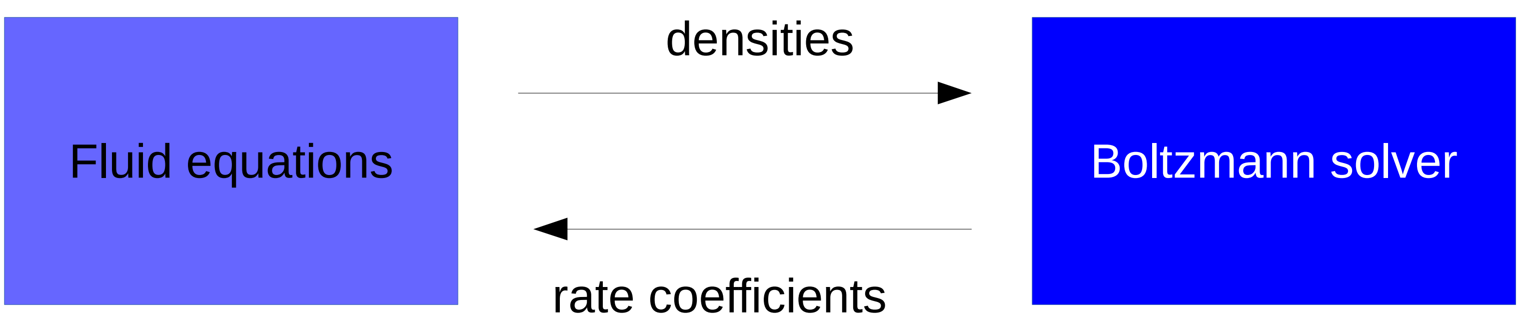
Monte Carlo Model:

Needs cross sections data for the collision frequency:

$$\nu(v) = n_{partner} \sigma(v) v$$

Cross sections in fluid models

- Electron temperature is calculation using the energy balance equation
- Rate coefficients are calculated from the cross sections either for Maxwellian distributions or EEDFs from a Boltzmann-solver. Cross sections are also used in the collision term of the Boltzmann equation.
- Rates are assigned to mesh cells according to the local electron temperature



$$k = \int v \sigma(v) f(v) dv$$

Cross sections in fluid models

Cross sections are also found in the transport parameters (mobility and diffusion coefficient) used in the flux calculation via the collision frequency for momentum transfer

$$\Gamma = -\mu n E - D \nabla n$$

$$\mu = \frac{e}{m\nu} \qquad D = \frac{k_b T_e}{m\nu}$$

Uncertainties in cross sections affect both particle generation and transport!

Cross sections in particle models

Obvious model: check for collision for each particle after each time step; computational expensive

$$P = 1 - \exp\left(-n\sigma(v)v\Delta t\right)$$

To save computational time: Null-collision method: check for collision after random time step based on maximum collision frequency.

$$\sigma_{tot}(v) = \sum \sigma_i(v) + \sigma_{null}$$

Often this is not done for each individual particle. Instead, each time step $P_{max}N$ particles are randomly selected as candidates for collisions.

Cross sections in global models
Electron density

The plasma density is given by the power balance equating the absorbed power with power losses by charged particles:

$$n_0 = \frac{P}{e u_B A \epsilon_T}$$

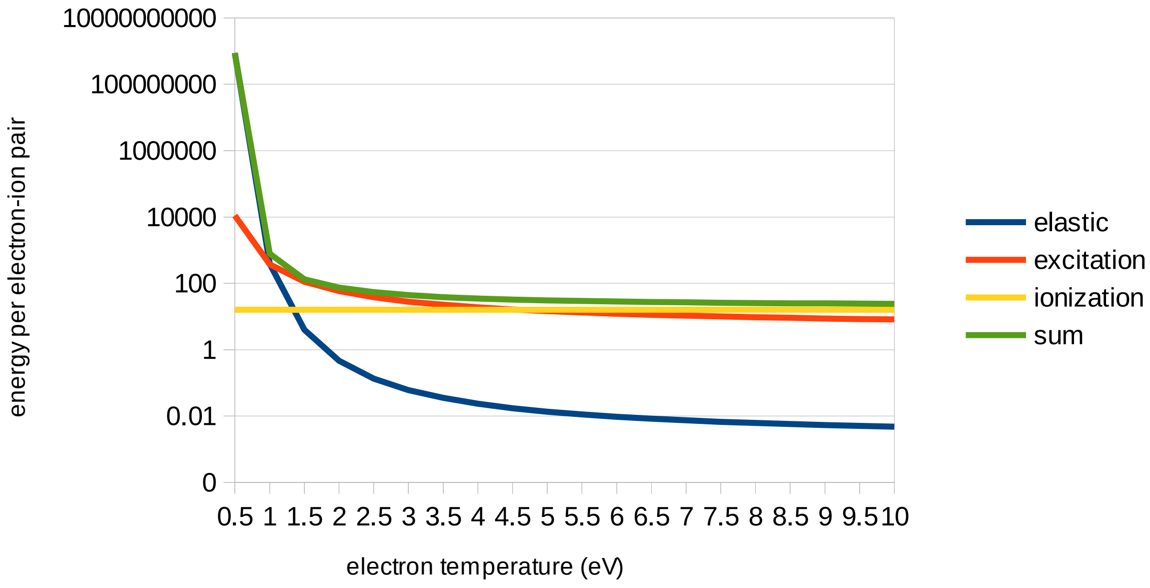
with the energy loss per ion-electron pair ε_T which can be spilt up into collisional losses and losses at the wall.

$$\epsilon_T = \epsilon_{coll} + \epsilon_e + \epsilon_{ions}$$

$$\epsilon_{coll} = \epsilon_{ion} + \sum \frac{\epsilon_i k_i}{k_{ion}}$$

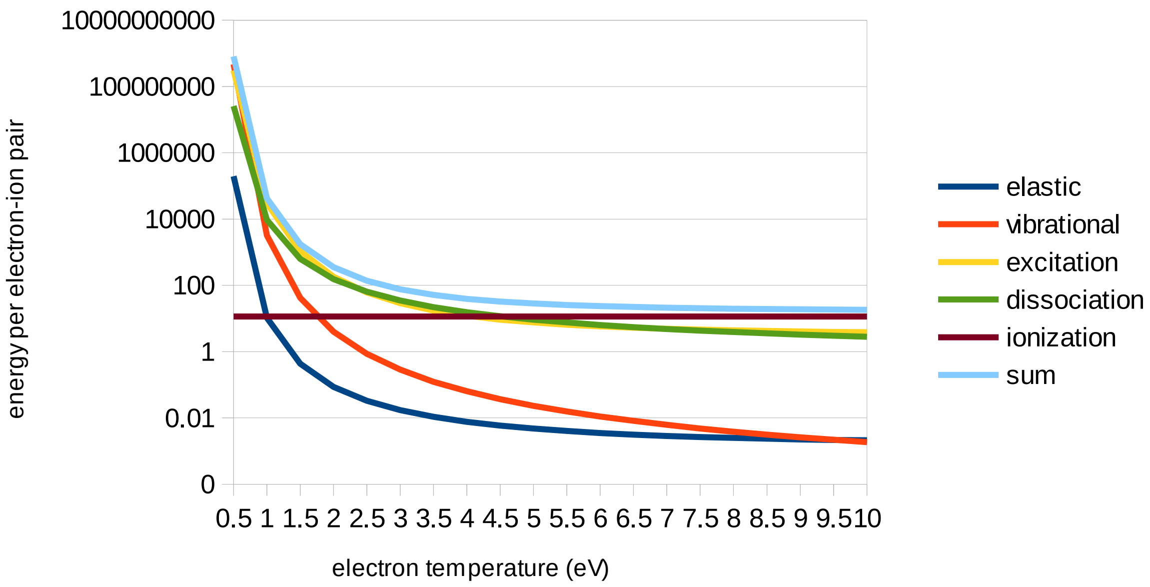
Thus, the plasma density does not only depend on the ionization cross sections, but also on the cross sections for elastic collisions, excitation, dissociation etc.

Examples



In argon, energy losses are dominated by excitation. So these reactions need to be included even if the excited states themselves are not taken into account.

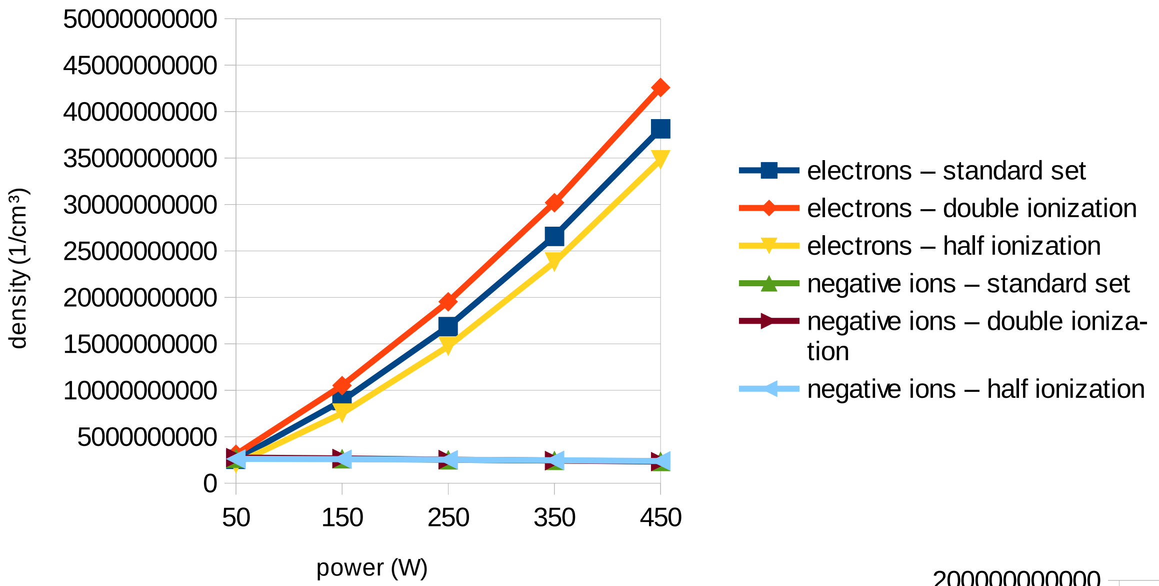
In molecular gases, dissociation dominates. At low electron temperatures, vibrational excitation also contributes significantly.



Note that although elastic collision do not contribute significantly to the energy loss they are vital to calculate the shape of the EEDF and trajectories in particle models.

Ionization of O_2

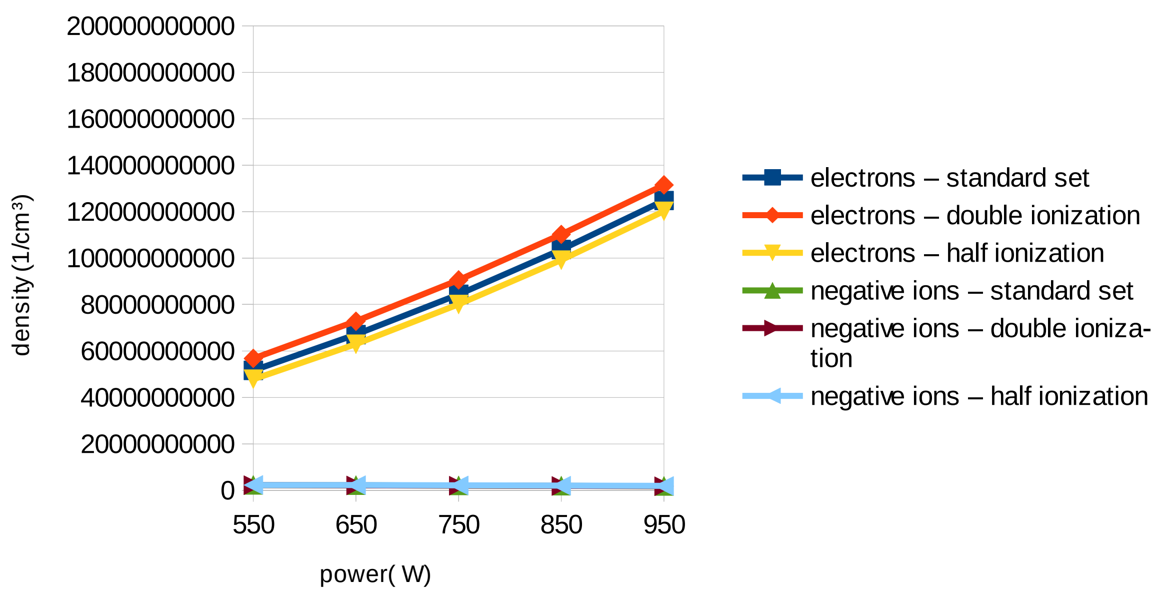
Influence of uncertainties



ICP discharge at 50 mTorr simulated with Q-VT

Large difference (about 30%) at low powers/low degrees of dissociation

Smaller difference (about 10%) at high powers/high degrees of dissociation

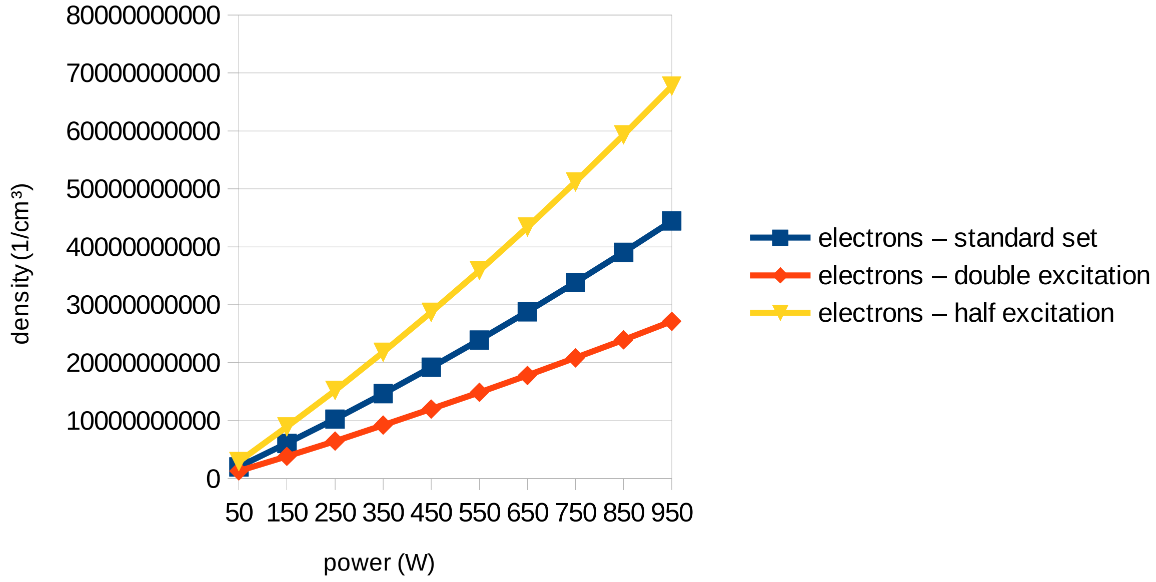


In reactive plasmas, cross sections for the dissociation products are often more important than for the feed gases.

But also harder to obtain.

Excitation of O_2

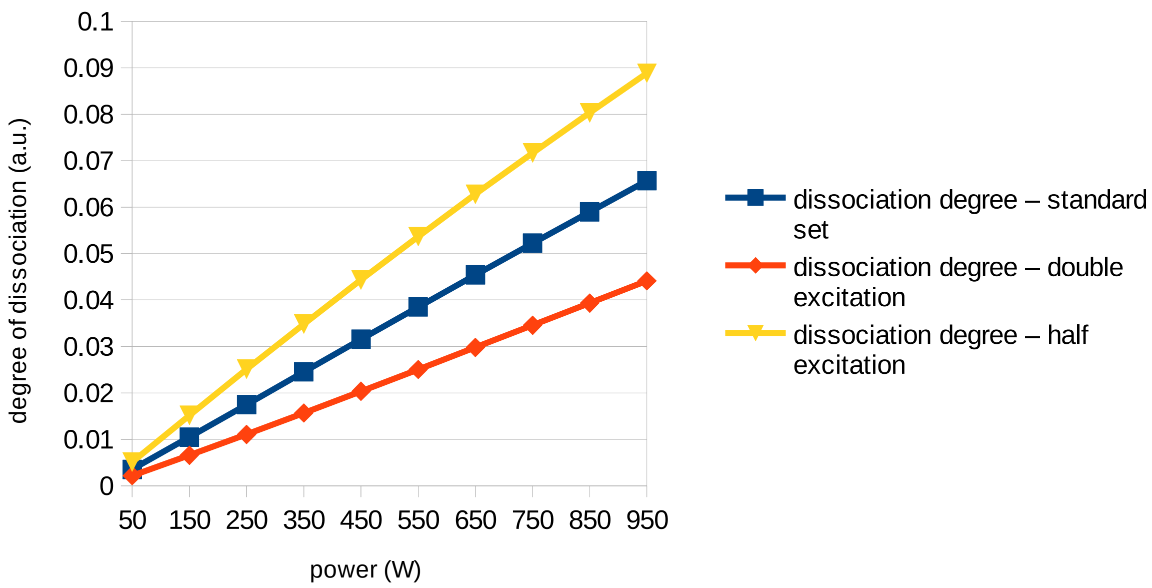
Influence of uncertainties



The excitation cross sections have a larger impact on the electron densities than the ionization cross sections! The difference is more than 100%.

The same is seen in connected parameters such as the degree of dissociation.

Consequences of uncertainties in cross sections are not always straight forward.



Cross sections in global models
Electron temperature

The electron temperature is given by the particle balance equating electron gains with electron losses:

$$V n_e \Sigma k_{ion,i}(T_e) n_i = \Gamma_e A = n_e u_b(T_e) A$$

This equation is only valid for electropositive gases with diffusion as the only loss mechanism and electron impact as the only source. In this case, the electron temperature is independent from the electron density and thus the power. With regards to cross sections, there is only a dependence on the ionization cross section.

For more complicated gas mixtures or high pressures, we would need to include other terms such as dissociative attachment, dissociative recombination, Penning ionization, which may introduce a dependence on the plasma density and other cross sections.

Attachment

$$k_{DA}(T_e) n_e n_g V$$

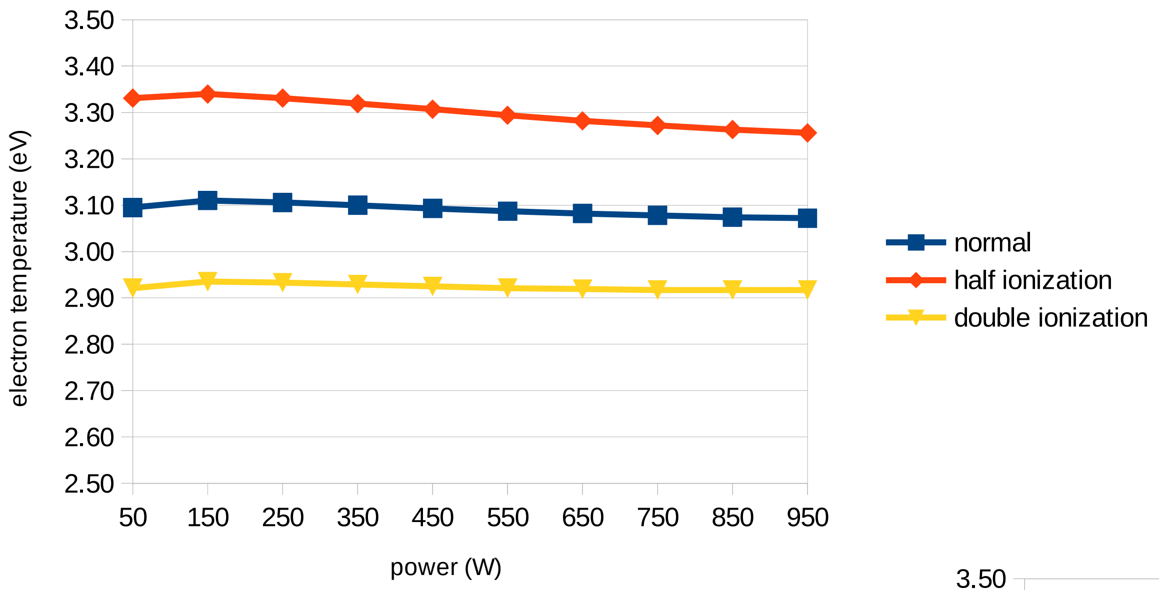
Recombination

$$k_{DR}(T_e) n_e n_i V$$

Penning ionization

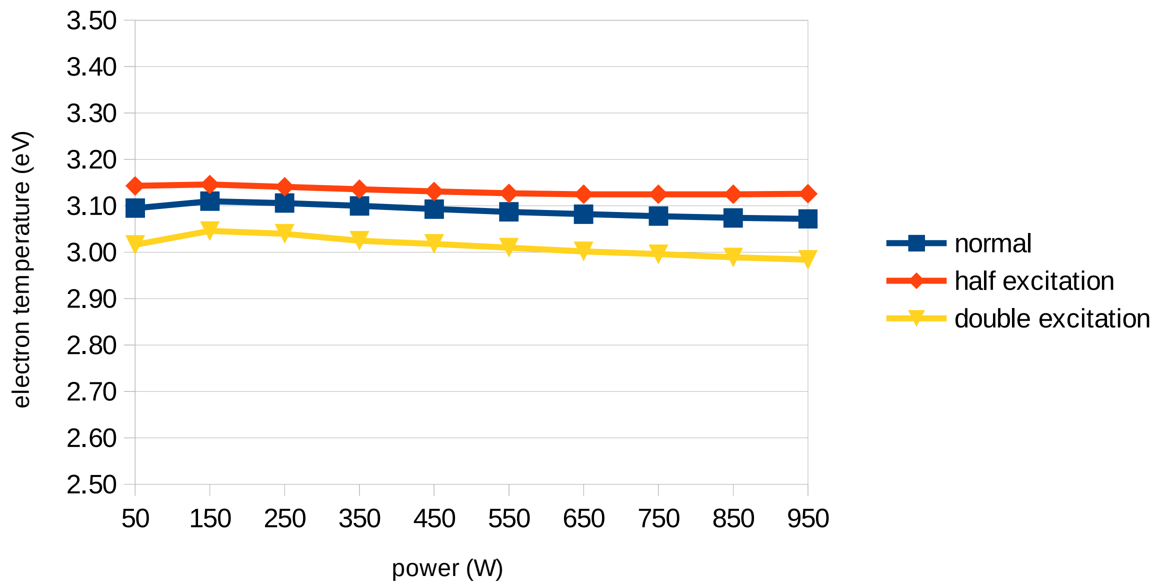
$$k_{penn} n_m (n_e, T_e)^2$$

Influence of uncertainties
Electron temperature



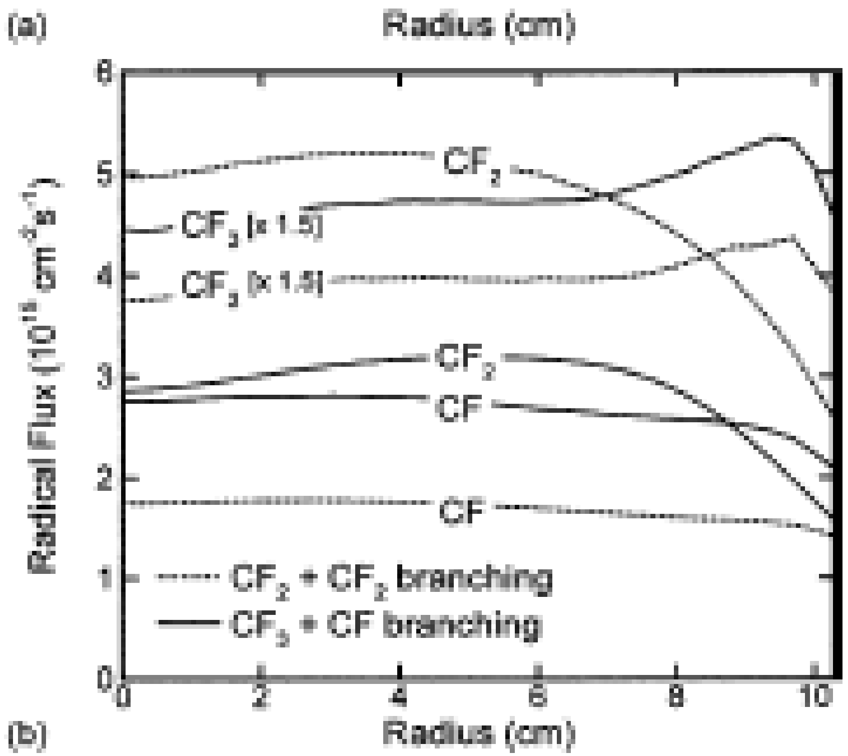
Uncertainties in the ionization cross section do indeed affect the electron temperature.

On the other hand, uncertainties in the excitation cross sections only have a minor influence.



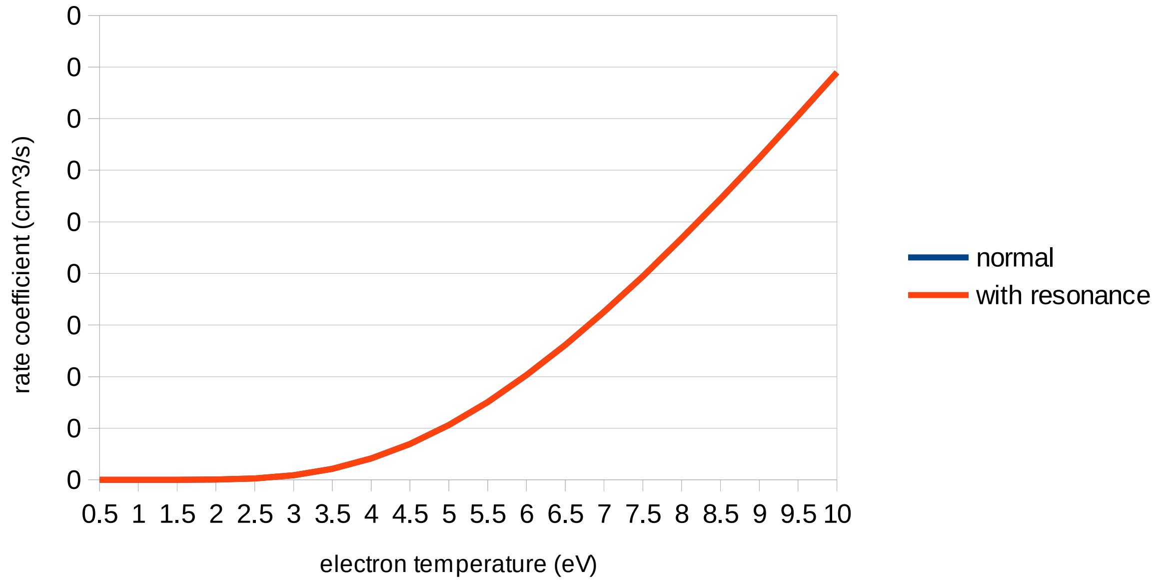
Other uncertainties
Branching ratios

Branching ratios for dissociative ionization can be estimated based on experimentally obtained mass spectra. Branching ratios for neutral dissociation have to be guesstimated when unknown.



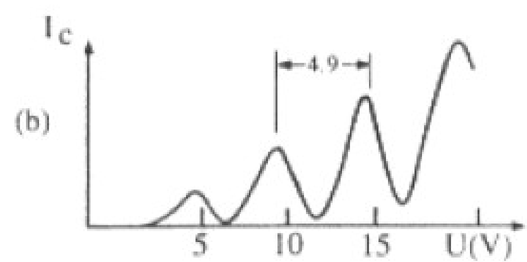
A V Vasenkov and Mark J Kushner, *J. Appl. Phys* **95** (2004)

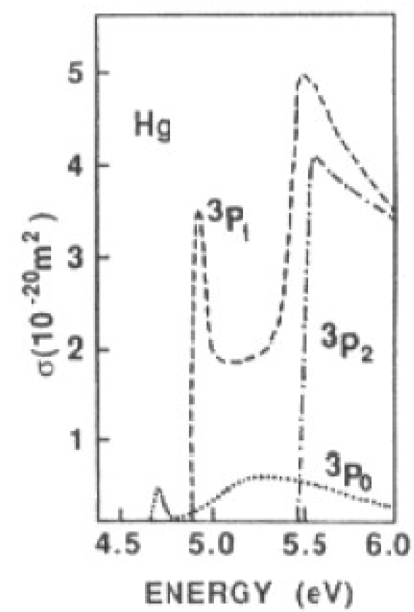
Other uncertainties
Resonances



Resonances do not play such a large role when using rate coefficients as the information about them is lost by the integral.

If cross sections are used directly, they can have a substantial influence. Think of the Franck-Hertz experiment which only works so well because of a resonance in the mercury excitation cross section.





G F Hanne, *Amer. J. Phys.* **56** (1988) 696

Summary

- “Crash source” in plasma modelling focused on usage of cross sections
- The in general not straightforward influence of uncertainties in cross section values was demonstrated.
- Uncertainties in branching ratios and resonances were shortly discussed.

Thank you for your attention