Quantemol Global Model as a tool for plasma chemistry analysis and optimisation

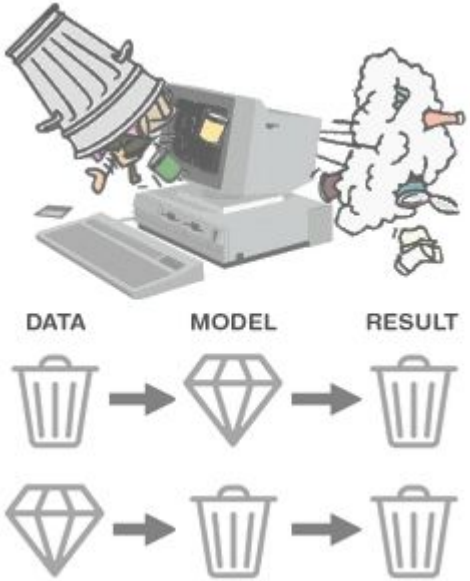
Dr Sebastian Mohr

Introduction

Simulations are widely used in both academic and industrial settings to gain insight into and optimize plasma processes.

The success of such investigations hinges on having good data for the chemical processes in form of:

- Cross sections
- Rate coefficients
- Coefficients for surface processes

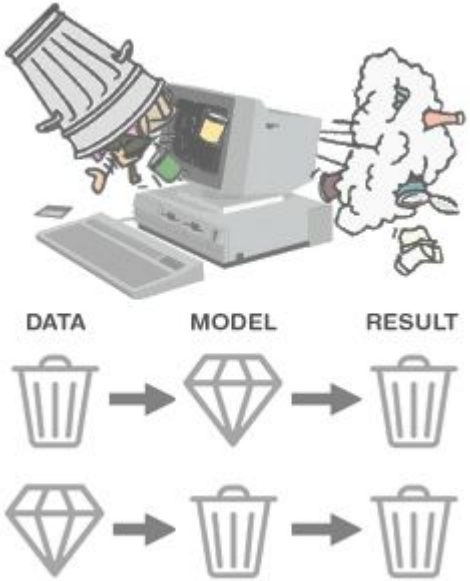


Data can be found in individual publications or databases such LXCat, UMIST,KIDA,NFRI,NIFS, or QuantemolDB.

Introduction

Important questions for a set construction:

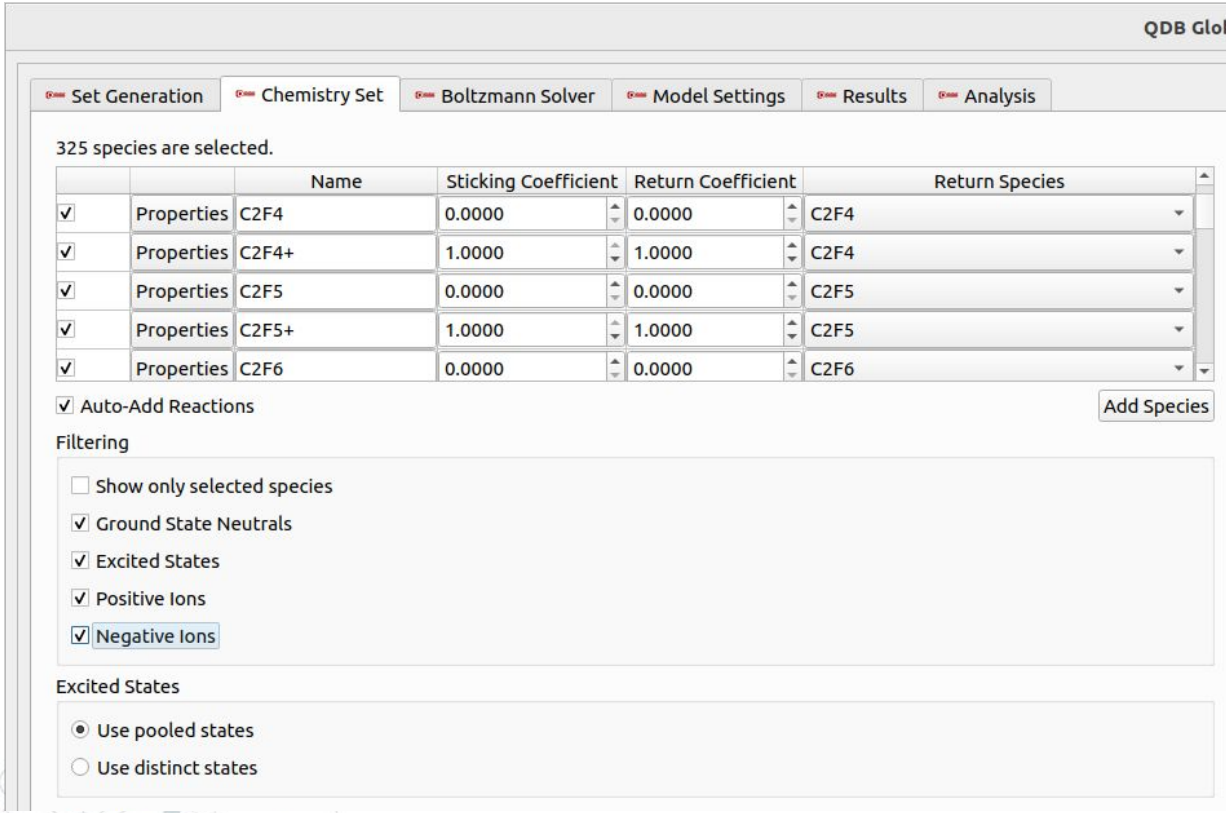
- Does it cover all important species and reactions?
- Are there species/reactions which can be neglected to save computational resources?
- How do uncertainties impact the simulation result?



Constructing a set with the QDB desktop app

Choose feed gases; this will download all species and reactions in QDB which can originate from these feed gases in up to 5 reaction steps.

Selecting species

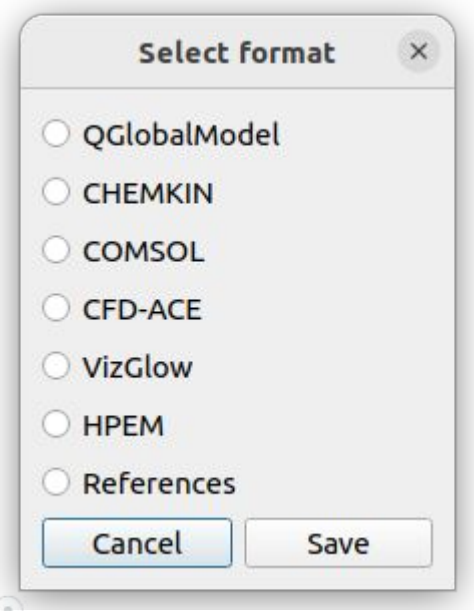


You can then select the species you want to include in your model. For example, you can exclude species which only form at high pressures (Ar_2^+, O_3) or minor ions (O_2^-).

You can add species (and reactions) which are not (yet) part of QDB to complement your set, e.g. to investigate unstudied feed gases.

The app also checks for important missing reactions such as ion-ion recombination and gives the option to add these automatically.

Export your custom set



The chemistry sets can be exported in formats compatible with widely used multi-dimensional plasma simulations.

If you are interested in a specific additional format, we are happy to add it to the selection.

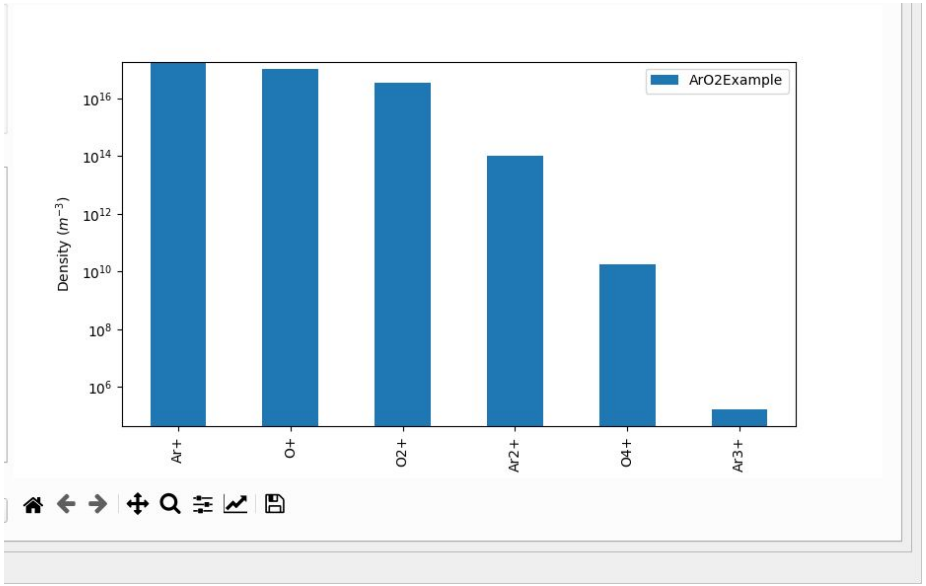
Testing your set with a global model

quantemol

To check whether the set is suitable for given process parameters, you can run it through global model with these options:

- Use rate coefficients from Maxwellian EEDFs or calculated by a Boltzmann solver
- Constant power supply or pulsing between two power levels
- Set gas temperature or self-consistent calculation
- Automatic parameter variation, e.g. power, pressure, flows

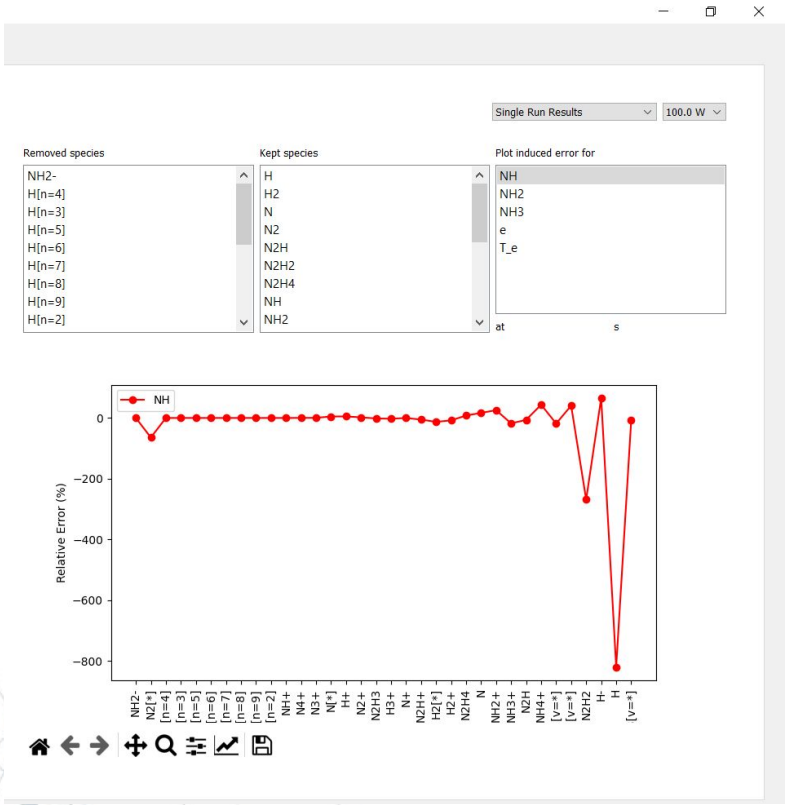
Optimizing sets - Manual reduction



For simple sets, running tests and looking for species with low densities can be the easiest way to identify negligible species. For more complex sets, this approach, however, suffers from:

- Manually removing lots of species and running tests
- “Hidden” reactions of low density species

Optimizing sets - Automatic reduction



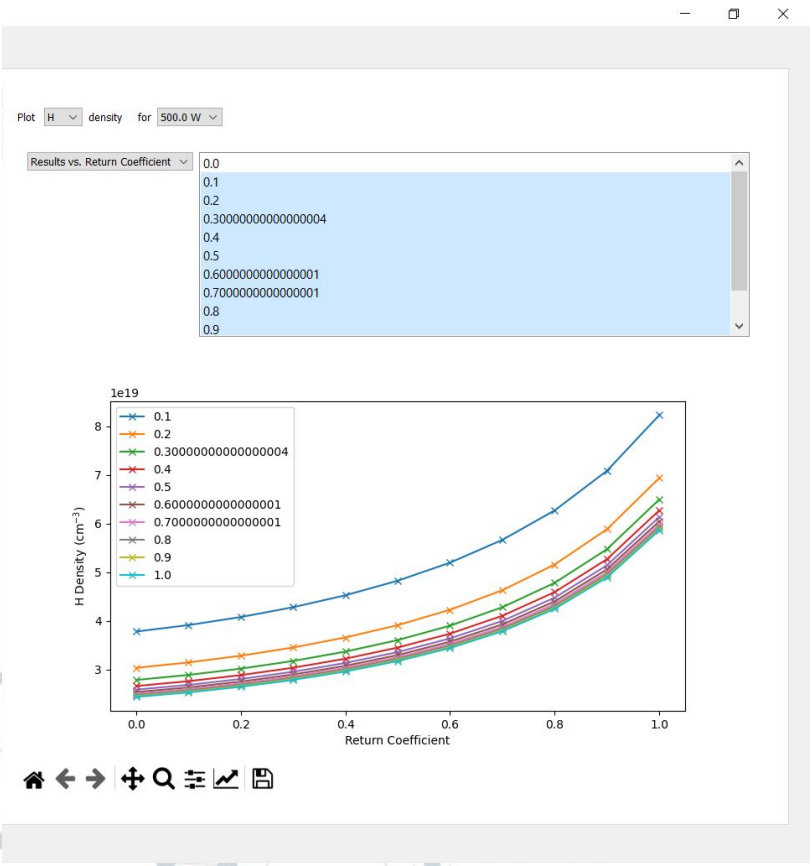
The desktop app offers an automatic reduction; this first ranks the species based on the reaction network with regards to their influence on the densities of key species. In a second step, test runs with single removed species are done and the results checked against an allowed error.

Optimizing sets - Automatic reduction

	100.0 W	200.0 W	300.0 W	400.0 W	500.0 W
H[n=9]	0.46 % in e	-0.87 % in NH3	-3.89 % in NH2	-6.08 % in NH3	-4.89 % in NH3
H[n=2]	0.93 % in e	-1.98 % in NH3	-6.63 % in NH3	-12.04 % in NH3	-22.75 % in NH3
NH+	0.96 % in e	-2.87 % in NH	-3.32 % in NH2	-5.21 % in NH3	-2.53 % in NH3
N4+	0.84 % in e	-2.08 % in NH	-5.77 % in NH3	-2.99 % in NH3	-4.96 % in NH3
N3+	0.87 % in e	2.06 % in e	-6.88 % in NH3	-5.22 % in NH3	-8.75 % in NH3
N[*]	4.81 % in NH	9.55 % in NH2	32.23 % in NH2	47.23 % in NH2	56.28 % in NH2
H+	5.08 % in NH	9.98 % in e	11.18 % in e	-14.38 % in NH3	-31.26 % in NH3
N2+	6.72 % in e	7.20 % in e	8.28 % in e	17.76 % in NH3	27.80 % in NH3
N2H3	6.74 % in e	-2.76 % in NH	-1.82 % in NH	-1.32 % in NH	-1.30 % in NH2
H3+	6.76 % in e	10.10 % in e	8.33 % in e	2.03 % in e	2.59 % in NH2
N+	12.40 % in e	-13.20 % in NH2	-11.13 % in NH3	-10.62 % in NH3	-17.47 % in NH3
N2H+	6.93 % in e	10.13 % in e	27.73 % in NH3	68.75 % in NH3	68.36 % in NH3
H2[*]	-12.91 % in NH	-11.64 % in NH	11.63 % in NH3	5.72 % in NH2	6.92 % in NH2
H2+	15.56 % in e	21.85 % in NH2	19.82 % in e	10.66 % in NH2	11.16 % in NH2
N2H4	-17.37 % in NH2	-9.83 % in NH2	-5.20 % in NH2	-2.50 % in NH2	-2.52 % in NH2
N	-28.06 % in NH2	-164.16 % in NH2	-197.43 % in NH2	-281.46 % in NH2	-365.95 % in NH2
NH2+	25.67 % in NH	28.90 % in NH	-31.16 % in NH2	-28.32 % in NH2	-27.42 % in NH2
NH3+	22.87 % in e	27.04 % in NH2	-40.12 % in NH3	-71.12 % in NH3	-111.64 % in NH3
N2H	-11.82 % in NH2	7.30 % in e	-22.20 % in NH	-20.64 % in NH	21.36 % in NH2

The desktop app offers an automatic reduction; this first ranks the species based on the reaction network with regards to their influence on the densities of key species. In a second step, test runs with single removed species are done and the results checked against an allowed error.

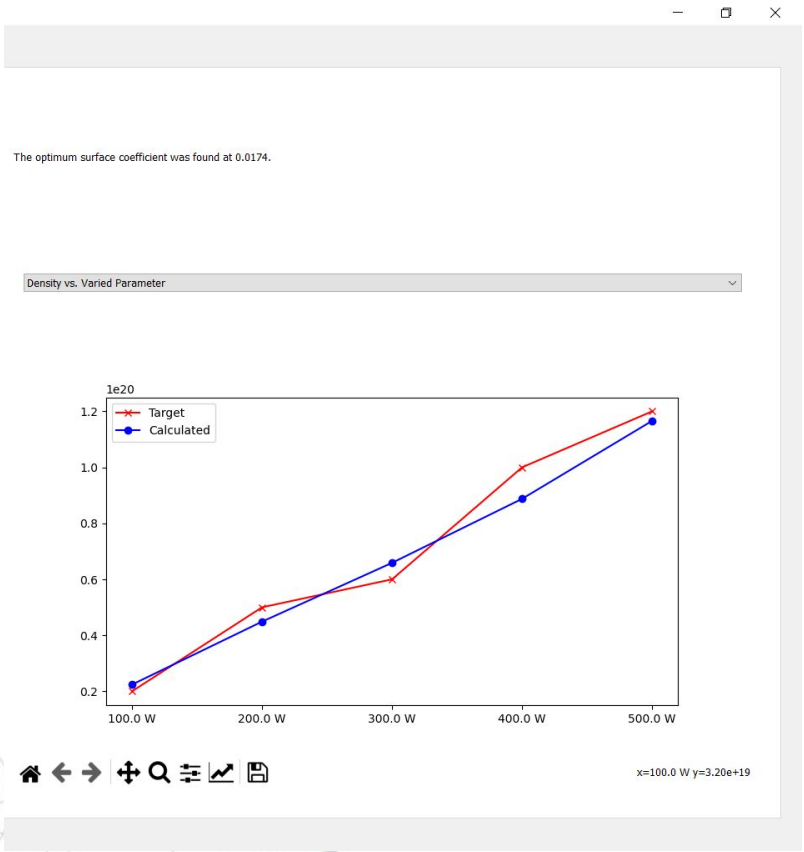
Optimizing sets - Investigating uncertainties



It is quite unlikely to find precise data for all possible reactions in both gas phase and at surfaces. Especially probabilities for surface reactions are notoriously uncertain.

The QDB desktop app offers an automatic variation of surface coefficients to get some insight how uncertainties can influence the results of a simulation

Optimizing sets - Investigating uncertainties



It is quite unlikely to find precise data for all possible reactions in both gas phase and at surfaces. Especially probabilities for surface reactions are notoriously uncertain.

If densities for a set of parameters are known, you can also find the surface probabilities which best fit the known densities.

Summary and Outlook

The QDB app offers:

- Fast generation of comprehensive sets based on data in QDB
- Option to add missing species/reactions
- Checks for vital missing reactions
- A global model/Boltzmann solver to make test runs
- A reduction tool to quickly find species which can be neglected for specific parameters
- Automatic variation/calibration for surface coefficients
- Export to commonly used simulation software (COMSOL, ChemKin, HPEM, VizGlow,CFD-ACE+)

We will add:

- More export options (ZDPlaskin, Tech-X)
- Additional checks (asymmetric charge exchange)
- Additional coefficient variation and calibration
- Tools for missing data estimation, e.g. ML algorithm for heavy particle reactions.
- API to LiDB to automatically add radiative decay of excited states

Hands on session

quantemol

Please use this key to start the desktop app:

PT6JFSCQ4W4FQTHL