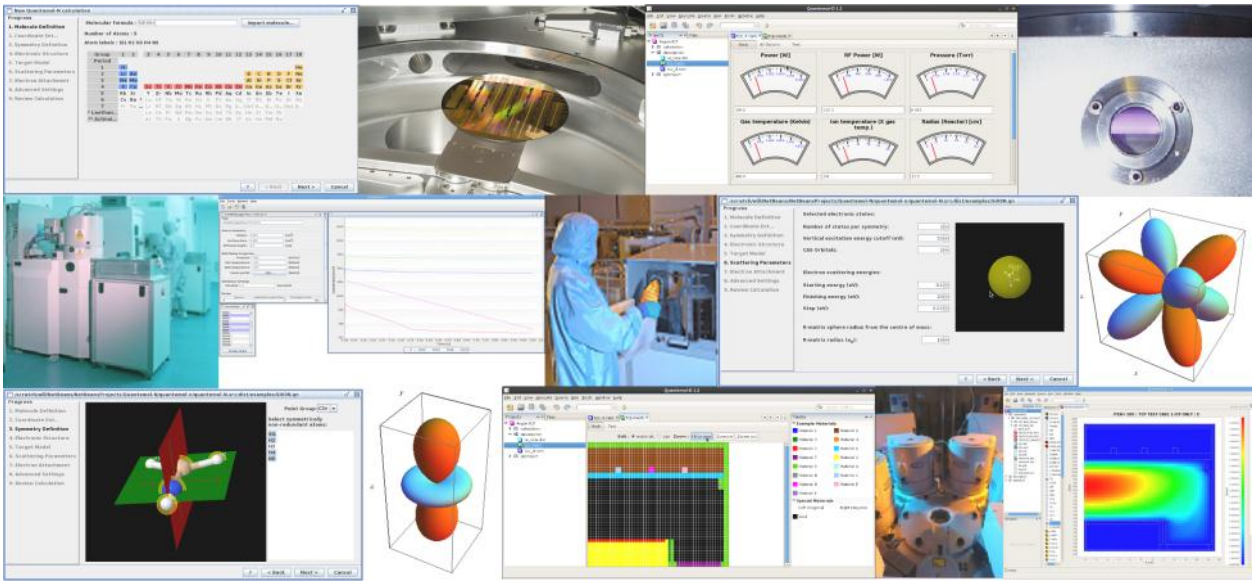
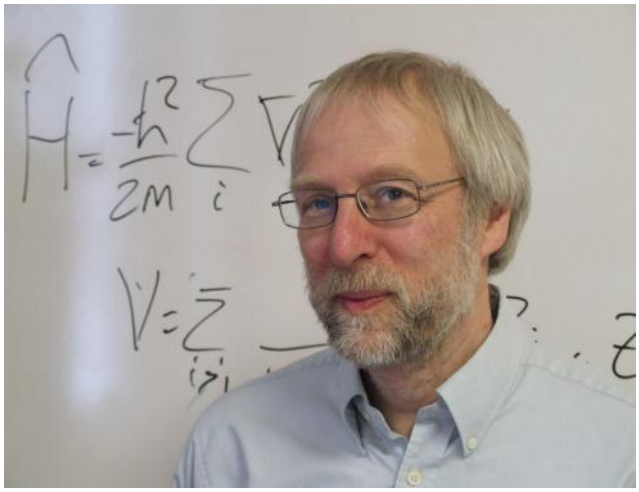
Quantemol



2012 Brochure

Company Profile

Quantemol is based at University College London and was initiated by Prof. Jonathan Tennyson FRS (right) and Dr. Daniel Brown. The company develops unique software tools that bring accessibility to highly sophisticated research codes. Quantemol-N allows the UK molecular R-matrix code, which is used to model electron polyatomic molecule interactions, to be employed quickly with reduced set up times. Quantemol-D brings an unsurpassed user experience to the world-renowned plasma simulation codes of Prof. Mark Kushner from the University of Michigan. With an expanding research team Quantemol is also able to offer consultancy projects which are carried out by world leading scientists in their respective fields.



Company's mission statement is:

"To serve our users in industry and academia to simulate complex processes more efficiently, reliably, accurately and cost-effectively and thereby accelerate technological and scientific innovation".

Client Testimonials

Prof. Nigel Mason OBE, Department of Physics and Astronomy, The Open University:

"Quantemol-N provides much needed electron-molecular scattering data, particularly for molecules and molecular species that are difficult to isolate and study experimentally — such as the fluoro-carbon radicals. Such molecular data is in high demand from both academia and industry. Quantemol-N's uniqueness lies in the fact that one does not have to be a specialist in the underlying scattering theory in order to utilise it."

Dr Tom Field, Centre for Plasma Physics, School of Maths and Physics, Queen's University Belfast:

"Good software for finding low energy electron-molecule scattering resonances with excellent user support."

Quantemol-N

Background

Collisions of low-energy electrons with molecules control many aspects of the environment and modern technologies. For example:

- Initiating plasma etching processes.
- Controlling the action of lasers.
- Controlling the ignition of internal combustion engines.
- Determining edge effects in fusion plasmas.
- Causing radiation damage in biological tissue.
- Dictating the behaviour of the earth's ionosphere.

Measurements of these collisions are both expensive and difficult to perform, and their theoretical determination requires the use of sophisticated procedures based on the application of quantum mechanics.

The new Quantemol-N code provides an expert interface for driving the sophisticated UK molecular R-matrix code. By specifying a few easily determined molecular parameters the user can obtain collision cross sections, excitation cross sections and rates for electron

Quantemol-N Products:

Quantemol-N is available in both standard (SE) and enterprise (EE) editions. Enterprise edition includes all the features of the standard edition with the addition of a batch job facility, and a parallel version of SCATCI (which significantly reduce calculation times on multicore machines). It also includes an even larger suite of molecular examples (currently ~40) so the user can get started immediately.

What does Quantemol-N do?

Calculates a variety of observables for electron molecule collisions including:

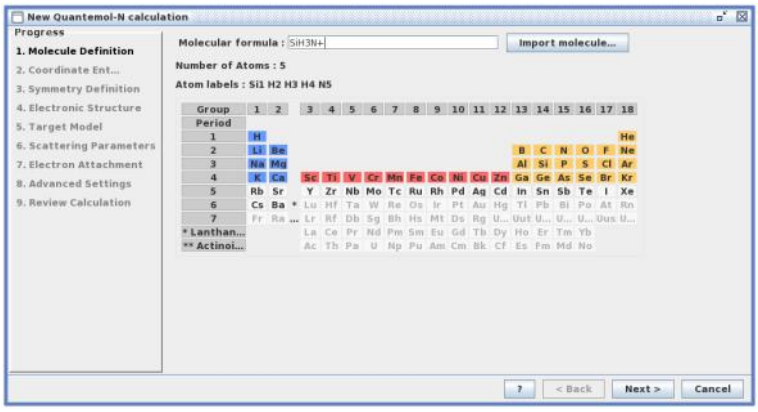
- Total cross-sections
- Electronic excitation and dissociation cross sections
- Resonance parameters
- BEF ionisation cross-sections
- Dissociative attachment cross-sections estimator
- Differential cross-sections
- Momentum-Transfer cross-section

The key advantages of Quantemol-N?

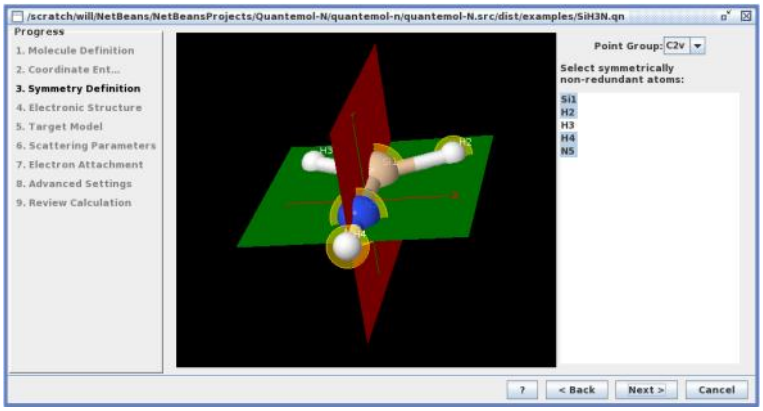
- Based on the world leading UK molecular R-matrix code
- Easy to use graphical interface
- Results presented in a flexible, user friendly form
- Can run on a desktop machine or laptop

What range of problems can be tackled with Quantemol-N?

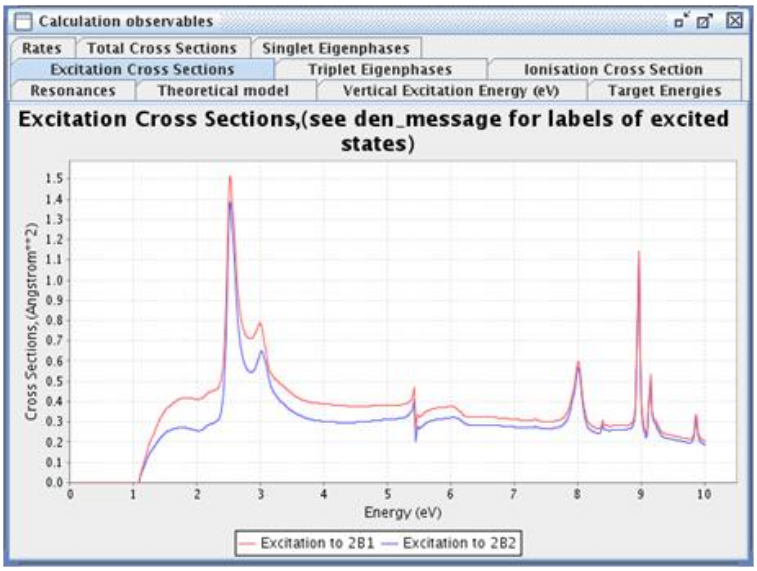
- Closed shell molecules.
- Open shell molecules, radicals.
- Neutral and positively charged species.
- Molecules with up to 17 atoms tested.



Quantemol-N provides a simple to use graphical interface for easy simulation set up.



The user is guided through the input stage with a series of easy to complete fields. This is aided by the use of a step by step wizard and tutorial system.



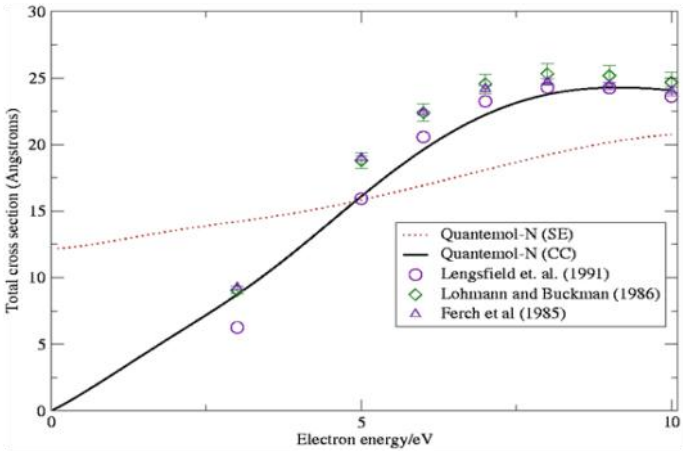
Results are automatically plotted and presented in a tabbed results window. These can be quickly called up again at a later date in the exact same format. The data is also available as text files for post analysis and use in models.

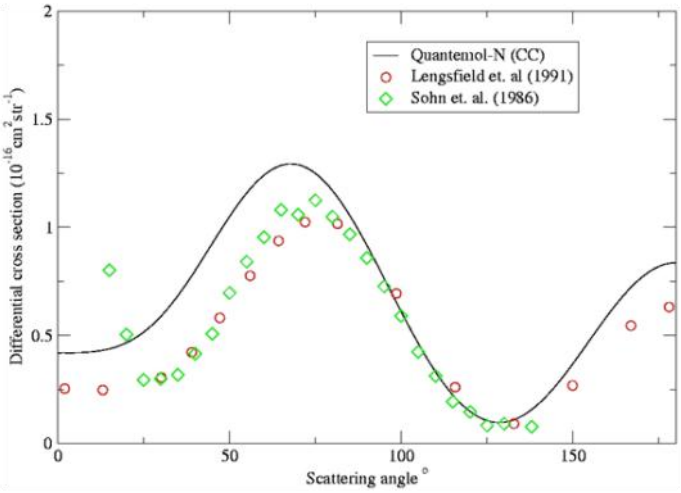
Please note all Quantemol software requires at least: Linux x86, 1 GB RAM (2GB for large calculations), 10 GB free disk space, Installation of the official Java virtual machine and JRE v.1.6.0.

Quantemol-N

TRUSTED RESULTS

Total cross-sections of CH_4. Here the Quantemol-N results (black & red lines) are shown with theory (Lengsfield et. al., circles) and experiment (Lohmann & Buckham, diamonds, Ferch et.al., triangles)

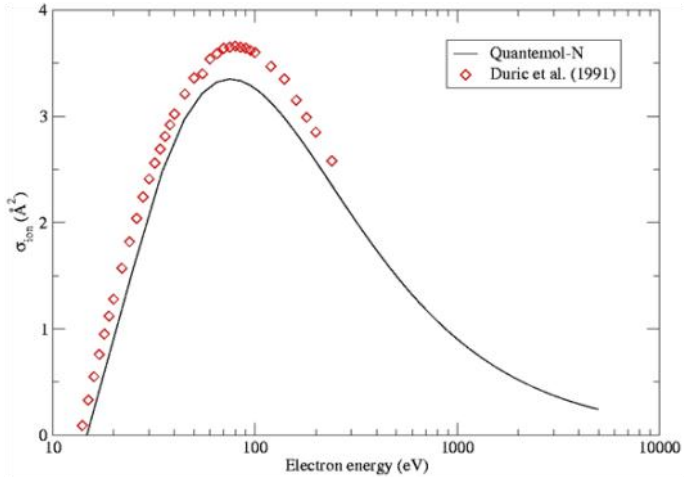




Differential cross-section of CH_4, derived from Q-N data. Here we can see the Quantemol-N (black) results when compared to theory (Lengsfield et. al., red) and experiment (Sohn et.al., green).

Note: Differential cross-sections can be produced from Q-N directly upon user based consultation.

BEB ionisation cross-section of CH_4. Here the Quantemol-N data is compared with experimental data (Duric et.al., red).



Quantemol-D

Background

More and more emphasis is now being placed upon people to save, with industry looking to become more efficient both in terms of waste products and costs. This is particularly applicable to huge scale world-wide sectors such as silicon chip manufacturing.

The development of new machinery underpins the production of new technology, as without newer, more advanced machines large scale manufacturing is not possible. Traditionally the development of such machinery is costly and wasteful, with many iteration cycles throughout the design process.

With the Quantemol-D software the machine design can be driven by high-level physics based simulation, leading to fewer physical iterations of the machine. Thus a cheaper, more efficient design process is created that also has less impact on the environment.

What does Quantemol-D do?

Quantemol-D is an expert software system for the simulation of industrial plasma processes. Quantemol-D builds upon the respected Hybrid Plasma Equipment Model (HPEM) codes developed by leading plasma physicist Professor Mark Kushner, adding a number of needed systems for both expert and non-expert users.

With Quantemol-D it is possible to:

- reduce wafer start ups
- develop more efficient etch and deposition processes
- model the design of new plasma sources

In other words it can create a cheaper and more efficient machine optimization process.

What are the advantages of Quantemol-D?

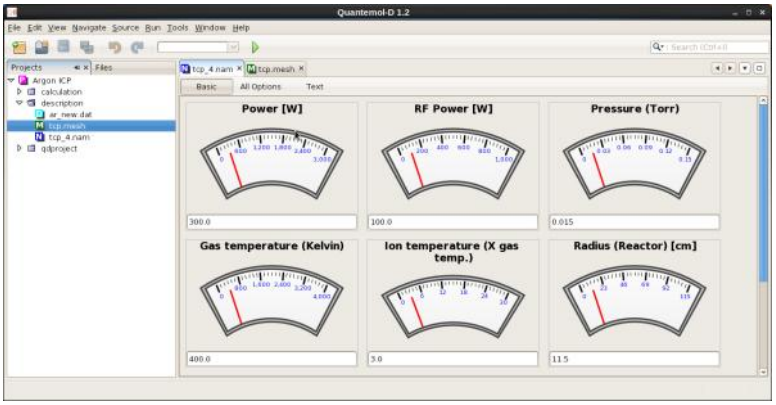
- Hybrid Plasma Equipment Model simulation system driver
- Full HPEM and Tecplot file compatibility
- 1D visualisation of wafer fluxes and plasma kinetics
- 2D reactor scale visualisation of species and plasma properties
- Reactor “painter” for machine design
- Live, syntax checked, colour-coded views of HPEM input files
- Job runner with single and simultaneous queuing and execution of simulations
- Project views, for managing multiple machines & simulations
- Example library including numerous reactors and chemistries

Applications

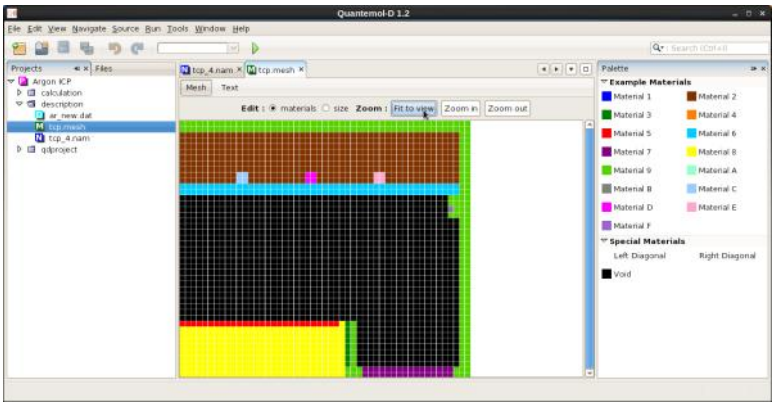
- Plasma reactors
- Plasma assisted deposition
- Deep reactive ion etch

Requirements

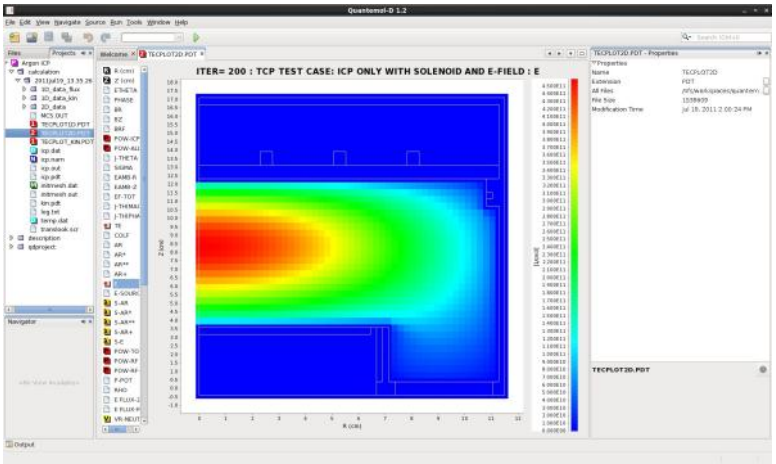
Please note that Quantemol-D is an expert system for the HPEM codes. If you currently do not have access to the HPEM codes, we can provide you with them. Please contact us for more details at sales@quantemol.com



Machine settings can be edited either via text files or by use of the intuitive design view, aiming to replicate the feel of a physical machine.



Graphics palette style mesh design, paint your machine design with materials of your choice, each will have its own individually designed properties.



View simulation outputs directly within Quantemol-D. This allows faster analysis and thus dramatically reduces the initial set up times.

Advanced views are available for the experienced HPEM users. Full documentation is included to help user learn the more advanced features of the program.

Please note all Quantemol software requires at least: Linux x86, 1 GB RAM (2GB for large calculations), 10 GB free disk space, Installation of the official Java virtual machine and JRE v.1.6.0, **Quantemol-D** requires HPEM

Quantemol-P

Background

The etching of silicon wafers using gaseous plasmas underpins the rapid advance in computer technology that has powered the global economy, and will continue to do so for the foreseeable future. Currently, experimental testing is used to establish the relevant plasma mixes to generate the desired etch. Such testing is an expensive and time-consuming process even for relatively minor improvements in the processes. With Quantemol-P much of this process can be done outside of the reactor at reduced cost and improved efficiency.

One of the key fundamental processes in etch plasmas are collisions of low-energy electrons with molecules. But for many years the associated molecular data has been missing from the plasma researchers toolkit. Measurements of these collisions are both expensive and difficult to perform, and their theoretical determination requires the use of sophisticated procedures based on the application of quantum mechanics.

The key advantages of Quantemol-P?

- Contains a large database of molecular data.
- Can utilises Quantemol-N and the R-Matrix method to obtain molecular data.
- The expert system has a sophisticated understanding of the plasma chemistry.
- Requires only basic input, equivalent to the definition of a plasma recipe.
- Easy to use graphical interface.
- Very fast calculations
- Results presented in a flexible, user friendly form.

What does Quantemol-P do?

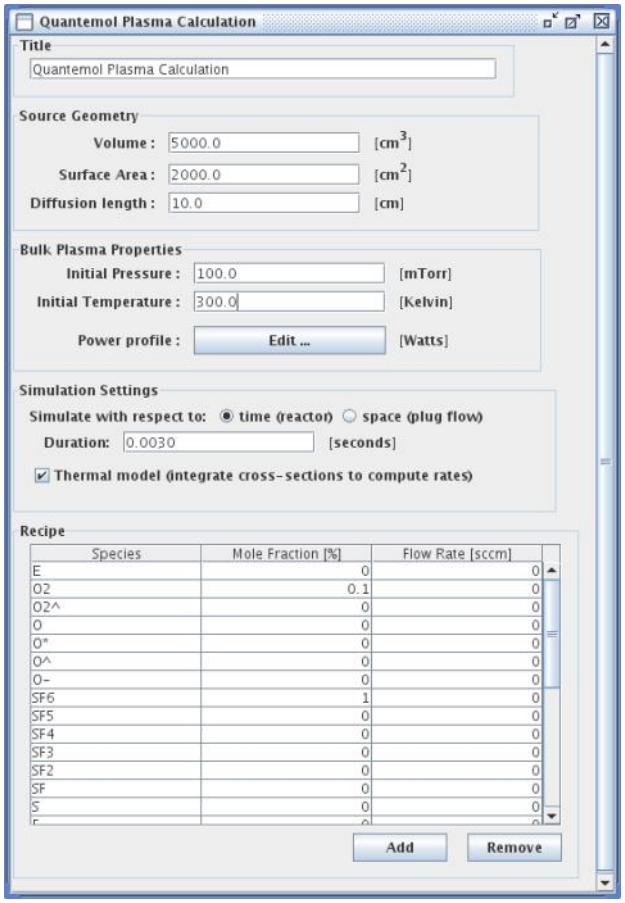
Quantemol-P assists in the research for new plasma recipes and optimizes given processes by simulating etch machines. The simulation inputs used by Quantemol-P match those of the plasma processing tools: e.g. power, pressure, gas flow rate, time, volume.

Quantemol-P couples molecular data with models of the plasma, providing full information of what is happening, giving the process engineers an insight into the problem.

A variety of technical plasmas can be simulated including plasma etch reactors, plug-flow reactors and well-mixed reactors.

Applications

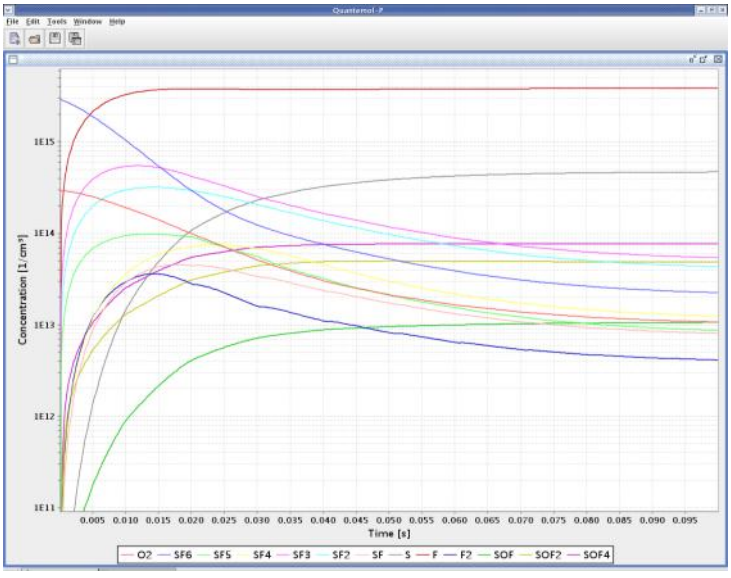
- Plasma reactors
- Plasma assisted deposition
- Deep reactive ion etch
- Atmospheric pressure plasma jets



Quantemol-P provides a simple to use graphical interface.

The user is guided through the input stage with a series of easy to complete fields.

The user needs only specify a few basic inputs on the plasma properties (volume, power, pressure, temperature) and on the plasma chemistry (initial chemical composition of the plasma, flow rates, mole fractions).



Results are automatically plotted, and are also available as text files for post analysis and use in models.

Standard outputs are produced and plotted automatically. These outputs comprise of concentration of the various species, gas temperature, gas pressure as a function of time (for a well-mixed plasma reactor) or space (for flowing plasmas).

Please note all Quantemol software requires at least: Linux x86, 1 GB RAM (2GB for large calculations), 10 GB free disk space, Installation of the official Java virtual machine and JRE v.1.6.0.

CONSULTANCY

Here at Quantemol as well as providing innovative user friendly software for clients we also offer a unique consultancy service. With our suite of software and highly skilled engineers we are able to provide complete and reliable research projects and studies. These can take the form of small quick calculations as well as large scale development projects. The typical types of consultancy work undertaken are as follows:

- Calculations of specific electron—molecule cross sections
- Industrial plasma tool design
- Plasma process parameter optimisation
- Plasma chemistry creation
- Plasma etching and deposition calculations
- General multiphysics problems (CFD, etc..)

Quantemol has successfully undertaken several large consulting projects. A Distinctive feature of our service is that we work with non-standard requests, using various computational methods and literature research in order to achieve the results within deadlines. We always strive to deliver a value to our customers and prioritise research tasks according to the clients development needs. A formal completion report is produced at the end of all work including the results (raw data, graphs, movies etc..) ready to be used and presented by customers. We work on a basis of complete confidentiality and understand the importance of protecting intellectual property.

Your opportunities with Quantemol

At Quantemol we take care to make sure the relationship between the company and the user is one which continues from the initial consultations through to the post-sales support. This has led to the development of many new features in our programs, and indeed the progression of the programs themselves. If you feel that our product suits your needs but you would like something in particular, please do not hesitate to contact us at sales@quantemol.com in order to start up a dialogue or make a query. We believe this is the best way to create and maintain strong company-user relations.

For **Quantemol-D** we can provide tailor-made tool designs upon consultation, as well as varying degrees of project work for your simulation. Alternatively we can provide training in the software to enable users to look for trends and optimization parameters on their own.

For any more information on any of our products or if you would like to arrange **a web-demonstration**, please feel free to contact us using the details given below.

For more information, or to order a license, please contact:

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