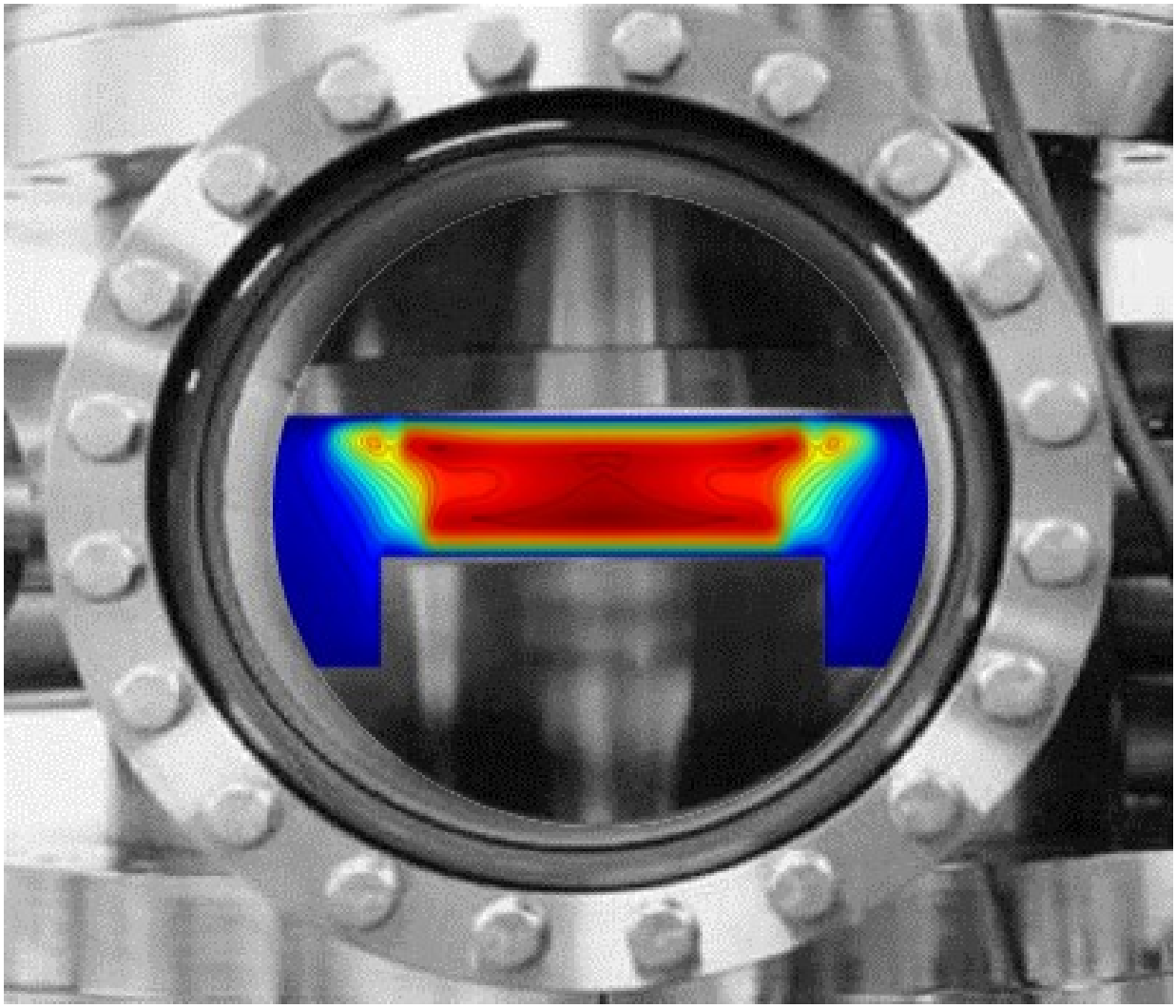
QVT

Virtual Tool



The Plasma Simulation System 2022 Brochure

Quantemol

www.quantemol.com

Company Profile

Quantemol was founded by Prof. Jonathan Tennyson FRS (right) and Dr Daniel Brown in 2004. We develop unique software tools that bring accessibility to highly sophisticated research codes.

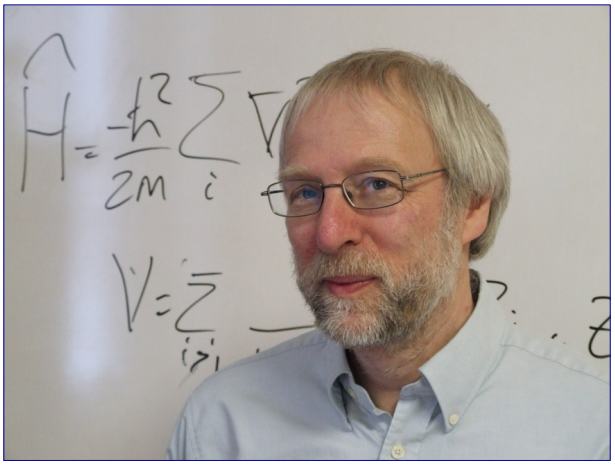
Quantemol-N allows the UK molecular R-matrix code, used to model electron-polyatomic molecule interactions, to be employed quickly with reduced set-up times.

Quantemol-EC is a new generation highly-automated software. It calculates electron-molecule scattering cross sections using a suit of new R-matrix codes alongside Molpro, a quantum chemistry program.

Quantemol-VT brings an unsurpassed user experience to the world-renowned plasma simulation codes of Prof. Mark Kushner from the University of Michigan.

Quantemol-DB (QDB) is a leading sustainable database, representing the chemical and radiative transport properties of a very wide range of plasmas. The database contains chemistry data for plasma chemistry modelling with pre-assembled and validated chemistry sets, and is regularly updated with the most recent and relevant data.

With an expanding research team, Quantemol is able to offer consultancy projects that are carried out by world leading scientists in their respective fields.



Prof. Jonathan Tennyson, FRS, UCL

Our mission statement

"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."

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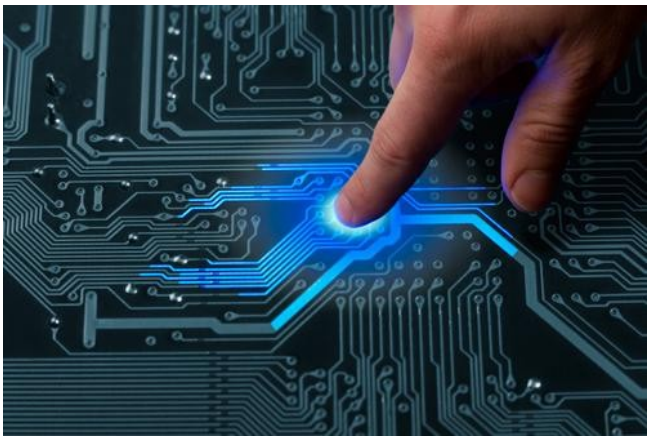
Virtual Tool

What does Q-VT do?

Quantemol-Virtual Tool is an expert software system for the simulation of industrial plasma processing tools. Q-VT builds upon the comprehensively validated Hybrid Plasma Equipment Model (HPEM) codes developed by the renowned plasma physicist Professor Mark Kushner for simulating non-equilibrium low pressure plasma processes. Q-VT includes an intuitive user interface, data visualisation and analysis capabilities, and convenient job/batch management.



"*I have enjoyed using the Quantemol Virtual Tool (QVT) as a user-friendly front end to the Hybrid Plasma Equipment Model (HPEM) of Professor Mark Kushner. It is easy to define geometries to be modelled by the software. All of the features of the HPEM are available and the settings for these features are integrated into one user interface. After the definition of the geometry of a plasma reactor, the workflow includes setting the input parameters to the system, such as those necessary for the coupling of electromagnetic energy into the reactor, as well as initial gas compositions in the chamber, gas flow rates and data for chemical reactions occurring in the plasma. Finally, a large range of output plasma parameters such as concentrations, fluxes, and temperatures of species can be displayed over the computation domain*."

Dr. Mark Stamminger, Heraeus Conamic

Benefits of Q-VT

- Trust in your results: An experimentally validated simulation system focused on modelling plasma tools.
- Reduced learning curve: Intuitive interface created for plasma physicists.
- Time saved on chemistry data search: Vast library validated cross-sections is provided with the licence.
- Model your complex process: Plasma chemistry sets can be directly imported from QDB and QVT can handle chemistry of hundreds of reactions.
- Learn quickly: Examples of commonly used ICPs and CCPs are included in the examples library.
- No fuss tool geometry mesh: Object oriented mesh drawer (NEW) drawing tool for chamber design and modification: a tool simulation set-up service can be provided.
- Do not dismiss complex plasma phenomena, get additional modules (radiation transport, ion kinetics, external circuits, etc.).
- Save time and use multi–jobs run management system for managing large numbers of simulations, saved and labelled in orderly manner (can work on a cluster).
- Save money on data visualisation programs: Built in advanced reactor scale visualisation of scalar and vector plasma properties
- Save time on comparing data within the interface: possibility to import experimental results
- Create a tailored solution for your process: add user reaction database, so no need to add the same reactions over and over manually
- API link to QDB database
- API to add your species and cross sections to HPEM library (previously you can only use hard coded species and cross sections)

What can Q-VT model?

- Plasma tool geometry alterations
- Advanced volume and surface chemistries
- Variation of key plasma state variables with process parameter changes
- Ion flux on wafer level: ion and energy neutral energy/angular distribution functions, and fluxes of all species along the wafer
- Non-Maxwellian electron dynamics
- Complex electromagnetic plasma interactions (current coils, permanent magnets, multi-frequency power supply, plasma circuit interactions, electrodynamic effects on CCPs)
- Pulsed plasma discharges

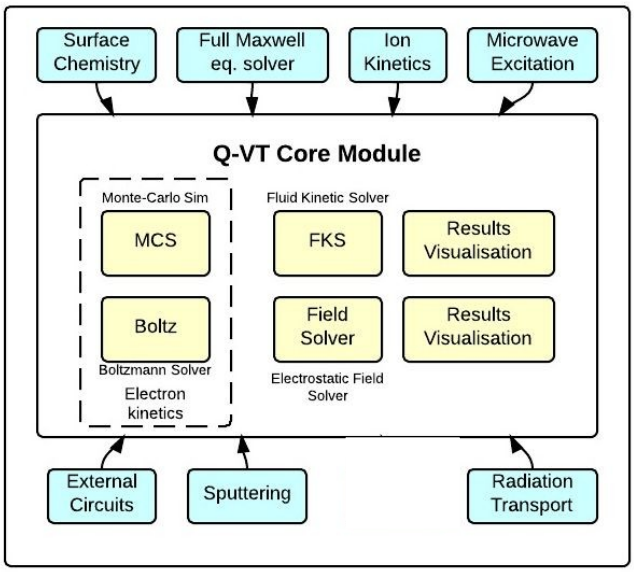
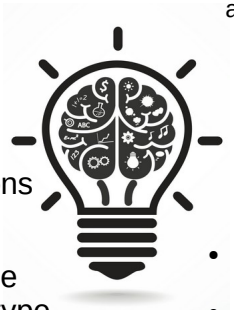


Fig.1 The simulation consists of a core simulation module, the HPEM, which can be extended with additional add-on modules to incorporate the physics of interest in a given plasma process.



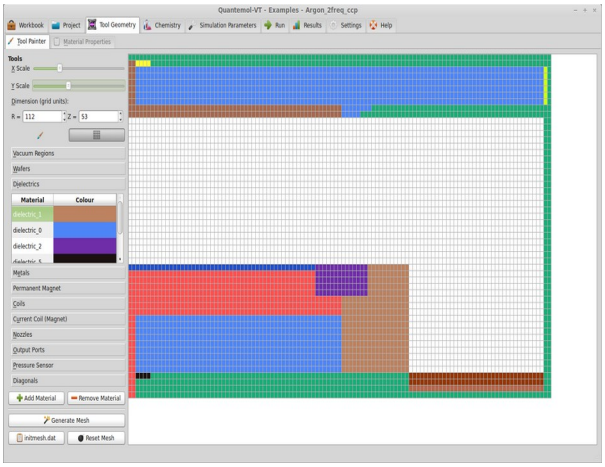
Latest release v 2.0 features:

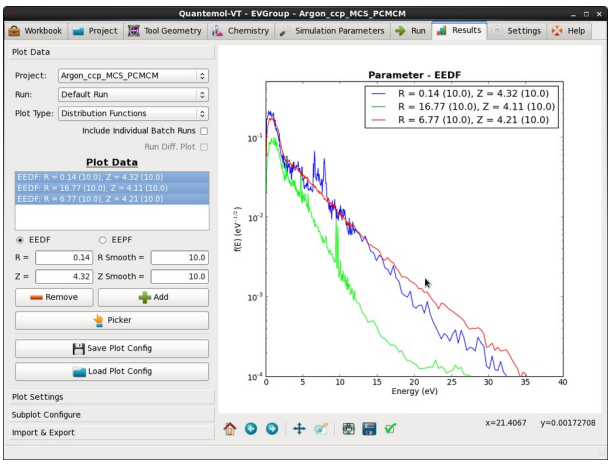
- Update to Python 3 and recent versions of python modules
- Displayed species and reactions in the chemistry tab can now be filtered by type, name etc.
- There are now chemistry consistency checks accessible via the Chemistry/Species tab. These check for example for missing ion-ion recombination or symmetric charge exchange reactions.
- Enabled custom species and cross-section imports
- QDB API: There is now also a link to the QDB Chemistry Generator

Applications of Q-VT

- Tool design and development
- Modelling of discharge and wafer level chemistry kinetics
- Modelling etch/deposition uniformity
- Examining tilting effects (when used with an additional scale profile model feature, specifically compatible with Synopsys TCAD software)
- Large wafer size simulation (12 inches and more)

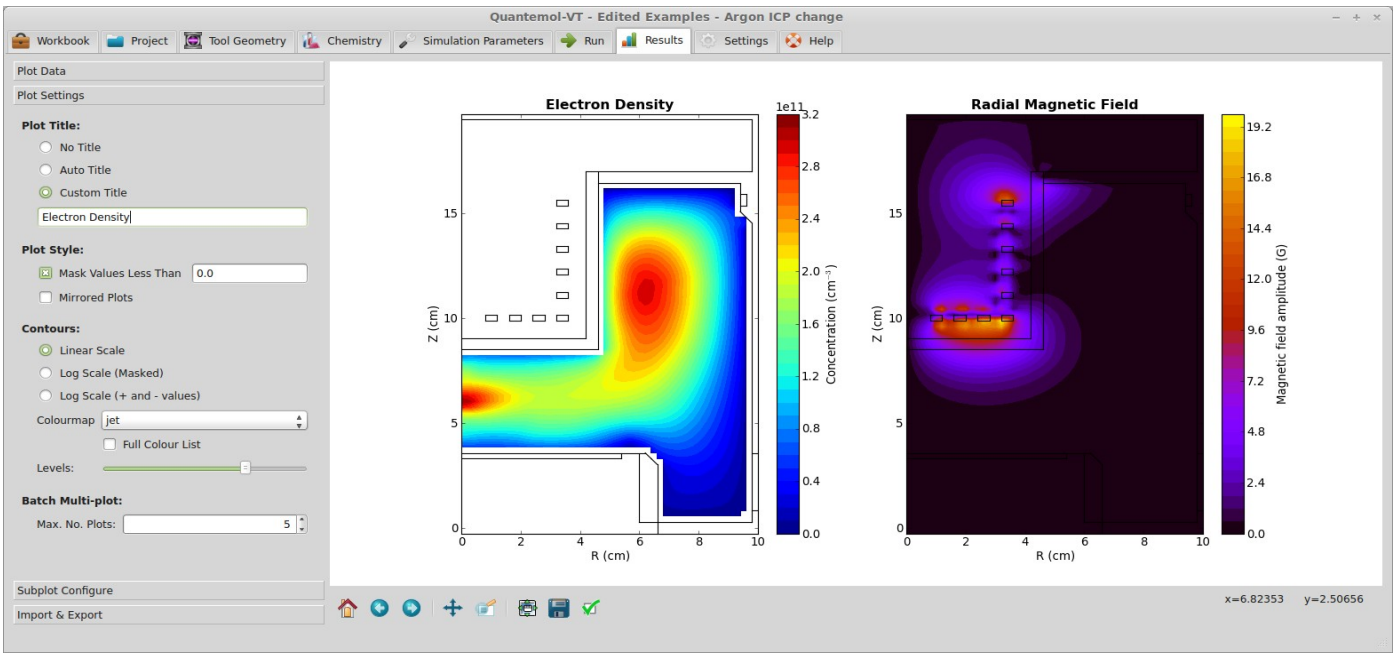
In Quantemol-VT, tool settings can be easily modified through the intuitive design viewer. The simulation projects are organised and structured with a workbook management system.
With the help of an object oriented meshing tool, the chamber design can be drawn with materials of your choice in 2D (planar) and 2.5D (axisymmetric cylindrical geometry).
Results can be plotted and analysed within Q-VT or exported as data files.
Outputs from Q-VT include: 2D distributions of species densities, temperatures, fluxes, fields and power depositions, surface fluxes, time-resolved kinetics, spatially resolved EEDFs, and ion/neutral energy/angle distributions.





Citations for the underlying simulation

- J. Shoeb, M. M. Wang and M. J. Kushner, "Damage by Radicals and Photons During Plasma Cleaning of Porous low-k SiOCH. I. Ar/O2 and He/H2 Plasmas", *J. Vac. Sci. Technol. A* **30**, 041303 (2012).
- S. Tinck, W. Boullart and A. Bogaerts, "Modeling Cl2/O2/Ar inductively coupled plasmas used for silicon etching: effects of SiO2chamber wall coating", *Plasma Sources Sci. Technol.* **20**, 045012 (2011).
- Y. Yang, M. Strobel, S. Kirk and M. J. Kushner, "Fluorine Plasma Treatments of Polypropylene Films: II. Modeling Reaction Mechanisms and Scaling", *Plasma Proc. Polymers* **7**, 123 (2010).



The core physics behind Q-VT is a comprehensive model (Hybrid Plasma Equipment Model) developed by Professor Mark Kushner and others for modelling low pressure plasma processing reactors.

The core simulation module includes:

- Simulation of gaseous phase chemistry and surface sticking reactions
- Fluid transport model for species in the gaseous phase
- Heat transport due to reactions, conduction, diffusion and flow
- Electrostatic field solvers with the ability to apply DC and RF potentials to surfaces and coils
- Boltzmann solutions of electron kinetics
- Extensive database of cross-section reactions developed by Prof. Mark Kushner and his group
- Calculation of inductively coupled electromagnetic fields

Additional add-on modules available

1	EMC	Electron Monte Carlo
2	SKM	Surface Kinetics Module
3	MAXWELL	Maxwell Equation Solver for CCPs
4	PCMC	Plasma Chemistry Monte Carlo Simulation
5	MICROWAVE	Finite Difference Time Domain Microwave Module (FDTDM)
6	CIRCUIT	RF circuit module.
7	SPUTTER	Sputtering
8	HV	Photon beam injection
9	RADTRANS	Radiation Transport Module (MCRTM)
10	IMCS	Ion Monte Carlo Simulation

Consultancy

As well as providing advanced modelling software, Quantemol delivers a unique consultancy service. With our suite of software and a team of highly skilled engineers, we provide extensive and in depth analysis tailored to specific customer requirements. Consultancy projects range from small quick calculations work to comprehensive plasma chemistry development. Typical types of consultancy work provided are:

- Calculations of specific electron-molecule cross sections including:
- Electron impact dissociation cross-sections producing specific products
- Electron impact ionisation dissociation producing specific products
- Vibrational excitation cross-section calculation molecules and ions
- Industrial plasma tool simulations
- Plasma process parameter optimisations
- Plasma chemistry designs
- Plasma etching and deposition calculations
- General multiphysics problems (CFD, etc.)

Training (NEW)

Quantemol team offers bespoke training courses for individuals or research groups. Our experts will prepare material to suit your needs and knowledge level. We can deliver it online, or with on site visit or if you come to our offices.

For more information please contact us:
+44 208 133 51 03
info@quantemol.com

Price list

Use Case	Type of Licence	Version	Licence term		
			1 year	3 years	Annual Support
Non-commercial research	Single Workstation	SE	£7,600	£15,200	£3,400
		NE	£10,100	£19,000	£4,300
	Research group	SE	£12,600	£25,300	£5,500
		NE	£16,400	£31,600	£6,000
	Institution	SE	£20,200	£39,200	£6,700
		NE	£25,300	£43,000	£7,000
Commercial research	Single Workstation	SE	£22,600	£45,100	£6,500
		NE	£30,100	£56,400	£7,100
	Site	NE	£37,600	£69,000	£8,400

General terms

Commercial research - Research by commercial organisations or for commercial organisations with results not disclosed to public access.
Non-commercial research - Research by not-for-profit organisations producing publishable results.
All licences are floating type licences and can be moved from one PC to another.
SE - Standard Edition
NE - Network Edition,
Single workstation licence - To be used on a single workstation with a possibility to be used by multiple users.
Research group licence - Includes up to 5 workstations used by researchers in one group, can be installed on the cluster but the number of users should be limited to 5 within one group only.
Institution licence - Covers an unlimited number of users across different groups within an institution.
Site licence - Covers an unlimited number of users within a company.
HPEM database - An extensive electron impact cross-sections database is included.
Min spec:
Quantemol-VT software Linux x86, 64 bit operating system, 4 GB RAM (large calculations will require more RAM), 10 GB free disk space

Training costs The prices quoted are estimates based on generic materials and an online format. The cost will increase if you require a very specific material to be developed. An in person training format will incur an additional fee to cover our expert's travel costs.

*** - perpetual licences for academic institutions include only five years of HPEM licence. If intending to continue using the software, academic institutions are required to purchase a support for the sixth year of licence in order to get HPEM licence extension.*

Add-on module prices

Use Case	Type of Licence	Licence term*	
		1 year	3 years
Non-commercial research	Single Workstation	£250	£500
	Research group	£310	£630
	Institution	£380	£750
Commercial research	Single Workstation	£1,900	£3,800
	Site	£3,800	£7,500
Proprietary chemistry data space in HPEM (NEW)	Any above	30% extra to the licence price	

Standard Edition on single workstation can use any number of cores to be run
Network Edition of single workstation licence allows you to submit jobs across the network, but user will still have to share the work space
Annual support includes initial training, e-mail and telephone support, bug fixes throughout the year.
Add on modules should be purchased separately and we can advise which ones you might need
The HPEM cross section library is included free of charge, additionally customers can upolad proprietary chemistry data and upload your own species and cross sections (new) or connect to QDB database via API (subject of QDB gold membership).
Contact us on **sales@quantemol.com** for more details

Training

Group Size	Duration		
	1 day	2 days	3 days
1 to 1 tutorial	£420	£780	£1000
Small group (up to 5 ppl)	£460	£860	£1100
Large group (up to 15 ppl)	£500	£940	£1300