

QuantemolDB

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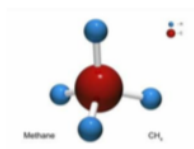
²Quantemol Ltd., London, UK.

November 15, 2018

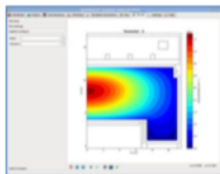
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- 3 Integration with QVT
 - Reactions
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 - Reduce Chemistries
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ABOUT QUANTEMOL

2004



2015



2016



Quantemol-DB

Trusted chemistries for plasma research.

SEARCH

LATEST NEWS

08 Oct 2018

[COMSOL and VizGlow formats >](#)

12 Sep 2018

[Workshop on Designing and Reducing Complex Chemistry >](#)

31 Jul 2018

[Quantemol is organising Workshop in September! >](#)

15 Feb 2018

[How to design a plasma chemistry set-ground up >](#)

29 Sep 2017

[QDB with QVT Tutorial >](#)



Current Status

17505 Reaction data sets

[LEARN MORE >](#)

Advisory board team

Quantemol-DB

LATEST NEWS

08 Oct 2018
COMSOL and
12 Sep 2018
Workshop on
Chemistry >
31 Jul 2018
... is
2018
design a plasma chemistry sets ground up
2017
QVT Tutorial >

Complex
September

Ranjan A.



J. Tennyson



M. Goekner



Y. Itikawa



Z. Petrovic



A.



K. Bartschat



N. Mason



M. Turner



U. Czarnetzki



Y-K Pu



C. Whitehead



J-S Yoon



J-P Booth



B. J. Braams



J. Schulze



A. Laricchiuta



S. Rauf



K. Hassouni



K. Hamaguchi



A. Bogaerts



S.C. Pande



E. Krishnakumar

- Trustworthy and validated data for plasma modelling.
- Time saved on chemistry set search, comparison and validation.
- Easy to use interface importing and exporting data in flexible formats.
- Active customer support.
- Help with referencing publications.
- Compatibility with the most commonly used plasma modelling software: QVT (HPEM), COMSOL, VizGlow, CHEMKIN, CFD-ACE+.

Rating	ID	Mixture	Reactions
★★★★☆	C3	N ₂ /H ₂ chemistry	135
★★★★☆	C4	Ar/H ₂ chemistry	64
★★★☆☆	C5	O ₂ /H ₂ chemistry	107
★★★★☆	C6	SF ₆ /O ₂ chemistry	142
★★★★☆	C7	CF ₄ /O ₂ chemistry	163
★★★★☆	C8	SF ₆ chemistry	60
★★★★☆	C9	CF ₄ chemistry	81
★★★★☆	C10	CF ₄ /O ₂ /H ₂ /N ₂ chemistry	296
★★★☆☆	C11	C ₄ F ₈ chemistry	146
★★★☆☆	C13	SiH ₄ chemistry	59
★★☆☆☆	C14	SiH ₄ /NH ₃ chemistry	77
★★★★☆	C15	Ar/O ₂ chemistry	49
★★★☆☆	C16	Ar/O ₂ /C ₄ F ₈ chemistry	414
★★☆☆☆	C17	SiH ₄ /Ar/O ₂ chemistry	175
★★☆☆☆	C18	Ar/Cu chemistry	43
★★★★☆	C19	Cl ₂ /O ₂ /Ar chemistry	55
★★★★☆	C20	Ar/BCl ₃ /Cl ₂ chemistry	58
★★★☆☆	C21	Ar/NH ₃ chemistry	157
★★★★☆	C22	CH ₄ /H ₂ chemistry	182
★★☆☆☆	C23	C ₂ H ₂ /H ₂ chemistry	79
★★☆☆☆	C24	CH ₄ /NH ₃ chemistry	259
★★☆☆☆	C25	C ₂ H ₂ /NH ₃ chemistry	165

Standard

- Database search for reactions and species.
- **New!** Use chemistry generator app to make the reaction list for new chemistry.

Silver

- Database search for reactions and species.
- **Flexible graphs for cross-section data.**
- **Access to the chemistry sets and download of Ar, H₂, O₂.**
- **New!** Use chemistry generator app to make the reaction list for new chemistry.

Gold

- Database search for reactions and species
- **Access to over 40 pre-assembled chemistry sets.**
- **New!** Use chemistry generator app to make the reaction list for new chemistry **and download it in a flexible format.**
- Flexible graphs for cross-section data.
- **Download data in flexible software formats: COMSOL, CHEMKIN, VisGlow, CDF ACE+, QVT.**
- **Customer support on working with chemistry data.**

INTEGRATION WITH QVT

From QVT can select to import reactions or chemistry set from QDB directly.

The screenshot shows the Quantemol-VT interface with a table of reactions. The table has columns for Reaction, A [cgs units], n, E [eV], Exothermicity [eV], Special Number, and Comment. The 'Connect to QDB' button is highlighted with a red box. A red line connects this button to a dialog box on the right.

Reaction	A [cgs units]	n	E [eV]	Exothermicity [eV]	Special Number	Comment
1 O ⁺ + O > O + O ⁺	8e-10	0.0	0.0	0.0	1	EST.
2 O2 ⁺ + O2 > O2 + O2 ⁺	5.2e-10	0.0	0.0	0.0	1	ION_TABLES_NEW
3 O2 ⁺ + O2* > O2* + O2	2e-17	0.0	0.0	0.0	1	NIST
4 O2* + O2 > O2 + O2	2e-18	0.0	0.0	0.0	1	NIST
5 O2* + O* > O2 + O	1e-11	0.0	0.0	0.0	1	NIST
6 O2* + AR > O2 + AR	1e-18	0.0	0.0	0.0	1	NIST
7 O + O ⁺ > O + O	1e-07	0.0	0.0	0.0	1	
8 O + O2 ⁺ > O + O2	1e-07	0.0	0.0	0.0	1	
9 O + O > O2 + E	3e-10	0.0	0.0	0.0	1	
10 O + AR ⁺ > O + AR	1e-07	0.0	0.0	0.0	1	
11 O ⁺ + O2 > O + O2	3.8e-11	0.0	0.0	0.0	1	NIST
12 O ⁺ + O* > O* + O	1e-11	0.0	0.0	0.0	1	EST
13 O ⁺ + O > O + O	5e-12	0.0	0.0	0.0	1	NIST
14 O ⁺ + AR > O + AR	5e-13	0.0	0.0	0.0	1	NIST
15 O + O + M > O2 + M	8e-33	0.0	0.0	0.0	1	NIST

Buttons at the bottom: Save Reactions, **Connect to QDB**, Find Reaction(s), Add Reaction, Remove Reaction(s), Show Cross Section

Choose an Option

Find Reactions

Get Chemistry

Cancel OK

INTEGRATION WITH QVT / REACTIONS

Select species → Retrieve Reactions → Select reactions → OK

Search and Import Reactions from QDB

Species

O2^
O-
O*
M
AR^
O^
AR
O2*

Retrieve Reactions

Reactions

	Reaction	A	n	E	Exothermicity	Comment
1	O- + AR^ + M > AR + O + M	2e-25	-2.5	0.0	0.0	
2	E + E + O2^ > E + O2	7.18e-27	-4.5	0.0	0.0	
3	E + O2^ + M > O2 + M	4.31e-34	-1.5	0.0	0.0	
4	E + O^ + M > O + M	4.31e-34	-1.5	0.0	0.0	

Note: Electron collisions present in the HPEM library are not displayed.

Cancel OK

INTEGRATION WITH QVT / CHEMISTRY SETS

Import a Chemistry from QDB

Chemistries

N2/H2 chemistry
Ar/H2 chemistry
O2/H2 chemistry
SF6/O2 chemistry
CF4/O2 chemistry
SF6 chemistry
CF4 chemistry
CF4/O2/H2/N2 chemistry
C4F8 chemistry
SiH4 chemistry

Reactions

	Reaction	A	n	E	Exothermicity	Comment
1	$\text{N}_2 + \text{N}^* > \text{N}_2 + \text{N}$	5e-12	0.0	1620.0	0.0	
2	$\text{H}_2 + \text{N}^* > \text{H} + \text{NH}$	4.6e-11	0.0	880.0	0.0	
3	$\text{H}_2 + \text{N} + \text{NH}_3 > \text{NH}_3 + \text{NH}_2$	1e-36	0.0	0.0	0.0	
4	$\text{H} + \text{NH}_2 + \text{M} > \text{NH}_3 + \text{M}$	6e-30	0.0	0.0	0.0	
5	$\text{E} + \text{H}_2^{\wedge} > \text{E} + \text{E} + \text{H}^{\wedge} + \text{H}^{\wedge}$	2.12e-09	0.31	23.3	0.0	
6	$\text{E} + \text{H}^- > \text{E} + \text{H}^-$	0.0	0.0	0.0	0.0	

- show omitted species
 show omitted reactions

Cancel

OK

FUTURE DEVELOPMENTS / CHEMISTRY GENERATOR

Input: feed stock gas mixture

Species possibly present in the plasma (based on QDB species)

The user chooses which species they want to include in their set

$AB_4/XY_3/Z_2$

Neutrals	Excited States	Positive Ions	Negative Ions
A_2 ✓	A^+ ✓	A^+ ✓	A^- ✓
B_2 ✓	B^+ ✓	X_2Y^+ ✓	ZY_3^- ✓
X_2 ✓	A_2^+ ✗	Y^+ ✓	A_2^- ✓
X ✓	X_2^+ ✗	Y_2^+ ✓	Y^- ✓
YX_2 ✓	X^+ ✗	ZB^+ ✓	Z^- ✓
Z_2B ✗		Y_2^+ ✓	
B ✗		Y^+ ✓	
ZA ✗		ZY_3^+ ✓	

FUTURE DEVELOPMENTS / CHEMISTRY GENERATOR

List of reactions from QDB
including chosen species
via cascade algorithm



User chooses which reactions
to form the set and download
(post optimization)

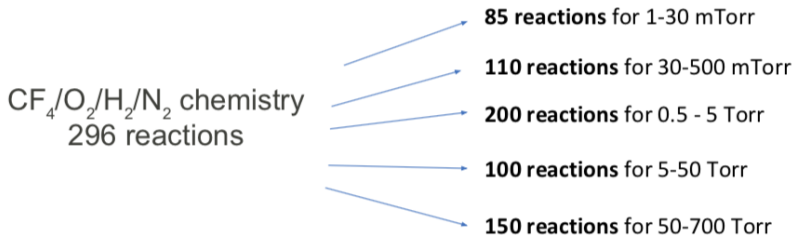
electron collisions	ion-ion reactions	ion-neutral reactions	neutral-neutral reactions
$e^- + A_2 \rightarrow A + A^-$ ✓	$A^- + A_2^+ \rightarrow A_2 + A$ ✓	$A + A^- \rightarrow e^- + A_2$ ✓	$X + YX_3 \rightarrow X_2 + YX_2$ ✓
$e^- + YX_2 \rightarrow e^- + YX_2$ ✓	$A^+ + A_2^- \rightarrow A_2 + A$ ✓	$A^+ + A_2 \rightarrow A + A_2^+$ ✗	$X + YX_2 \rightarrow X_2 + YX$ ✗



- QVT (HPEM)
- COMSOL
- VizGlow
- CFD-ACE+

FUTURE DEVELOPMENTS / REDUCE CHEMISTRIES


Chemistry sets need to be optimised for external conditions like system pressure using a combination of techniques



* The above is an example of the dynamic optimization of chemistry sets at different plasma conditions

FUTURE DEVELOPMENTS / STOICHIOMETRIC ANALYSIS

Chemistry set optimization would occur via the identification of dominant reaction pathways using master chemical kinetics equations and Stoichiometric Matrices.

$$\frac{dy_i}{dt} = g(y_i) = \sum_{j=1}^R s_{ij} F^j(y_i)$$


	R1	R2	R3	R4	R5	R6	R7	R8
S1	s_{11}	s_{12}	s_{13}	s_{14}	s_{15}	s_{16}	s_{17}	s_{18}
S2	s_{21}	s_{22}	s_{23}	s_{24}	s_{25}	s_{26}	s_{27}	s_{28}
S3	s_{31}	s_{32}	s_{33}	s_{34}	s_{35}	s_{36}	s_{37}	s_{38}
S4	s_{41}	s_{42}	s_{43}	s_{44}	s_{45}	s_{46}	s_{47}	s_{48}
S5	s_{51}	s_{52}	s_{53}	s_{54}	s_{55}	s_{56}	s_{57}	s_{58}
S6	s_{61}	s_{62}	s_{63}	s_{64}	s_{65}	s_{66}	s_{67}	s_{68}
S7	s_{71}	s_{72}	s_{73}	s_{74}	s_{75}	s_{76}	s_{77}	s_{78}

A combination of integrated 0D modelling and sensitivity analysis would ensure that a smart chemistry app would output optimized chemistry sets.

Please sign up!
www.quantemoldb.com

Some useful youtube videos:

- QDB basic tutorial
<https://www.youtube.com/watch?v=iE9dzQcQj-A>
- QDB with QVT tutorial
<https://www.youtube.com/watch?v=YEELYrprZI>

Thank you!

Workshop
24-26 June 2019
UCL, London, UK.
UK-Rmol codes and QN

