QuantemolDB

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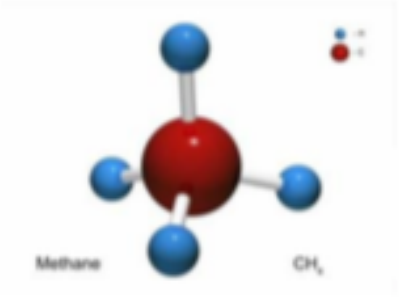
QDB plasma chemistry

About Quantemol

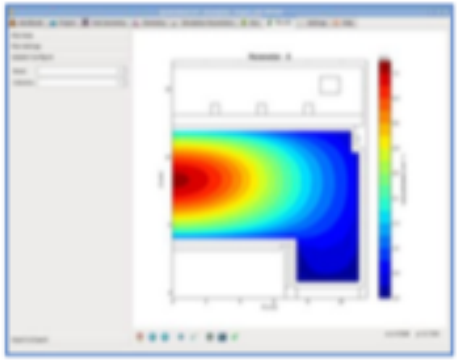
2004

Electron Scattering



2015

Virtual Tool



2016

plasma chemistry

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 »

QDB plasma chemistry SPECIES REACTIONS CHEMISTRIES CONTACT ABOUT GOLD LOG IN SIGN UP

Advisory board team

Quantemol-DB

Trusted ch… …asma research.

LATEST NEWS

08 Oct 2018 COMSOL and …

12 Sep 2018 Workshop on Chemistry >

… Complex … September!

…design a plasma chemistry set- ground up …

… QVT Tutorial >


J.Tennyson


M.Goekner


N. Mason


Y. Itikawa


M. Turner


Z.Petrovic


A. Ranjan


K.Bartschat


C. Whitehead


J-S Yoon


J-P Booth


B. J. Braams


J. Schulze


U.Czarnetzki


Y-K Pu


E. Krishnakumar


A. Laricchiuta


S. Rauf


K. Hassouni


K. Hamaguchi


A.Bogaerts


S.C.Pande

QUANTEMOLDB / BENEFITS

- 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_4F_8 chemistry	146
★★★☆☆	C13	SiH_4 chemistry	59
★★☆☆☆	C14	SiH_4/NH_3 chemistry	77
★★★★☆	C15	Ar/O_2 chemistry	49
★★★☆☆	C16	$Ar/O_2/C_4F_8$ 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_2H_2/H_2 chemistry	79
★★☆☆☆	C24	CH_4/NH_3 chemistry	259
★★☆☆☆	C25	C_2H_2/NH_3 chemistry	165

QDB plasma chemistry

QUANTEMOLDB / MEMBERSHIP

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, H_2, O_2.**
- New! Use chemistry generator app to make the reaction list for new chemistry.

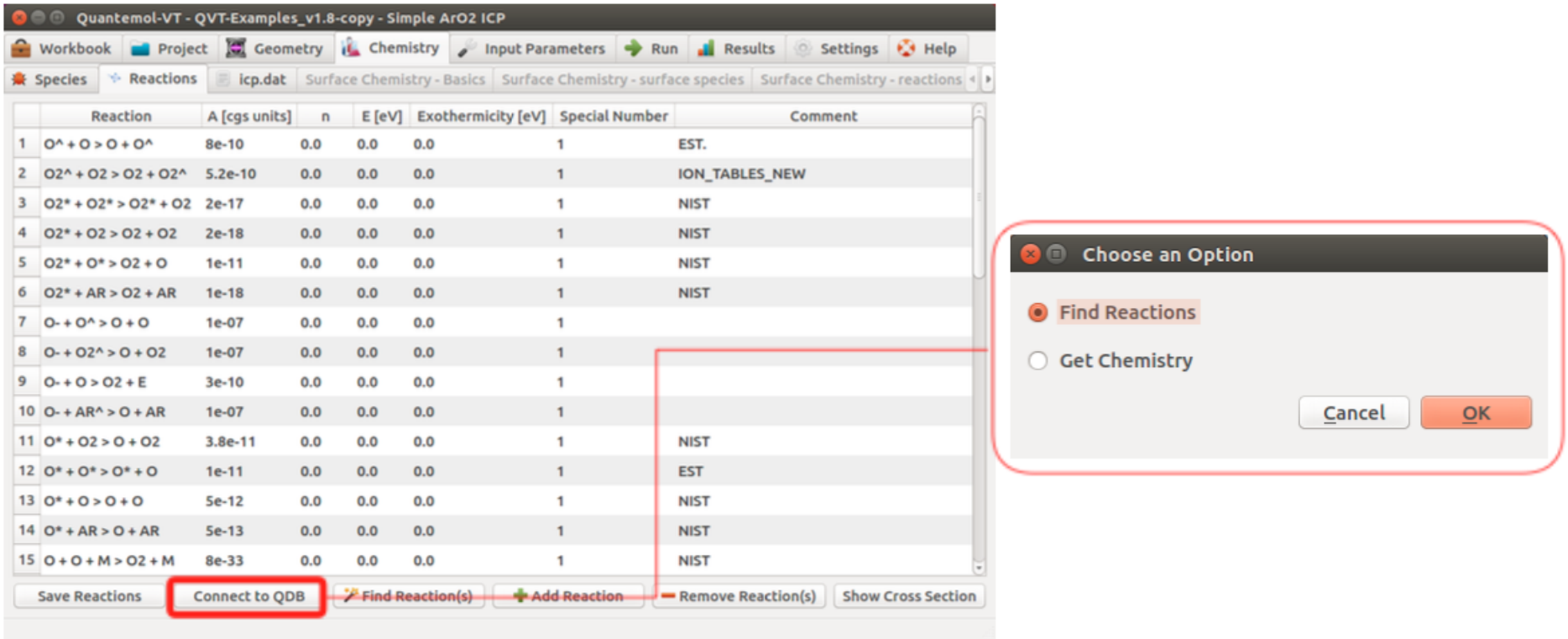
Gold

- 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.**

QDB plasma chemistry

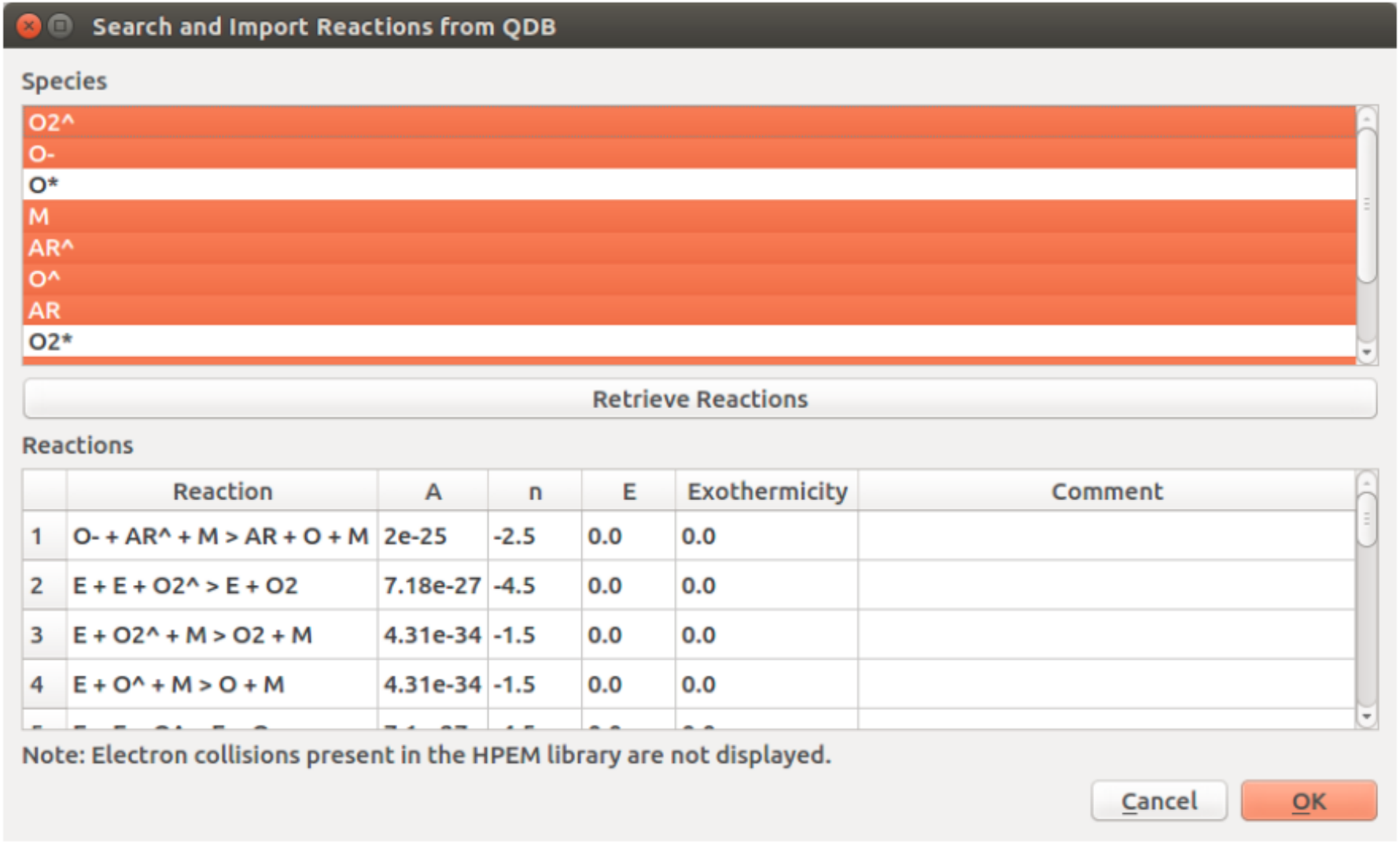
Integration with QVT

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

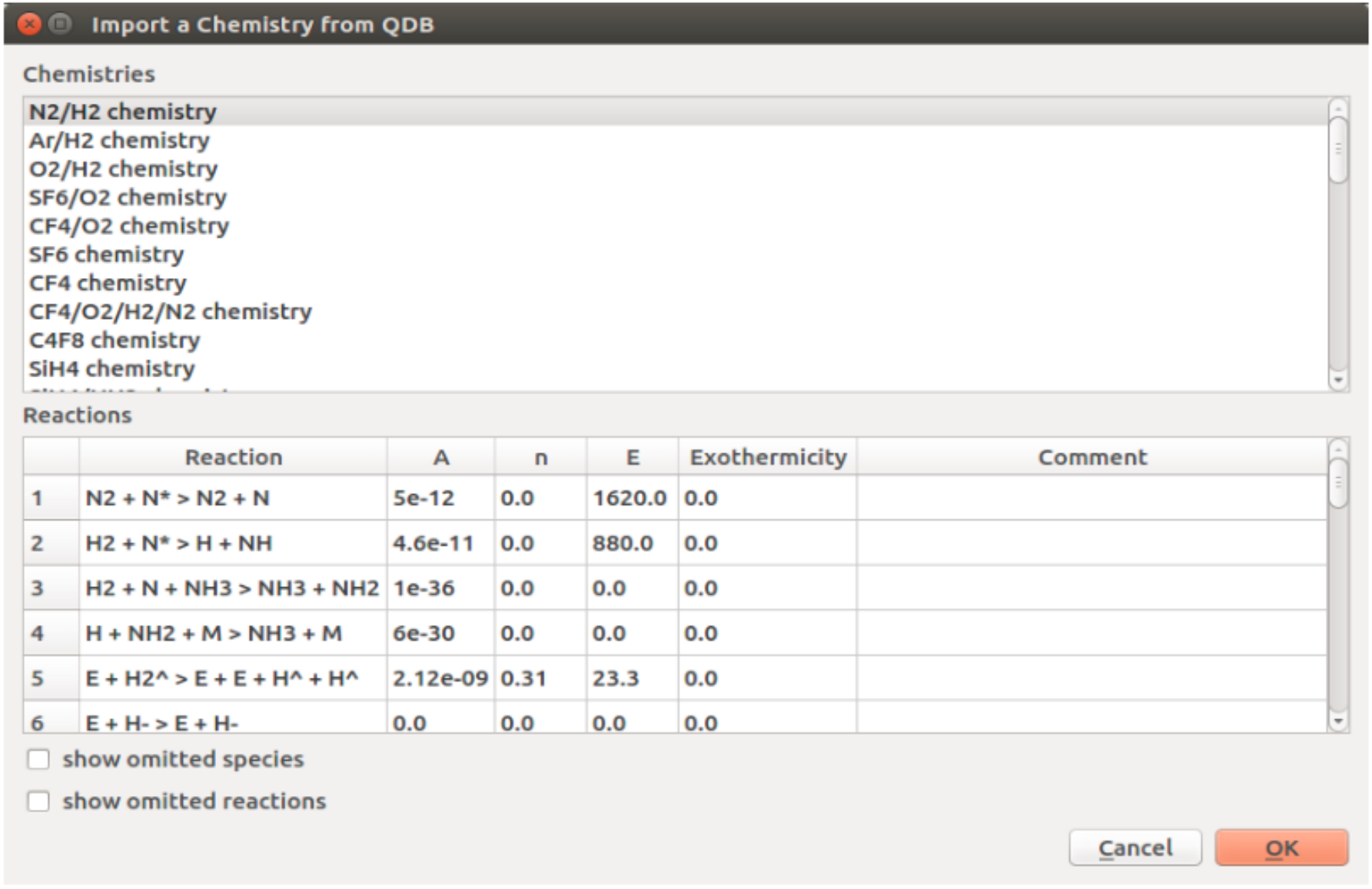


Integration with QVT / Reactions

Select species → Retrieve Reactions → Select reactions → OK



Integration with QVT / Chemistry Sets



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

$CF_4/O_2/H_2/N_2$ chemistry
296 reactions

- **85 reactions** for 1-30 mTorr
- **110 reactions** for 30-500 mTorr
- **200 reactions** for 0.5 - 5 Torr
- **100 reactions** for 5-50 Torr
- **150 reactions** for 50-700 Torr

*** 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.

SignUp

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=YEELYYrprZI

Thank you!

SignUp

Workshop

24-26 June 2019

UCL, London, UK.

UK-Rmol codes and QN