JÜLICH FORSCHUNGSZENTRUM

Status of Be, BeH and BeH^+ electron and proton collision data used in fusion

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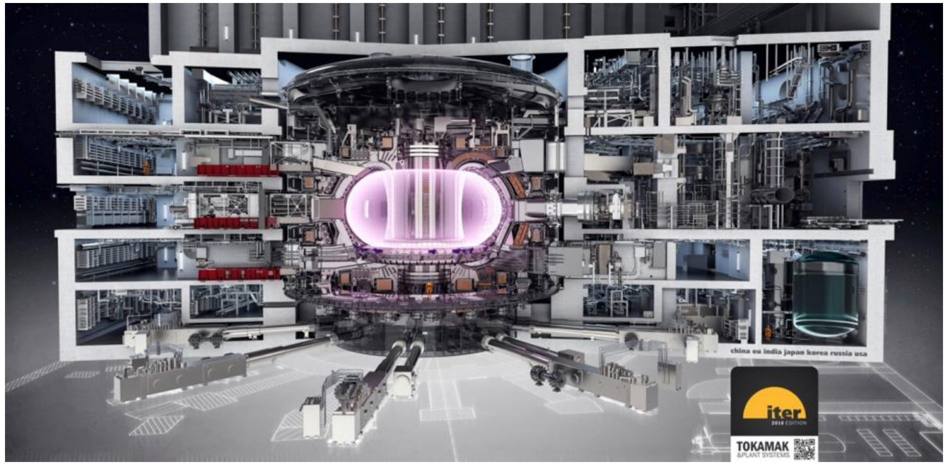
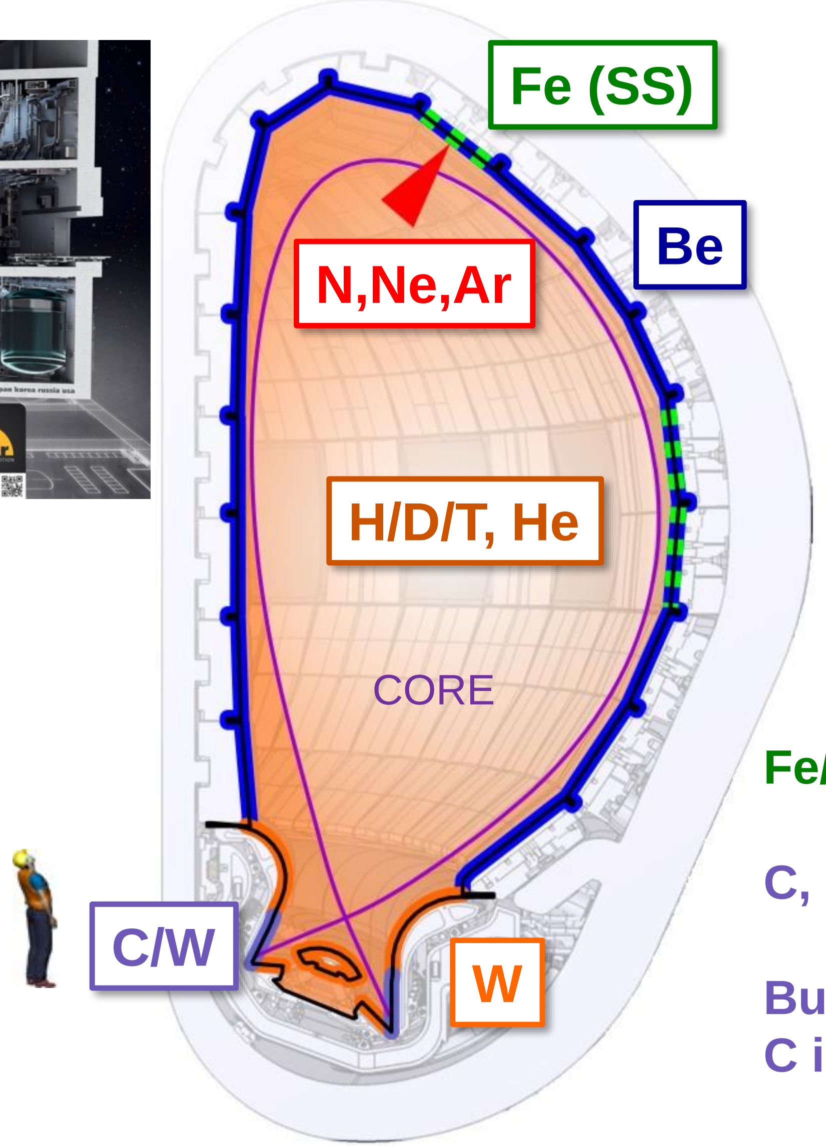
IAEA Consultancy Meeting on Evaluation of Fundamental Data on Beryllium-containing Species for Edge Plasma Modelling, Vienna, IAEA Headquarters, June 6-7, 2019

List of the main elements relevant to the ITER plasma





Fe/SS, 2011: armour at diagnostics port plugs

C, in 2013: replaced by all W divertor

But:

C in: W7X (2016), JT-60SA (2019),…

MOLECULAR PROCESSES CONSIDERED IN FUSION:

- e,p + $H_2(v_i)$ → …, e+$H_2^+(v_i)$ → H + H* divertor detachment dynamics,

www.amdis.iaea.org, data center network, Atoms 2016, D. Wuenderlich, U.Fantz, IPP Garching, K. Sawada, M.Goto, NIFS, and Fursa et al, PRL 2016

e+$H2^+$(v) : Int. Conference series: Dissociative Recombination 1-9 (1988 -2012)

- e,p + C_xH_y →…., e+$C_xH_y^+$ → …. C erosion and migration, tritium retention,….

Excited states of products (CH(A→X)) ?

R. Janev et al., Phys. Plasma (2002, 2004) 11, IAEA: www.amdis.iaea.org, APID Vol 16 (2012)

- e+H_3^+(v3) → …., DR, DE,…. H_3^+ probably irrelevant in fusion plasmas

M. Larsson et al., PRL (1993) 70, S. Datz et al., PRL (1995) 74, and: Conference series: DR 1-9

- e+ BeH/BeH^+ → …. possible role on spectroscopy and on material migration:

Formation rates ?? 10% of Be sputtering? Volumetric particle exchange reactions ?

J.B. Roos et al. Phys. Rev A (2009) 80, IAEA Atomic Molec. data unit CRP 2012-2015

Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre, J. Tennyson et al. (Quantemol), R. Celiberto et al. (Bari)

Multiple aspects solved, but data scattered in literature, not jet compiled into a single comprehensive database.

- e+ N_2, N_2^+ → …. N_2-seeding, plasma cooling: Ammonia formation. So far mostly: only resulting atomic ions N, N^+, N^{++},…. but first plasma chemistry databases emerge

See planetary atmospheric entries research, e.g. A. Bultel et al, Universite de Rouen, France

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e+$H2^+$(v) : Int. Conference series: Dissociative Recombination 1-9 (1988 -2012)

Rapid progress in molecular H_2 data, often tested against experimental results in small (linear) plasma devices

Recommended entry point to the data-bases used here (and in other edge codes):
3 recent reviews (2016) from an IAEA “coordinated research project”
(CRP) 2011-2016

atoms MDPI www.mdpi.com/journal/atoms

Dirk Wünderlich and Ursel Fantz

Atoms 2016,4,26;doi:10.3390/atoms4040026

Keiji Sawada and Motoshi Goto

Atoms 2016,4,29;doi:10.3390/atoms4040029

Roberto Celiberto, Mario Capitelli et al.

Atoms 2017,5,18;doi:10.3390/atoms5020018

First ab initio electron-molecule CCC calculations now become available (one of the golden standards for electron collision processes in small systems) for the e+H_2 and e+H_2^+ systems: Curtin Univ. Perth, Australia

Zammit, Savage, Fursa & Bray, Phys. Rev. Lett. 16 (2016) 233201 and
Phys. Rev. A 90,022711 (2014), and Phys. Rev. A 95,022708(2017)

MOLECULAR PROCESSES CONSIDERED IN FUSION:

- e,p + C_xH_y → …., e+$C_xH_y^+$ → …. C erosion and migration, tritium retention,….

Excited states of products (CH(A→X)) ?

R. Janev et al., Phys. Plasma (2002, 2004) 11, IAEA: www.amdis.iaea.org, APID Vol 16 (2012)

Fusion had not progressed very far until carbon based plasma facing components were used (mid eighties of last century).

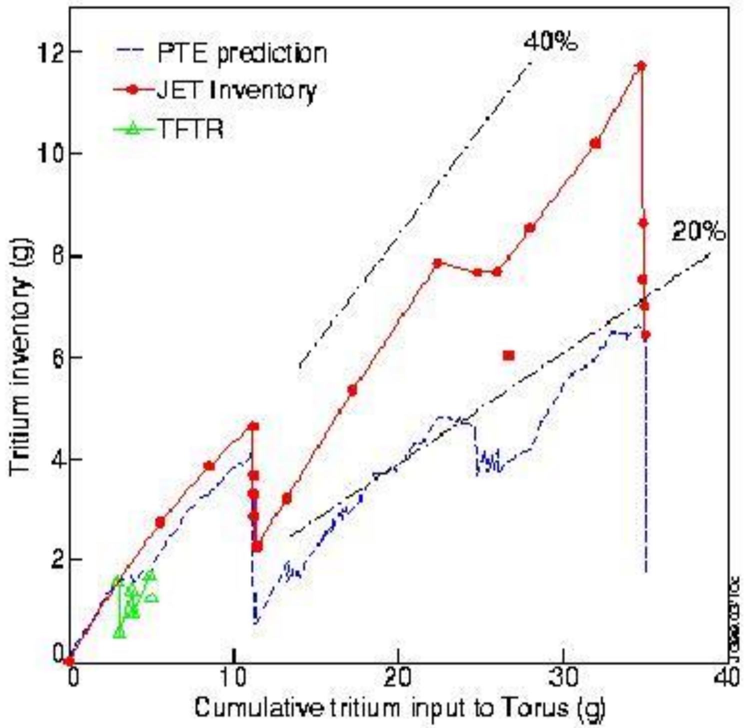
Mostly studied then: atomic C spectroscopy and transport,
little interest in carbon containg molecules, initially.

This changed in the years following 1997: the tritium experiments at JET

The tritium retention issue:

On JET, operated with tritium (1997), the tritium inventory built up without saturation limit.

JET: Retained Tritium

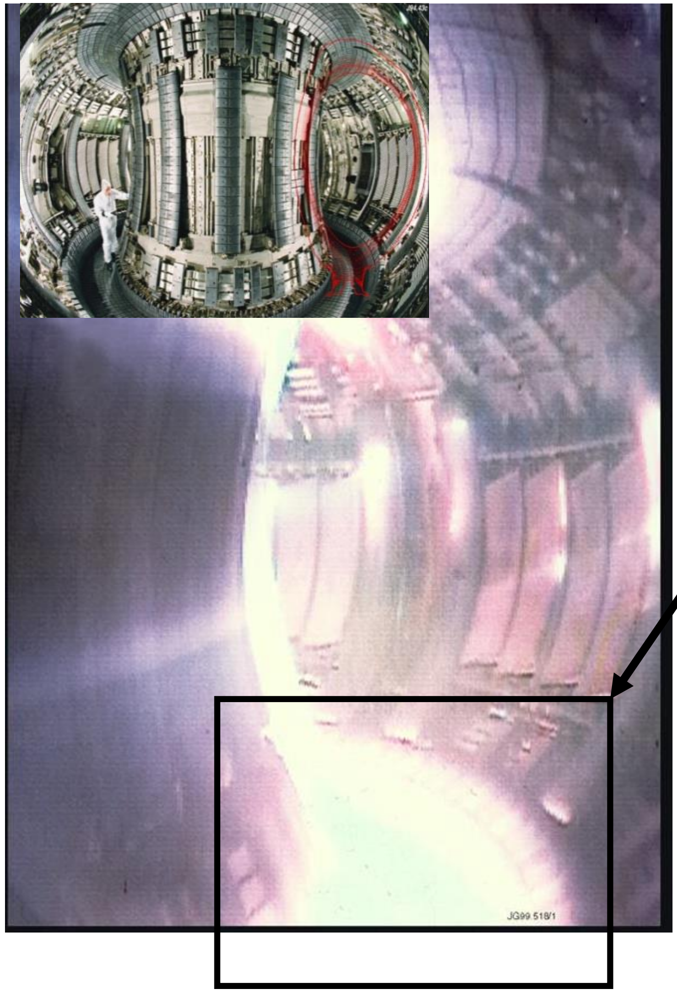


The rate of T retention in JET during DTE1 was 40% of input, reducible to 17% after cleanup in D, without sign of saturation.
P. Andrew, et al, FED 47 (1999) 233.

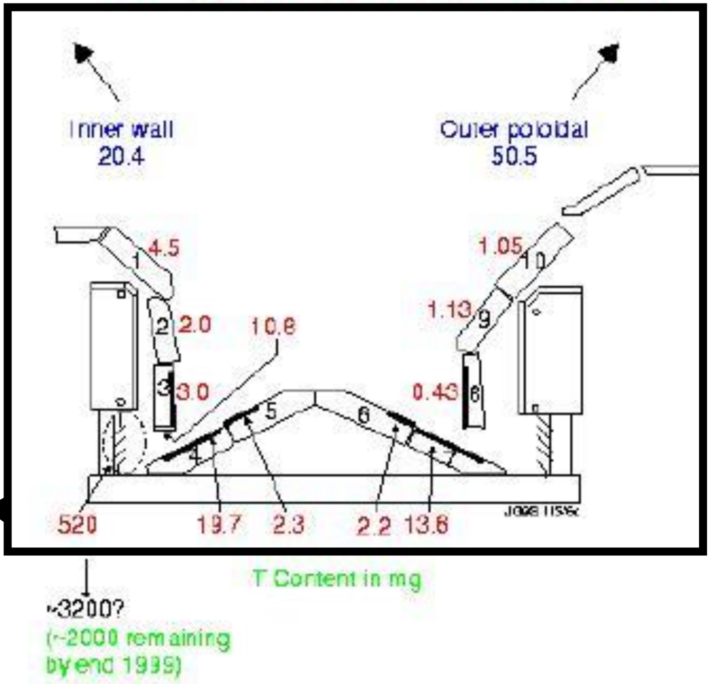
Extrapolation to ITER: the permitted in-vessel T inventory, 0.7 kg, could be reached in 100 shots

Carbon re-deposition, tritium co-deposition in JET

JET, Joint European Torus



Location of tritium in JET vessel during the post-DTE1 shutdown

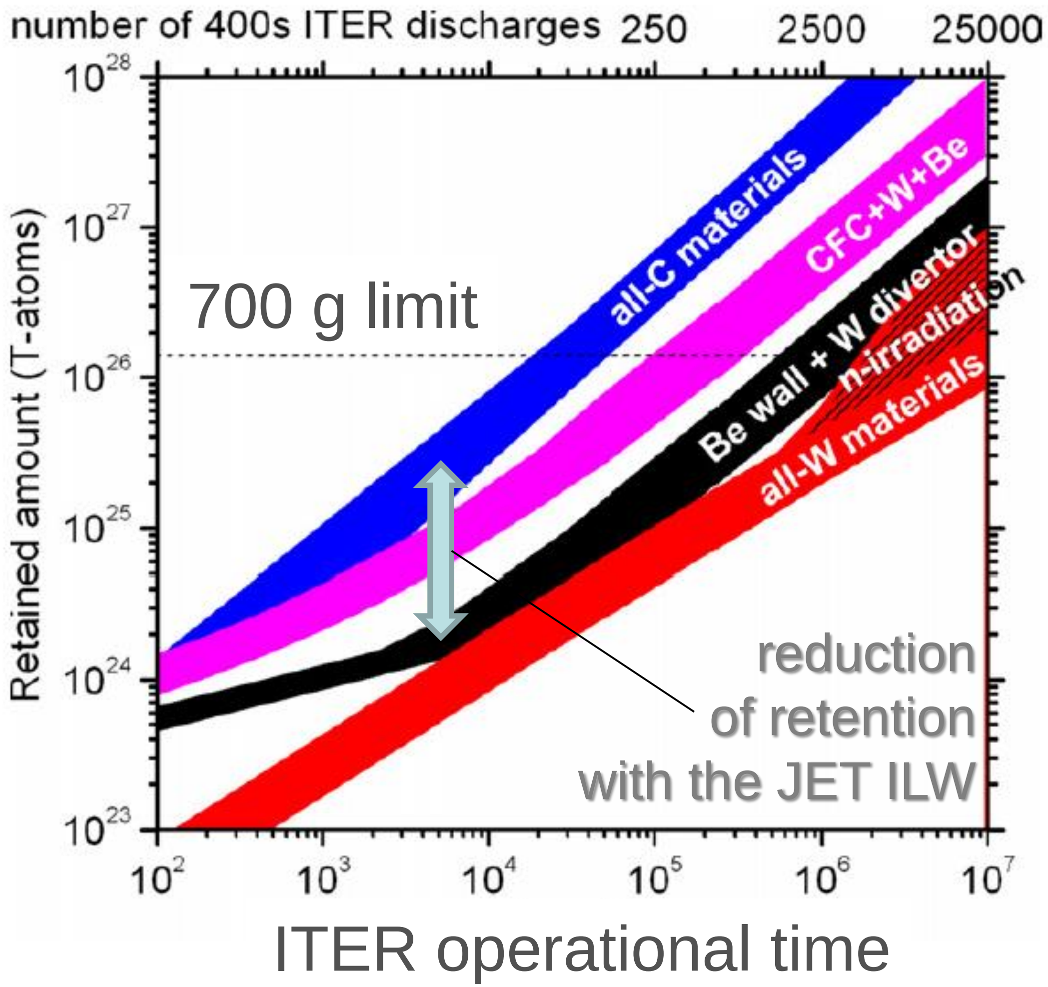


The location of the deposition is surprising: only a few mgs were found on typical tiles, but 520 mg were vacuumed up from the cooled, out-of-sight louvers, suggesting up to 3200 mg also that have fallen through to the vessel floor.

J.P. Coad, et al, J Nucl Mater 290-293 (2001) 224.

Predictions of fuel retention in ITER

fuel retention in C versus W



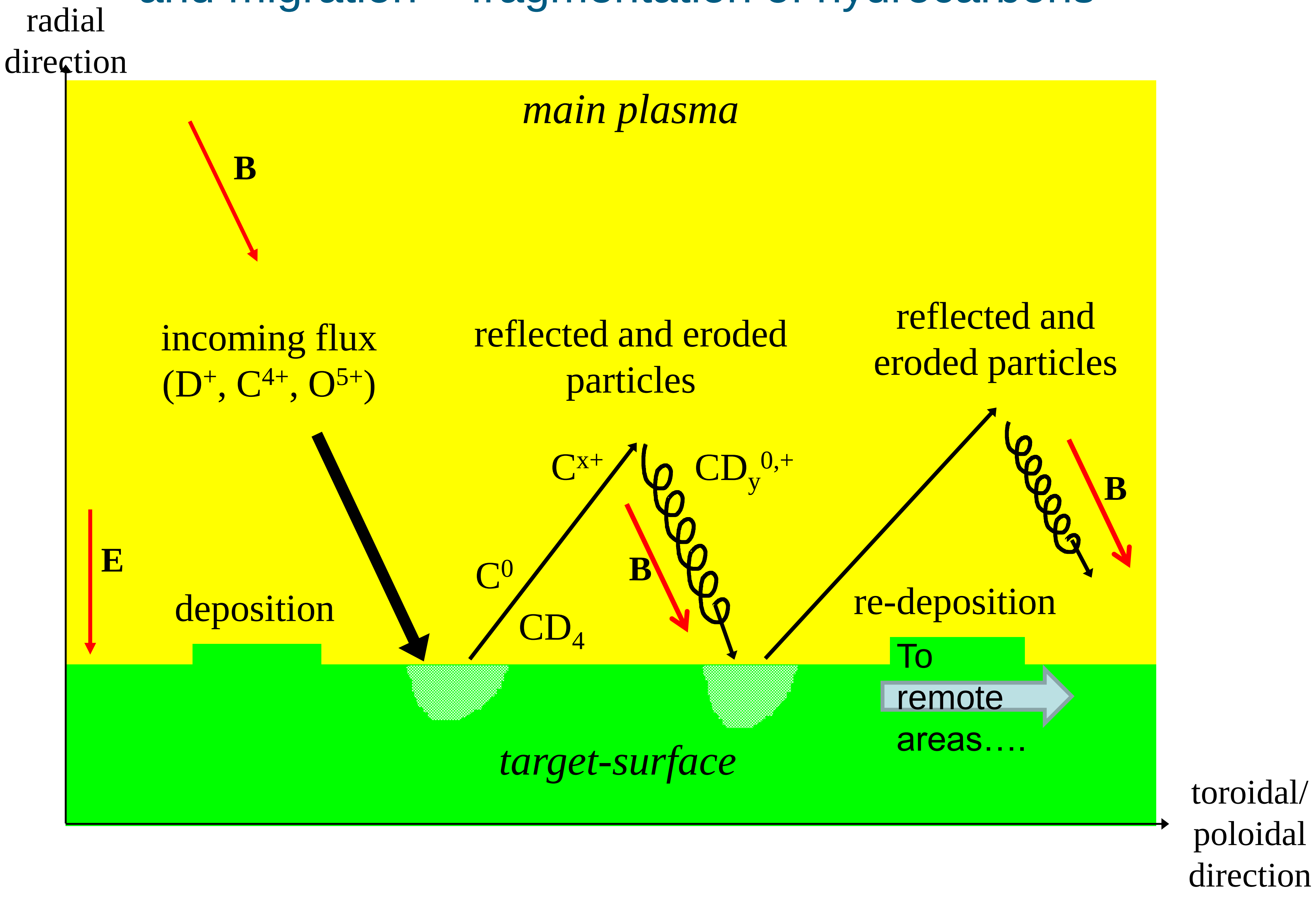
J. Roth et al., Plasma Phys. Cont. Fus. 50 (2008)

Data derived from empirical results obtained at **AUG, JET** and **PISCES** and modelling of erosion & re-deposition

Conclusion:

Fuel retention with carbon divertor is unacceptably large

Release (chem. sputtering) and migration + fragmentation of hydrocarbons



Courtesy: A. Kirschner, FZ Jülich

SEPARATING KNOWN FROM UNKNOWN: COMPUTATIONALLY

In most applications of A&M data in low temperature plasma chemistry:

$$\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i\right) \approx \frac{n_i}{\tau} = S_{n_i}$$

Plasma transport: known A&M unknown

Well stirred conditions,
Near equilibrium, homogeneous,
isotropy

In magnetically confined fusion plasmas:

$$\frac{\partial}{\partial t} n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i\right) = S_{n_i}$$

Plasma transport: unknown known

Anomalous transport
Drifts, electrical currents,
Kinetic corrections

“If we are confident in a plasma state, then we can quantify A&M processes in it”.

The generic equation, for all A&M effects „S“ in plasma (or in any other given inhomogeneous medium): „Boltzmann (linear) transport equation“, solved with conventional Monte Carlo transport codes. In fusion: e.g. EIRENE code, ERO code, etc

$$\frac{1}{v}\frac{\partial\phi(\mathbf{r},\mathbf{\Omega},E,t)}{\partial t}+\mathbf{\Omega}\cdot\nabla\phi(\mathbf{r},\mathbf{\Omega},E,t)+\Sigma(\mathbf{r},E,t)\phi(\mathbf{r},\mathbf{\Omega},E,t)$$
$$=\int\int\Sigma(\mathbf{r}',\mathbf{\Omega}',E'\rightarrow\mathbf{r},\mathbf{\Omega},E)\phi(\mathbf{r}',\mathbf{\Omega}',E',t)d\mathbf{\Omega}'dE'+Q,$$

Neutrons: nuclear science and engieering → linear, or nonlinear: MC - T- H **(e.g.: MCNP)**

Radiation: astro and laser physics → linear, or nonlinear: MC – temp. fields

Neutrinos:

Electrons: solid state physics applications

Neutral atoms/molecules: magnetic fusion → linear, or nonlinear: MC – plasma (transport) dynamics

And many more….

Here go the data (e.g. nuclear data)
In fusion: AM&S data

→ requires: balanced, internally consistent, complete, convenient,…A&M data sets

$$\frac{1}{v}\frac{\partial\phi(\mathbf{r},\boldsymbol{\Omega},E,t)}{\partial t}+\boldsymbol{\Omega}\cdot\nabla\phi(\mathbf{r},\boldsymbol{\Omega},E,t)+\Sigma(\mathbf{r},E,t)\phi(\mathbf{r},\boldsymbol{\Omega},E,t)$$
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And many more….

Ludwig Boltzmann: S=k log W

Vienna Central Cemetery, May 2019

PLASMA CHEMISTRY DATABASES: FAR SOL, SUB-DIVERTOR

C_xH_y as a role model for other Hydrides (Be_xH_y, HeH^+,….systems?)

- Already done SiH_y: Janev, Reiter, Contr. Plasma Physics, 2003,43,401-417

Chemistry | Physics

Extensions, evaluations, new exp. and theor. results

1987

2002-2004

2012

Plasma chemical rate constants (Arrhenius form) for well stirred, equilibrium, low T conditions

A.B. Ehrhardt, W. D. Langer, Report PPPL-2477, Princeton (1987).

Comprehensive set.
Cross sections already, but universal fit expression for all types of processes
→ poor asymptotic behaviour

R.K. Janev, D. Reiter
Phys. Plasmas, Vol 9, 9, (2002) 4071
Phys. Plasmas, Vol 11,2, (2004) 780

Classification of processes,
Asympt. correct fits, separate form for each category of reactions

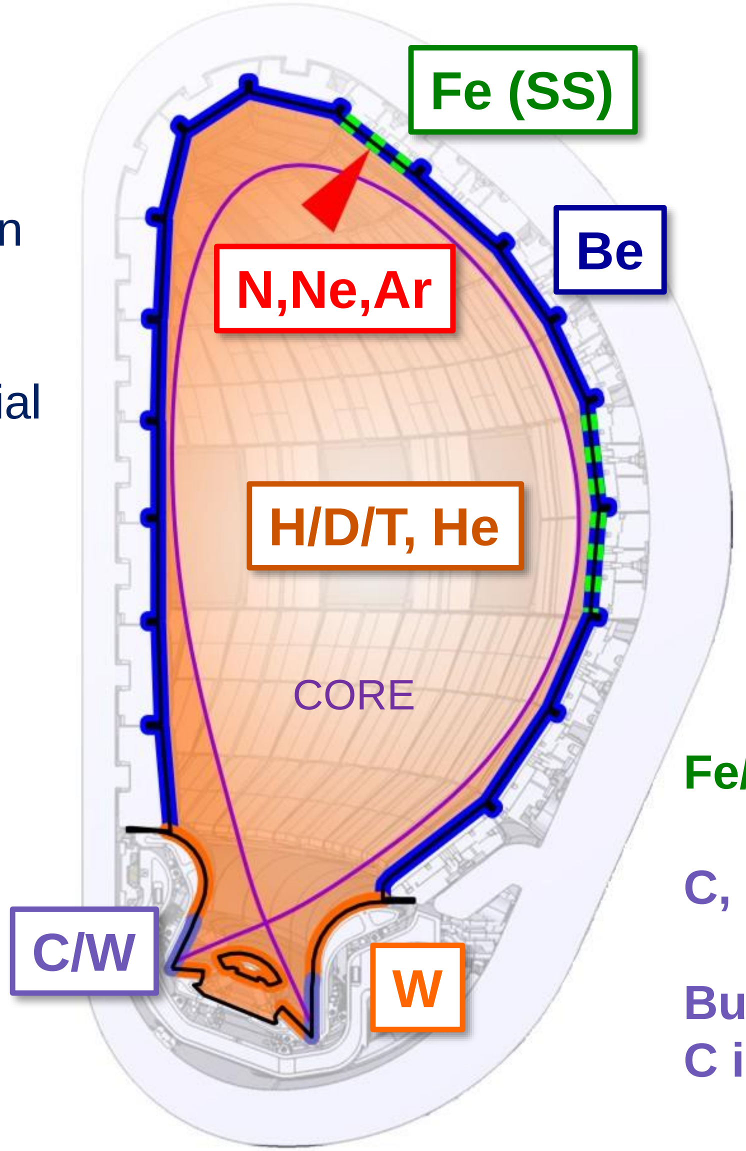
APID 16,
IAEA AMD unit

List of the main elements relevant to the ITER plasma

Because of T-retention and migration Carbon was removed from ITER design in 2013.
I.e. the material we knew most about in fusion, and the most forgiving material too (does not melt), was removed.

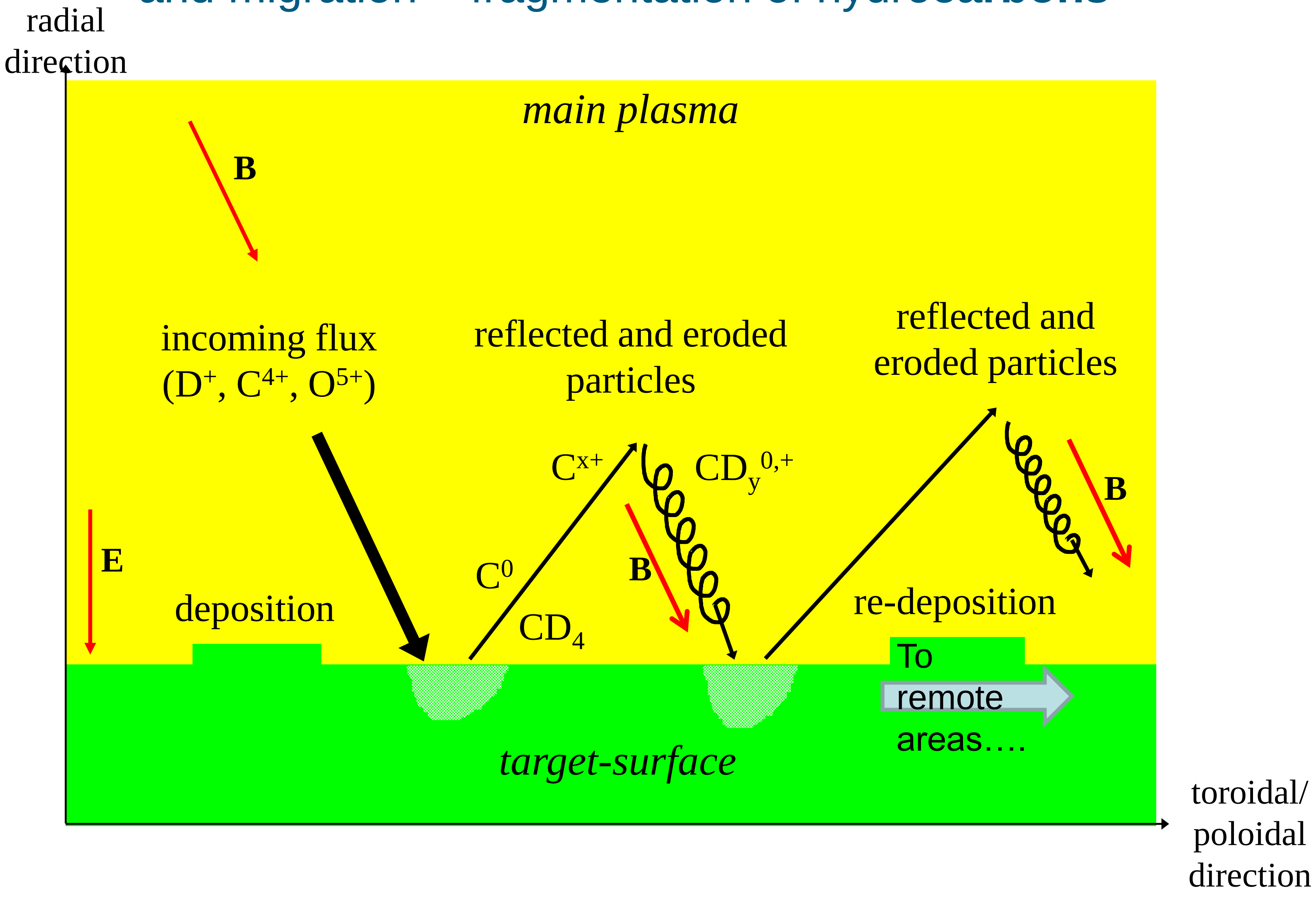
This puts BeH, BeH_2 into focus, wrt. its tritium issues:

- Transport modelling of pathways
- spectroscopical wall erosion rate quantification

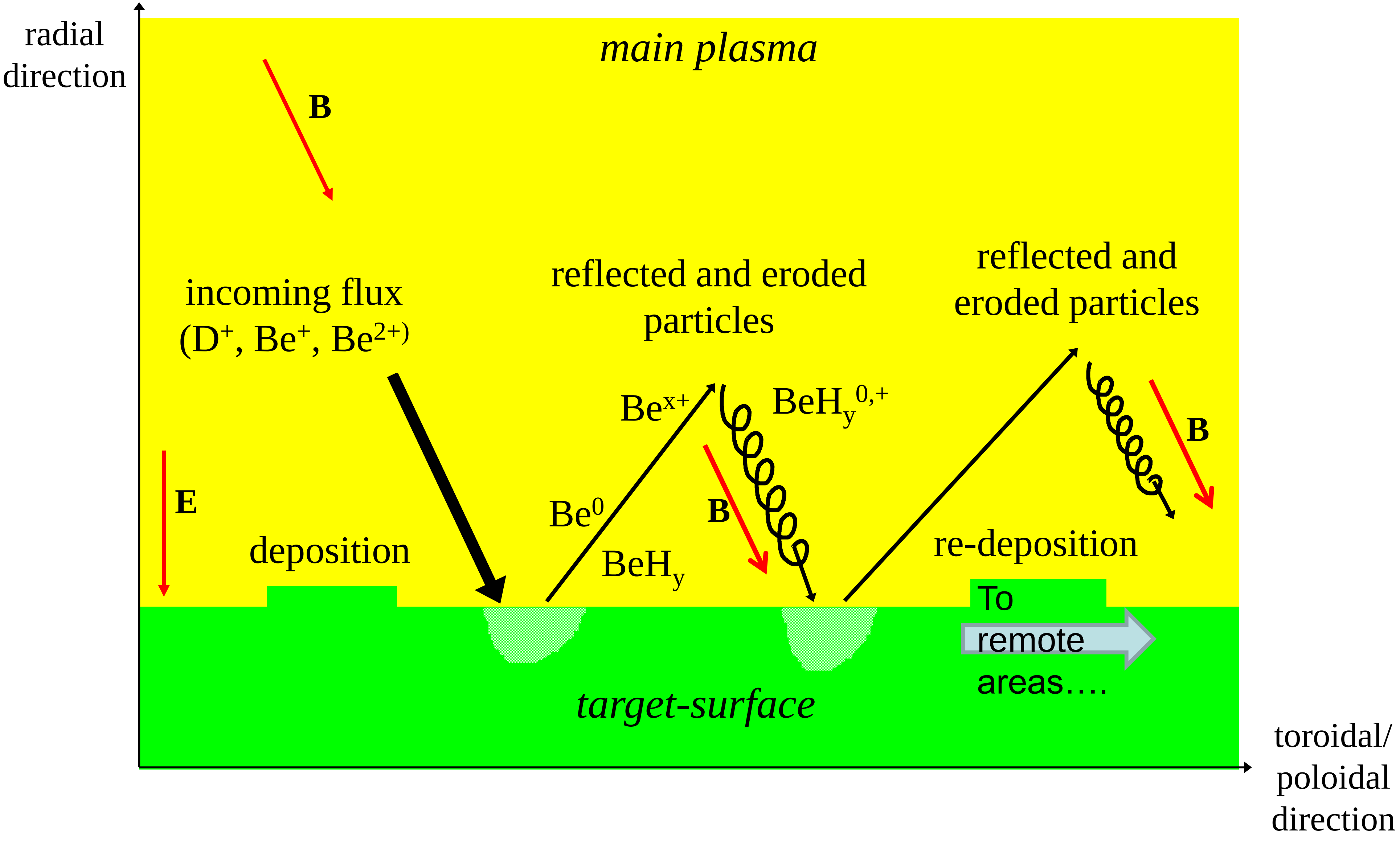


Fe/SS, 2011: armour at diagnostics port plugs
C, in 2013: replaced by all W divertor
But:
C in: W7X (2016), JT-60SA (2019),…

Release (chem. sputtering) and migration + fragmentation of hydro**carbons**



Release (sputtering, volumetric formation/fragementation) and migration + fragmentation of **beryllium** hydrides



MOLECULAR PROCESSES CONSIDERED IN FUSION:

- e+ BeH/BeH^+ → .... possible role on spectroscopy and on material migration:

Formation rates ?? 10% of Be sputtering? Volumetric particle exchange reactions ?

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Exp.: UC Louvain, Theory: I. Schneider et al., Univ. Du Havre, J. Tennyson et al. (Quantemol), R. Celiberto et al. (Bari)

Multiple aspects solved, but data scattered in literature, not jet compiled into a single comprehensive database.

Be, BeH, ..status (notes by B. Braams, 2013, IAEA, „light element CRP“)

- From both PISCES and JET BeH is measured spectroscopically without any special effort to inject it.
- It is found in deuterium plasma where it is presumed to be **produced on the walls** and it is found in experiments where beryllium is seeded into deuterium plasma and there it would be **produced by volumetric formation**

  ($Be^{+} + H_2 \rightarrow p + BeH$?? particle transfer).
- In PISCES the release of BeH can be dominant form of beryllium release, up to 100% it is claimed. See Section 4 in the article by D. Nishijima et al., "Properties of BeD molecules in edge plasma relevant conditions“ [1], http://iopscience.iop.org/0741-3335/50/12/125007. I believe that it is not known **how much is released in the form of BeH_2** and maybe some of the measured BeH is a breakdown product of BeH_2. Note that the breakdown chain for BeH_2 does not need to pass through neutral BeH, it may go direct to BeH^{+} and it may even by-pass that ion.
- (D.R., added 2019:) The primary source of information on Be, BeH in fusion relevant plasmas today is **PISCES [1]and JET [2] experiments**. The primary tool for transport analysis and interpretation are Monte-Carlo codes such as **ERO [3]**.

2011: Construct a BeH_y breakup model, similar to the C_xH_y database? How hard can it be ?

April 2012 (from notes of R. Janev, at that time):

"There are not much cross sections available in the literature for e-impact processes with BeH. I was not able to find anything even for the ionization cross section. The only available source for calculating this cross section is the Gryzinsky formula (GBB) **having an unspecified uncertainty"**.

IYMG (If you must guess):

2013: C. Björkas, …,R. Janev, et al.: Journal of Nuclear Materials 438 (2013) ERO code [3]:

"The **ADAS database** […] was here used to describe the electron collision rates for Be reactions in the plasma and the cross-section (σ) for non-dissociative ionization of BeD was calculated using the **Gryzinski–Bauer–Bartki** approximation […]. The dissociative excitation (via a series of pre-dissociating BeD excited states) was evaluated by the **Born–Bethe (BB)** approximation, appropriately corrected in the low-energy region and with proper account of pre-dissociation probabilities. After dissociating, Be is most probably in the ^3P metastable state. The dissociative recombination cross section of BeD+ was taken from Ref. […]. …The rates were calculated assuming that BeD is in its first excited vibrational level, v= 1 (in accordance with observations […]). The excitation cross section for BeD ($X^2\Sigma^+;v_i=0 \rightarrow A^2\Pi;v_f= 0$) transition was also calculated using the **BB approximation,** corrected at low energies with the R-matrix results […] and then scaled to the $v_i=1 \rightarrow v_f=1$ transition. Assuming that all excited molecules promptly radiatively return to the BeD ($X^2\Sigma^+;v_i=1$) state, a photon emission coefficient emerges that agrees well with the experimental lower limit estimation of Ref. […] (illustrated in the inset of Fig. 2)."

This appears to be all about BeH, BeH+ collision data, that has arrived in practical fusion applications today.

(reconfirmed last week with the ERO group in Jülich)

- Despite being **entirely obsolete**, and furthermore only a small subset of that database being actually used in ERO,

at least the underlying cross section data can now be **publicly exposed**

(I found Ratko‘s original notes (2011), when recently clearing my office in Jülich, March 2019)

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BeD Database

A. e - BeD collision PROCESSES AND $A^2\Pi_{v'} \to X^2\Sigma$, RAD. TRANSITIONS

A.1. Ionization (non-dissociative)

$$e + BeD(X^2\Sigma^+; v) \to e + BeD^+ + e \quad , \quad v = 0, 1, \dots 7$$

v - vibrational level

Cross section (BBG model):

$$\sigma_{ion}(v) = \frac{6.515}{[I_p(v)]^2} G(x) \quad (\times 10^{-14} cm^2)$$

$$G(x) = \frac{1}{x} \left(\frac{x-1}{x+1} \right)^{3/2} \left\{ 1 + \frac{2}{3}\left(1 - \frac{1}{2x}\right) \ln\left[e + (x-1)^{1/2}\right] \right\}$$

$e = 2.718281828, \dots$

$$x = \frac{E}{I_p(v)} \;; \; E, \; I_p(v) \text{ in eV units}$$

E - electron energy
$I_p(v)$ - ionization energy of $BeD(v)$

Table A.1.: Values of $I_p(v)$, in eV units:

v	$I_p(v)$ [eV]
0	8.21
1	8.03
2	7.85
3	7.67
4	7.50
5	7.34
6	7.18
7	7.01

A.2. Excitation of $A^2\Pi$ state

$$e + BeD(X^2\Sigma^+; v) \to e + BeD(A^2\Pi; v') \quad , \quad v, v' = 0, 1, \dots 7.$$

Cross section (Born-Bethe approximation):

$$\sigma^{X-A}_{v,v'} = \frac{2}{3} \frac{\pi}{E} g \left| D_{X-A}(R_{ex}) \right|^2 S^{X-A}_{v,v'} \cdot \ln\left(\frac{4 E I_p(v)}{\Delta E^2_{vv'}} \right) a_0^2 \qquad (a)$$

$g = 2$ - stat. factor

$|D_{X-A}(R_{ex})| = 0.872164$ a.u. - dipole transition moment for X-A at $R = R_{e,X}$

$S^{X-A}_{v,v'}$ - Frank-Condon factor for $X(v) \to A(v')$

$\Delta E_{vv'}$ - transition energy for $X(v) - A(v')$

$I_p(v)$ - ionization energy of $X(v)$ [Table. A.1.]

$$\sigma^{X-A}_{v,v'} = \frac{2.4286}{E_{(eV)}} S^{X-A}_{vv'} \cdot \ln\left(\frac{4 E I_p(v)}{\Delta E^2_{vv'}} \right) \quad (\times 10^{-15} cm^2)$$

$E, I_p(v), \Delta E_{vv'}$ - in eV units ; E - electron energy

$I_p(v)$ - given in Table A.1. (p. 1)

$\Delta E_{vv'}$ - given in Tabe A.2. (next, p. 3)

$S_{vv'}$ - given in Table A.3. (next, p. 3)

Note: Eq. (a) is writen in Frank-Condon approximation for the electric dipole (transition) moment:

$$\left| \langle \chi_{Av'} | D_{XA}(R) | \chi_{Xv} \rangle \right|^2 \simeq \left| D_{XA}(R_{eX}) \right|^2 S^{X-A}_{vv'}$$

Table A.2. Values of $\Delta E_{vv'}$ in eV units

v	v'=0	v'=1	v'=2	v'=3	v'=4	v'=5	v'=6	v'=7
0	2.4843	2.6709	2.8518	3.0269	3.1968	3.3591	3.5189	3.6762
1	2.2998	2.4864	2.6673	2.8424	3.0123	3.1746	3.3344	3.4887
2	2.1203	2.3069	2.4878	2.6629	2.8328	2.9951	3.1549	3.3122
3	1.9461	2.1327	2.3136	2.4887	2.6586	2.8209	2.9807	3.1380
4	1.7765	1.9631	2.1440	2.3191	2.4890	2.6513	2.8111	2.9684
5	1.6139	1.8005	2.0714	2.1565	2.3264	2.4887	2.6485	2.8058
6	1.4532	1.6398	1.8207	1.9958	2.1657	2.3280	2.4878	2.6451
7	1.2947	1.4813	1.6622	1.8373	2.0072	2.1695	2.3293	2.4866

Table A.3. Values of $S^{X-A}_{vv'}$ (Frank-Condon factors)

v	v'=0	v'=1	v'=2	v'=3	v'=4	v'=5	v'=6	v'=7
0	1.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	(0.0022) 0.0022	0.9960	0.0010	0.0005	0.0002	0.0001	0.0	0.0
2	0.0010	0.0022	0.9940	0.0015	0.0008	0.0003	0.0002	0.0
3	0.0005	0.0015	0.0025	0.9920	0.0018	0.0010	0.0005	0.0002
4	0.0002	0.0008	0.0015	0.0030	0.9900	0.0025	0.0015	0.0003
5	0.0003	0.0010	0.0025	0.0035	0.0050	0.9810	(0.0350) 0.0350	0.0025
6	0.0005	0.0015	0.0030	0.0055	0.0010	0.0170	0.9280	0.0130
7	0.0010	0.0020	0.0040	0.0070	0.0012	0.0200	0.0350	0.875

* Note the large values of $S^{X-A}_{v=v'}$, coming from closeness of R_{eA} and R_{eX} of potential curves for $X^2\Sigma^+$ and $A^2\Pi$ states. (R_e - equilibrium nuclear distance)

A.3. RADIATIVE $A^2\Pi; v' \to X^2\Sigma^+; v$ TRANSITIONS

Radiative transition probability (in atomic units): a.u.

$$A^{v'\to v}_{A\to X} = \frac{2}{c^3} \Delta E^2_{vv'} \left| f^{v'v}_{AX} \right| \frac{1}{g}$$

$\Delta E_{vv'}$ – transition energy (in a.u.)

$c \approx 137.04$ speed of light (= 137.0360... a.u.)

$g = 2$ stat. factor

$f^{vv'}_{AX}$ – oscillator strength

$$f^{vv'}_{AX} = \frac{2}{3} g \, \Delta E_{vv'} \left| \langle \chi_{v'} | D_{XA}(R) | \chi_v \rangle \right|^2$$

$$A^{v'\to v}_{AX} = \frac{4}{3} \left(\frac{\Delta E_{vv'}}{c} \right)^3 \left| D_{AX}(R_{e,x}) \right|^2 \cdot S_{vv'} \quad \text{(in a.u.)}$$

(in Frank-Condon approx. for $M_{XA} = |\langle |D| \rangle|^2$)

$D_{AX}(R_{eX}) = -0.87216$ a.u. (−0.87216)?

$t_e = 2.4188884326 \cdot 10^{-17}$ sec (atomic unit for time)

$$\Delta E_{vv'}(\text{a.u.}) = \frac{\Delta E_{vv'}(\text{eV})}{27.21}$$

When $\Delta E_{vv'}$ is expessed in eV units and $A^{v'\to v'}_{AX}$ in sec^{-1}:

$$A^{v'\to v'}_{AX} = 8.087806 \cdot 10^5 \, \Delta E^3_{vv'} \, S_{vv'} \; (\text{sec}^{-1})$$

(8.087806)?

For v, v' = 0 – 7, the values of $\Delta E_{vv'}$ (in eV) and $S_{vv'}$ are given in Tables A.2. and A.3., respectively (p. 3).

- 5 -

Diss. Exc. / RKJ

A.4. (PRE)DISSOCIATIVE EXCITATION: (VIA) $C\Sigma^+ (\equiv 2\Sigma^+)$ STATE

$$e + BeD(X^2\Sigma^+; v) \to e + BeD(C\Sigma^+) \to e + Be(^3P) + D(^2S)$$

$v = 0, \ldots 7$

~~presspredissociation~~

Bethe-Born cross section:

$$\sigma_{X-C}^{diss} = \frac{6.515}{E \cdot \Delta E_{vc}} \cdot g \cdot f_{XC} \cdot \ln\left(\frac{4 E I_p(v)}{\Delta E_{vc}^2}\right) \quad (\times 10^{-15} cm^2)$$

$g = 1$, stat. factor; E - electron energy, in eV units

$f_{XC} = 0.0523$, oscillator strength

$I_p(v)$ - ionization energy (in eV) of $X^2\Sigma^+; v$ (Table A.1)

ΔE_{vc} - transition energy (in eV) (Table A.4 bellow).

$I_p(v)$, in eV, given in Table A.1

Table A.4.: Values of $\Delta E_{v,c}$ (in eV)

v	$\Delta E_{v,c}$ (eV)
0	5.4834
1	5.2985
2	5.1194
3	4.9452
4	4.7756
5	4.6130
6	4.4523
7	4.2938

TOTAL KINETIC ENERGY of PRODUCTS:

$E_K = 0.524$ eV

DISTRIBUTION OF E_K:

$$E_{Be} = \frac{2}{11} E_K, \quad E_D = \frac{9}{11} E_K$$

- 6 -

A.5. (PRE-)DISSOCIATIVE EXCITATION: (VIA) $3, 4, 5\,^2\Sigma^+$ STATES

$$e + BeD(X^2\Sigma; v) \to e + BeD(F; v') \to e + Be(^3P) + D(^2S)$$

$v, v' = 0, 1, \ldots 7$

$F = 3^2\Sigma^+, 4^2\Sigma^+, 5^2\Sigma^+$

Cross section:

$$\sigma_{v-v'}^{X-F} = \frac{2}{3} \frac{\pi}{E} g \left| D_{X-F}(R_{e,X}) \right|^2 S_{vv'}^{X-F} \ln\left(\frac{4 E I_p^X(v)}{[\Delta E_{vv'}^{X-F}]^2}\right) P_F^{LZ}(v')\, a_0^2$$

$g = 1$, stat. factor, E - electron energy

$|D_{X-F}(R_{e,X})|$ - transition dipole moment for X-F at R_{eX}

$S_{vv'}^{X-F}$ - Frank-Condon factor

$I_p^X(v)$ - ionization energy of $(X^2\Sigma; v)$ (Table A.1)

$\Delta E_{vv'}^{X-F}$ - transition energy for $X; v \to F; v'$

$P_F^{LZ}(v')$ - predissociation probability of $(F; v')$ state

When E, $I_p(v')$ and $\Delta E_{vv'}^{X-F}$ are expressed in eV units:

$$\sigma_{vv'}^{X-F} = \frac{1.596}{E} \left| D_{X-F}(R_{eX}) \right|^2 \cdot S_{vv'}^{X-F} \cdot \ln\left(\frac{4 E I_p^X(v)}{[\Delta E_{vv'}^{X-F}]^2}\right) \cdot P_F^{LZ}(v') \quad (\times 10^{-15} cm^2)$$

$I_p^X(v)$ - (Table: A.1) (in eV)

Table A.5.: Values of dipole transition moments $D_{XF}(R_{eX})$:

F	$D_{X-F}(R_{eX})$ a.u.
$3\Sigma^+$	0.14971
$4\Sigma^+$	0.59826
$5\Sigma^+$	0.76147

$S_{vv'}^{X-F} \approx S_{vv'}^{X-A}$

↳ given in Table A.3. (p. 5)

Values of $\Delta E_{vv'}^{X-F}$ and $P_F^{LZ}(v')$ given in the following pages,

Also on following pages are given the E_K values

Table A.6. Values of $\Delta E_{vv'}^{X-F}$ (in eV) for $F = 3^2\Sigma^+$

v	v'=0	v'=1	v'=2	v'=3	v'=4	v'=5	v'=6	v'=7
0	5.6454	5.9090	6.0993	6.2711	6.4310	6.5851	6.7263	6.8522
1	5.4609	5.7245	5.9148	6.0866	6.2465	6.4006	6.5418	6.6677
2	5.2814	5.5450	5.7353	5.9071	6.0670	6.2211	6.3623	6.4882
3	5.1072	5.3708	5.5611	5.7329	5.8928	6.0469	6.1881	6.3140
4	4.9376	5.2012	5.3915	5.5633	5.7232	5.8773	6.0185	6.1444
5	4.7750	5.0386	5.2289	5.4007	5.5606	5.7147	5.8559	5.9818
6	4.6143	4.8779	5.0682	5.2400	5.3999	5.5540	5.6952	5.8211
7	4.4558	4.7194	4.9097	5.0815	5.2414	5.3955	5.5367	5.6626

Table A.7. Values of $\Delta E_{vv'}^{X-F}$ (in eV) for $F = 4^2\Sigma^+$

v	v'=0	v'=1	v'=2	v'=3	v'=4	v'=5	v'=6	v'=7
0	6.2035	6.4295	6.6470	6.8475	7.0334	7.2033	7.3576	7.4974
1	6.0190	6.2450	6.4625	6.6630	6.8489	7.0188	7.1731	7.3129
2	5.8395	6.0655	6.2830	6.4835	6.6694	6.8393	6.9936	7.1334
3	5.6653	5.8913	6.1088	6.3093	6.4952	6.6651	6.8194	6.9592
4	5.4957	5.7217	5.9392	6.1397	6.3256	6.4955	6.6498	6.7896
5	5.3331	5.5591	5.7766	5.9771	6.1630	6.3329	6.4872	6.6270
6	5.1724	5.3984	5.6159	5.8164	6.0023	6.1722	6.3265	6.4663
7	5.0139	5.2399	5.4574	5.6579	5.8438	6.0137	6.1680	6.3078

Table A.8.: Values of $\Delta E_{vv'}^{X-F}$ (in eV) for $F = 5^2\Sigma^+$

v	v'=0	v'=1	v'=2	v'=3	v'=4	v'=5	v'=6	v'=7
0	6.7716	6.9349	7.0890	7.2364	7.3822	7.5273	7.6711	7.8138
1	6.5871	6.7504	6.9045	7.0519	7.1977	7.3428	7.4866	7.6293
2	6.4076	6.5709	6.7250	6.8724	7.0182	7.1633	7.3071	7.4498
3	6.2334	6.3967	6.5508	6.6982	6.8440	6.9891	7.1329	7.2756
4	6.0638	6.2271	6.3812	6.5286	6.6744	6.8195	6.9633	7.1060
5	5.9012	6.0645	6.2186	6.3660	6.5118	6.6569	6.8007	6.9434
6	5.7405	5.9038	6.0579	6.2053	6.3511	6.4962	6.6400	6.7827
7	5.5820	5.7453	5.8994	6.0468	6.1926	6.3377	6.4815	6.6242

Table A.9. Predissociation probabilitie ($P_F^{LZ}(v')$) and total kinetic energies of dissociation products $E_K^F(v')$ for $F = 3^2\Sigma^+, 4^2\Sigma^+, 5^2\Sigma^+$ states

	$P_F^{LZ}(v')$			$E_K^F(v')$ [eV]		
v'	$3^2\Sigma^+$	$4^2\Sigma^+$	$5^2\Sigma^+$	$3^2\Sigma^+$	$4^2\Sigma^+$	$5^2\Sigma^+$
0	0.97	0.4 [0.8]	0.5 [0.7]	0.686	1.244	1.812
1	0.98	0.6 [0.9]	0.7 [0.8]	0.950	1.470	1.976
2	0.99	0.7 [1.0]	0.7 [0.9]	1.140	1.688	2.130
3	1.0	0.9 [1.0]	0.95	1.312	1.888	2.277
4	1.0	1.0	1.0	1.472	2.074	2.423
5	1.0	1.0	1.0	1.626	2.244	2.568
6	1.0	1.0	1.0	1.767	2.398	2.712
7	1.0	1.0	1.0	1.893	2.538	2.855

Total kin. energy distribution: $E_{Be} = \frac{2}{11} E_K$, $E_D = \frac{9}{11} E_K$

* Values for $P_F^{LZ}(v')$ in [ ] are preferred

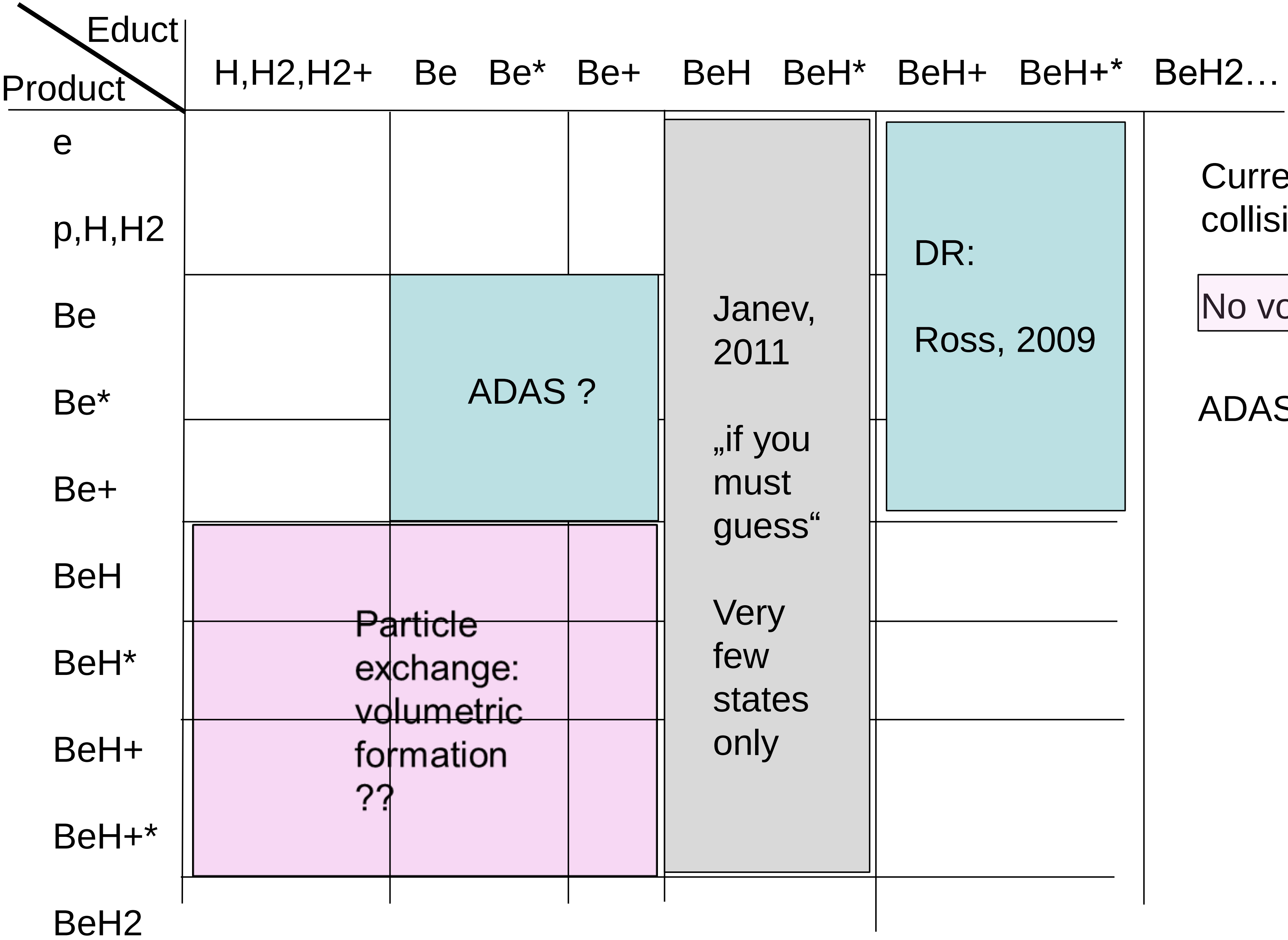
This IYMG ("if you must guess") model, together with early models for atomic Be, Be+ in www.HYDKIN.de online: 2012-2017.
HYDKIN is not maintained anymore at FZJ and disabled for online use (2017).
As of today: all data are still saved, available from FZJ (M.Rack@fz-juelich.de),
but at least the BeH, BeH+ and the 2003 Be CCC data **are obsolete today.**
BeH data are still kept mainly because some of them are still being used in ERO code.

Select type of process

	IAEA		Adas		
Be	**FLYCHK**	**Be CCC**	**Open Adas**	**Adas 89**	**Adas 93**
	☐$Be^{k+}_{I,ci}$, k=0,3 ☐$Be^{k+}_{I,ea}$, k=0,3	☐Be_I	☐Be^{k+}_{I}, k=0	☐Be^{k+}_{I}, k=0,3	☐Be^{k+}_{I}, k=0,3
		☐Be_E			
	☐$Be^{k+}_{R,rr}$, k=1,4 ☐$Be^{k+}_{R,dr}$, k=1,4	☐Be_R		☐Be^{k+}_{R}, k=1,4	☐Be^{k+}_{R}, k=1,4
BeH					
☐$BeH_{y\ I\text{-}DI}$					
☐$BeH_{y\ E/DE}$ ($BeH(X\ ^2\Sigma^+;v)$ <-> $BeH(A\ ^2\Pi;v')$) ☐$BeH_{y\ E/DE}$ ($BeH(X\ ^2\Sigma^+;v)$ -> Be(2s12p13P) + H(1s) via C Σ^+) ☐$BeH_{y\ E/DE}$ ($BeH(X\ ^2\Sigma^+;v)$ -> Be(2s12p13P) + H(1s) via 3 $^2\Sigma^+;v'$) ☐$BeH_{y\ E/DE}$ ($BeH(X\ ^2\Sigma^+;v)$ -> Be(2s12p13P) + H(1s) via 4 $^2\Sigma^+;v'$) ☐$BeH_{y\ E/DE}$ ($BeH(X\ ^2\Sigma^+;v)$ -> Be(2s12p13P) + H(1s) via 5 $^2\Sigma^+;v'$) ☐$BeH_{y\ E/DE}$ ($BeH(X\ ^2\Sigma^+;v)$ <-> $BeH(3\ ^2\Sigma^+;v')$) ☐$BeH_{y\ E/DE}$ ($BeH(X\ ^2\Sigma^+;v)$ <-> $BeH(4\ ^2\Sigma^+;v')$) ☐$BeH_{y\ E/DE}$ ($BeH(X\ ^2\Sigma^+;v)$ <-> $BeH(5\ ^2\Sigma^+;v')$)					
☐$BeH^+_{y\ E/DE}$ ($BeH^+(X\ ^1\Sigma^+;v)$ <-> $BeH^+(A\ ^1\Sigma;v')$) ☐$BeH^+_{y\ E/DE}$ ($BeH^+(X\ ^1\Sigma^+;v)$ <-> $BeH^+(B\ ^1\Pi;v')$)					
submit					

www.HYDKIN.de (2017): Be/BeH main entry page

Used (2019), ERO: CR Matrix for the Be – BeHy system



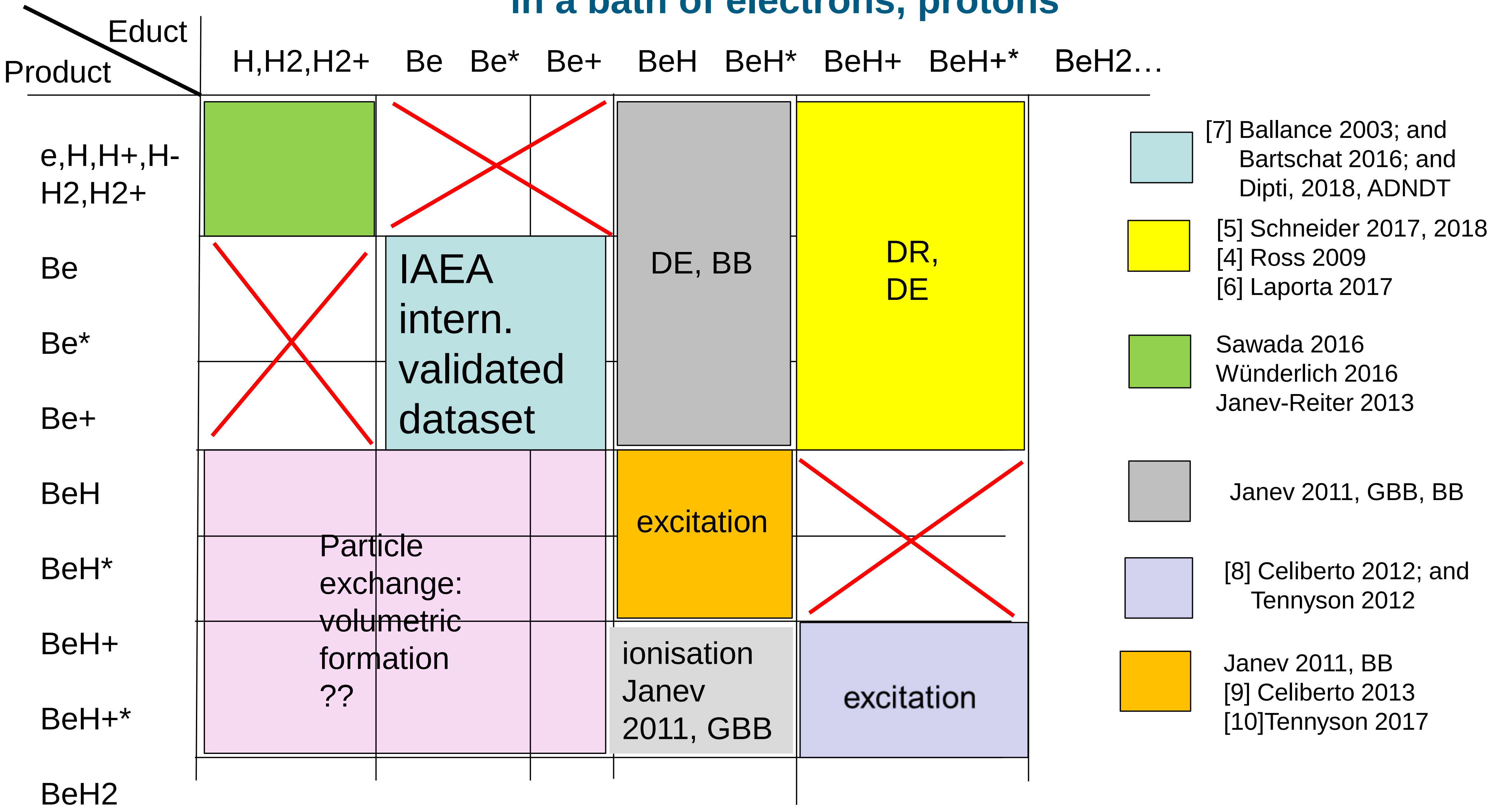
Current usage of Be, BeH collision data in fusion codes ?

No volumetric BeH_y formation ?

ADAS underlying raw data ?

Available (2019): CR matrix for the Be – BeH_y system

in a bath of electrons, protons



Issues:

Many individual data now, spread all over the place.

- Overlapping energy range, temperature range ?
- Resolution wrt. vibr., rot., electr. states within each block ?
- Detailed balance ?
- Near threshold and asymptotic behaviour of cross sections, and rate coefficients ?
- Reaction kinetics (KER: kinetic energy releases), branching ratios?
- Heavy particle collisions: particle exchange – charge exchange
- Surface processes: formation of BeH_y ?

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Thank you for your attention!