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# of atomic data for kinetic modelling of fusion plasma edge

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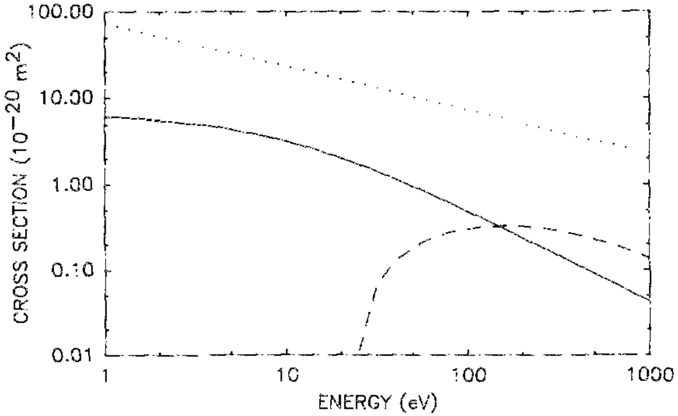
Outline

- Introduction
- Non-Maxwellian EDF effects on plasma-neutral and plasma-impurity rates in a stationary SOL
  - i. electron i,mpact processes
  - ii. ion impact processes
- Evolution of rate coefficients in the ELM-ing SOL
- Energy and angular DF of ions absorbed at the divertor plates
- New developments and list of cross-sections needed urgently for kinetic modelling of the SOL
- Conclusions

Introduction

History of implementation of plasma-neutral/impurity interactions in edge kinetic codes



1. **Primitive approach** (~30 years ago): linear model,
   transitions from ground state, qualitative CS

2. **Advanced approach** (~20 years ago): nonlinear model,
   transitions from ground and/or averaged states,
   multiple channels including 3 target and 4 product
   particles *[e.g. Matyash/Tacogna/Tskhakaya]*

3. **Model following selected state** (recent): selected excited states of particle species are followed *[e.g. Mijin, SOL-KiT, CPC 2021, Laricchiuta this meeting].*
   Applicable to simplified systems: "exponentially" increase of the number of required CS for
   more realistic cases including complex types of interactions (***N*** states requires ***N(N-1)***/2 CS)

4. **Dressed CS** approach (under development).

Do we really need a cross-section against Maxwell-averaged rate coefficients?

Stationary SOL: 1D flux tube model (BIT1)

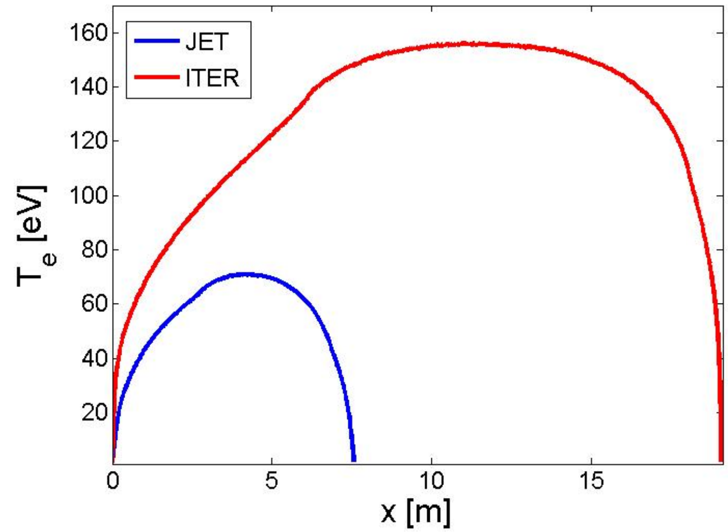
Ne seeded shots at JET and ITER,

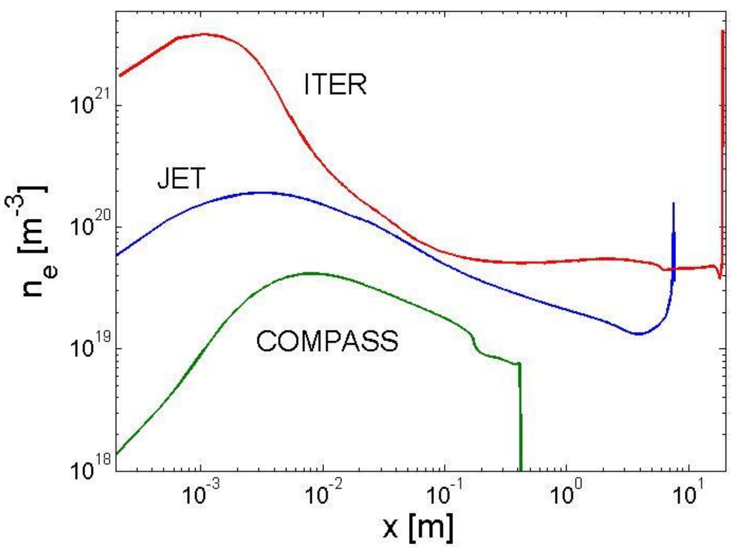
carbon divertors at COMPASS

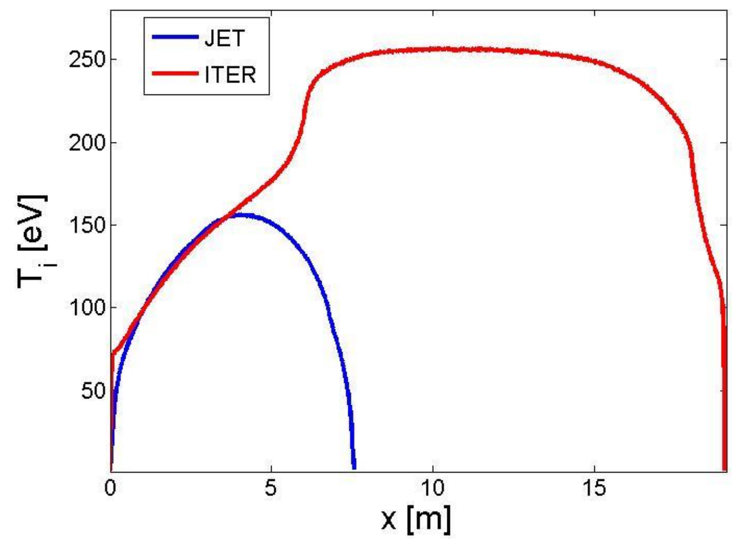
2320 points with E- and V-DF

$$R_{PIC} = \langle \sigma V \rangle_{f_{PIC}}$$

$$R_{Maxw} = \langle \sigma V \rangle_{f_{Maxw}}$$



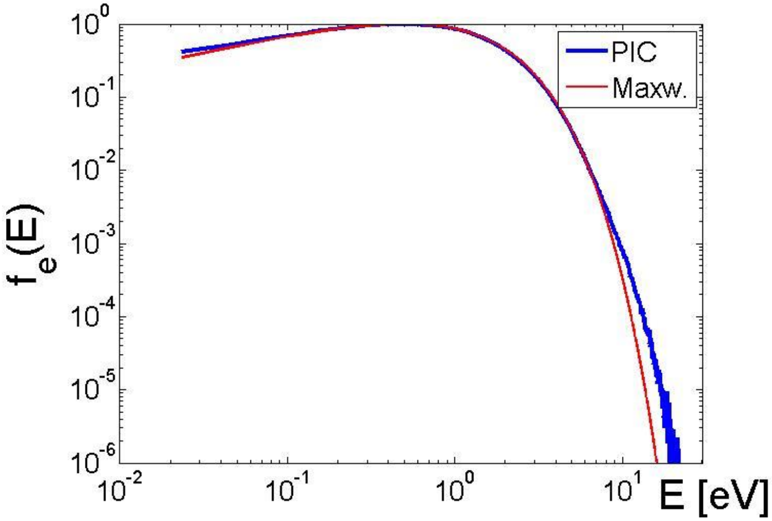


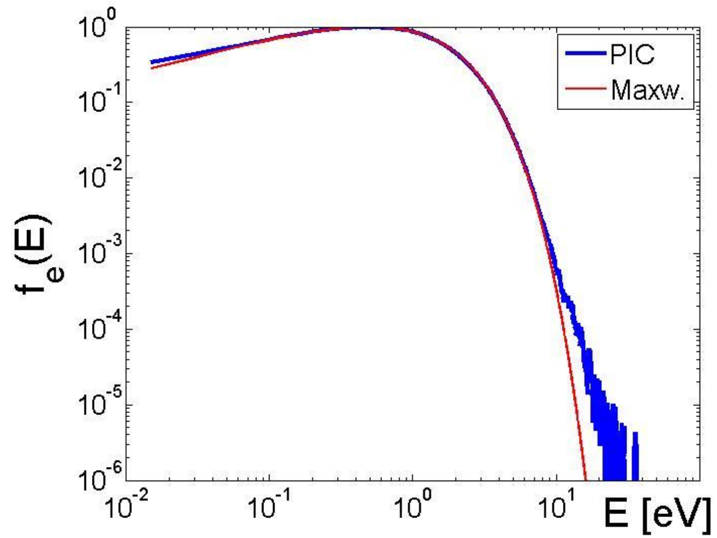


Stationary SOL: electron impact collisions

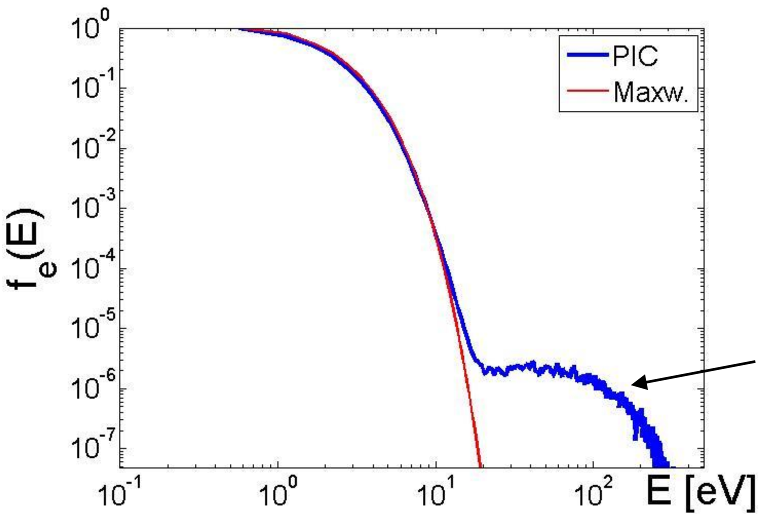
JET | **ITER**

1m from ID

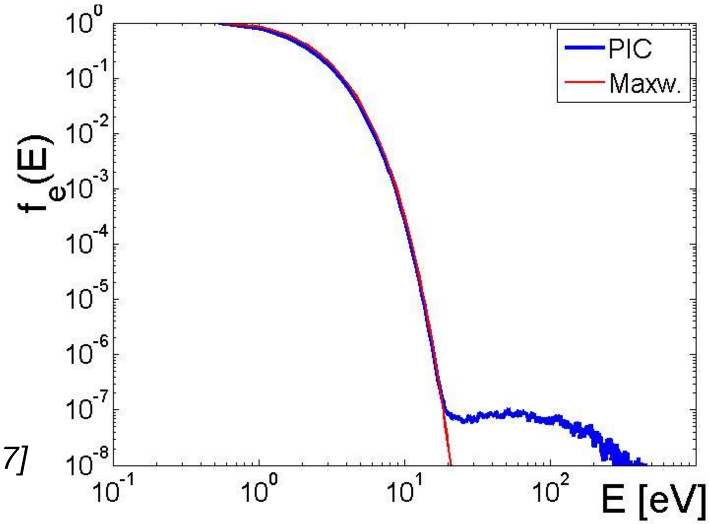




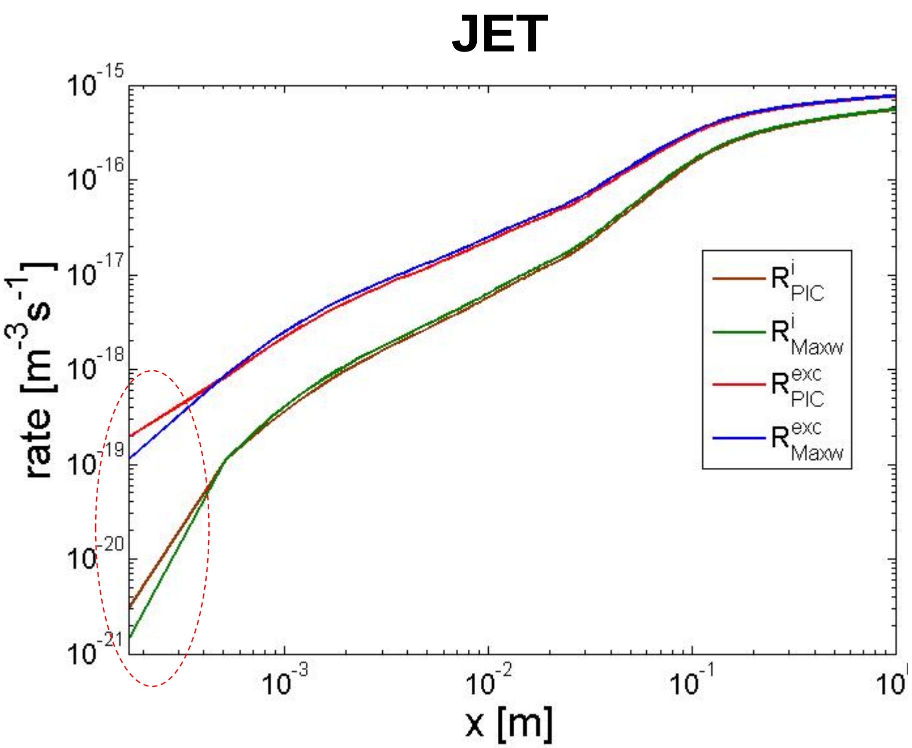
At the ID

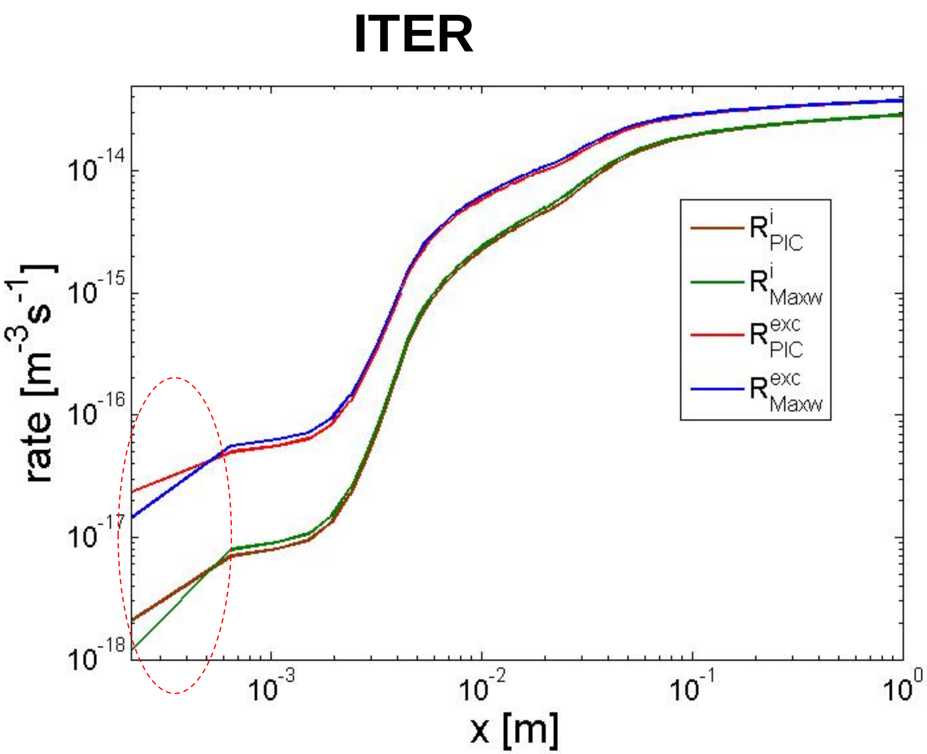


Collisionless super-thermal electrons *[Tskhakaya PPCF 2017]*



Stationary SOL: e + D collision rates

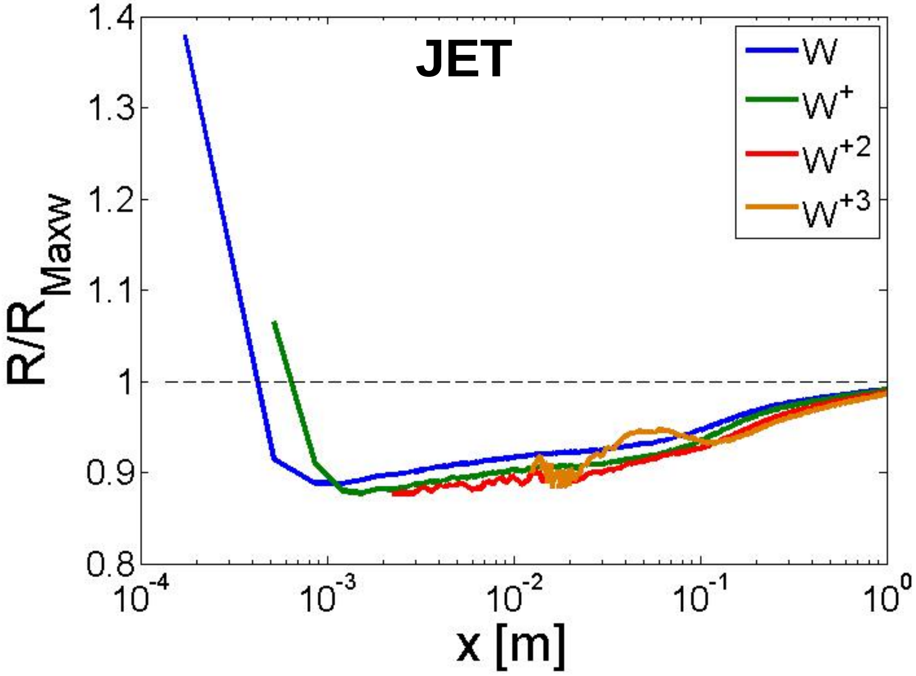


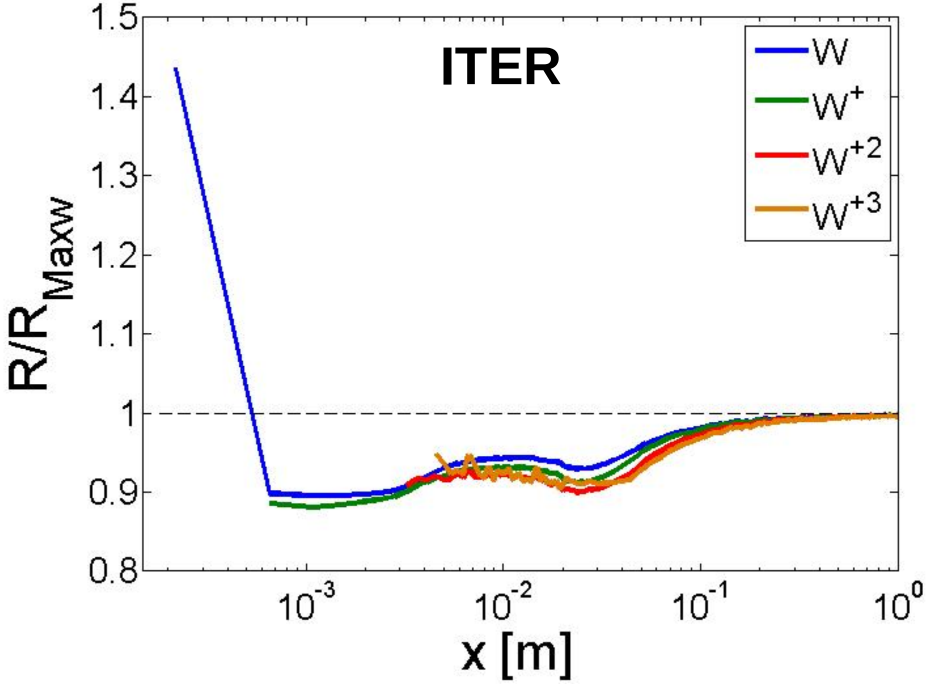


PIC vs Maxwellian-average RC **difference is negligible**

Cross-sections are from *[Janev (Ed.), Atomic and Molecular Processes in the Fusion Edge Plasmas, (1995)]*

Stationary SOL: e + W^{+i} ionization rates





There is some deviation **inside the sheath**

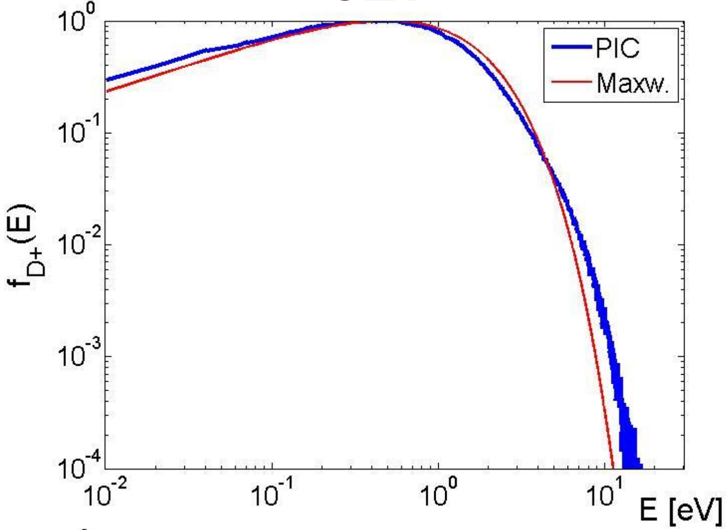
Can be important for **prompt re-deposition**

Actual for COMPASS-U: T_{div} 20 – 50 eV

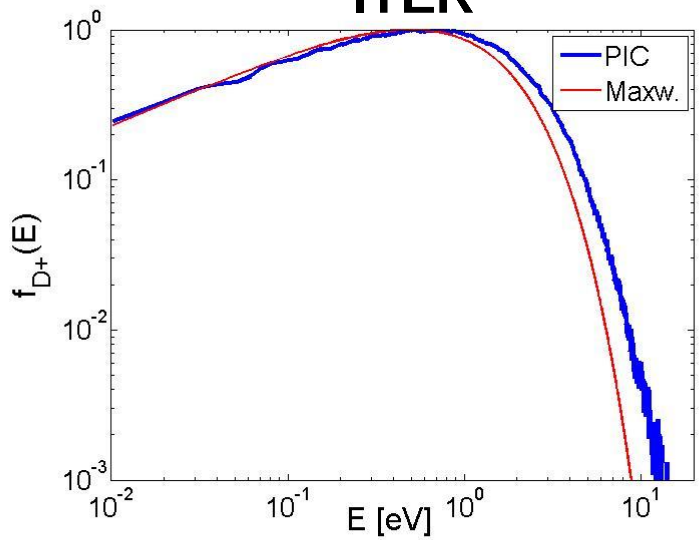
Cross-sections are taken from *[Vainshtein, et al., J. Phys. B: At. Mol. Opt. Phys., 44 (2011) 125201]*

Stationary SOL: ion impact collisions

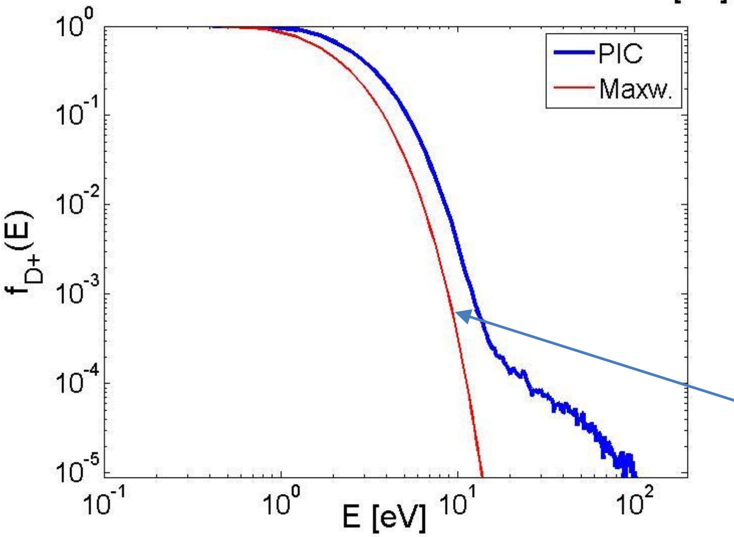
JET



ITER



1m from ID



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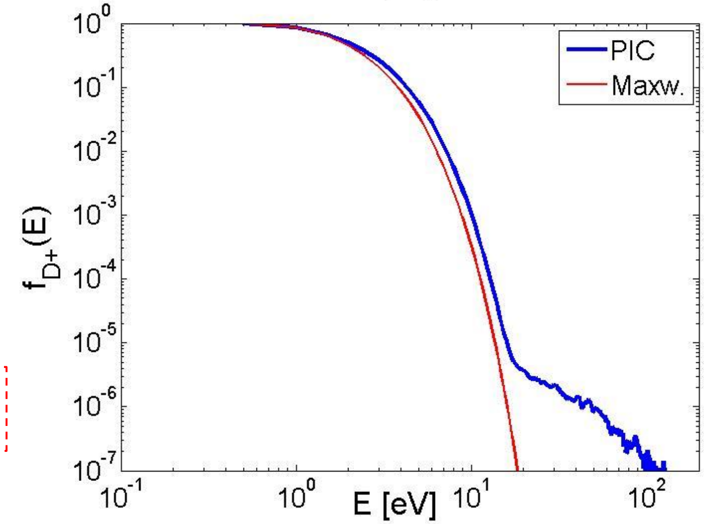
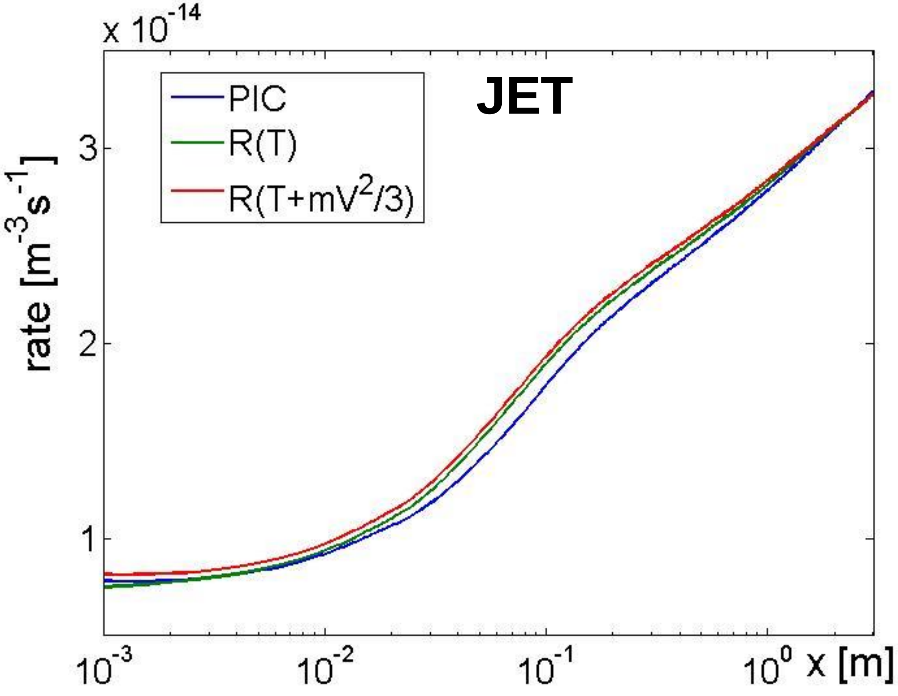
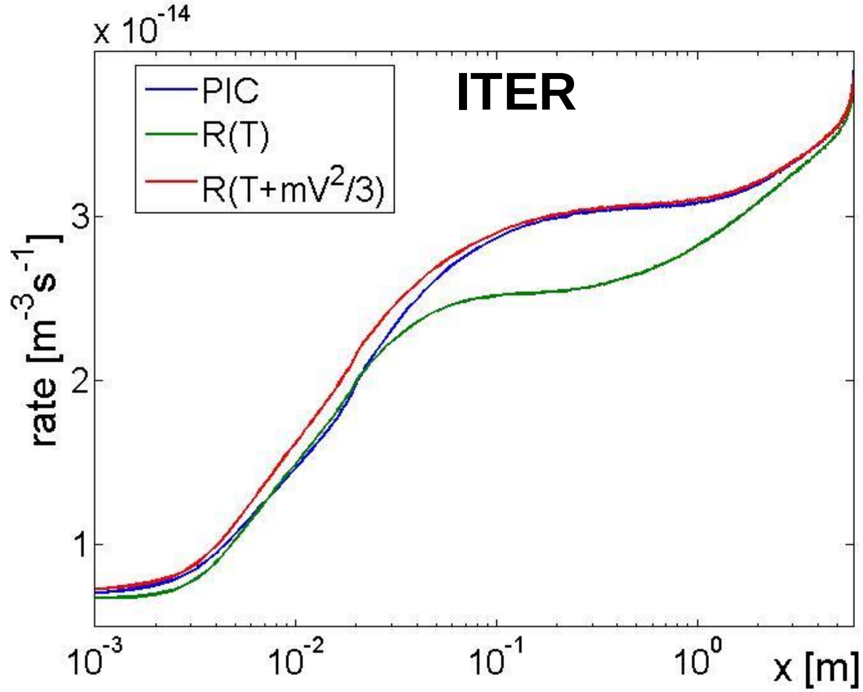
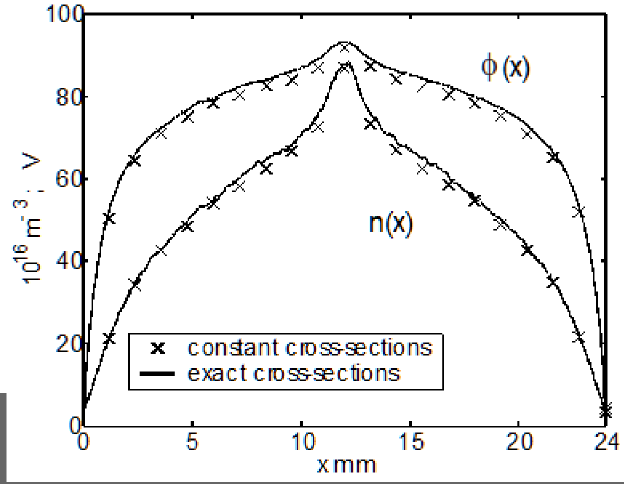


$V_{||} \sim C_s \sim V_T$

Stationary SOL: D + D$^+$ CX rates



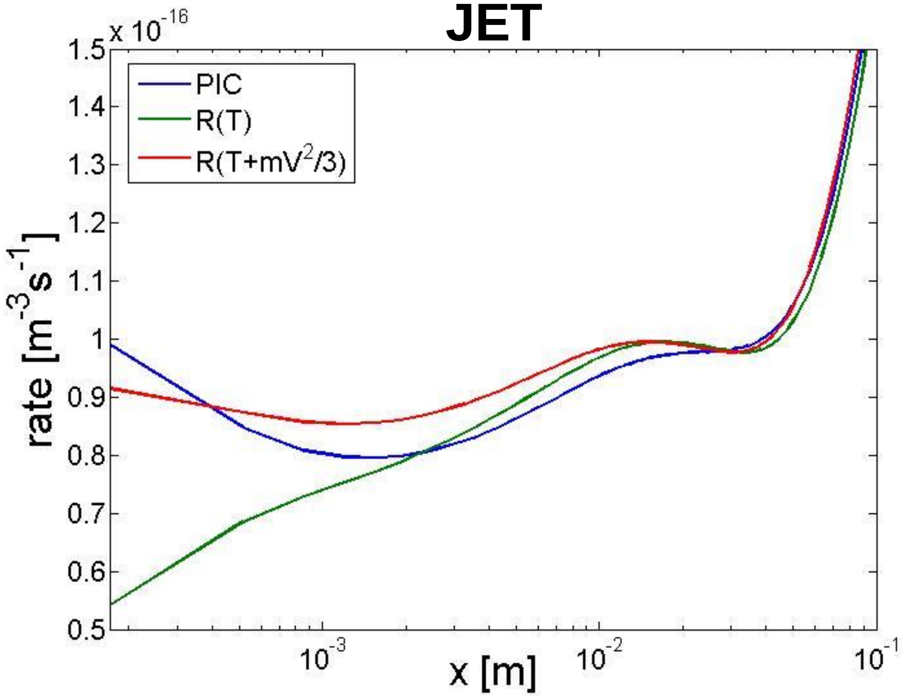


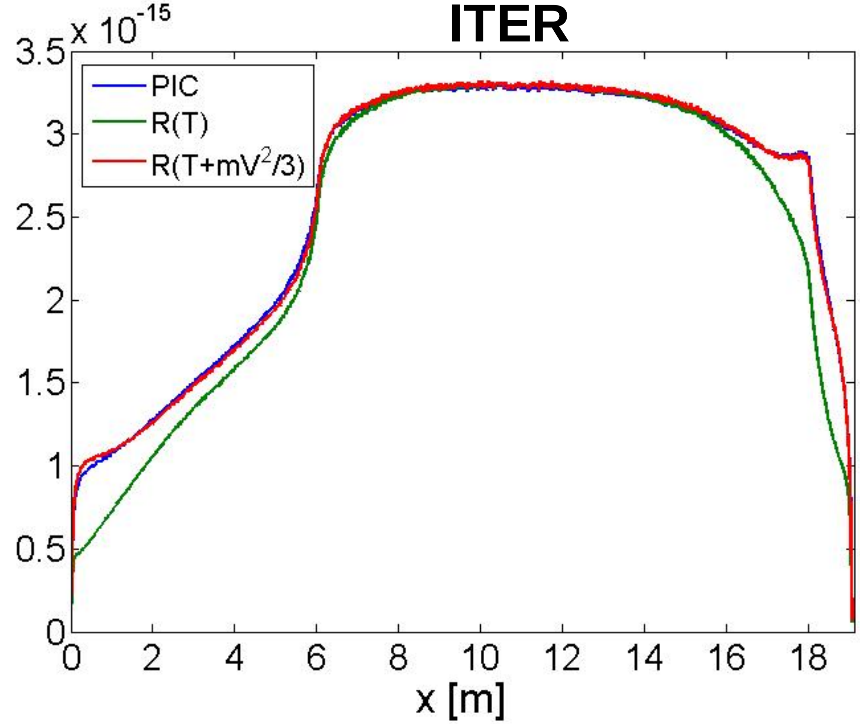


Linear vs exact CS
[D. Tskhakaya EPS-29 2002]

Cross-sections are from *[Krstic/Schultz, Nucl. Fus. Suppl. 8 (1998).; Janev (Ed.), Atomic and Molecular Processes in the Fusion Edge Plasmas, (1995)]*

Stationary SOL: $D^2 + D^+$ CX rates



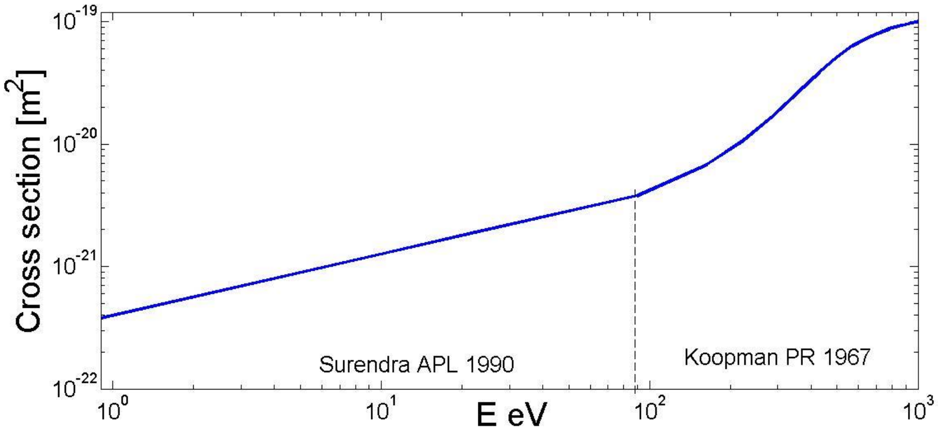


Deviation can be reduced by following substitution

$$R(T) \rightarrow R(T + 2E_{\parallel}/3), \quad E_{\parallel} = \frac{mV_{\parallel}^2}{2}$$

Cross-sections are from *[Janev, et al., Collision Processes in Low-Temperature Hydrogen Plasmas, 2005]*

Stationary SOL: Ar + D^+ CX rates

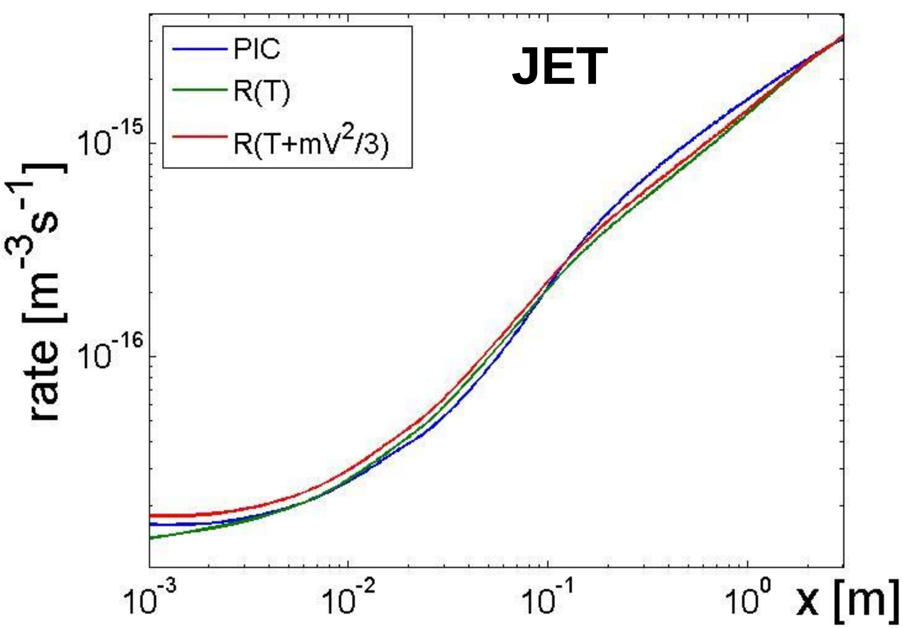


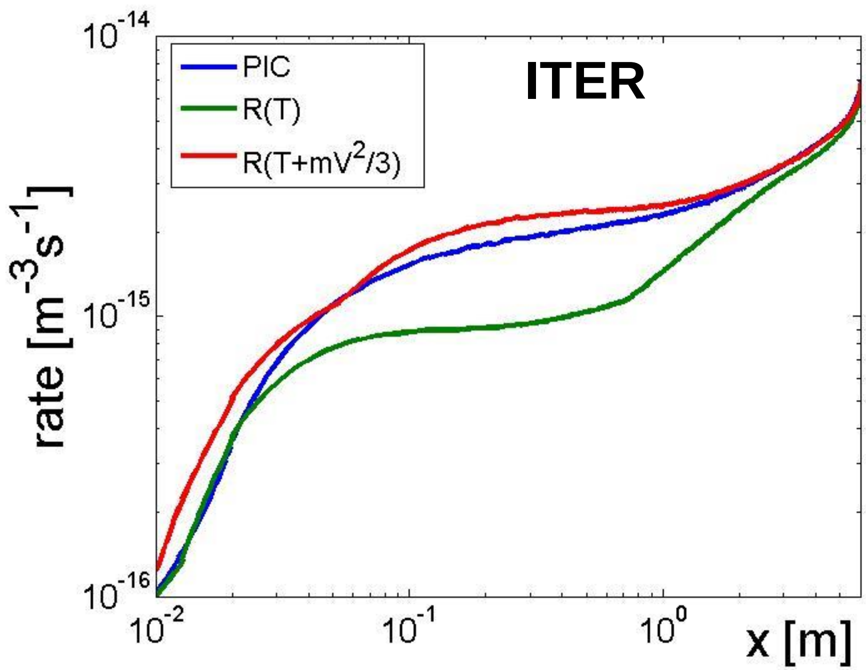
Cross-section for Ar + D^+ → D^+ + Ar charge-exchange collisions.

No CS data is available for impurity CX collisions *E* < 1 keV; exceptions: *C*, *Ar*

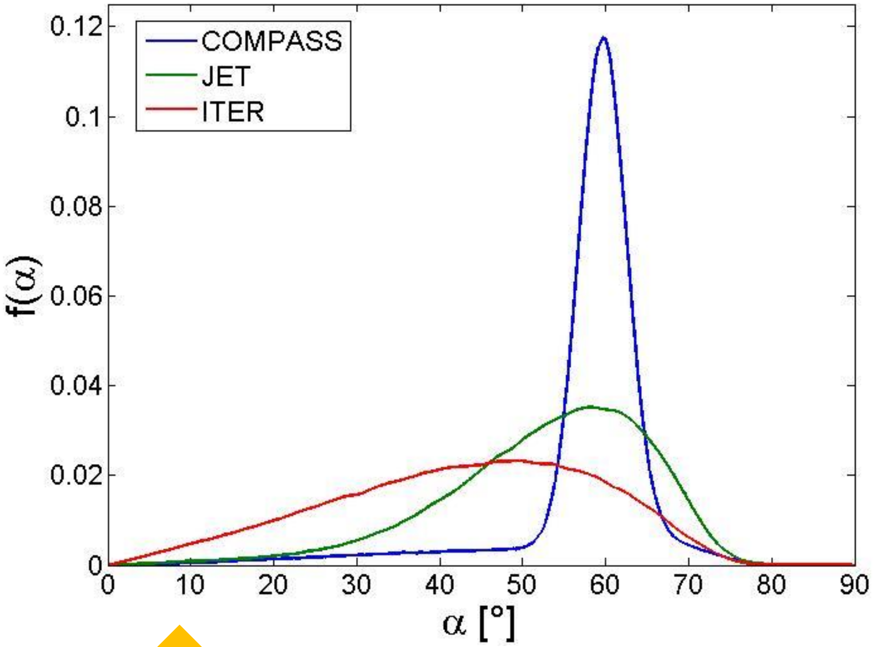
Deviation can be reduced by substitution

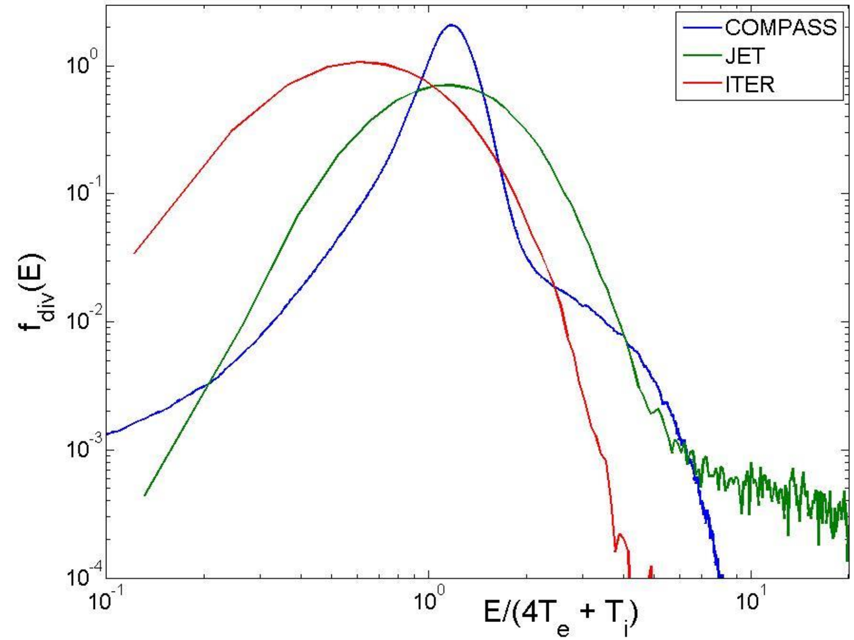
$$R(T) \rightarrow R(T + 2E_{\|}/3), \quad E_{\|} = \frac{mV_{\|}^2}{2}$$





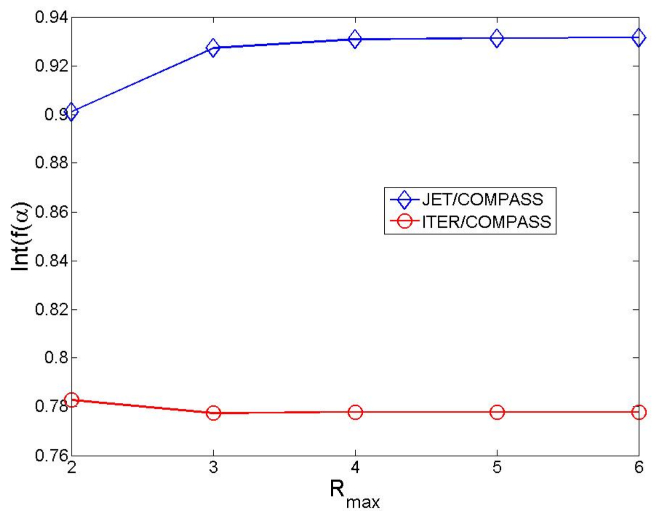
Stationary SOL: DF of absorbed ions



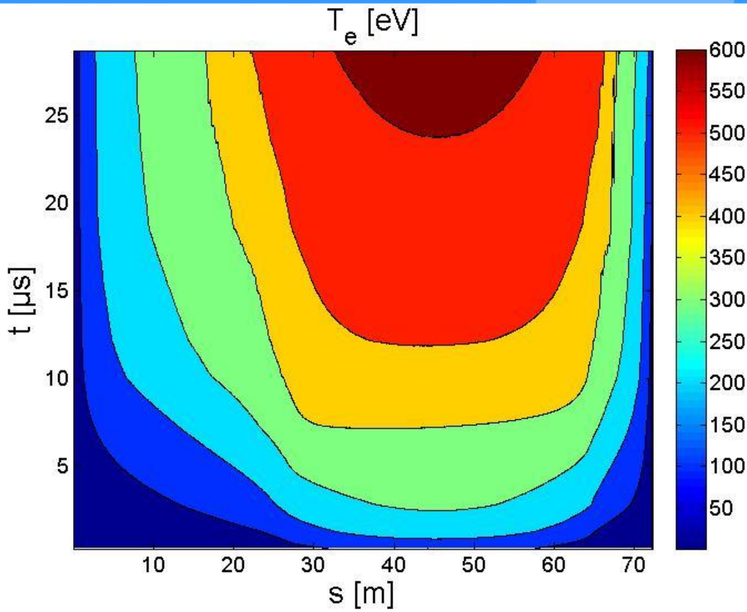


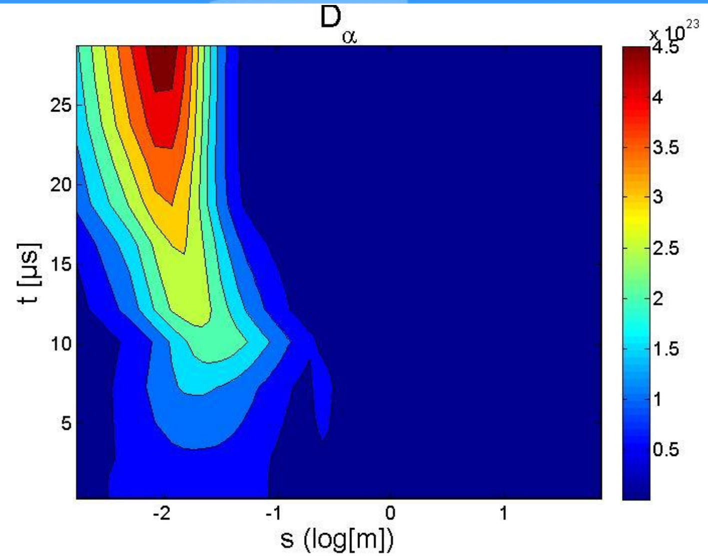
$$R_{em}(\alpha)=\begin{cases}\dfrac{1}{\cos(\alpha)} & if\ \leq R_{\max}\\ else,\ R_{\max}\end{cases}$$

$$\int_{\alpha} R_{em}(\alpha)d\alpha$$

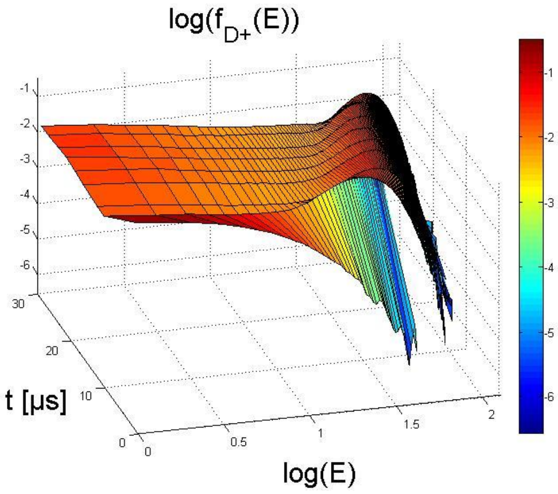


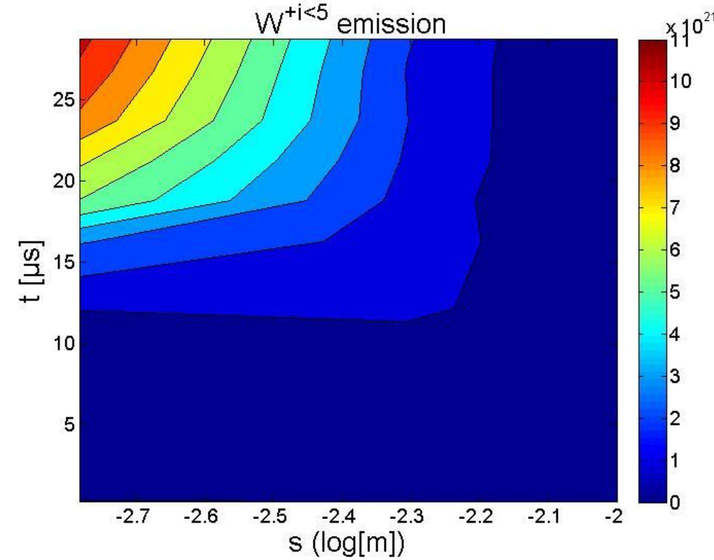
220 kJ ELM-ing SOL (JET)



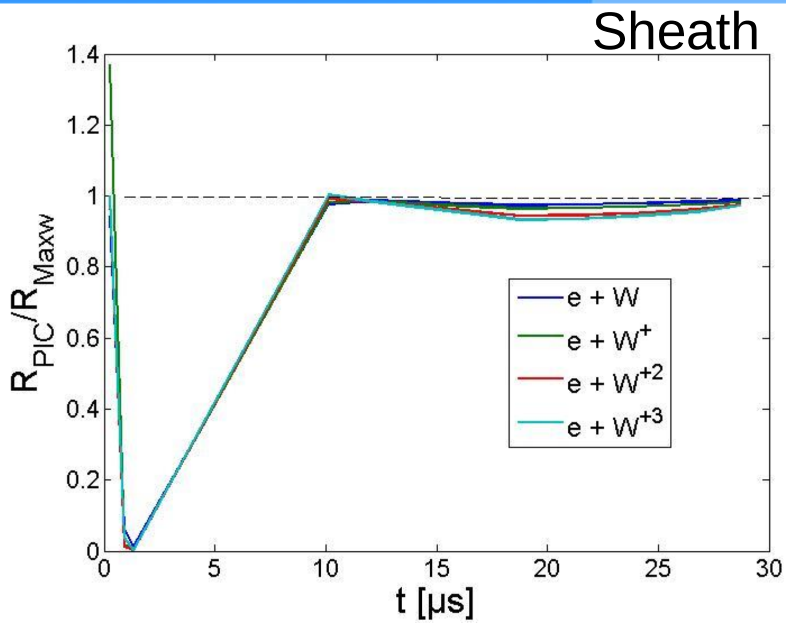


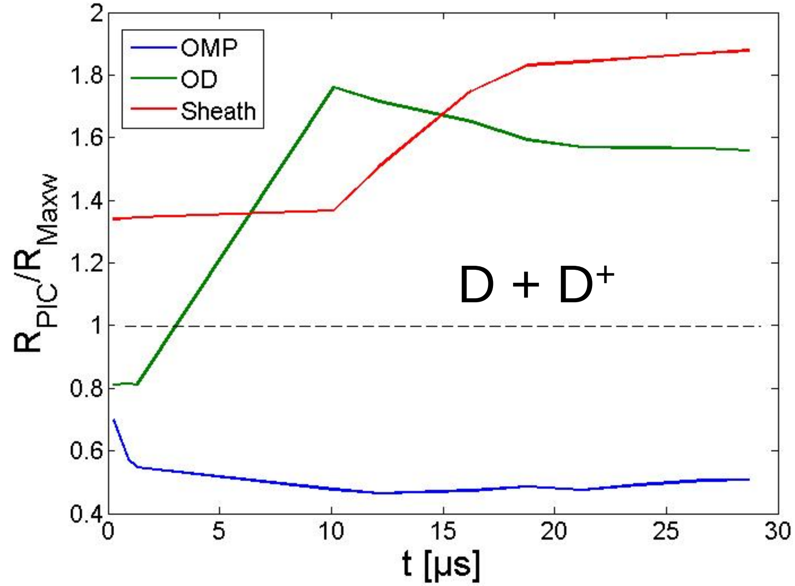
D⁺ EDF at
1cm from OD

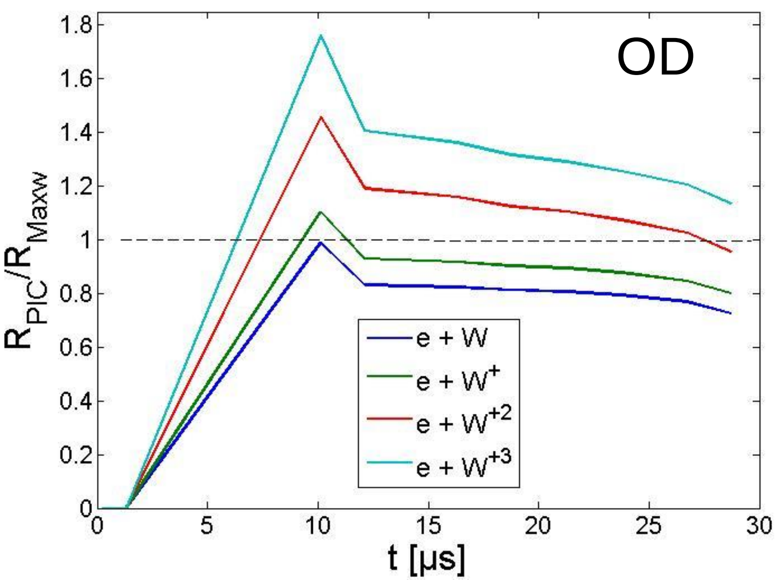


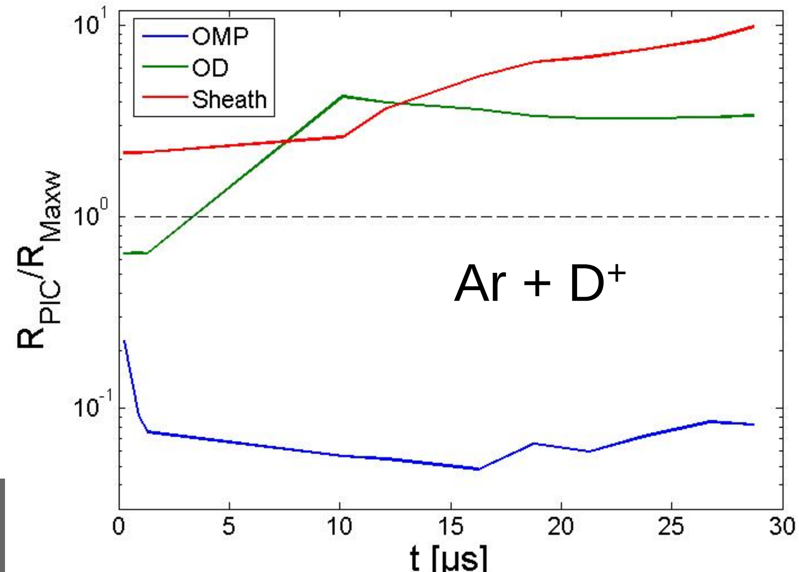


ELM-ing SOL: ionization and CX rates









New developments: motivation

Data for fluid and liner kinetic modelling

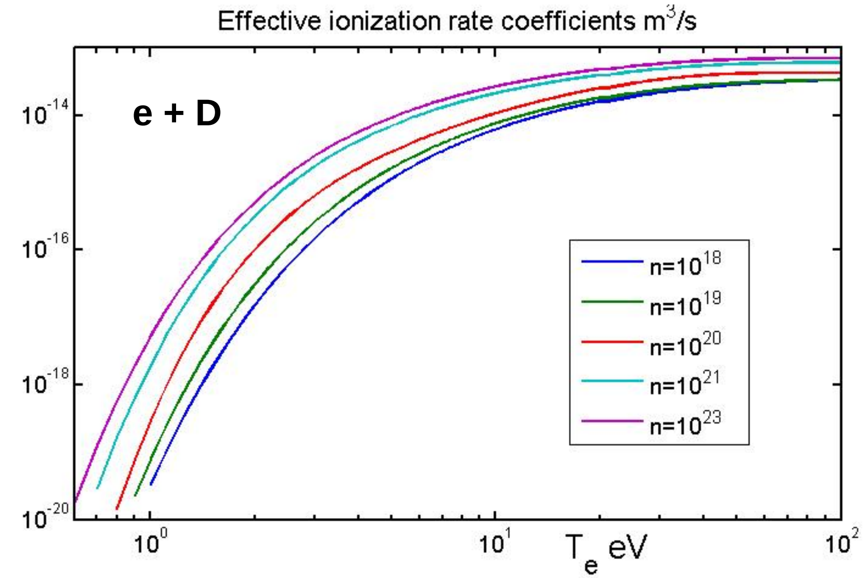
Collisional radiative model (CRM) $$\sum_{i,j}\langle\sigma V\rangle_{ij}^{a} n_i n_j + \sum_i S_i^a n_i = \left(\sum_{i,j}\langle\sigma V\rangle_{ia}^{j} n_i + S_a\right) n_a, \quad i,j=1,\dots,N$$

$$A+B\to A^*+B^*,\quad \underline{R_{AB}=R_{AB}(n_B,T_B)},\quad \lim_{n_B\to 0} R(n_B,T_B)=\langle\sigma V\rangle_{AB}(T_B)$$

Can one develope a kinetic CRM?

Example from ADAS: $e + Ne^{+i} \rightarrow e + Ne^{+i,(v)}$

Target	states	Number of CS
Ne	89	3 916
Ne^{+}	279	38 781
Ne^{+2}	554	153 181
Ne^{+3}	668	222 778
Ne^{+4}	564	158 766
Ne^{+5}	147	10 731
Total		**~ 6x10^5**



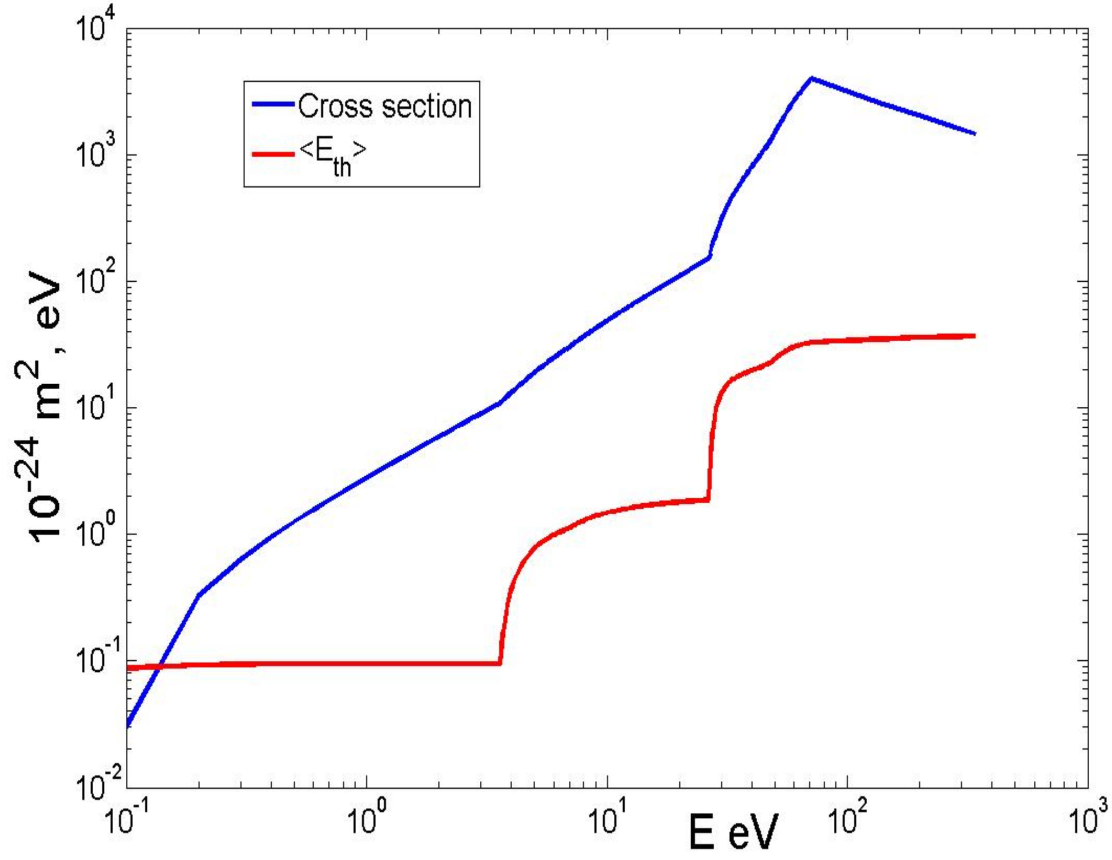
New developments: averaged transitions

Transition from *given* to some *average* state (and vv)

$$\sigma(E) = \sum_i \sigma_i(E),$$

$$\langle E_{th}(E) \rangle = \frac{\sum_i E_{th}^i \sigma_i(E)}{\sigma}$$

Cross-section and threshold energy for e + Ne excitation collisions ***from ground state*** *averaged over* ***84 resulted states***.



bundling of ionized states?

Still too expensive for nonlinear kinetic modelling!

New developments: dressed CS

$$\sigma(E,T,n)=\underline{\sigma_{n=0}(E)}\frac{R(T,n)}{R_{n=0}(T)},$$

$$R(T,n)=\int f_m V\sigma(E,T,n)d\vec{V}$$

$$\sigma(E,T,n\to 0)=\sigma_{n=0}(E)$$

Advantage

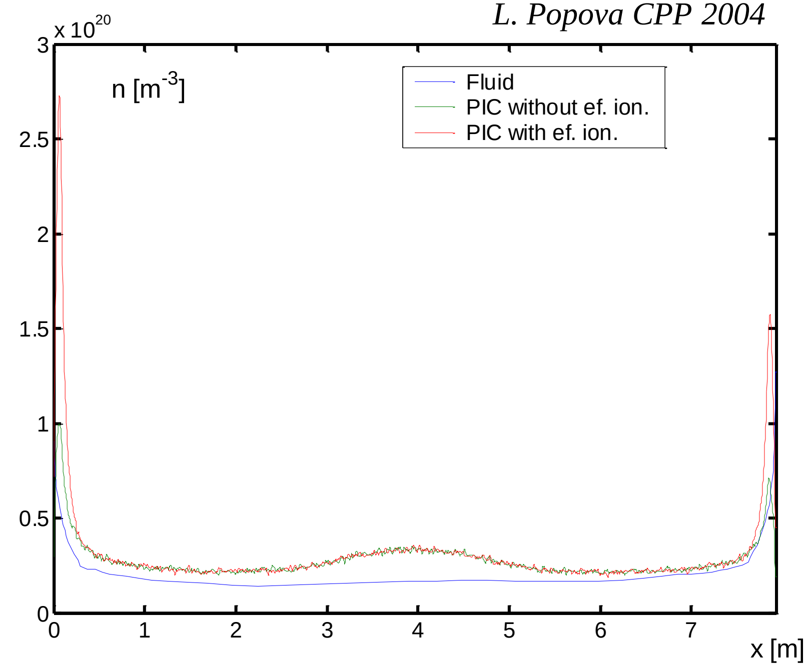
cross-sections and rate coefficients are available

Disadvantage

i. needs calculation of temperature – speed reduction (~10%)

ii. It is unclear how to obtain E_{th} for $E < E_{th,n=0}$?

L. Popova CPP 2004



Density profile in the JET SOL obtained from different models

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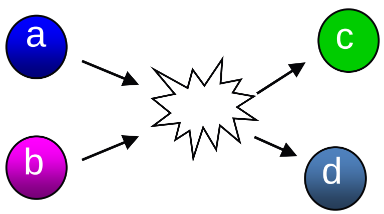
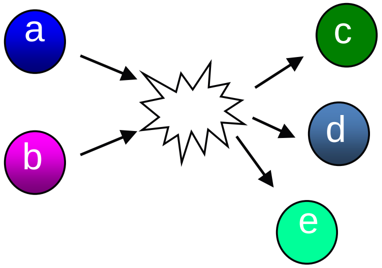
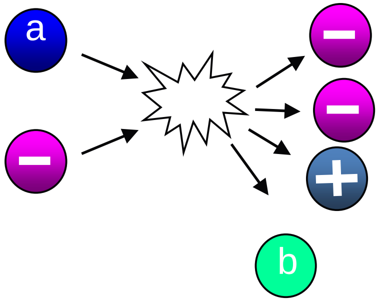
Nonlinear models used in kinetic codes

[Matyash], [Taccogna], BITn, DIVGAS…







Data needed

$$\sigma(E,\theta) \qquad \sigma(E,E_1,\theta_1,\theta_2) \qquad \sigma(E,E_1,E_2,\theta_1,\theta_2,\theta_3)$$

Data provided

$$\sigma(E)$$

$$\sigma(E,E_1,\theta_1)$$
$$\sigma(E,E_1)$$

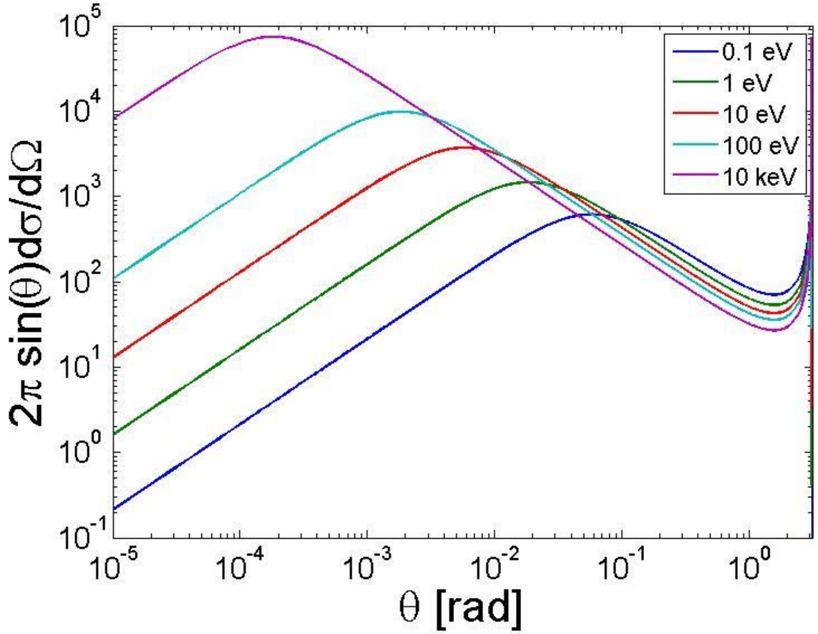
$$\sigma(E,E_1,E_2)$$
$$\sigma(E,E_1),\ \sigma(E)$$

Differential CS might be important for elastic collisions!

Missing data (CS)

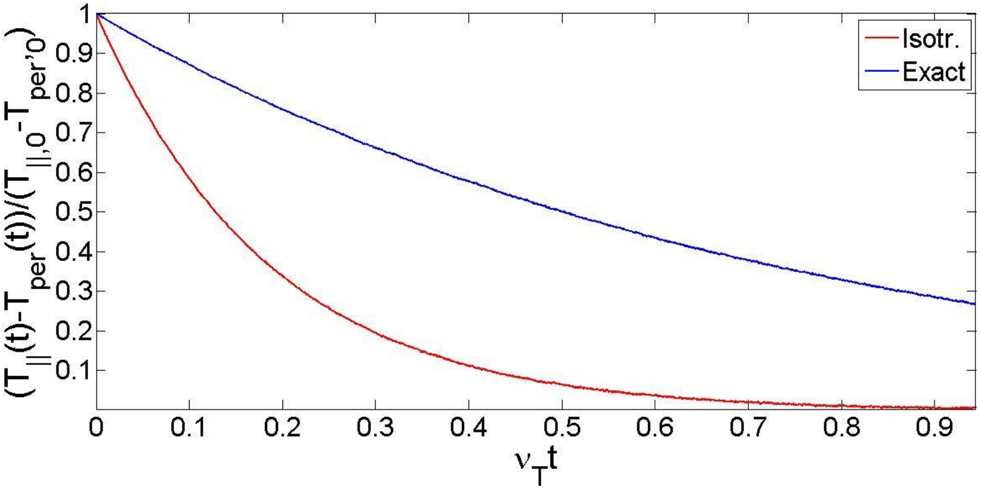
$$e+W^{+i} \rightarrow W^{+(i-1)} + \nu h,\ \ W+H^{+} \rightarrow W^{+} + H,\ \ AW$$

Differential CS for elastic D+D



Differential cross-sections (CS) for D+D elastic collisions for different relative energies implemented in BITn.
CS are from [Krstić / Schultz, NF, 1998].

Temperature isotropization of D atoms with exact and isotropic differential CS.



Proper linear treatment requires (at least) **two rate coefficients** – momentum and energy transfer RC

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Conclusions

- Stationary SOL

i. electron impact collisions: **no significant deviation** of rate coefficients from Maxwell-averaged values (R_{Maxw}) **except** *W* ionization rates in the sheath

ii. ion impact collisions: **deviation** observed for CX collisions with impurity atoms and H_2 molecules; this deviacion **can be reduced** by substitution

$$\boxed{R(T) \to R(T + 2E_{\parallel}/3), \quad E_{\parallel} = \frac{mV_{\parallel}^2}{2}}$$

- ELM-ing SOL: **significant** time and space dependent **deviation** of rate coefficients from Maxwell-averaged RC

- Impurity – main ion CX data (CS) for low energies **is missing** (e.g. $W + D^+ \rightarrow W^+ + D$;

required **accuracy**: case dependent; a "dream" value is ~ **20%**

- PSI: small variation of angular dependent part, EDF broadens with the divertor collisionality

- Development of **reduced kinetic** collisional radiative model is ongoing