Update on OPEN-ADAS
and
Recent work on excitation data and population modelling

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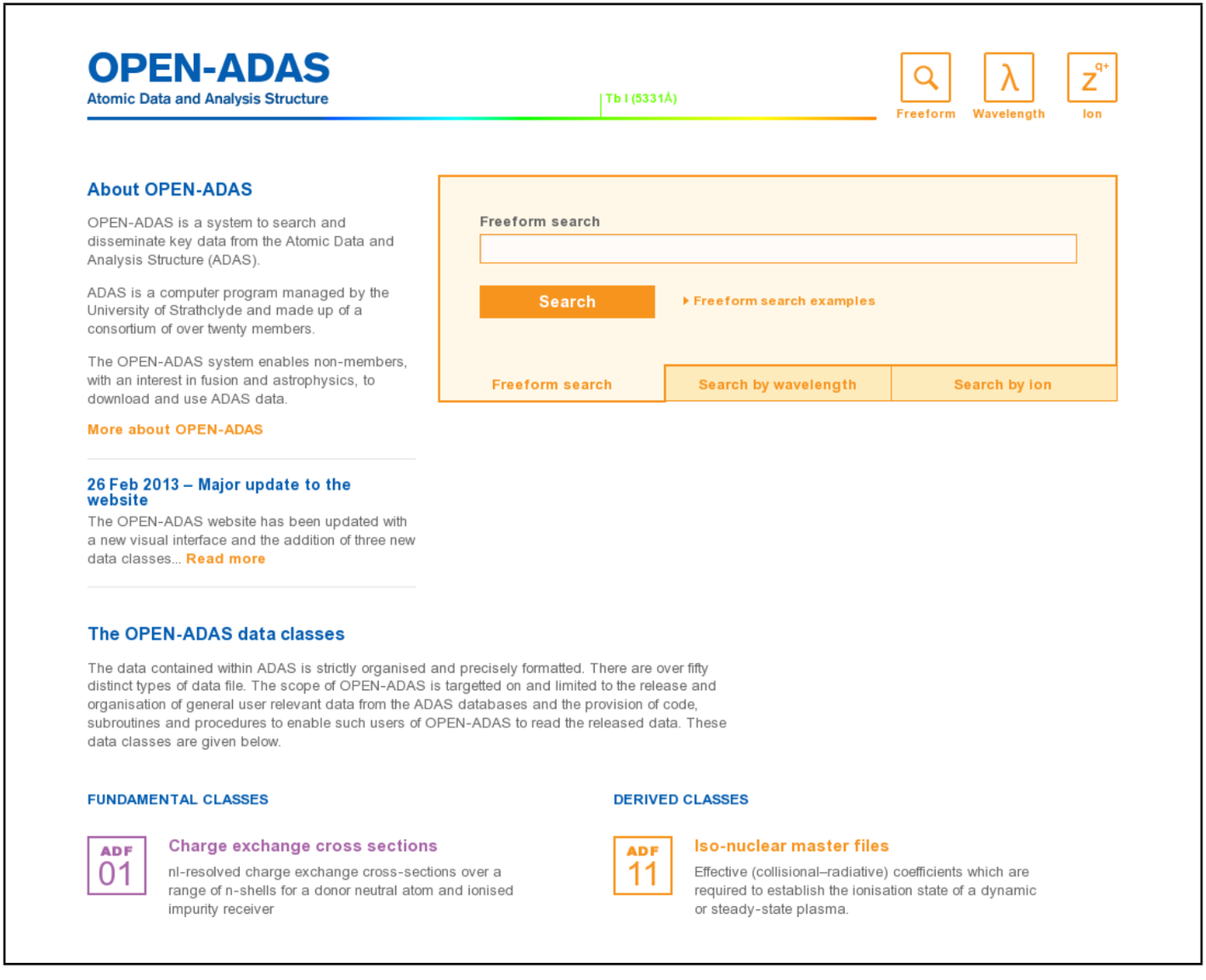
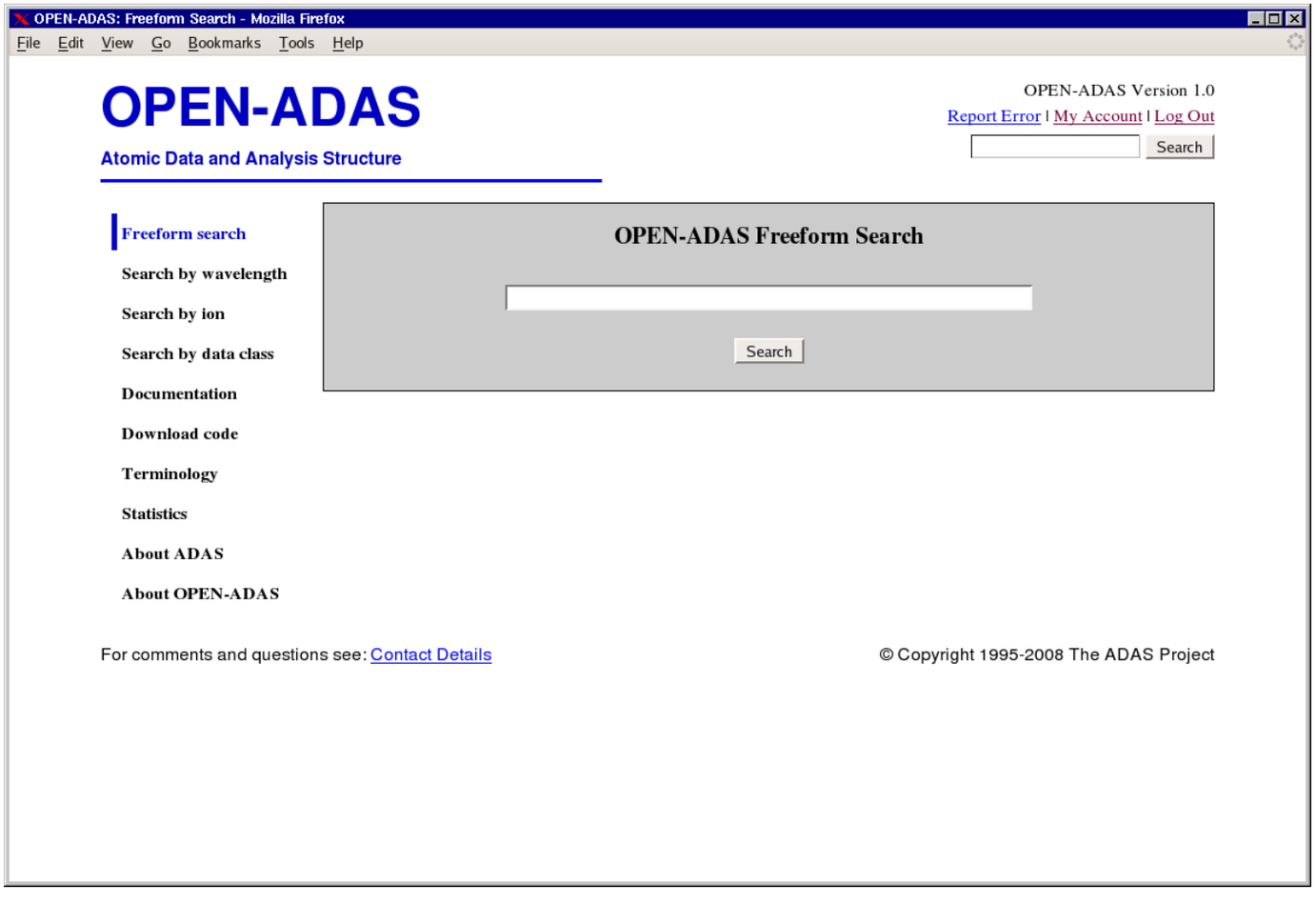
OPEN-ADAS has a new look

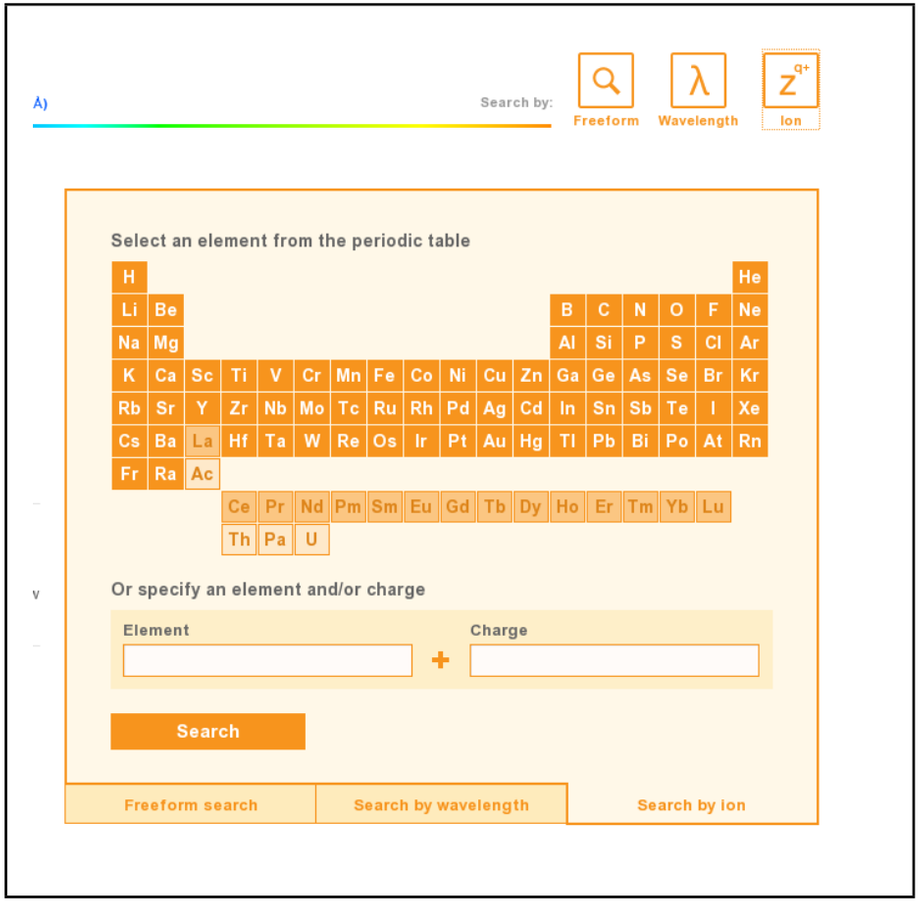


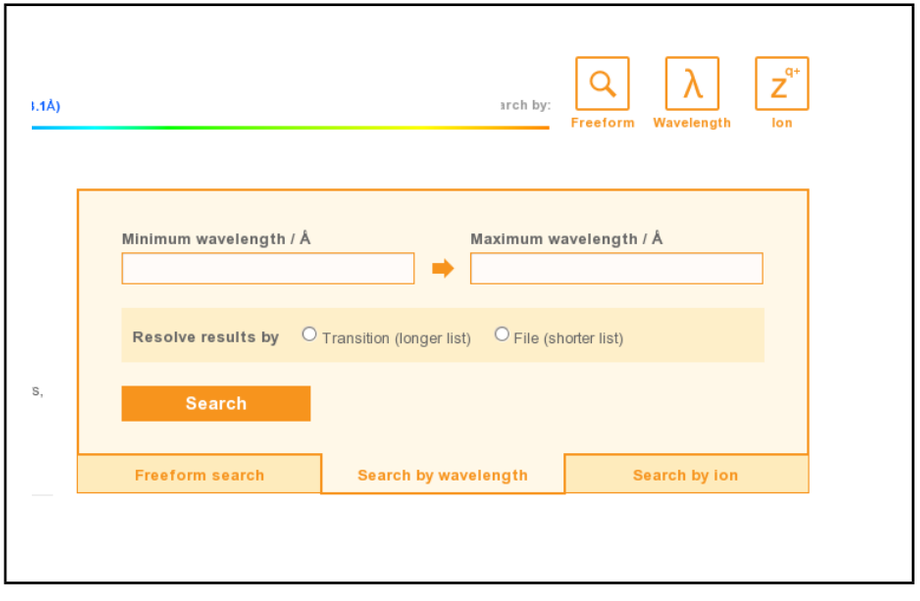
OPEN-ADAS has a new look

A reminder of the previous incarnation:



OPEN-ADAS: new search dialogues

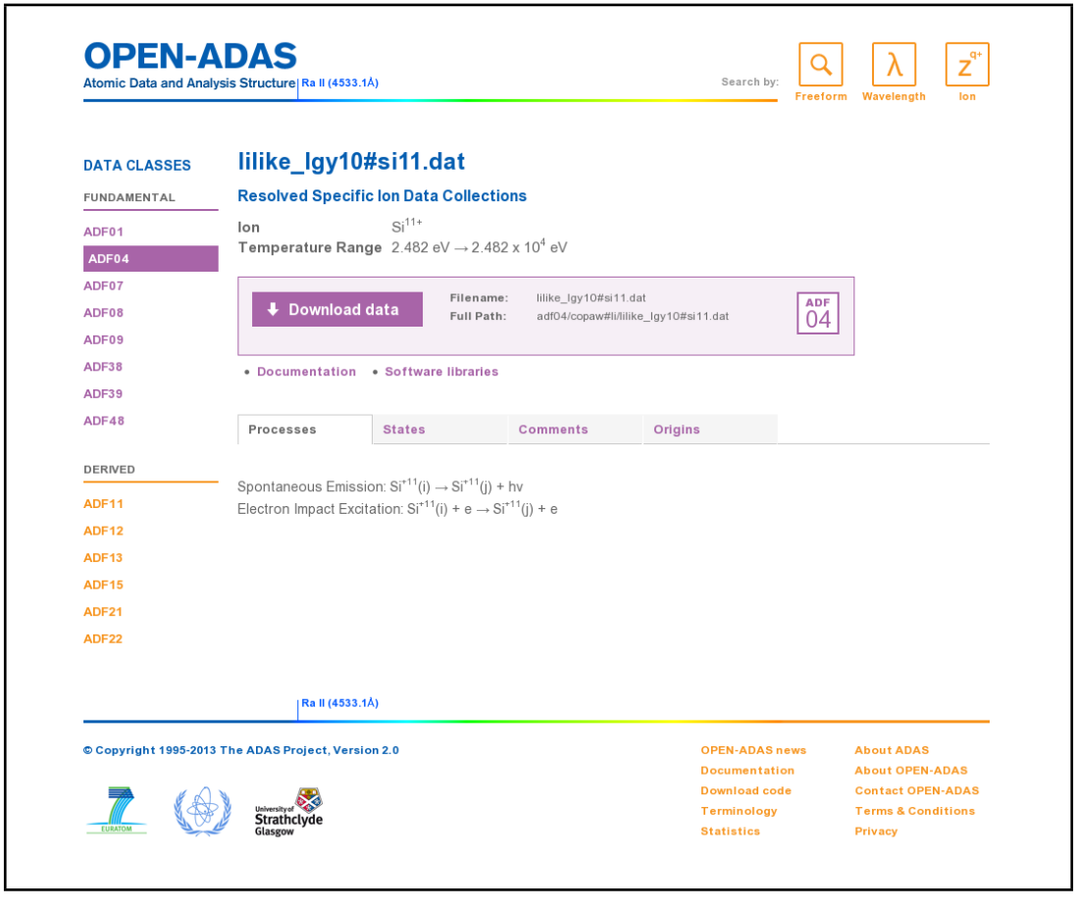




- Functionality remains broadly similar.
- Always available — can pop-over the current screen.

OPEN-ADAS: download a dataset

- Delivery of a complete *adf* dataset remains the paradigm.
- Actual use of ADAS data is via direct use of its complete datasets — *not* via web access.



OPEN-ADAS: reasons for upgrading

- The ADAS-EU Project placed a strong emphasis on knowledge exchange.
- OPEN-ADAS is a key (data) dissemination route.
- A new server for OPEN-ADAS was installed.
- The internet is becoming an even more hostile environment — security hardening was essential.
- A significant quantity of new data has been produced during normal ADAS activities since the first version.
- New classes of data — photo-excitation and photo-ionisation needed an authoritative distribution method.
- Internal tool chain streamlining to make OPEN-ADAS updates a simpler process.

OPEN-ADAS: fundamental and derived data

FUNDAMENTAL CLASSES

ADF 01 — Charge exchange cross sections
nl-resolved charge exchange cross-sections over a range of n-shells for a donor neutral atom and ionised impurity receiver

ADF 04 — Resolved specific ion data collections
Coefficient data for a given ion which includes spontaneous emission coefficients and electron impact collisional rates and other optional processes.

ADF 07 — Electron impact ionisation coefficients
Collections of Maxwell averaged electron impact ionisation rate coefficients for both direct ionisation and excitation/autoionisation.

ADF 08 — Radiative recombination coefficients
Maxwell-averaged radiative recombination coefficients i.e. spontaneous free-bound transitions of Maxwellian electrons excluding dielectronic recombination.

ADF 09 — Resolved dielectronic recombination coefficients
Collections of state-selective dielectronic recombination coefficients of Maxwellian free electrons resolved by initial and final metastable and captured n-shell.

ADF 38 — Photoexcitation-autoionisation rate coefficients
Fundamental data for inner shell excitation followed by autoionisation

ADF 39 — Photoionisation cross-sections
Fundamental data for direct (including and especially inner shell) photoionisation.

ADF 48 — Radiative recombination rate coefficients
Partial final-state resolved radiative recombination rate coefficients from both ground and metastable levels.

DERIVED CLASSES

ADF 11 — Iso-nuclear master files
Effective (collisional–radiative) coefficients which are required to establish the ionisation state of a dynamic or steady-state plasma.

ADF 12 — Charge exchange effective emission coefficients
Collections of effective emission coefficients for spectrum lines emitted by ions of elements following charge transfer from neutral beam donor atoms.

ADF 13 — Ionisation per photon coefficients
Data collections useful in analysis of a spectrum line from an ionisation stage of an element, which is inflowing into a plasma from a surface.

ADF 15 — Photon emissivity coefficients
Fully density dependent and metstable resolveed effective emissitivy coeffeicients from a collisional–radiative model.

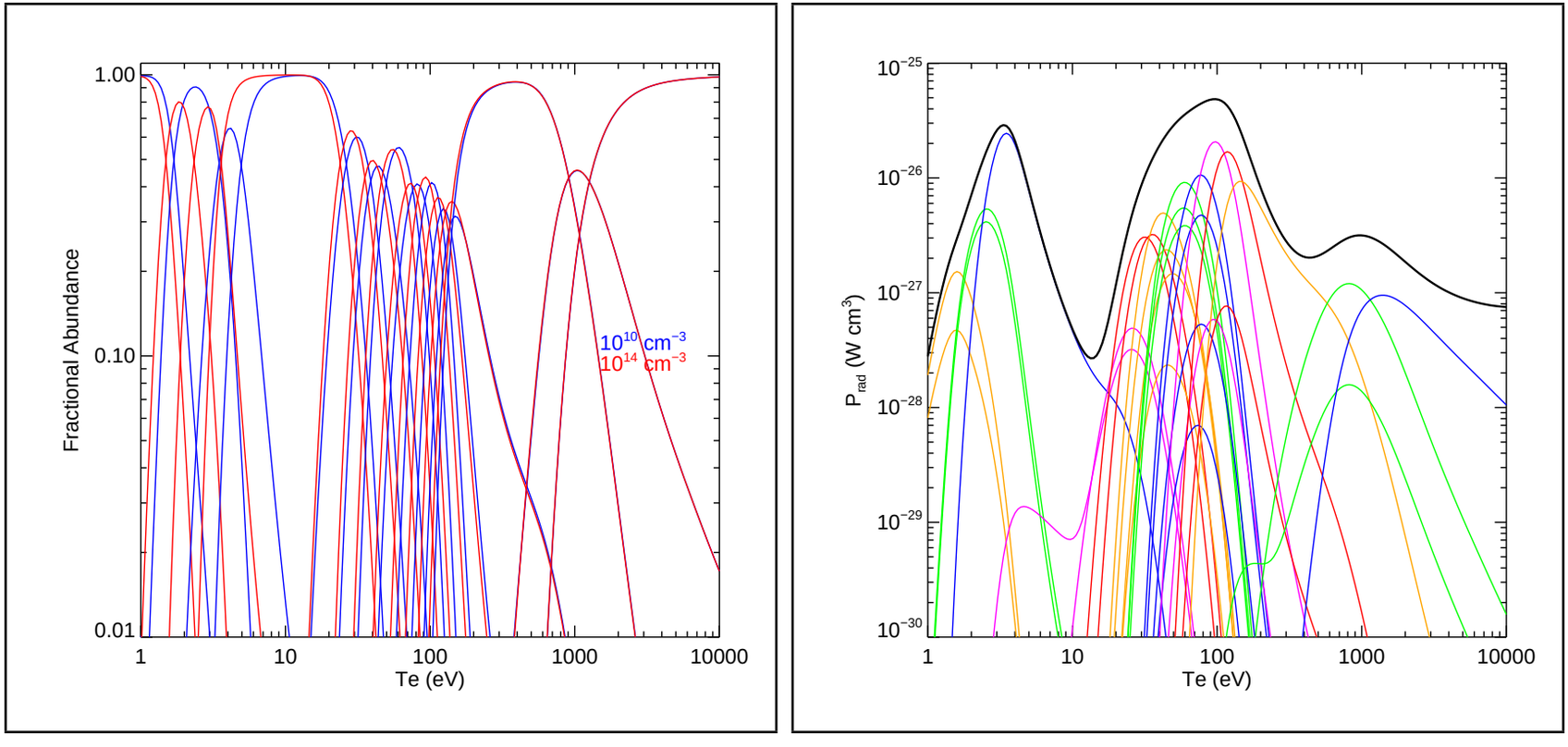
ADF 21 — Effective beam stopping/excitation coefficients
They are effective ionisation coefficients, including charge transfer losses, which leave the beam atoms ionised.

ADF 22 — Effective beam emission/population coefficients
Coefficients for the emission from a beam when it enters an ionised plasma including impurities. Results are fully density dependent output from a collisional–radiative model.

OPEN-ADAS: new data classes

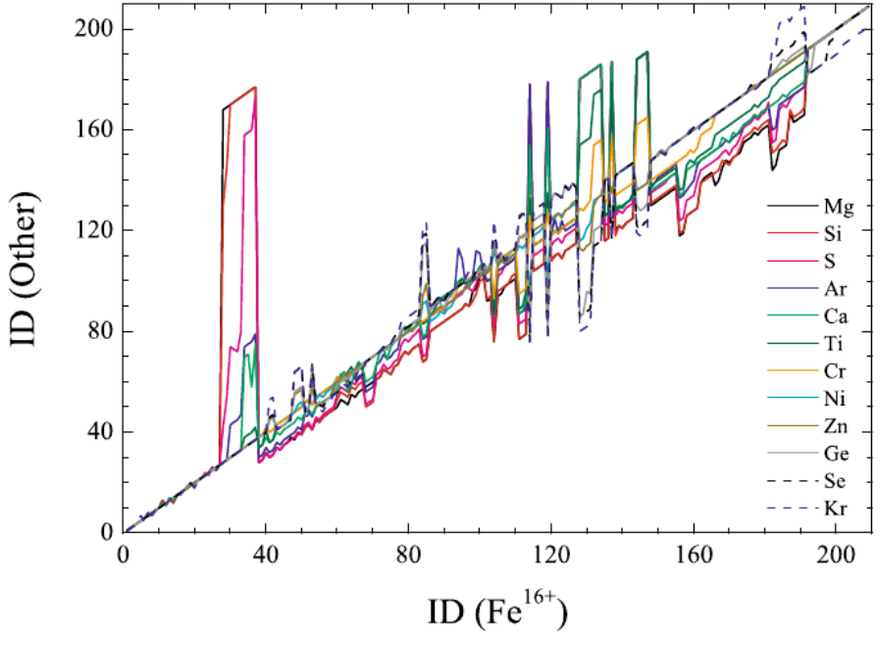
- *adf38* state resolved photo-excitation cross sections.
  - Inner- and outer-shell final-state resolved partial dipole photoionization cross sections for all states of the initial ground complex.
- *adf39* state resolved photo-ionisation rates.
  - Inner-shell final-state resolved partial photoexcitation-autoionization data for all states of the initial ground complex.
- *adf48* state resolved radiative recombination rates.
  - Final-state resolved partial RR rate coefficients for ground and metastable initial states.
- Bare ion to Mg-like sequences.
- Elements considered are: Hydrogen to Zinc (and Xenon).

Silicon GCR data



- Metastable-resolved and density dependent ionisation balance for silicon.
- Work is progressing on Magnesium, Aluminium and Argon.
- Re-formulating to an intermediate coupling ion state description with the target plasma determining the metastables.

R-Matrix sequence data



G Liang, N R badnell, M Witthoeft

- Work programme to maximize utility of R-matrix codes.
- He, Li, F, Na, Ne sequences.
- Elements up to Zinc.
- Neutral and singly ionized are excluded.
- Be-like and B-like under way.
- H-like has somehow dropped between the cracks.
- Preparing a repository for the resonance-resolved OMEGA files is under consideration.

Improving ADAS baseline excitation data

- Completness is important for fusion models
  — Iso-nuclear rather than iso-electronic!
- *adf04* produced with Cowan code was the ADAS baseline method
  — very good structure
  — but no inter-system rates
- Extend AUTOSTRUCTURE with distorted wave method.
- H-like to Ar-like sequences produced.
- H to Zn with selected higher Z — increases database by 10Gb.
- Collision strengths and effective collision strengths produced.

Non-Maxwellian population modelling: rate coefficients

Consider the reaction $A^{+z}(i) + e(\varepsilon_i) \rightleftharpoons A^{+z}(j) + e(\varepsilon_j)$

Maxwellian: detailed balance

$$\Upsilon_{ij}(T_e) = \int_0^\infty \Omega_{ij}(\varepsilon_j) \exp\left(-\frac{\varepsilon_j}{kT_e}\right) d\left(\frac{\varepsilon_j}{kT_e}\right)$$

$$q_{i\to j}(T_e) = 2\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_e}\right)^{1/2} \frac{1}{\omega_i} \exp\left(-\frac{\Delta E_{ij}}{kT_e}\right) \Upsilon_{ij}(T_e)$$

$$q_{j\to i}(T_e) = 2\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_e}\right)^{1/2} \frac{1}{\omega_j} \Upsilon_{ij}(T_e)$$

same

Non-Maxwellian: no detailed balance

$$\Upsilon_{i\to j}(T_{eff}) = \frac{\sqrt{\pi}}{2} \exp\left(\frac{\Delta E_{ij}}{kT_{eff}}\right) \int_0^\infty \Omega_{ij}(\varepsilon_i) \left(\frac{\varepsilon_i}{kT_{eff}}\right)^{-1/2} f(\varepsilon_i)\, d\varepsilon_j$$

$$\Lambda_{j\to i}(T_{eff}) = \frac{\sqrt{\pi}}{2} \int_0^\infty \Omega_{ij}(\varepsilon_j) \left(\frac{\varepsilon_j}{kT_{eff}}\right)^{-1/2} f(\varepsilon_j)\, d\varepsilon_j$$

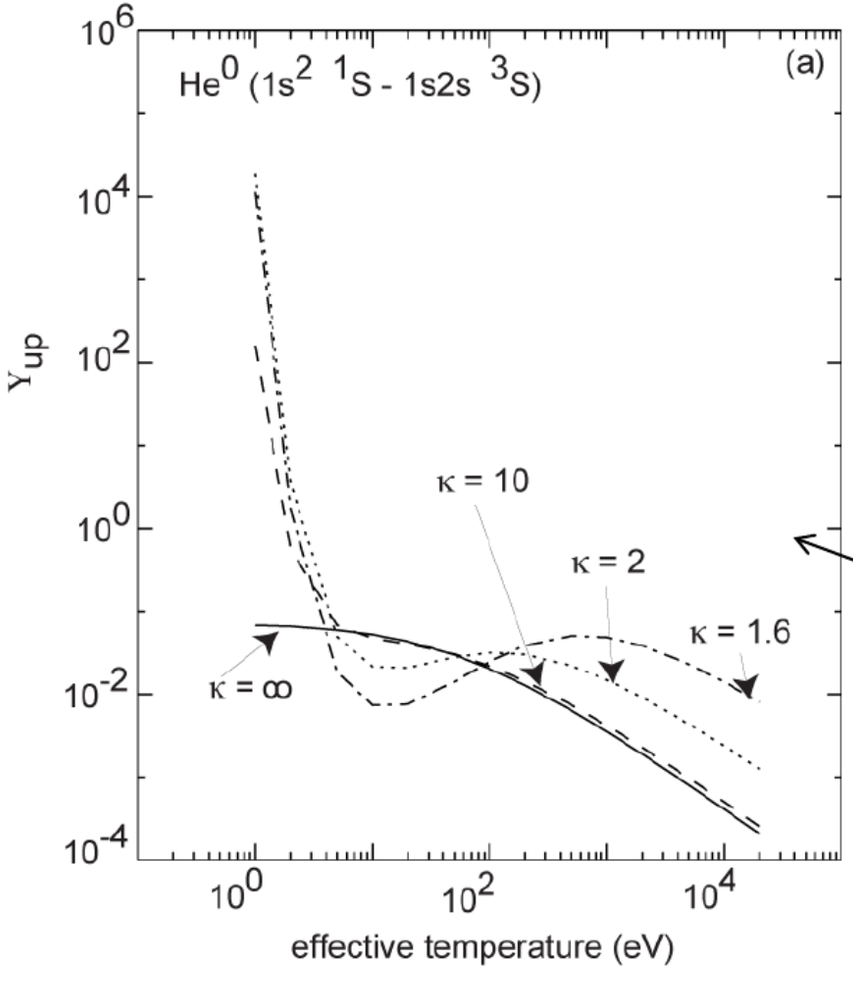
$$q_{i\to j}(T_{eff}) = 2\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_{eff}}\right)^{1/2} \frac{1}{\omega_i} \exp\left(-\frac{\Delta E_{ij}}{kT_{eff}}\right) \Upsilon_{i\to j}(T_{eff})$$

$$q_{j\to i}(T_{eff}) = 2\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_{eff}}\right)^{1/2} \frac{1}{\omega_j} \Lambda_{j\to i}(T_{eff})$$

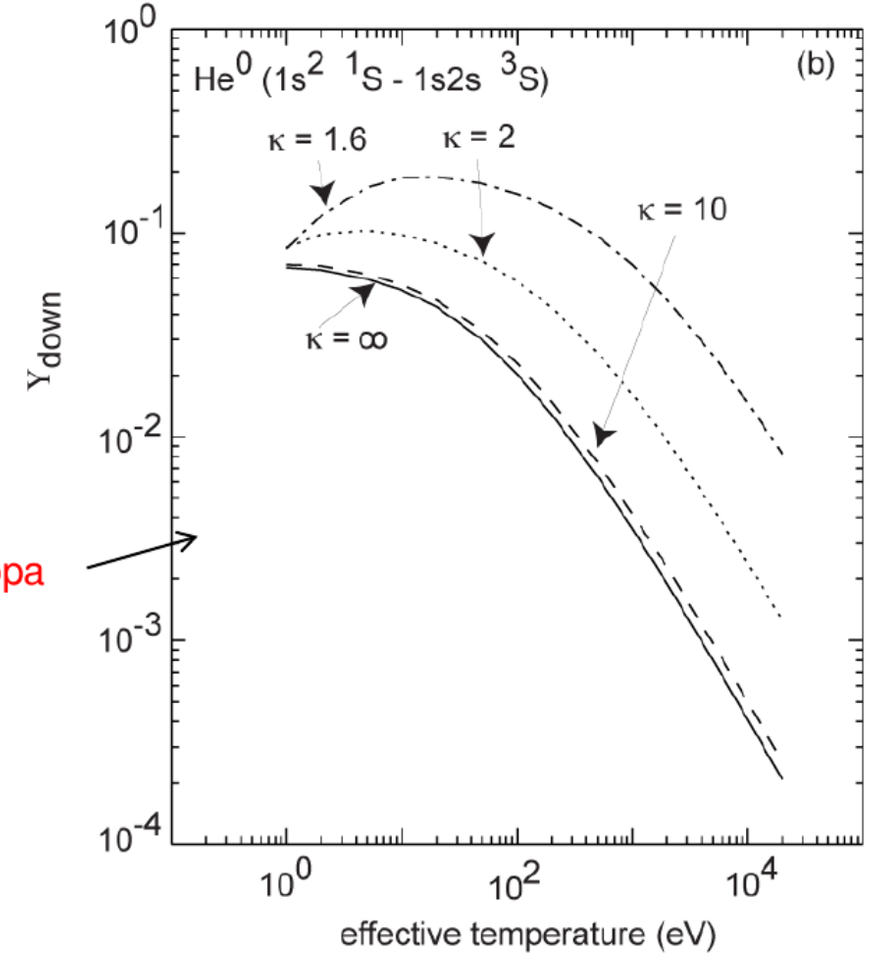
different

Effective mean energy parameter

Non-Maxwellian upsilons and downsilons



Kappa



Non-Maxwellian population modelling: other rates

Dielectronic recombination and radiative recombination coefficients are straightforward.
Electron impact ionisation and three-body recombination are more complicated.

Fowler relation is the starting point

$$\omega_i E Q_{i\to+}(E;E',E'') = \frac{16\pi m}{h^3}\omega_+ E' E'' Q_{+\to i}(E',E'';E)$$

Collisional ionisation →

$$q_{i\to+} = \int_{I_i}^{\infty}\sqrt{\frac{2E}{m}}Q_{i\to+}(E;E',E'')f(E)\,dE\int dE'\int dE''$$

E is the incident energy, E' and E'' the scattered and ejected energies

Three-body recombination →

$$\alpha^{(3)}_{+\to i} = 8\left(\frac{\pi a_0^2 I_H}{kT_{eff}}\right)^{3/2}\frac{\omega_i}{2\omega_+}e^{I_i/kT_{eff}} \times\int_{I_i}^{\infty}\sqrt{\frac{2E}{m}}Q_{i\to+}(E;E',E'')f(E)\,dE \times\int\int\left[\frac{\sqrt{\pi}}{2}(kT_{eff})^{3/2}e^{-I_i/kT_{eff}} \times\sqrt{\frac{E}{E'E''}}\frac{f(E')f(E'')}{f(E)}\right]dE'\,dE''$$

Thompson cross-section allows evaluation ↓

$$Q_{i\to+}(E;E',E'') = 4\pi a_0^2\zeta I_H^2\frac{1}{EE'^2}\delta(E-E'-E''-I_i)$$

Non-Maxwellian population modelling: diagnostic potential

Non-Maxwellian populations evaluated using code ADAS218.

Differential variation of populations according to enhancement or depletion of regions of the appropriate distribution functions.

The numerical non-Maxwellian is from a JET simulation near the divertor plate by Tskhakaya.

The non-Maxwellian adf04 datasets were prepared for the appropriate distribution functions using offline_adas/adas7#3/adf04_om2ups