University of Strathclyde Glasgow

Data and issues for ADAS

Martin O'Mullane

ADAS – Atomic Data and Analysis Structure

- ADAS is a (mostly) atomic modelling framework for producing and manipulating atomic data.
- The goal is to provide – by generating or collating – atomic data for diagnostic interpretation and emission modelling of fusion plasmas.
- ADAS began at JET, the Joint European Tokamak experiment.
- It has evolved into a large database in widespread use but retained the capacity to originate and produce atomic data.
- ADAS also has an astrophysics (solar and nebulae) heritage which explains choice of units and extension of population codes to low temperatures.
- OPEN-ADAS is the pathway for ADAS data to be made publicly available and was a joint project between ADAS and IAEA.
- Effective coefficients, characterizing finite density conditions, are required for modelling and diagnostic interpretation. Collections of fundamental, individual process data, are needed to produce the derived, effective data.
- All data, fundamental, derived and driver files (internal use) are defined in ADAS Data Format files. These are human-readable ASCII files arranged in sub-directories.
- OPEN-ADAS has also been used to provide a public data store to satisfy data management plans (needed for UK and other national funding bodies).
- ADAS will not become a database for data without a plasma (fusion/astro/lab) application.

Data in ADAS

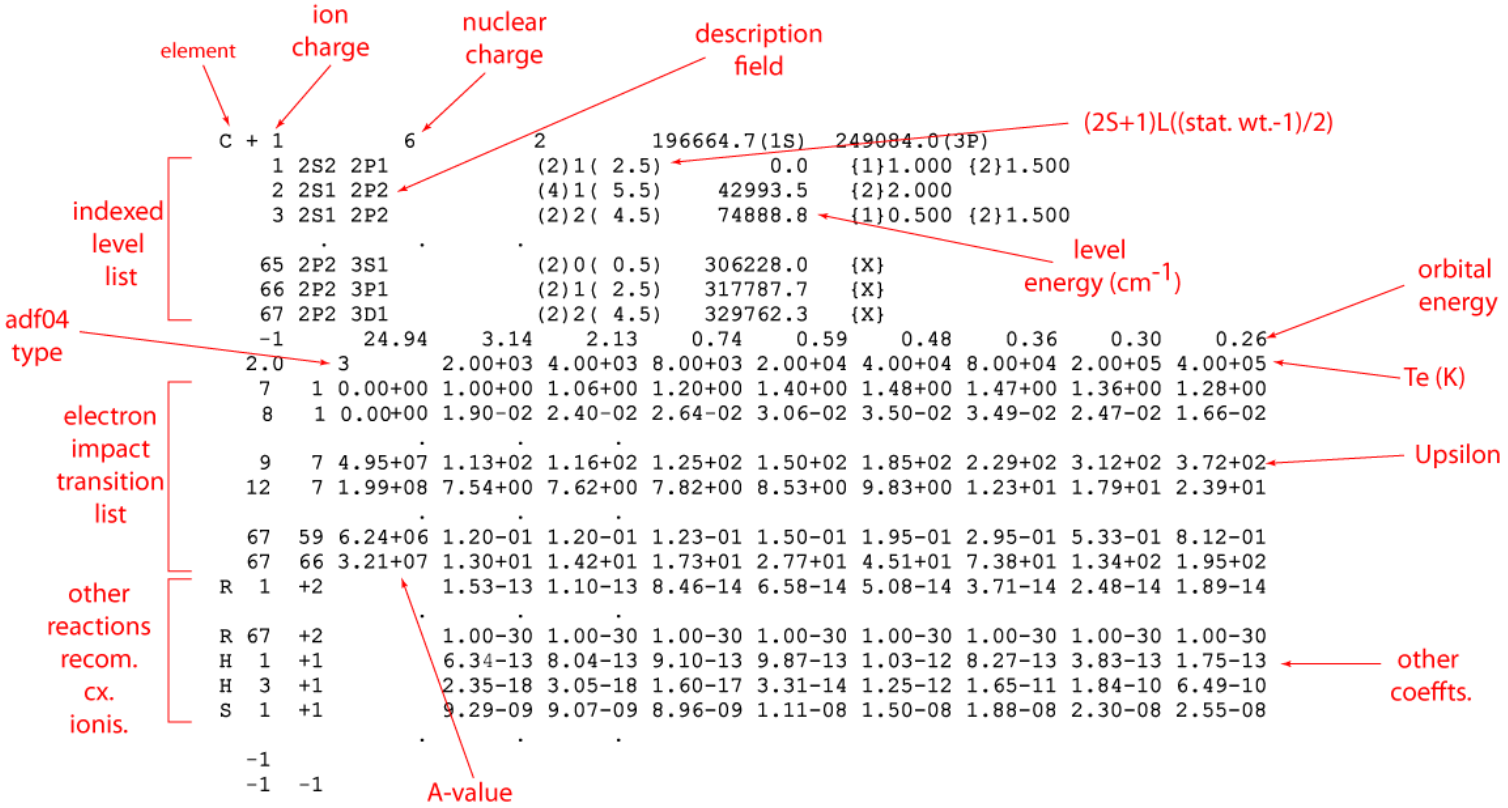
Data in ADAS is grouped and is stored in well-defined, plain-ASCII files
ADAS Data Format, adf files:

adf00	Ground configurations and ionisation potentials	156	1.5M
adf01	Charge Exchange Cross Sections	136	2.5M
adf02	Ion impact cross-sections	7	372K
adf03	Empirical parameter sets for baseline 89 adf11	38	548K
adf04	Specific Ion Data for e-impact population	5853	29G
adf05	General z excitation data collections	32	880K
adf06	Specific Ion Data for ion-impact	2	96K
adf07	Electron Impact Ionisation Coefficients	103	1.4M
adf08	Radiative Recombination Coefficients	114	1.4M
adf09	Dielectronic Recombination Coefficients	2238	1.7G
adf10	Iso-electronic master files	772	11M
adf11	Iso-nuclear Master Files	1021	81M
adf12	Charge Exchange Effective Emission Coefficients	58	1.9M
adf13	Ionisation Per Photon Coefficients	171	44M
adf14	Thermal charge exchange coefficients	19	296K
adf15	Photon Emissivity Coefficients	595	147M
adf16	Generalised contribution functions	1	32K
adf17	Condensed projection matrices	106	487M
adf18	Cross-referencing data	247	2.2M
adf19	Zero density radiative power	9	140K
adf20	G(Te) functions	643	75M
adf21	Effective Beam Stopping/excitation Coefficients	223	2.9M
adf22	Effective Beam Emission/population Coefficients	410	5.3M
adf23	State selective electron impact ionisation rates	158	2.3M
adf24	State selective charge transfer cross-sections	24	196K
adf25	Driver data-sets for ADAS204	64	788K
adf26	Bundle-n and bundle-nl populations of beam atoms	41	204M
adf27	Driver data-sets for ADAS701 (AUTOSTRUCTURE)	8642	84M
adf28	Driver data-sets for ADAS702 (AS post-processing)	5111	40M
adf32	Driver data-sets for ADAS802 (CADW ionisation)	113	924K
adf34	Driver data-sets for ADAS801 (Cowan code)	248	1.2M
adf35	Energy/spectral filter data (+Henke data)	3	2.3M
adf37	Non-Maxwellian EEDF distributions	2	60K
adf38	Photoexcitation-autoionisation Rate Coefficients	940	40M
adf39	Photoionisation Cross-sections	1480	69M
adf40	Envelope feature photon emissivity coefficients	370	251M
adf42	Driver data-sets for ADAS810 (PEC/plt/fPEC prod.)	1	16K
adf48	Radiative Recombination Rate Coefficients	900	408M
adf49	State-selective CX universal fit data	2	52K
adf54	General excitation promotional rules	9	468K
adf56	General ionisation promotional rules	1	64K
mdf00	Basic molecular data and constants	539	3.6M
mdf02	Intermediate molecular rate coefficients	3	396K

fundamental atomic data in OPEN-ADAS
derived atomic data in OPEN-ADAS

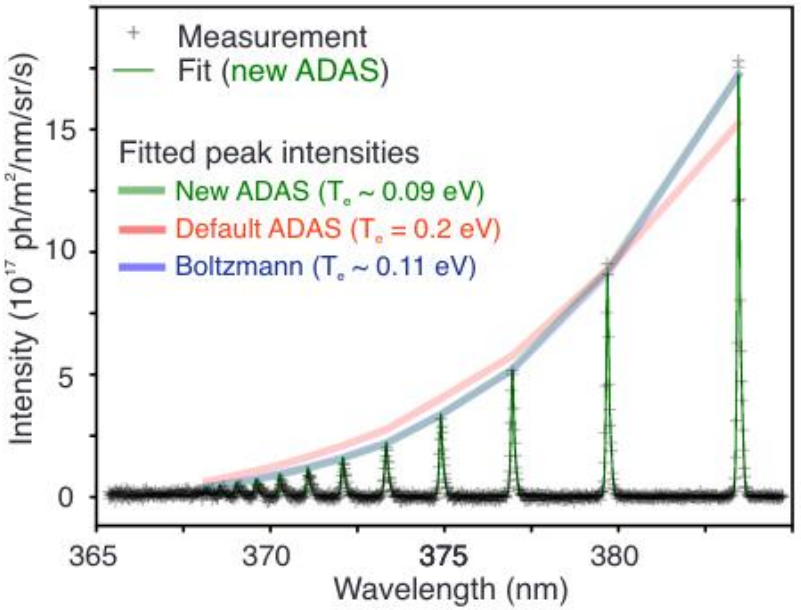
Not all data is in OPEN-ADAS

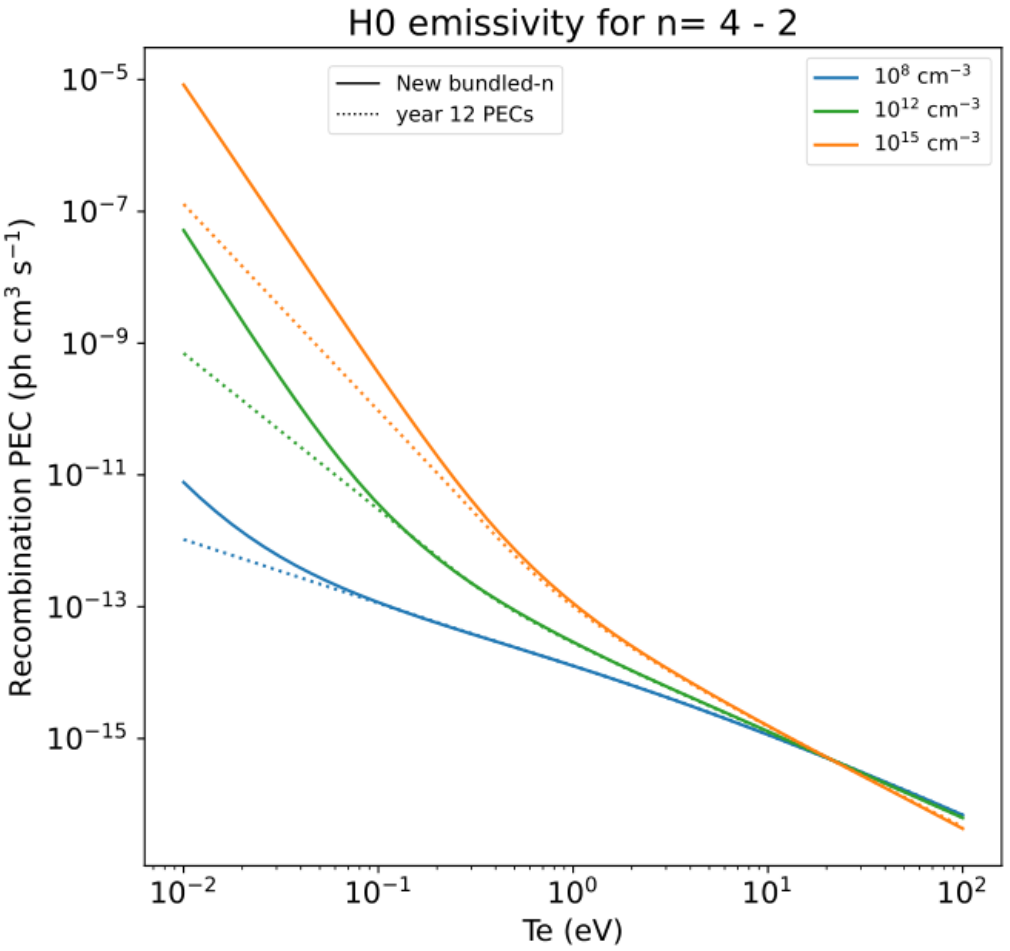
adf04 example



A free-format comment section at the end detailing source and responsible person.

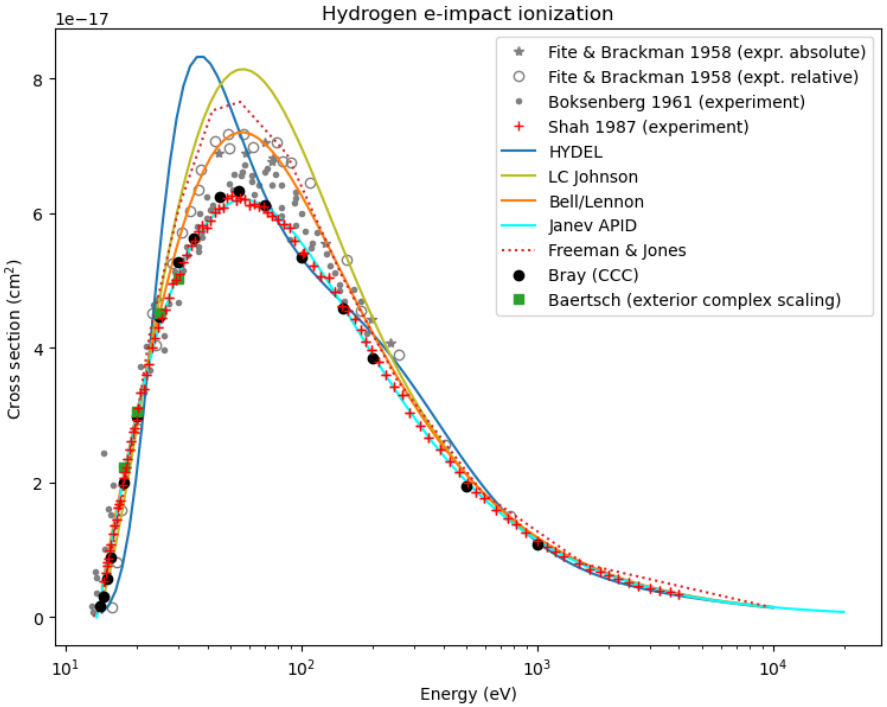
Hydrogen can still surprise – models must be appropriate for plasma conditions

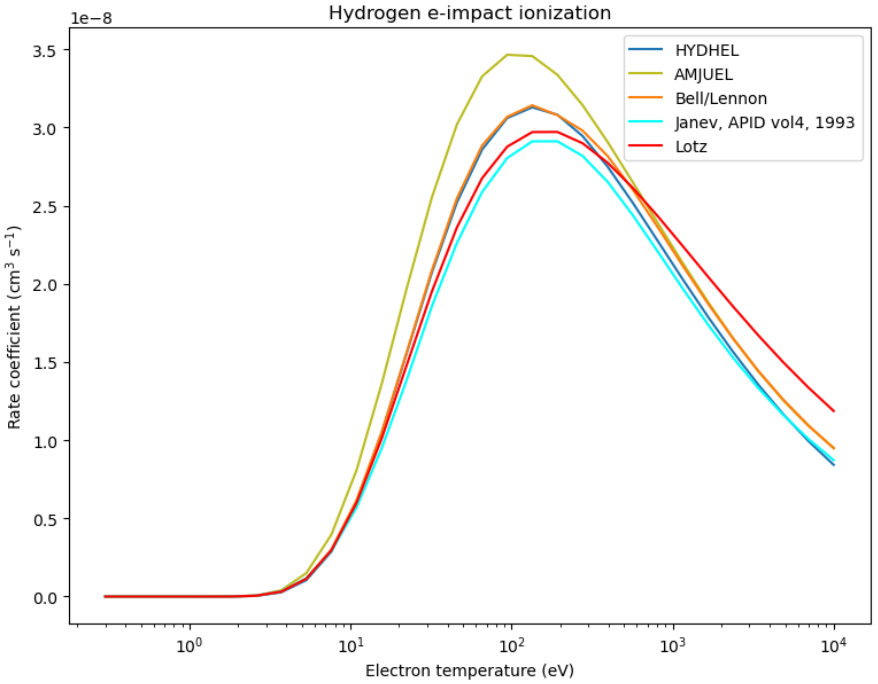




When 3-body is important it must be modelled correctly – not badly extrapolated !

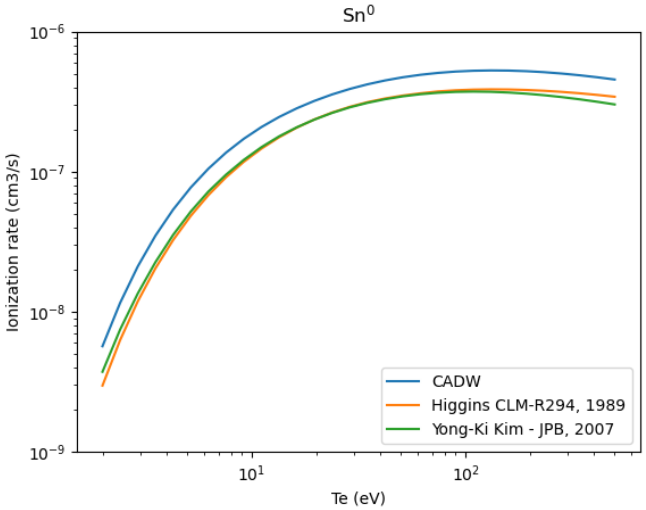
Hydrogen can still surprise – e-impact ionization

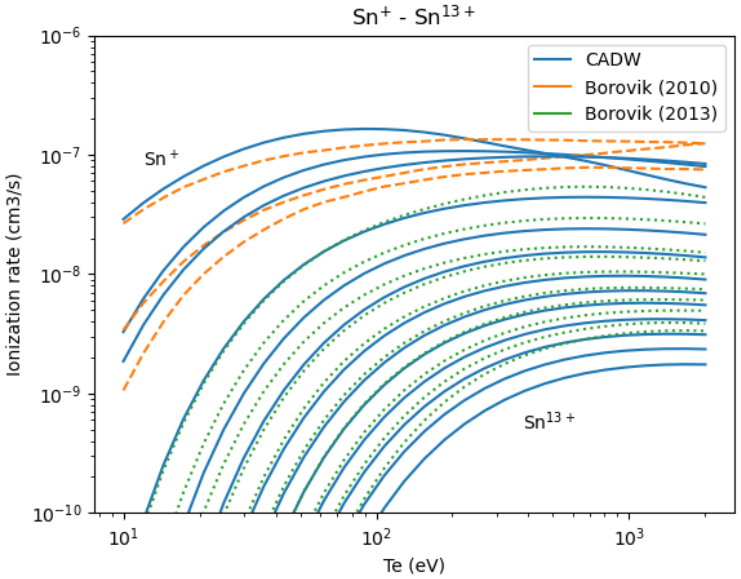


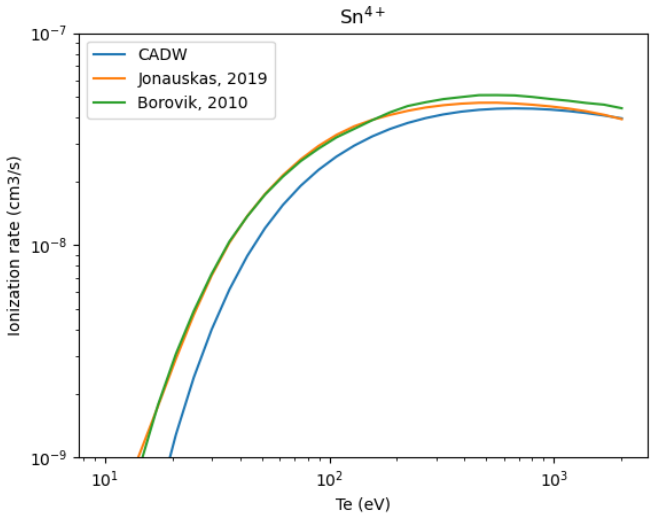


Completeness – Sn ionization

Current ‘best’ ionization data for tin – how to archive and recommend this?

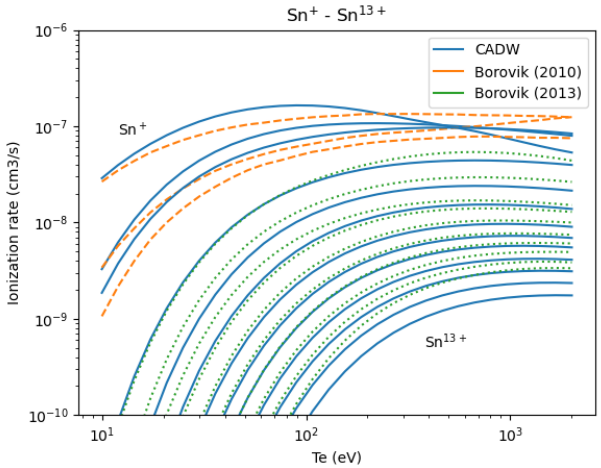




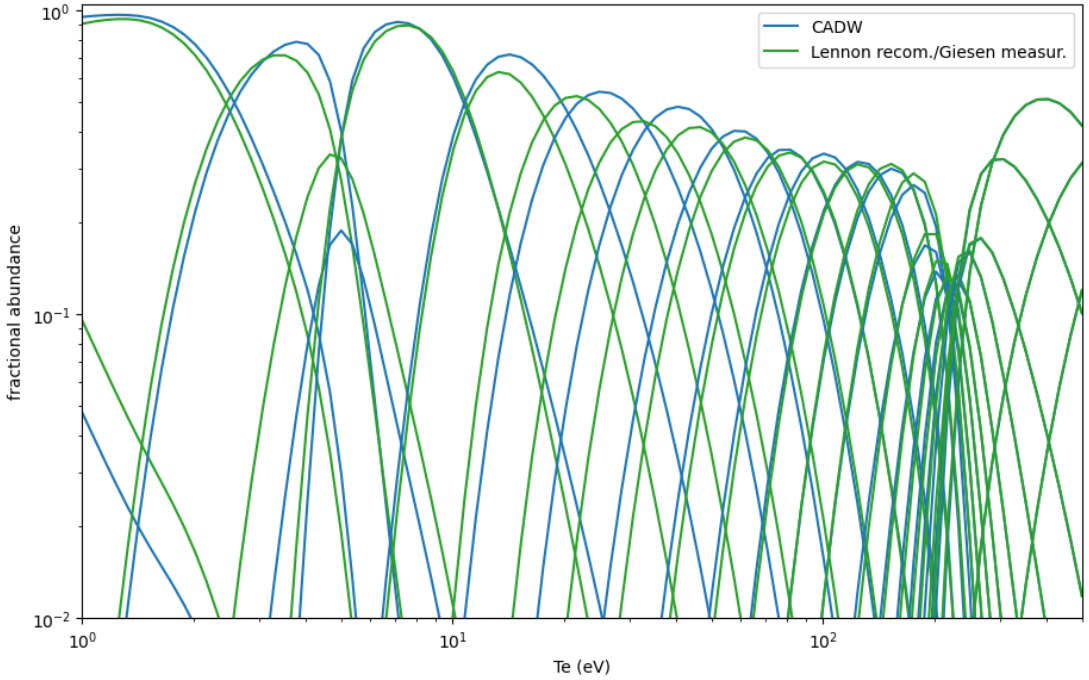


- Some good data/measurements for some ions.
- More than one calculation for others.
- The CADW baseline is reasonable but may need optimization.
- No fully assessed/validated data for all ions which leave a gap.
- But waiting until they are filled is also ‘wrong’.

Completeness – Sn ionization



- Do not have the luxury of waiting.
- UQ assignation here will be more opinionated out of necessity.
- The ionization balance is affected.



Issues for ADAS

- Increasing requests for different licencing of OPEN-ADAS data.
- Requests for use of ADAS library codes in open source products.
- How to engage with private fusion companies – database or whole system have different implications.
- Licencing – how to prevent/discourage fracturing of data and ADAS name.
- Is CC-BY-ND too restrictive? Probably.
- How to not paint ourselves into a corner by licence choice.

- Change from centrally managed computing – user is expected to provide own software (either container/pull from github) with little expectation of centrally provisioned software.
- Recognize that the database is more useful/practical to most users than the entire structure.
- When to switch language? Keep fortran but move to modern fortran. Switch from IDL to python. What about Julia?
- How to continue existing and to maintain a useful role.
- How to survive consequences of Brexit.