Mar4-11 **ADAS Bulletin**

Items:

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5. Code and data updates in release v3.1.

1. This is the first bulletin, since I took over from Hugh as director of the ADAS Project. It is three months later than intended, which I trust will not be repeated. However it has been a busy time, with a number of developments and implications for ADAS which I wish to expand upon. Firstly though I am glad that all seem to have survived the ADAS Workshop in Armagh at the beginning of October. It was nice to be in Armagh under the auspicies of the Armagh Observatory and the meeting was progressing well until we all started to go down in turn with food poisoning. A bit upsetting really, but just one of those things I guess. Anyway, the ADAS Workshop is in the USA for 2011 for the first time. So that is a date for your diaries – 6-8 Oct. 2011 at Auburn University in Alabama (see the ADAS website for details as they become available). Stuart Loch is leading the local organising at Alabama.

   Under ADAS-EU, we held the second (2010) ADAS training course at the EFDA-JET Facility from 7-15 Oct 2010. In fact the provision of more training in ADAS seems to be a need for us to try to fulfill, particularly for those who find it less easy to travel to Europe for the annual ADAS-EU course or are unable to commit so much contiguous time. Thus we held a slightly shorter version of the course at Auburn in the Summer of 2010 and also a special one at ITER at the beginning of December 2010. I think these were quite successful and effective in that somewhat stronger focus on local interests was possible. The next course (ADAS-EU 2011) will be in October 2011, but we have not decided between Cadarache, Juelich or back at Garching or JET yet.

   This brings me to ITER and the preparations for ITER, which have contributed to my slowness in getting the present ADAS release (v3.1) out. ITER of course joined the ADAS Project at the end of 2009, and this year I have spent a significant amount of time at ITER both getting ADAS working effectively and helping to integrate its use into some of the diagnostic instrumentation evaluation. I hope this will be of benefit to us all, since eventually ITER will be operating and we shall all wish to interprete the results from it using these same spectrometric diagnostic systems. I should perhaps add that I have also been engaged in implementing the ADAS atomic data links to the European 'Integrated Tokamak Modelling' project, which I trsut will also be time well spent. But these efforts do mean that ADAS itself has some overdue developments to put in place.

2. ADAS release v3.1 is a mixture of code and data items. There are no major new codes, but a series of corrections, adjustments and subroutine/procedure additions which improve ADAS handling. These have by and large arisen from working the heavy species capabilities of ADAS, but also from a fresh surge of activity on full generalised collisional-radiative modelling of light elements. The latter stems from our intention to take the ADAS light element modelling up from neon to argon. In this context, the data base extensions are also to be noted with some quite large collections, for example adf04 data sets for many members of the He-like, Ne-like and Na-like isoelectronic sequences. Note also C50 of section 4, enabling the IDL virtual machine. This makes 90% of ADAS functional and so should help those for whom IDL licences are a problem.

3. I wish to outline our expected travel associated with ADAS and ADAS-EU over the next nine months. Firstly, on ADAS-EU, we are at the point of starting to bring the external benchmark studies at the first group of partipating Universities into a completed state for incorporation in ADAS. To this end I will traveling to Mons, Hugh to Giessen and Madrid and Nigel to Giessen and Vilnius in the next few months. Also, I should add that we have got the electron collision working party moving again with Nigel now leading that. We lost our way for a bit with Allan's departure. Our next meeting of the working party will be around the end of this month, which should then establish the long term pattern of our intentions and computations. Still on ADAS-EU, we now have Francisco and Luis ready to make visits in Europe, so please let me know if a visit would be helpful for you and I shall try to schedule one in. We would particularly like to engage with some of the other European countries who particpate in the European fusion programme, but do not yet have ADAS links. Turning to ADAS, with the Workshop being in Auburn in 2011, our ADAS team who will be at the Workshop will take the opportunity to make visits in the USA. That includes certainly San Diego, Madison and Princeton and will be in late September, early October. I shall be in India in December for a conference and will use that opportunity to visit our ADAS members there. Finally, we are overdue visits to Japan and China. For these Stuart Loch will join me. These are of course all subject to being able to settle on dates. This is so difficult now with so many conferences and everyone so busy.

4. I plan to follow this release with another quite soon. This is because we now are close to completion on a number of substantial developments. Firstly, Christopher Nicholas has finished his work on establishing the ADAS capability for special feature modelling. You will recall that the pedagogical part of it (AFG) was in the previous release as adas605. Chris has been exercising the spectral fitting part (FFS) extensively over the last months on a wide range of spectra – multi-line UV spectra, spectra with distorted line shapes (from SOHO-CDS), He-like satellite line spectra, molecular bands, field perturbed features etc. We plan to get the complete system into ADAS for the next release and of course get Chris' PhD thesis onto the website. Then Alessandra Giunta has been moving the full GCR modelling of light species up as far as silicon and hopefully with the recipes to take it on to argon. Alessandra has been using these results to analyse solar spectra from SUMER, CDS and EIS and the results of using such high precision modelling data are very encouraging. So that is a lot more data to into ADAS (especially adf11 and adf15, but with new adf04, adf07, adf08, adf09, adf23 etc. data to go with them). Alessandra's thesis will also appear on the website in due course. Nigel and Hugh's work on extending dielectronic recombination to heavy species exploiting BBGP is also nearly ready for release. On the hydrogen molecular front, Francisco's data and collisional-radiative model should be ready for the next release too. So there has been a lot of development and I am optimistic that we shall get it all embedded and released soon – I am aiming for completing within six months.

5. The list of code and data updates in v3.1 follows:

Corrections and updates to code (ADAS v3.00 to ADAS v3.01)

C.1 Now use *xxdata_04* in ADAS412 to read data from adf04 files – the newer adf04 datasets are not as rigidly formatted. Remove ADAS412 routines which duplicated central ADAS routines.

Note that in ADAS412, the reading of adf11 data still uses old access routines which cannot parse partition information.

C.2 For the same reason use *xxdata_04* in ADAS215 to read data from adf04 files. Note that the orbital energies are not written to the re-gridded adf04 file.

C.3 When returning the fulldata structure from *read_adf04.pro* make the dimensions usable with the current (large) values set by the heavy species work.

C.4 *read_adf22.pro* is a wrapper around *read_adf21.pro* as the adf21 and adf22 data formats are effectively identical. However it passed *fulldata* to *read_adf21* whether or not it was requested thus disabling its use. This has been corrected. Recall that the *read_adf* routines either return all the data in the file (via *fulldata* output structure) or interpolated/extrapolated data at requested conditions.

C.5 Some S/XB (adf15) data produced in the early days of the GCR project contained zeros at low temperatures. These data are not incorrect but their presence can cause the splining routines to fail. The zeros have been excluded from the spline fitting *Fortran* routines.

C.6 adf14 datasets generated by adas302 could put un-initialised values as the producer. It now returns the real name of the user.

C.7 An incorrect/misleading warning message was printed to screen if the element name was either missing, or inconsistent with the atomic number, in the adf11 dataset. THis has been corrected.

C.8 Options to control the on/off setting of ion impact ionisation and charge exchange have been added to *run_adas310.pro*. Note that these are specialised options and have not yet been made available in the interactive GUI of ADAS310.

C.9 Now allow temperature and density to be supplied as vectors, rather than be specified as min/max number values in *run_adas408.pro*.

The interactive GUI does not allow this flexibility yet.

C.10 ADAS416 no longer forces the output filenames, specified in the driving script file, to be lowercase.

C.11 When specifying the element by user identifier in *run_adas405.pro* and *run_adas406.pro* the central ADAS (for default data) and user adas directories are no longer assumed to be on the same file system.

C.12 *preview_natural_partition.pro* now allows the fractional abundances to be returned as values, as well as producing figures.

C.13 Add the ability to use partitioned adf11 datasets in ADAS405 and ADAS406.

C.14 In adf11, modify the checks of the iz1/is1 stage/partition index to account for the extra stage present in *zcd*, *ycd* and *ecd* data classes relevant to superstages.

C.15 Add *iprate.for* to ADAS804 (and *libadas8xx*). This routine provides a calculation of the electron collisional excitation and de-excitation rate coefficients for dipole transitions in the impact parameter approximation.

C.16 The bremsstrahlung and dielectronic recombination power returned from *cgbnhs.pro* were reversed. This has been corrected

C.17 The stand-alone *merge04.x* program no longer required the "-1" terminator for the transition list of the adf04 file to be in columns 3 and 4. It can now process the more flexibly formatted adf04 files.

C.18 Newer compilers, such as *gfortran*, are less sanguine about legacy *Fortran* constructs. A number of *Fortran IV* era methods have been updated to (at least) *Fortran 77* standards – in ADAS804 function definitions, in ADAS603 and in the various configuration string parsing routines (of the form *<>pars.for*, *<>prs1*.for). In particular, *integer*4* was replaced by *integer*.

In ADAS416 the minimum allowed integer should be one less than -2^31 which causes an overflow when compiling with *gfortran*.

In ADAS701, ADAS702 and ADAS801 some integer variables were set to character constants in data statements. This is apparently an IBM extension to the *Fortran 66* standard. The correct, *Fortran 77*, way is to use Hollerith constants in the data statement (eg, 'F' should be set using 1hF). One should not forget to call *gfortran* with the "*-std=legacy*" option! Character variables can/should be set using literals. Note that *g77*, the *Portland* Group, *Intel* and *Lahey* compilers are not as restrictive.

Offline ADAS8#1 has been modified also.

C.19 An IDL function, *split_multiplet.pro*, returns the relative intensities of the *J-J'* lines that make up the multiplet. The inputs are *S*, *L*, *S'* and *L'* and it is split according to formulae in Condon and Shortley (Chapter 9).

C.20 The IDL routines to read and write adf11 data have been updated. The data classes, *acd*, *scd* etc., are now returned as a string in addition to the old method of an integer. The size of the temperature set had been omitted.

The *write_adf11.pro* routine will now write the correct class specific header line for each stage. It will cope with the different numerical format required for the *ecd*, *zcd* and *ycd* classes. The arguments have been changed to bring them into line with the other *write_adf<nn>.pro* routines. The ADAS8XX routines which use it have been changed but routines outside central ADAS which call it should be modified.

C.21 The IDL version of *r8necip.pro* passed a wrong value for the ion charge to the underlying *fortran* code. This arose from using the *fix()* function rather than *long()* function to clean up the values to be passed to *fortran*.

C.22 In ADAS314, the data output to the adf01 file was mis-labelled. Effective cross sections are output, ie rate / velocity where the velocity is *1.384e6 * sqrt(te)*, but these were incorrectly labelled as rates in the adf01 file. A stronger warning is also set in the comments.

C.23 The IDL function, *xxeiz0.pro*, which returns the atomic number when the element symbol is given, has been vectorized.

C.24 *read_adf04.pro* did not act like the other *read_adf* routines when returning the values from a selected transition. It returned the temperature and effective collision strength in the dataset and did not interpolate/extrapolate onto a given temperature. Extracting this data is

better performed via the fulldata structure method.

The routine has been modified to interpolate onto Te and the excitation and de-excitation rates are now returned as additional, optional, outputs. The Burgess-Tully transformed variables are also interpolated.

If Te is not input the old behaviour is retained. However note that subsequent calls to *read_adf04* may now have a valid Te declared.

C.25 Some minor changes have been made to routines in ADASLIB, ADAS215, ADAS310 and ADAS801 to enable compilation with the *Lahey* (*lf95*) compiler. Commas before the first variable in read and write statements and assuming 1.0E-99 will be interpreted as real*8 are not valid. The rarity of such errors across the ADAS codebase is heartening.

C.26 A new utility IDL routine which takes a list of adf23 ionisation data files and generates an iso-nuclear adf07 file has been added. This is imaginatively named *adf23_to_adf07.pro*.

C.27 New utility routines have been added to ADASLIB. *xxcsaz.for* analyses pairs of Eissner configurations to determine whether they differ by one orbital. The *i4ldec.for* function returns the *L* quantum number given its decimal order.

C.28 Extra analysis outputs have been added to *xxdtes.for*, the routine which determined whether a configuration string is in Eissner or standard notation. In addition to handling arbitrary length configurations, the new outputs return a 19 character string covering the valence end of the configuration string and another string for the core. It also outputs and indication as to whether the configuration is in bundled or parent form. The previous version returned just the principal quantum number of the outer n-shell, but the updated routine returns the l-shell as well.

This means the the argument list of *xxdtes* has changed so routines which use it need to be updated.

C.29 Two general purpose IDL routines which may be useful have been added to ADASLIB:

upcasefirst	: capitalises the first letter of a string (or array).
wheresubarray	: returns the indices (and count) of where a sub-array matches a larger array.

C.30 A utility routine, *split_adf07.pro*, which splits an unresolved adf07 ionisation rate file into a metastable resolved adf07 file has been added. Ionisation stages up to Ar-like can be split. Note the pathways are defined in a spreadsheet. The routine acts on this information when it is exported as a colon separated text file. Many assumptions are made when post-processing the spreadsheet data so strict adherence to its format is required.

C.31 The IDL-only *xxuser.pro* function relies on a valid LOGNAME environment variable being present. The routine now checks that this valid before proceeding.

C.32 The transition identification in the ADAS303 processing panel was blank because of an 'upgrade' in the adf12 reading routine. It now indicates the n-n' transition as before.

C.33 Four fortran routines, providing cross-sections and rates for ion impact excitation and ionisation of hydrogen and hydrogenic ions, have been made accessible to IDL. The Lodge-Percival-Richards ionisation and Percival-Richards excitation formulations are used for the higher-n levels in ADAS series 2 and 3 codes. These are in:

idl/adas3xx/adas310/qlpr.pro
qipr.pro

rqlnew.pro
rqinew.pro

Although these are in the linkable libraries this continues the policy of providing IDL access on an as-needed or as-requested basis.

C.34 An IDL version of *cxqntb* has been added. This gathers data from an adf01 charge exchange file and returns the beam driven rate coefficients on a requested energy vector and representative n-shell set. It optionally returns an average rate coefficient over fractionally weighted beam energies.

C.35 The */ecipcalc* option to *read_adf04.pro* occasionally failed when generating rates from excited parents. It has been rewritten to be more robust.

C.36 In the *fulldata* structure returned from *xxdata_09.pro*, the total dielectronic coefficient (*diel_tot*) is tabulated on the set of initial parents, and not on the set of total parents. The returned array now only contains the correct data.

C.37 An error in logic was discovered in *r8yip.for*, the routine which evaluates the impact parameter cross-section second Bessel integral (*Y*); see Burgess and Summers, MNRAS (1976) 172, 345. This routine is used in calculating the ECIP ionisation rates and ion impact rates in the series 3 codes.

Fortunately this branch of the code is rarely triggered and the electron impact ionisation rates used in the GCR work. The central ADAS adf11 and adf15 datasets are unchanged. Similarly no errors are introduced in the adf12 CX emissivity coefficients generated with ADAS309.

This is one of the older errors found in ADAS – being present since 1993!

C.38 Two IDL utility routines for manipulating adf04 data have been added to the *adaslib/proc_adf/* directory. These are:

bundle_adf04.pro : bundles levels in an adf04 file according to an input map
merge_adf04.pro : merges two adf04 files according to an input map.

The *bundle_adf04.pro* routine complements adas209.

C.39 When extrapolating adf11 *acd* data using *read_adf11.pro* a more appropriate extrapolation option is used. This brings *read_adf11.pro* into line with ADAS401 and ADAS404.

C.40 The command line *filter04.x* routine, which sanitises adf04 files, can now accept comments up to 150 characters in length – increased from 80 which cut off some of the more verbose comments.

C.41 The latest adf09 files, produced as part of the DR Project, are on an extended temperature range. ADAS204 has been updated to use these newer data. Extra checks for numerical stability, when substituting high quality zero-density ionisation rates, were added.

C.50 A version of the interactive system which runs under the IDL virtual machine has been added. This is accessed via command line switches:

adas -vm

or

adas --virtual-machine

Nearly all ADAS programs will function in the virtual machine although there are a few exceptions. However it does allow ADAS to be used when IDL licenses are not available.

C.51 There were minor inconsistencies between the adf08 specification, the ADAS211 generation code and the *read_adf08* reading routine. The documentation and ADAS211 have been updated. The data from adf08 files can now be read into a *fulldata* structure from *xxdata_08.pro* (or *read_adf08.pro*). A number of datasets were updated to bring them into line with the adf08 specification.

Corrections and updates to data (ADAS v3.00 to ADAS v3.01)

D.1 The adf00 datasets for Li, Be, Br and Rn had a positive iz0 but they did include ionisation potential data.

D.2 Identify the table used from ORNL6086/V1 for the Maxwell average charge exchange coefficients in *adf14/tcx#h0/tcx#h0_h.dat*.

D.3 Add the missing XENON element name to the first line of the 89-set adf11 files. This supresses an annoying error message from *xxdata_11*.

D.4 Add specific ion data for calcium from CHIANTI v6. These data are converted to adf04 format. The configuration labelling and numerical data is that of the original CHIANTI data. A naming convention is adopted: the data are stored as

adf04/copch#20/chv6_ic#ca<z1>.dat

where *ch* represents CHIANTI, v6 the version used and *<z1>* is the ion charge of interest.

D.5 The documentation for adf14, thermal charge exchange rates, gave the incorrect order for donor and receiver temperatures. This has been corrected.

D.6 The adf03 parameter file for Al (the historical van Maanen one, *atompars_vm#al.dat*) had more sub-shells included for Al^{+2} and Al^{+3} ionisation than indicated, which caused adas408 to crash.

D.7 Add metastable resolved adf00 datasets in LS coupling for elements Mg and Si. The datasets include excitation energies in addition to ionisation energies as required in the preparation of resolved adf11/ecd data. The datasets take the form '*<elem symb>_ls.dat*'.

D.8 R-matrix calculations for various ions have been added:

adf04/nelike/nelike_dcg08#kr26.dat - Griffin et al, J Phys B41, 215201 (2008)
nilike/nilike_cpb06#w46ic.dat - Ballance et al, J. Phys. B39, p3617-3628 (2006)
culike/culike_cpb07#w45ic.dat - Ballance et al, J. Phys. B40, p247-258 (2007)
znlike/znlike_cpb07#w44ic.dat - Ballance et al, J. Phys. B40, p247-258 (2007)

D.9 PEC data for Na-like krypton (Kr25+) has been added to the adf15/transport/ directory to support transport analysis.

D.10 New adf04 files in intermediate coupling with the collisional rates computed with R-matrix have been archived. These are for: He-like C^{+4} to Kr^{+34} by Allan Whiteford ; Ne-like Na^{+} to Kr^{+26} by Guiyun Liang; Na-like Mg^{+} to Kr^{+25} by Guiyun Liang. These are named respectively as

adf04/copaw#he/helike_adw05#<el.sym.><ioncharge>.dat
adf04/copaw#ne/nelike_lgy09#<el.sym.><ioncharge>.dat
adf04/copaw#na/nalike_lgy09#<el.sym.><ioncharge>.dat

D.11 In the *adf04/copsm#li* collection of Zhang and Sampson Li-like data, the volume of the referenced paper in ADNDT has been corrected. The paper can be found in vol 44, p31 (1990) and not vol 42.

D.12 The ionisation potentials for Mg^{+3}, Si^{+5}, Ar^{+9} and Fe^{+17} have been corrected to the NIST values since they differed by 1-5%.

D.13 A non-printing *CTRL-Z* appeared in some *adf04/coppm#li* datasets. Others in this collection had non-standard comments. All datasets now conform to ADAS standards.

D.14 The adf04 specific ion data for magnesium and iron generated from CHIANTI data was unsatisfactory in two respects.

The temperature range of the adf04 files has been changed to the standard ADAS one rather than the fixed range in the first version. This ensures that the adf04 file contains data which is centered at the temperature of maximum abundance.

More seriously, a number of transition probabilities were omitted from the adf04 files. There is no accompanying effective collision strengths in the CHIANTI database, which have been set to zero in the adf04 file. The exclusion of these A-values would lead to misleading results when calculating the excited populations.

Note that these files are significantly different from the previous set which are no longer recommended for use. In this case the error was sufficiently serious that these datasets were replaced rather than adding newer data to the central adf04 collection.

D.15 A number of datasets were updated to bring them into line with the adf08 specification. No values were changed. A missing separator line after the temperatures was omitted in some data. A few other files had index columns aligned incorrectly.

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4 Mar. 2011