mar18-97 **ADAS Bulletin**

This is the first bulletin in the new maintenance phase of the ADAS Project. To keep you up-to-date, after consultations, we agreed it would be best value for money to make a full-time computer support officer appointment here at the University rather than buying 8 weeks per year of Tessella time for ADAS support. Our ADAS maintenance funds would allow us 4/7 of the time of the appointee. I placed a post-doctoral computational physicist (Ricky Martin) in the position temporarily for three months while negotiations with the University authorities were completed. Ricky has been covering ADAS maintenance and development since 1 Feb. 1997 and has already announced himself to you. The University has agreed to the creation of an open-ended computer officer position in my department for as long as it is fully funded. The position must be advertised in the public domain and this is being done now. We hope to have completed interviews and made the permanent appointment within about six weeks. ADAS maintenance is indeed allocated 4/7 of the time and the appointee will be under my line management. I think this will secure long term solid support for ADAS. Ricky is of course applying for the permanent position.

A substantial number of the ADAS programs and datasets have been exercised heavily over the last few months. It was of course our intention and hope since this way the programs harden rapidly. In this bulletin therefore I wish to notify the corrections and adjustments to the programs and data, arising from the experience gained, which are in the new release (release 1.10). I should say that we have also three new programs in preparation for release but I wish to hold these off until release 1.11 (planned for June) since I would like some feed-back on what facilities to put in them. I shall return to this point at the end of the bulletin.

1. **ADAS211** Nulls characters were being placed at the end of certain lines in the comments section of the output data04.pass file. This as a problem appeared only with particular editors and systems. The fault has been corrected by Ricky.
2. **ADAS212**
   - 2.1. The code, which adds dielectronic recombination data lines to the end of specific ion files of data format *adf04*, had options set to prevent extrapolation of DR data beyond the temperature range of the input *adf09* datasets. The effect was to insert 1.0's in the problem locations in the *adf04* output file. This affected only very few cases where exceptional temperature ranges were chosen for the *adf04* file - in particular the /helike_kvil93he.dat file for helium gas puff and beam experiments. Controlled extrapolation is now allowed by setting the internal parameter IOPT=-1 to IOPT=1.
   - 2.2. A hard stop was present in the code if a *postllev.pass* file was not present in the user's pass directory. This has been amended.
3. **ADAS302**

   Note that there has been an alteration in formatting of the data class (*adf02*) interrogated by ADAS302. When using the old data sets, the information presented on the reaction selection widget of the processing screen is incomplete. Only the index numbers are given with *'s inserted in the other fields. This is not a fault but does make selection difficult. You need use the *Browse Comments* button to see what the index numbers refer to. Harvey Anderson has been reviewing and updating the *adf02* data. The revised data is in the new formatting which gives full information on the ADAS302 reaction selection widget.
4. **ADAS304**
   - 4.1. ADAS304 is an interrogation code, which accesses collections of beam stopping coefficients of ADAS data format *adf21*. There are separate datasets for each distinct impurity prepared by running ADAS310 for the 'pure' impurity case. Effectively this gives the stopping due only to the selected impurity and free electrons in proportion to the impurity's nuclear charge. These datasets are designed to allow rapid assembly of a composite impurity stopping by linear combination of the single impurity data. Such rapid assembly is necessary for efficient JET spectral data reduction. The precision of the linear superposition is the point in question in comparison with a true composite impurity stopping coefficient calculation by ADAS310. This has been under investigation by Harvey. It was noted that central IBM ADAS304 and IDL

ADAS304 lacked the implementation of the optimum effective electron density in the interpolative search for the density dependent stopping coefficient. The correct prescription was in the ADAS User Manual and had been entered in the JET analysis (KS4FIT) but overlooked in the IBM and IDL programs. This has been corrected.

4.2. The second issue concerns the definition of the stopping coefficient. The generating program ADAS310 defines the coefficient with respect to the electron density. Thus the stopping rate (cm-3 s-1) is $N_e N_B S^{(e)}$ with N_B the neutral beam atom density. This applies even if the stopping is calculated for the case of a pure impurity with all free electrons assumed contributed by the impurity in charge balance. An alternative philosophy is to write the stopping coefficient in terms of the impurity ion density since impurity ions are responsible for the most important stopping collisions. Thus for impurity number density N_I, the stopping rate is $N_I N_B S^{(I)}$. For a pure impurity of nuclear charge Z, then $S^{(e)} = S^{(I)} / Z$. The program ADAS304 interrogates collections of pure species stopping coefficients generated by ADAS310. Originally however ADAS304 assumed it received, as input, stopping coefficients defined in terms of impurity ion density and returned a composite coefficient also in terms of total impurity ion density. That is according to the expression $S^{(I)}_{final} = \sum f_i S^{(i)}$ with $N_I = \sum f_i N_i$. In the revised version of ADAS304 now being released, the quantity evaluated is $S^{(e)}_{final} = \dfrac{\sum Z_i f_i S^{(e)}_i}{\sum Z_i f_i}$ consistent with the ADAS310 calculation.

4.3. In the original version of ADAS304, the user specifies the total ion density although the electron density is returned in the output. This is now considered inconsistent with the internal treatment of the electron density as the primary density in ADAS310 and ADAS304. The revised version of ADAS304 now accepts user processing widget entry of the electron density rather than the total ion density.

4.4. The code ADAS310, with small adjustment of the post-processor section can generate beam emission coefficients, in particular for DI Balmer alpha. The organisation of output from the post-processor (*adf21*) for beam stopping is perfectly satisfactory for beam emission coefficients. We use the mnemonic '*bme*' for beam emission coefficients and store them in ADAS data format *adf22*. ADAS304 has been adjusted to interrogate *adf22* as well as *adf21*. It detects automatically which data class it is handling and adjusts graph titles accordingly.

5. ADAS310

5.1. A small discrepancy was observed by Harvey in the beam stopping coefficients produced by the JET IBM and UNIX versions of ADAS310. The extraction of the fundamental data and the formation of the rate coefficients was studied in depth and was satisfactory. It was found that the discrepancy was due to a simple programming error introduced when a NAG routine was removed from the IDL version of the code and replaced by an equivalent public domain routine. This produced a substantial error in the F3 column of the bundle-n population output tables (the first output data set from ADAS310). The influence of this is very small on the essentially linearly independent F1 column which determines the density dependent beam stopping . Nonetheless it was satisfying that the discrepancy was isolated. The error has amended and after running several simulations, the output from the IDL version of ADAS310 agree with the off-line version of the code and therefore the JET stopping data.

5.2. Note that ADAS310 executes repeated calculations of beam hydrogen population structure and collisional-radiative coefficients as one and two-dimensional scans over plasma and beam parameters. The primary output from these scans is post-processed in a section of ADAS310 to generate a compact tabulation of stopping coefficients in the ADAS data format *adf21* (the fourth output data set from ADAS310). This compact tabulation is the agreed form for direct utilisation in beam stopping analysis at JET.

5.3. In the course of correcting these discrepancies in the handling of electron and ion densities and mixtures of impurities between the series 3 ADAS codes, some associated errors were detected in ADAS310, most critically, an error occurred in certain situations when hydrogen itself was included as an impurity. Also in ADAS310, some additional protections for normalisation of mixed impurity fractions were included. The details are as follow:

5.4. Consider a mixture of impurities labelled by nuclear charge Z_i of number densities $N^{(Z_i)}$ and fractions f_i. Hydrogen nuclei may be one of these impurity species. In addition hydrogen nuclei may be specified as present in the plasma via a 'proton density' N_p. It is necessary that the two ways of including hydrogen nuclei are combined in a consistent manner. The procedure is to add the 'impurity' hydrogen nuclei to the 'protons' and delete it as an impurity from the impurity list. This is done internally in the code. ADAS310 accepts as input N_e, N_p and the set $\{Z_i, f_i .\}$. Write $N_I = (N_e - N_p) / \sum_i Z_i f_i$. Then $N_p' = N_p + f_{i_0} N_I$ where it is assumed that hydrogen impurity is given as the i_0 impurity. The new impurity fractions omitting the hydrogen are obtained as $f_i' = f_i / \sum_{i, i \neq i_0} f_i$ and the new total impurity number density becomes $N_I' = (N_e - N_p') / \sum_{i, i \neq i_0} Z_i f_i'$. Note that although the previous version of ADAS310 therefore gave incorrect results if hydrogen nuclei were included as an impurity, this was not the normal practice in generation of stopping data at JET.

6. **ADAS407** Martin O'Mullane has been working extensively on the JET baseline data for ionisation, recombination and radiated power. This is data of ADAS format (*adf11*), but specifically under the year number '89'. It is created by first generating parameter sets (*adf03*) from specific ion files (*adf04*) using ADAS407 and then running ADAS408 using these parameter sets. This has given us the opportunity to scrutinise ADAS407 and ADAS408 again quite thoroughly. One or two errors have been uncovered.

6.1. ADAS407 is normally used by cycling up through the members of an iso-nuclear sequence without leaving the routine. Thus a complete set of parameters of an element may be generated in one go. The specific ion files of the form */.../adf04/copmm#<nuclear charge number>/ls#...* have been specially created to feed ADAS407 in this operation. A fault condition occurred when the final case in the cycle, i.e. the hydrogen-like/bare nucleus was reached. The bare nucleus specific ion file you will notice is essentially a dummy file. The IDL file reading routine in ADAS407 was too strict and rejected it. This error has been trapped.

6.2. The configuration information on the specific ion files input to ADAS407 is used to determine the shell occupancy in the simple parameterisation of radiative recombination. The code was designed to assume that inner n-shells, not explicitly shown in the configuration, were full occupied. No assumption was made about omitted l-shells of the outer valence n-shell. In an isonuclear sequence of specific ion files, we had not noticed that in one or two cases an l-shell moved from being explicit to implicit. Rather than modifying the specific ion files, we thought it preferable to assume that l-shells of the valence n-shell with l less than the explicitly shown l-shells are fully occupied. ADAS407 has been so modified, **but bear this in mind with heavy species and complex configurations**.

6.3. When ADAS407 is building its parameterised approximation to the radiated power, it lists and allows bundling of allowed transitions with oscillator strengths above a minimum value (*FMIN= 0.01*). In our work with Ar^+, it was clear that this was too severe for $\Delta n=0$ transitions. We have reset *FMIN =0.003*.

7. **ADAS408** Martin has been looking at ADAS408 with radiated power filtering activated. Recall that ADAS408 allows production of radiated power tables both for the total

power and the power as seen through a filter. At the moment filters representing soft-X-ray cameras are allowed, namely, a simple cut-off filter or a beryllium coated glass (Be/Si) filter. There have been some inconsistencies and problems with the latter which we have corrected.

7.1. The units for the thicknesses of the Be and Si parts of the filter on the ADAS408 processing widget were incorrect. They should have been microns and mm respectively. The code assembles a filter name by taking two digits from each filter thickness part. as '*ft<nn><mm>* which insets in the output name structure of the power files, prb, plt as */.../adf11/prb<yr>/prb<yr>#<el>.ft<nn><mm>.dat*. The selection of two digits was ambiguous if decimals were included. We have forced integer thickness and have extended the Be part to 3 digits. Thus the total length of the filter name field is now seven characters. Blank filling of the name with zeroes is done. This file name length alteration has some wash-over effect on ADAS405 and ADAS406 - see below.

7.2. Ricky has picked up an error in the temperature conversions in ADAS408. This has not shown since we have been using the JET IBM codes for the main production runs. *adf11* data sets in the central ADAS database are not in error because of this fault. However the error has been corrected.

8. **ADAS405 & ADAS406**

In the light of the altered filtered power file name lengths of section 5.1 above, ADAS405 and ADAS406 have been modified to accept the longer names.

9. **ADAS501 & ADAS503**

9.1. Costanza has picked up a small error in the interrogation codes for ionisation per photon coefficients (*adf13*) and photon emissivity coefficients (*adf15*). The problem is with data sets which have data block entries of different temperature and density vector lengths. The program operates but then fails if you enter it again. The problem is in the */defaults* file which has to be deleted to operate the program again. The fault has not come to light before because normally we generate a complete *adf13* or *adf15* file at the one time from ADAS208 and do not 'pick and mix'. Ricky has corrected this error.

10. **ADAS601** Alessandro and David have continued working with the differential emission measure code ADAS601. One or two faults have been corrected and improvements added.

10.1. In a conversion from Roman spectroscopic notation for ions in the input *Intensity* file to ion charge notation, zero was returned. This has been corrected. Also alignment of the header titles in the DEM plot has been improved.

10.2. The theoretical line-of-sight intensities as calculated by the FORTRAN and IDL routines in ADAS610 were slightly different. The error has been traced and corrected.

11. **ADF02**

Note the alteration in the formatting of this data class. Harvey Anderson has reformatted and renamed the old hydrogen file as follows:

/.../adf02/ionatom/h.dat ----> */.../adf02/sia#h/sia#h_rfm#h.dat*

Note that we are moving to the use of *sia* as the mnemonic for ion/atom cross-section data. Harvey has carried out a very extensive review of the ion/atom collision cross-sections required for neutral hydrogen beam stopping and beam emission. This was due since the collection above dated form 1989 with some updates through to 1993. Also he has improved the data for Li^{+3} and Ne^{+10} in collision with neutral hydrogen. Two new files have been created. These are a new 'preferred JET' dataset

/.../adf02/sia#h/sia#h_j97#h.dat

and a dataset built on the above but with the cross-sections of the CCAO calculation of Toshima and Tawara (1995) substituted where they exist

/.../adf02/sia#h/sia#h_tos#h.dat

Use of these three data sets give a spread of results for beam stopping and beam emission coefficients which we consider gives a reasonable view of the 'working accuracy' of the latter coefficients. The */.../adf02/sia#h/sia#h_j97#h.dat* data set contains our preferred cross-section data at this time. It incorporates also data from the review of Janev and Smith (1993) (cf. the detailed report by Harvey - */.../adas/docs/bms-report*).

12. **ADF03**

Martin has been generating further collections of iso-nuclear parameter sets from ADAS407. These are by processing on the /.../copmm#<nuc. chg>/... specific ion files which Martin in turn generates from his off-line Cowan/Born structure code. The additional data sets are

/.../adf03/atompars/atompars_mm#c.dat
/.../adf03/atompars/atompars_mm#s.dat
/.../adf03/atompars/atompars_mm#ar.dat
/.../adf03/atompars/atompars_mm#kr.dat

Additionally there was a fault in the neon file which prevented it from running in ADAS408 (the first ionisation stage data was missing) and so it has been replaced, ie. there is a new

/.../adf03/atompars/atompars_mm#ne.dat

We have been looking in some detail at the accuracy of the parameter sets in representing the radiated power for Argon and krypton. Martin has a short report in preparation.

13. **ADF04**

13.1. Mathias Brix (KFA Jeulich) has been looking very carefully at the population structure of neutral helium for helium gas puff experiments on TEXTOR. In particular he has checked through the ADAS specific ion files and has found some errors. At the same time Ronnie Hoekstra, Fritz Bleik (KVI, Groningen) and I have been re-looking at the ADAS preferred specific ion file data in the light of the recent converged close-coupling results. Our new preferred data is dated 1997 ie. data sets

/.../adf04/helike/helike_kvil97he.dat
/.../adf04/helike/helike_kvih97he.dat

for low and high temperature respectively. Older data sets which have been amended in the light of Mathias' examination are

/.../adf04/helike/helike_kvil93he.dat
/.../adf04/helike/helike_kvih93he.dat
/.../adf04/helike/helike_tex93he.dat

There was also an error in the last two temperature values of the recombination lines on the extended adf04 file */.../adf04/helike/helike_kvih93he.dat* due to protections in the code ADAS212 against extrapolation. The restriction has been relaxed and the data set amended. (see

13.2. The statistical weights in the he-like specific ion files built on Sampson's Coulomb Born cross-sections, ie. in files of the form

/.../adf04/copsm#he/copsm#he_sm#<ion>l.dat

were in error. These have been corrected.

13.3. Massimo Landini (Arcetri Observatory, Florence)has passed over the data which he and Brunella Monsignori-Fossi prepared for the n-like sequence. Alessandro has converted this to adf04 files as follow:

/.../adf04/nlike/nlike_ml96#ar11.dat
/.../adf04/nlike/nlike_ml96#ca13.dat
/.../adf04/nlike/nlike_ml96#mg5.dat
/.../adf04/nlike/nlike_ml96#s9.dat
/.../adf04/nlike/nlike_ml96#si7.dat

Also Robert Frost (Technical University, Munich) has completed his extensive R-matrix calculations for the n=2 and n=3 shells of neutral nitrogen. These calculations were carried out on the Strathclyde University workstations under Nigel Badnell's initial direction

/.../adf04/nlike/nlike_rf97#n0.dat

13.4. Also Robert has completed similar calculations for the n=2 and n=3 shells of singly ionised nitrogen.

/.../adf04/blike/blike_rf97#n1.dat

13.5. Don Griffin (Rollins College, Winter Park, Florida) has completed a very large scale intermediate coupling R-matrix calculation for single ionised argon. This data has also been used to generate ionisation per photon data for Ar^+.

/.../adf04/cllike/cllike_dg97#ar1.dat

14. **ADF07** Don has added a new data set of state selective, zero density, direct electron impact ionisation rate coefficients for Ar^+. The data set is

/.../adf04/cllike/cllike_dg97#ar1.dat

15. **ADF09** Martin and Nigel have been working hard on creation of new large data sets for state selective dielectronic recombination coefficients for all the ions of the nitrogen and neon iso-nuclear sequences. These are complex background calculations using Nigel's AUTOSTRUCTURE code and post-processor. It has allowed us to revisit the older calculations for other first period elements and organise and systematise the actions required. A preliminary report is available but we shall add a little more to it concerning the special problems of recombination to form the neutral atom before the final version. The new data sets appear under the 96 year number and Martin's initials by iso-electronic sequence as

/.../adf09/mom96#<seq>/mom96#<seq>_<ion>ls<nn'>.dat

in the same manner as for Nigel's data. Note that there are some repeats over the *nrb93* data since these cases were executed as checks.

16. **ADF11**

16.1. A **serious error** has come to light for the

/.../adf11/<type>89/<type>89#ar.dat

data set. It is wildly wrong. Also it does not match the results from the parameter sets in *adf03* from which it was meant to have been produced. I have been unable to trace this fully, but it originates in a faulty parameter data set which was brought into JET about ten years ago. I recall that the faults were found and the parameters corrected. However, it appears that the *adf11* data sets were not then re-created (*mea culpa*). Argon was unfortunately, not a commonly used gaseous additive at JET. Martin has rechecked the consistency of all *adf03* parameter sets and *adf11* master files from them and this is the only inconsistency. The faulty *adf11* files for argon have been deleted.

16.2. Martin has created new iso-nuclear master files for the species argon and krypton using ADAS408. This is unresolved, state-to-stage data matching the '89' baseline year number. The data sets are archived as

/.../adf11/<type>89/<type>89#<element>.dat

16.3. Martin has been working extensively with filtered power data. We had not reached a conclusion as to whether such data should be put into the central IDL-ADAS database. I am open to suggestions on this, but in the meantime we have added some filtered power data for nickel as a sample. The files are

/.../adf11/plt89/plt89#ni.dat
/.../adf11/prb89/prb89#ni.dat
/.../adf11/prc89/prc89#ni.dat

17. **ADF18 & ADF25** We have been restructuring and adjusting the cross-referencing and driver data sets in these two data classes. These define the various mappings of data for codes ADAS204, ADAS208 and the preparation codes ADAS211 and ADAS212. At this time we are checking through ADAS204 to improve its operation at very low temperature and making some other improvements as we go. I therefore wish to postpone giving the details until the next release when these checks are finished.

18. **ADF21 & ADF22** Harvey has created the new 1997 data sets based on the new preferred ion/atom collision data (cf. *adf02*). The beam stopping coefficient data is in *adf21* and the Balmer alpha beam emission data in *adf22* as follow

/.../adf21/bms97#h/bms97#h_<ion>.dat
/.../adf22/bme97#h/bme97#h_<ion>.dat

where *<ion>* denotes *h1, be2, li3, be4, b5, c6, n7, o8, f9, ne10*. Note the extension to include *li3* and *f9* as stopping species in the plasma.

19.

20.

21. **Plans for ADAS508 and ADAS602**

21.1. There is a gap in the capabilities of ADAS in that the primary tabulations of G(Te) functions (*adf20*) have to be generated off-line. The code which does this was originally developed by Peter McWhirter at JET. Then Alessandro took it over, found the errors and made it more flexible. We have depended on Alessandro for running this code at suitable times to extend the G(Te) tabulations. However, now that the DEM code, ADAS601, is being used much more, with back checks etc. through the G(Te) functions to the specific ion files for problem lines, it will now be

helpful to have this G(Te) generator on-line. The code will be ADAS508 and Ricky is preparing it at this time. It will be ready for the next release.

21.2. Jim Lang (Rutherford Appleton) a few years ago prepared a very useful Gaussian spectrum line fitting program based on a maximum likelihood method. An important feature was that it provided a detailed error analysis. David has worked closely with Jim over the last year with the fitting code to orientate it for SOHO-CDS spectral data. Also David has worked with Davina Innes (MPAE Lindau) on using it for high velocity events in SOHO-SUMER data. Here at Strathclyde, we have also been using it. Two final year students, Gordon Fischbacher and Stuart Loch have been testing the code to destruction on SUMER data for opacity studies. We think the code is now quite robust and we have built up considerable experience with it on problem lines, overlapping multiplets, line shifts, background distortions, fixed patterning etc. I think this is a suitable time for David to put it up as ADAS602. However, the code and the subsequent processing linked to it is geared up to FITS format files for input. This would be a good time to specify other formats of experimental data input file orientated to fusion experiments if this is of interest. **Please let us know soon of special requests** which we may be able to accommodate.

H. P. Summers
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