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ADAS
Atomic Data and Analysis Structure

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Review of proton impact driven ionisation from the excited levels in neutral hydrogen beams

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Abstract: *The proton impact driven ionisation cross section data from excited states of hydrogen, used to model beam stopping and emission in ADAS, are incorrect. Both the source data and evaluation methods are found to be in error. The consequential effect on the derived coefficients (adf21 and adf22) used to model beam behaviour is examined. Recommendations for updating ADAS data are presented.*

1 Source of cross section data

The ADAS data used for modelling hydrogen beams was re-evaluated by Harvey Anderson in 1997 and reported in [1]. The ion-atom collision cross-section database is stored in the central ADAS dataset, `/home/adas/adas/adf02/sia#h/sia#h_j97#h.dat`. This is a composite dataset based on the earlier ADAS data but is strongly influenced by the review of Janev and Smith in 1993 [2] — referred to as JS93.

It has been pointed out by Mathias Brix [3] that the the cross section data for proton impact ionisation from the excited states of hydrogen (for $n = 2, 3, 4, 5$) are too large, particularly for energies above 10keV/amu. The JS93 review was the source of the ADAS data.

Resolving this anomaly in the ADAS data required both an examination of how the JS93 data was evaluated and, furthermore it was necessary to examine the original sources used in the JS93 review.

For $H^+ + H^*(n = 2) \rightarrow H^+ + H^+ + e^-$ the cross sections for energies below 10keV/amu are the result of adiabatic calculations of [4]. Above this energy the CDW-EIS cross sections of Fainstein [5] are used. The recommended cross section is given as an analytic fit,

$$\sigma_{ion} = 10^{-16} A_1 \left[\frac{\exp(-A_2/E)\ln(1 + A_3 E)}{E} + \frac{A_4 \exp(-A_5 E)}{E^{A_6} + A_7 E^{A_8}} \right] \tag{1}$$

with fitting parameters A_1–A_8, for energies in keV/amu giving σ in cm^2 (see appendix A). The recommended data can be extracted, and evaluated using the `HEXC3` routine, from the ALADDIN website [6].

For $H^+ + H^*(n = 3) \rightarrow H^+ + H^+ + e^-$ the cross section data is again from [4] for energies below 10keV/amu, while for higher energies the $n = 2$ values are scaled by

$$\sigma_{ion}(n = 3, E_3) = \left(\frac{3}{2}\right)^4 \sigma_{ion}(n = 2, E), \qquad E_3 = \left(\frac{2}{3}\right)^2 E. \tag{2}$$

A separate set of fitting parameters for evaluation with equation 1 is given (see appendix A).

For higher n the $n = 3$ result is scaled. As printed JS93 has the formula,

$$\sigma_{ion} = 10^{-16} \left(\frac{n}{3}\right)^4 A_1 \left[\frac{\exp(-A_2/E_n)\ln(1 + A_3 E_n)}{E_n} + \frac{A_4 \exp(-A_5 E_n)}{E_n^{A_6} + A_7 E_n^{A_8}} \right] \tag{3}$$

with $E_n = (3/n)^2 E$ in keV/amu. It uses the same fitting coefficients as the $n = 3$ case but uses a different ALADDIN evaluation routine, `HIONN`.

The first error occurs in the evaluation of the $n = 4$ and $n = 5$ cross sections. Harvey evaluated equation 3 using the collision energy rather than the reduced energy, ie by assuming E instead of E_n. Ironically there is a mistake in the printed equation 3 of JS93: the reduced energy should be $E_n = (n/3)^3 E$ as can be seen in the (canonical) `HIONN` fortran routine. Note that figure 2.2.4 of JS93 gives the correct curve. The discrepancy introduced by Harvey's error is shown in figure 1 which is not as large had the 'correct' evaluation method been followed.

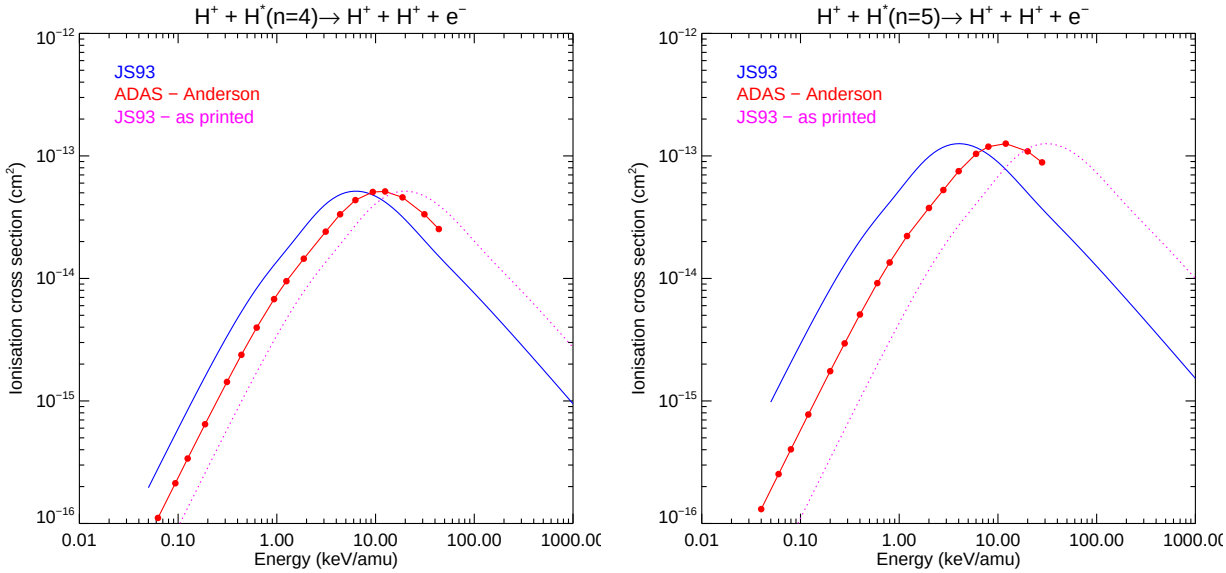

Figure 1: Ionisation cross sections from the $n = 4$ and $n = 5$ excited levels of hydrogen showing the ADAS data as calculated by Harvey Anderson, the JS93 review [2] the JS93 evaluation if the formula in the paper was followed. The symbols in the ADAS result show the range of energies archived in the dataset.

As can be seen in figure 1 the highest energy archived in the ADAS dataset is only 44keV/amu for $n = 4$ and 28keV/amu for the $n = 5$ cross sections. This just includes the turnover to the asymptotic high energy behaviour. In subsequent ADAS processing codes the extrapolation to higher energies assumes,

$$\sigma(E) = \sigma(E_{\rm last})\frac{E_{\rm last}}{E}. \tag{4}$$

No explanation for this low choice of cut-off energy can be uncovered this far removed from the production of the dataset.

There was another review, 10 years on from JS93, by Janev, Reiter and Samm [7] which also includes ionisation from excited levels of hydrogen. A slightly different fitting function was used but the results are essentially the same, since the source of the fundamental cross section data had not changed.

2 Validity of cross section data and a new fit

However the correctness of the high energy cross section data of [5] used in the JS93 review has been questioned. A short note in 1995, [8], showed that the CDW-EIS $n = 2$ cross section was too high by a factor of two. This was independently confirmed, using the same method, in [9]. It is noted that the cross section curves are scaled by n^2 in figure 1 of [8] and figure 5 of [9], presumably to distinguish the cross sections from each other.

In fact, another paper from the same group of Fainstein published a correction (of sorts), in the same year, when they extended their calculations to the $n = 3, 4, 5$ levels [10]. The correction

was given by way of a reference footnote and was not a prominent part of the paper. The curves in figure 3 of [10] are scaled in units of 10 to improve legibility.

However none of these works was considered in the 2003 review. It is important to note that the IAEA recommendation via ALADDIN has not changed — it remains that of the JS93 review.

Therefore a new dataset is required which should be based on the correct low energy data of the JS93 review and the corrected (and extended in n) CDW-EIS data of [10]. The 8 parameter fitting function of [7] (equation 40) was chosen:

$$\sigma_{ion}(n) = 10^{-16} b_1 n^4 \left[\frac{\tilde{E}^{b_2} \exp(-b_3 \tilde{E})}{1 + b_4 \tilde{E}^{b_5}} + \frac{b_6 \exp(-b_7/\tilde{E} \ln(1 + b_8 \tilde{E})}{\tilde{E}} \right], \qquad \tilde{E} = n^2 E. \qquad (5)$$

for σ in cm^2 given E in keV/amu. Figure 2 shows the fit and table 1 gives the parameters. The code used to produce the fit is listing in appendix B.

	$n = 2$	$n = 3$	$n = 4$	$n = 5$
b_1	3.9330(-03)	1.1076(-02)	1.1033(-02)	1.1297(-02)
b_2	1.8188(+00)	1.6197(+00)	1.6281(+00)	1.8685(+00)
b_3	1.8870(-02)	6.7154(-03)	5.5955(-03)	1.5038(-02)
b_4	6.7489(-03)	5.1188(-03)	7.2023(-03)	1.1195(-01)
b_5	1.3768(+00)	1.8549(+00)	1.7358(+00)	1.0538(+00)
b_6	6.8852(+02)	2.3696(+02)	2.2755(+02)	8.6096(+02)
b_7	9.6435(+01)	7.8286(+01)	8.6339(+01)	8.9939(+01)
b_8	5.6515(+23)	1.0926(+23)	3.9151(+29)	1.9249(+04)

Table 1: Fitting coefficients of equation 5 applied to the input cross section data of figure 2 ($a(b) \equiv a \times 10^b$). The IDL Levenberg-Marquardt least-squares fit routine MPFIT [11] was limited to 500 iterations without imposing a constraint on any parameter (see listing in appendix B).

A degree of subjective judgement on how to restrict the energy range of the low and high energy parts of the two sources for the fit procedure was required. The CDW-EIS model is not suitable for low energies thereby introducing a gap, unfortunately corresponding to JET beam energies[1]. Figure 2 shows the new fit to the fundamental cross section data, with the range of validity indicated by the filled-in symbols. The behaviour of the cross sections outside the range used in the fit is shown to indicate the degree of divergence. The gap in energy space between the two models motivates the use of equation 5 which is claimed to represent well the cross section shape [7].

It is interesting to note that the old ADAS data assessment agrees very well with the new fit in the region of interest for JET beam studies.

3 Does it matter?

Although a journey into reverse engineering ADAS data and demonstrating the pitfalls of using data from the publications of theorists is interesting as a historical exercise, a serious and germane

[1] This appears to be a perennial problem of ion-atom data.

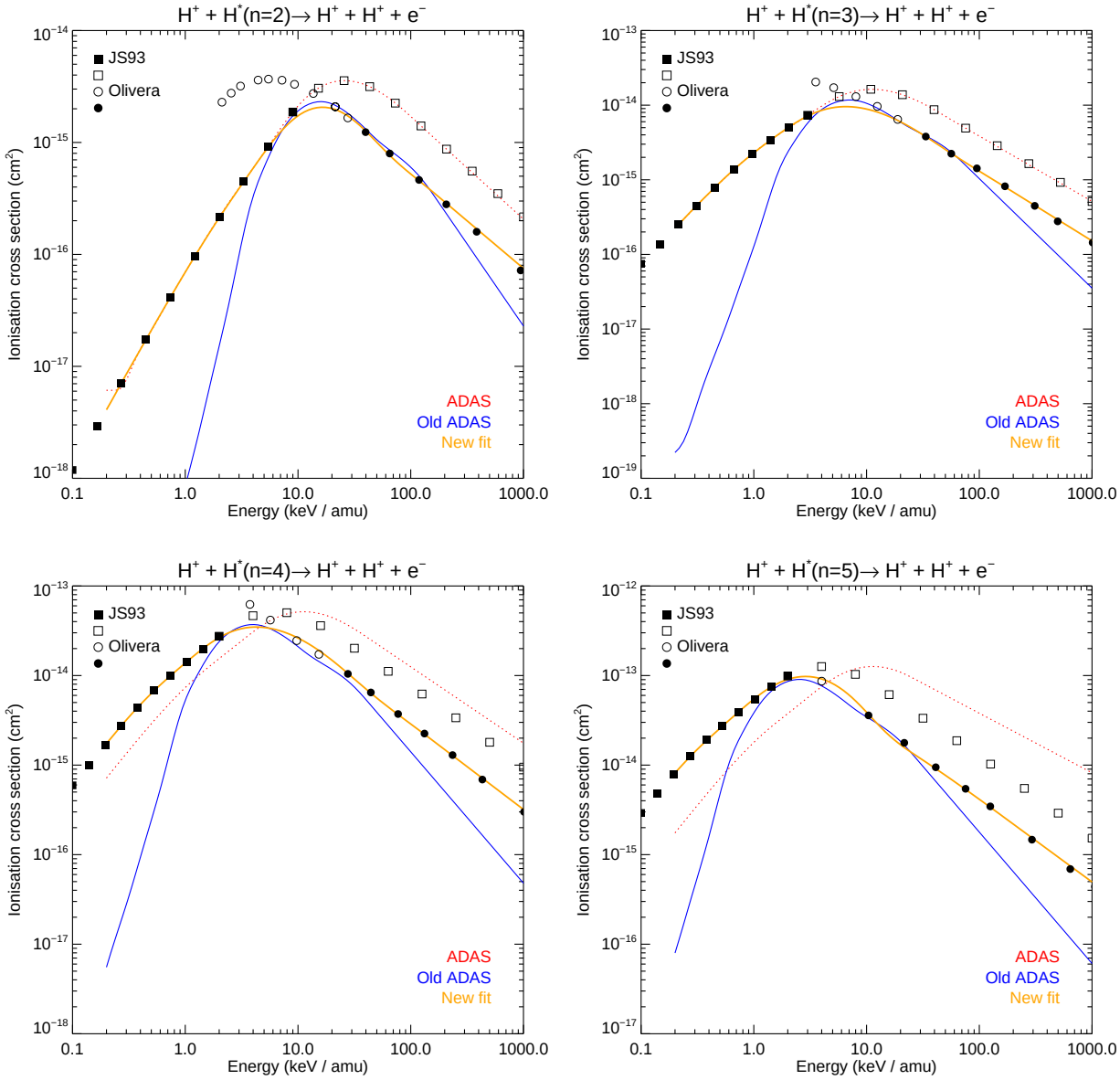

Figure 2: Proton driven ionisation cross section data. The three curves show the current ADAS data, the old (pre 1997) ADAS data and a new fit. The symbols show the cross sections used for the fits with filled symbols showing where the data is considered valid. The open symbols indicate where the JS93 data is in error and where the CDW-EIS approximation breaks down. The JS93 data were evaluated with the appropriate ALADDIN routine and the Olivera data were digitized from the graphs in their paper.

question arises: what is the effect of these mistakes when interpreting beam diagnostics?

These data are processed with the `adas310` code which is a very many n-shell bundle-n model of the hydrogen atom. For processes between low lying levels the in-built approximations are replaced by data drawn from the *adf02* set, which includes the proton impact ionisation from excited levels discussed here. Three derived coefficients are produced, viz: beam stopping, the population of excited levels in the beam and beam emission. The first two are used in CHEAP, so significant error here may require a re-evaluation of PPF data. The routine use of beam emission

measurements is less widespread.

Figure 3 shows the change in the stopping coefficients (*adf21*) as function of energy and density. At typical JET densities and beam energies the revised data differs from the current data by $\sim 3\%$. The consequences for a deposition profile are shown in figure 4 being less than 4% for $r/a > 0.3$. The simplified model assumes that there are no impurities present thus maximising the difference between the old and revised data.

Due to the amplification of errors in attenuation calculations an accuracy of $\sim 5\%$ should be expected for stopping coefficients. These are primarily dependent on ionisation (from ground) and charge exchange with significant contributions from stepwise processes. For excited levels the accuracy of the cross sections for excitation, charge exchange, ionisation are ranked at 20%–50%–100% [12].

Although the change introduced by this re-evaluation of four cross sections is at the 5% level, giving rise to some concern, the absolute accuracy is still within the original conservative range. Also despite the different energy dependence of the re-evaluated data, figure 3 shows that this structure is mostly washed out of the final stopping coefficients.

However the effect of the re-evaluation on the beam emission is expected to be greater given that they de-populate the upper levels of observed transitions. Figure 5 confirms this showing that the change in the $n = 2, 3, 4, 5$ populations ranges from 5–50%.

The differential changes between the 3–2 (6561Å) and 4–2 (4860Å) suggest that measurements can Further confirmation is possible if the 5–2 (4339Å) transition could also be observed.

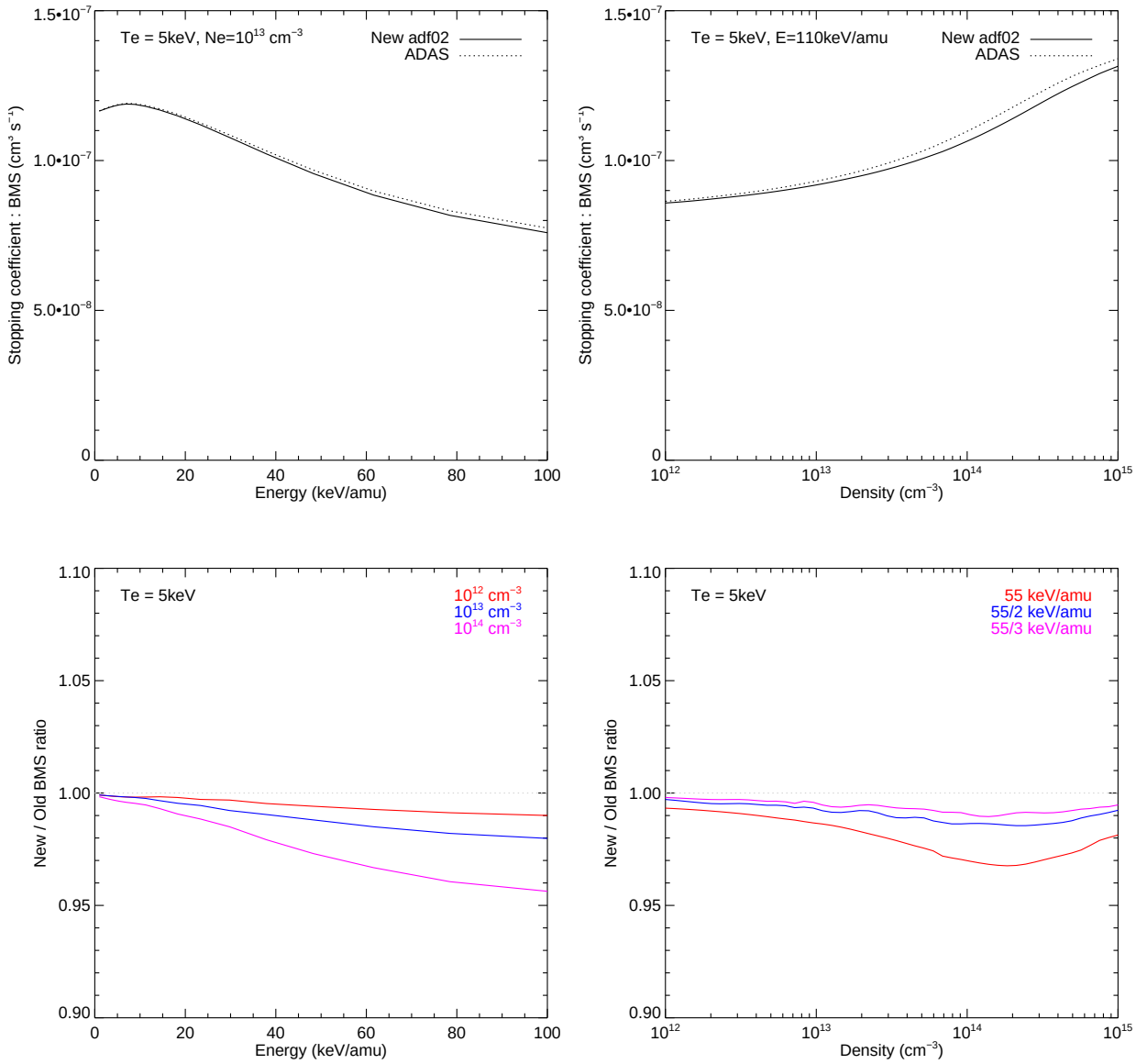

Figure 3: Effect on stopping coefficients of the new proton impact ionisation cross sections, as a function of energy (left) and density (right).

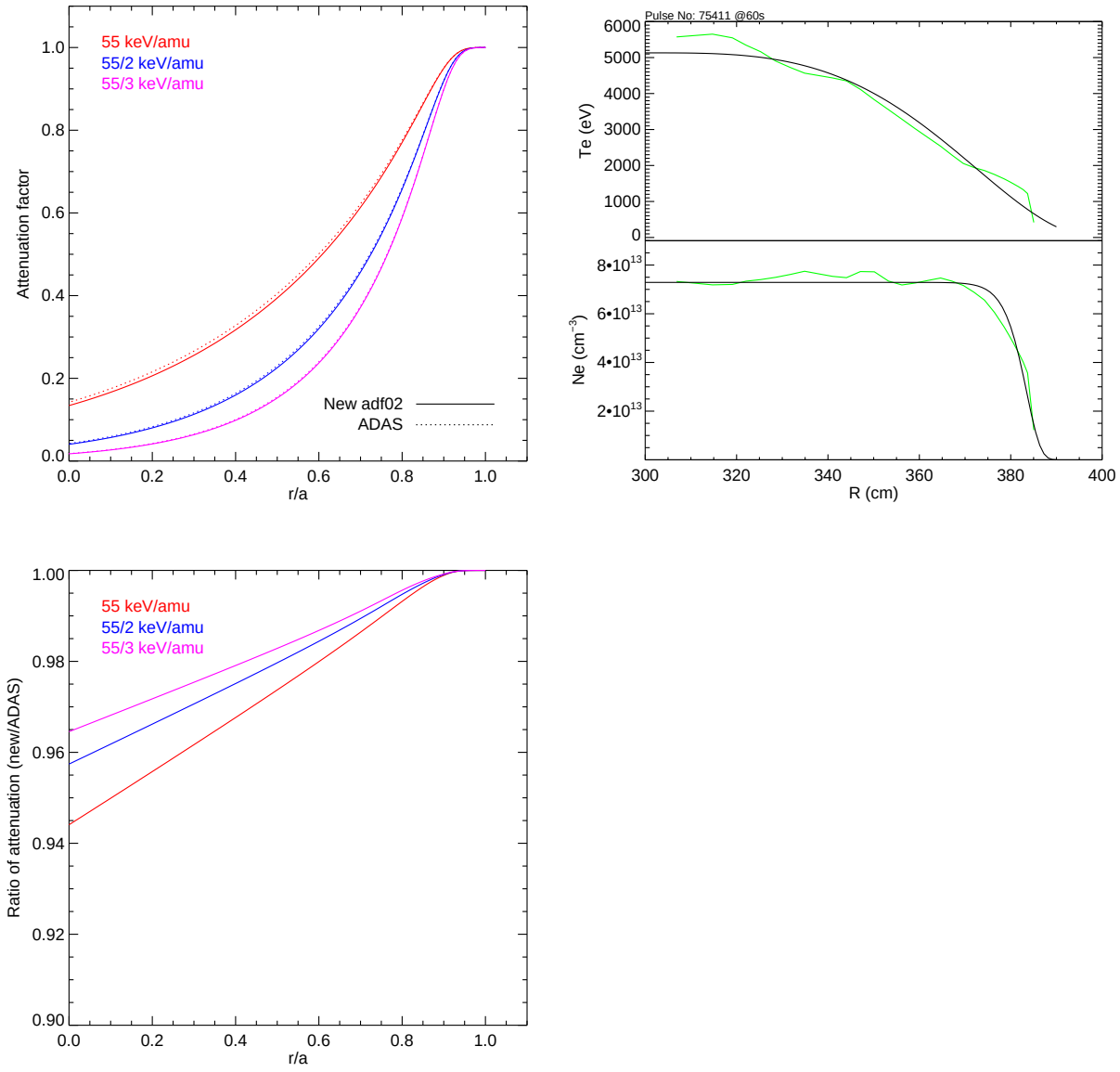

Figure 4: Attenuation profiles for a deuterium beam entering an idealised JET background plasma based on #75411. No impurities are assumed. The change is attenuation profile is best seen in the ratio of the new to old data.

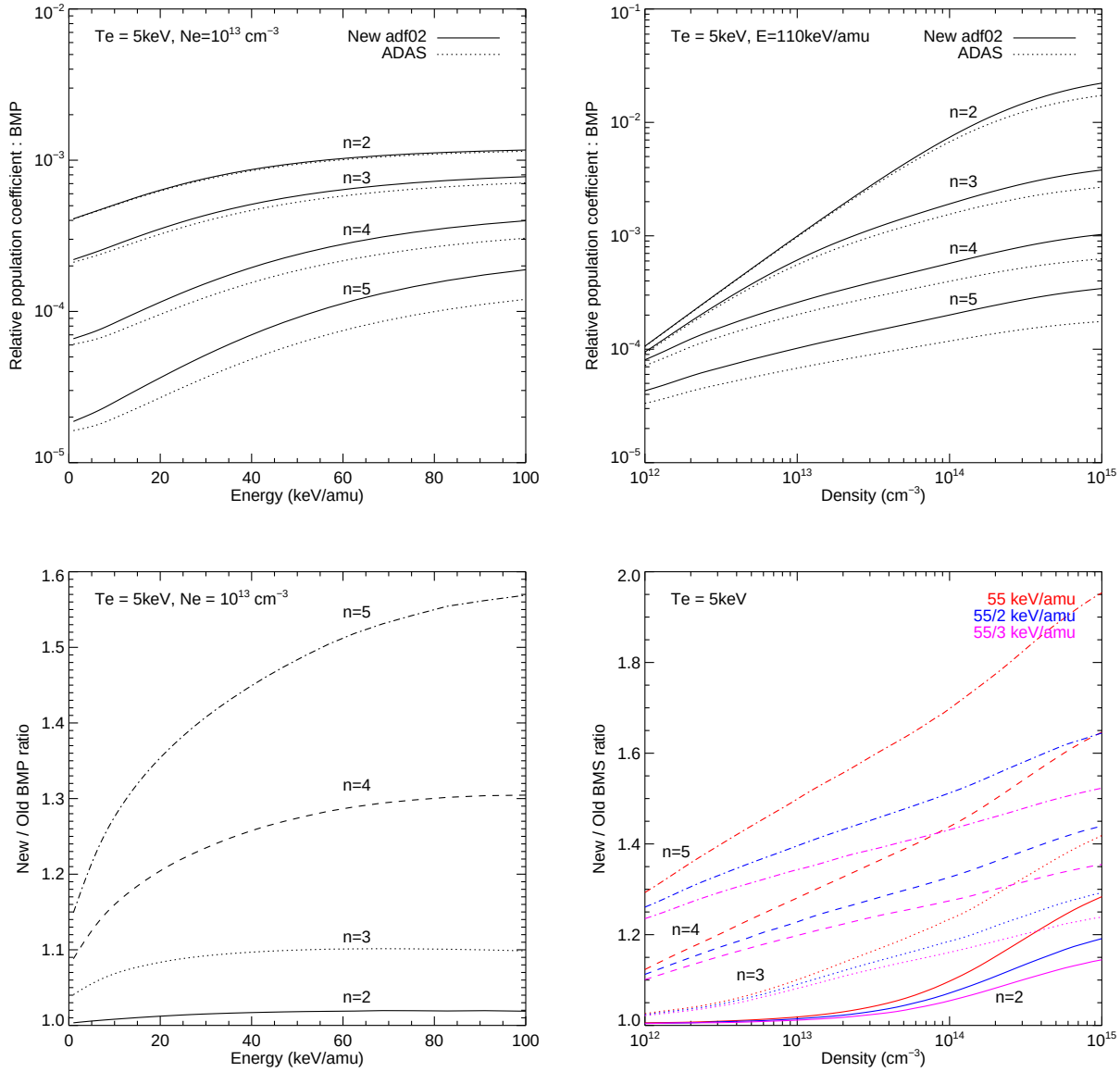

Figure 5: Relative populations of $n = 2, 3, 4, 5$ and ratio of new to old data as functions of energy (left) and density (right). The effect on full, half and third energy components of a typical 110keV deuterium beam.

4 New data in ADAS

There are implications for archiving ADAS data. The policy has been to replace datasets which have been in error and to add additional datasets when improved fundamental data becomes available. This revision blurs the distinction between straightforward error and improved data. It is not worthwhile to correct the $n = 4, 5$ cross section to bring all derived data into line with the JS93 review, given that these are no longer considered reliable.

The new fit for $n = 2, 3, 4, 5$ leads to the following updated/new files in ADAS:

- Add 4 new blocks to the end of the current recommended *adf02* dataset:
  — `adf02/sia#h/sia#h_j99#h.dat`.
- Add a note to the comments pointing out the flaws in the existing data.
- Modify *nsuph1.for* and recompile `adas310` to use the re-fitted data. This is an unfortunate side-effect of the way the beam population code works. There is a longer term plan to replace the built-in dependencies with a script driven way of running.
- Store tabular output of `adas310`:
  — `adf26/bdn98#h/bdn98#h_h1.dat`
- Generate new beam stopping coefficients with altered `adas310`:
  — `adf21/bms98#h/bms98#h_h1.dat`
  — `adf21/bms98#h_fast/bms98#h_fast_h1.dat`
- From the *adf26* data produce a new beam emission coefficient:
  — `adf22/bme98#h/bme98#h_h1.dat`
- And new beam excited populations:
  — `adf22/bmp98#h/bmp98#h_2_h1.dat`
  — `adf22/bmp98#h/bmp98#h_3_h1.dat`
  — `adf22/bmp98#h/bmp98#h_4_h1.dat`

The year is advanced (by one: to 98 from 97) in keeping with the standard ADAS conventions.

A Coefficients for cross section evaluation

For completeness the coefficients used to evaluate equation 1 given by ALADDIN, at the precision returned from the website are:

For equation 1:

```
A1 = 1.076350597E+02  A2 =  2.986018899E+01  A3 =  1.017653658E+06
A4 = 6.971359954E-03  A5 =  2.844794959E-02  A6 = -1.799099533E+00
A7 = 4.785196169E-02  A8 = -2.092295651E-01
```

For equation 1 ($n = 3$) and equation 3 ($n > 3$):

```
A1 = 3.362623069E+02  A2 =  1.360773100E+01  A3 =  4.990999998E+03
A4 = 3.056014519E-01  A5 =  6.436405625E-02  A6 = -1.492362852E-01
A7 = 3.152513859E+00  A8 = -1.631443524E+00
```

B IDL code for new fit

The IDL code used to produce the new *adf02* dataset by fitting to the JS93 data for lower energies and the Olivera data at higher energies is listed below. The code depends on four input files with the digitized cross-sections of Olivera.

```
FUNCTION janev_93, n_val, energy

; Evaluate JS93 cross section for given n and energy

n = n_val[0]

case n of
     1 : b = [1.289981741E+01, 6.189731817E+01,  9.273080765E+03, $
              4.974893565E-04, 3.989026160E-02, -1.589982457E+00, $
              3.183454734E+00, -3.715383993E+00]
     2 : b = [1.076350597E+02, 2.986018899E+01, 1.017653658E+06,  $
              6.971359954E-03, 2.844794959E-02, -1.799099533E+00, $
              4.785196169E-02, -2.092295651E-01]
     3 : b = [3.362623069E+02, 1.360773100E+01, 4.990999998E+03,  $
              3.056014519E-01, 6.436405625E-02, -1.492362852E-01, $
              3.152513859E+00, -1.631443524E+00]
  else : b = [3.362623069E+02, 1.360773100E+01, 4.990999998E+03,  $
              3.056014519E-01, 6.436425625E-02, -1.492362852E-01, $
              3.152513859E+00, -1.631443524E+00]
endcase

b    = double(b)
ered = double(energy/1000.0)

if n GT 3 then ered = double(energy/1000.0) * (n/3.0)^2

p1 = b[0]
p2 = (exp(-b[1]/ered) * alog(1.0d0 + b[2]*ered) ) / ered
p3 = (b[3] * exp(-b[4]*ered) ) / (ered^b[5] + b[6] * ered^b[7])

sigma = 1.0d-16 * p1 * (p2 + p3)

if n GT 3 then sigma = sigma * (n/3.0)^4.0

return, sigma

END
;-------------------------------------------------------------------------


FUNCTION sigma_proton, x, p

; Janev 2003 equation 40 (without n^4 multipler)

b    = double(p)
ered = x

p1 = b[0]
p2 = ered^b[1] * exp(-b[2]*ered) / (1.0d0 + b[3] * ered^b[4])
p3 = (b[5] * exp(-b[6]/ered) * alog(1.0d0 + b[7]*ered) ) / ered

sigma = 1.0d-16 * p1 * (p2 + p3)

return, sigma

END
;-------------------------------------------------------------------------


PRO fit_rate_one, lun, isel=isel, n=n, file=file

; Fit one n-shell ionisation cross section

; Set upper limit of low energy region - JS93 data

case n of
      2 : ehigh=9e3
      3 : ehigh=3e3
   else : ehigh=2e3
endcase

; Use 20 points at low energy for fit

e1 = adas_vector(low=100, high=ehigh, num=20)
s1 = janev_93(n, e1)


; Set low energy cut-off for Olivera high energy data - depends on n

case n of
      2 : elow=30e3
      3 : elow=20e3
      4 : elow=20e3
      5 : elow=8e3
endcase

; Read in Olivera data from digitized figures

mom_readdata, file=file, col_a=eng, col_b=sigma
e2 = eng*1000.0
i2 = where(e2 GE elow)
e2 = e2[i2]
s2 = sigma[i2] * 1e4


; 'known' values for fit

energy = ([e1, e2] / 1000.0) * n^2
sigma  = [s1, s2] / n^4


; Fit using Janev's 2003 formula on a 24 energy grid for adf02 dataset

e_02 = adas_vector(low=100, high=2.0e5, num=24)
e_in = (e_02 / 1000.0) * n * n

; Starting conditions

start = [1e-2, 2.0, 7e-3, 1e-2,1.5,3000, 100, 50]
start = double(start)
error = sigma / 50.0

res    = mpfitfun('sigma_proton', energy, sigma, error, $
                  start, maxiter=500)
mp_fit = sigma_proton(e_in, res)
s_02   =  mp_fit*n^4


; Write adf02 fragment

printf, lun, 'H + 0/H + 1  24/P=1.000D+00/S=1.000D+00/' + $
             'A=1.000D+00/E=0.000D+00/T=ION/ISEL=    ' +   $
              string(isel, format='(i2)')
printf, lun, e_02, format='(6E10.3)'
printf, lun, s_02, format='(6E10.3)'


; plot for checking

xmin = 100
xmax = 1e6
ymin = 1e-19
ymax = 1e-10
plot_oo, [xmin, xmax], [ymin, ymax], /nodata

oplot, e1, s1,  psym=sym(1)
oplot, e2, s2,  psym=sym(10)
oplot, e_02, s_02


END
;-------------------------------------------------------------------------


PRO fit_rate

; Open new adf02 dataset

openw, lun, 'adf02.tmp', /get_lun

fit_rate_one, lun, isel=1, n=2, file = 'olivera_fig1_n2.dat'
fit_rate_one, lun, isel=2, n=3, file = 'olivera_fig2_n3.dat'
fit_rate_one, lun, isel=3, n=4, file = 'olivera_fig2_n4.dat'
fit_rate_one, lun, isel=4, n=5, file = 'olivera_fig2_n5.dat'

free_lun, lun

END
```

References

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