

Use of ICRU-37/NBS Collision Stopping Powers in the EGS4 System.

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Abstract

An option has been added to the PEGS4 code in the EGS4 System for the Monte Carlo simulation of radiation transport. This option allows the user to input an arbitrary density-effect correction for use in calculating electron and positron collision stopping powers. A data base containing the relevant density-effect corrections for a large number of the materials in ICRU Report 37, as generated by the NBS (NIST) program EPSTAR (S.M. Seltzer, 1988), has been created. In conjunction with the code EPSTAR, one can therefore implement the latest electron/positron collision stopping powers for any material.

1 Introduction

The EGS4 system of codes does Monte Carlo simulations of the radiation transport of electrons and positrons in any material[1]. Part of the system is a stand alone code called PEGS4 which creates the necessary electron and photon data sets for use by EGS4 when doing the simulation. One important cross section is the collision stopping power for electrons or positrons. PEGS4 includes a large collection of data which allows the calculation of the collision stopping power for an arbitrary material. Aside from straightforward parameters such as the atomic number and material density, there are two more complex material-dependent physical parameters needed. These are the mean excitation energy I and the density-effect correction δ . The standard version of PEGS4 includes a table of I values for all elements (see section 2.13 of the EGS4 documentation[1]). These values are from the work of Berger and Seltzer at NBS[2] and have been adopted by the ICRU in their Report 37[3]. For a compound or mixture, PEGS4 determines the mean excitation by the standard procedure of taking a weighted average of the log of the I values of the elements in the compound. For an arbitrary material PEGS4 determines the density-effect correction using a formula due to Sternheimer and Peierls [4] which depends only on simple physical parameters plus the value of I for the material.

PEGS4 also contains an internal data base for 73 selected elements and materials for which both the I -value and Sternheimer *et als.* [5] parameterization of the density-effect correction used in ICRU Report 37 are included. Thus for these 73 materials, PEGS4 uses close to, but not exactly what is in ICRU Report 37. This is because the ICRU Report calculates the density-effect correction individually at each tabulated energy whereas the Sternheimer *et al.* five-parameter fit is just that, a fit to those data points. Figure 1 presents a comparison of the ratio to the ICRU values of the collision stopping powers calculated by PEGS4 for water using either the general formula of Sternheimer and Peierls to calculate the density-effect correction, or the tabulated five-parameter fit to the density-effect correction, and for comparison, the “old” (1964) standard values from Berger and Seltzer [6]. The differences between the stopping powers using the “best” fit values in PEGS4 and the ICRU values are quite small ($\leq 0.5\%$) but in some situations (e.g. the calculation of stopping-power ratios) this variation could introduce some uncertainty. Figure 2 presents a comparison of the density-effect corrections for water as presented in ICRU Report 37 and from the Sternheimer *et als* fit used in PEGS4. It is these small differences which cause the differences seen in Figure 1. The purpose of the present work was to allow PEGS4 to utilize an arbitrary density-effect correction.

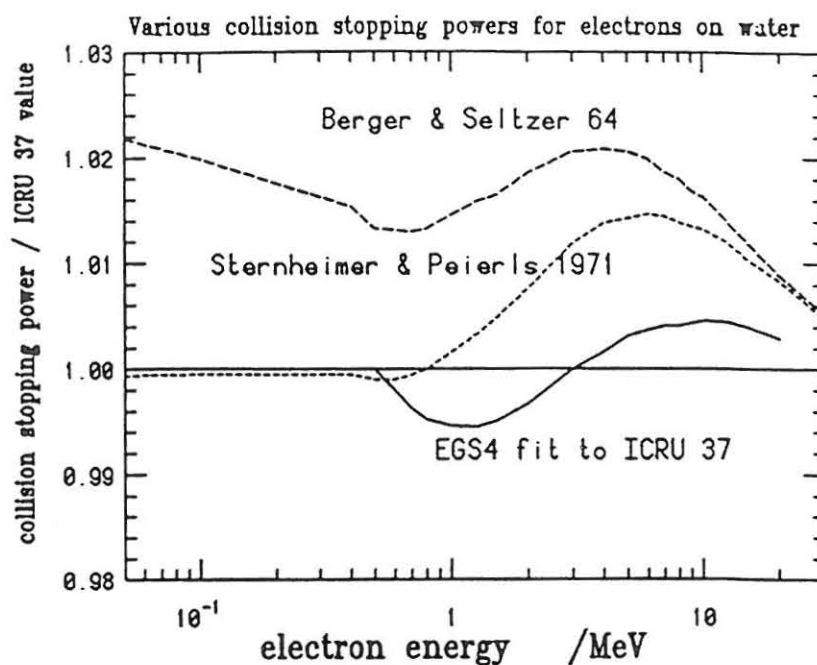


Figure 1: Comparison of collision stopping powers calculated using different density-effect corrections. Results are plotted as ratios to the values in ICRU Report 37.

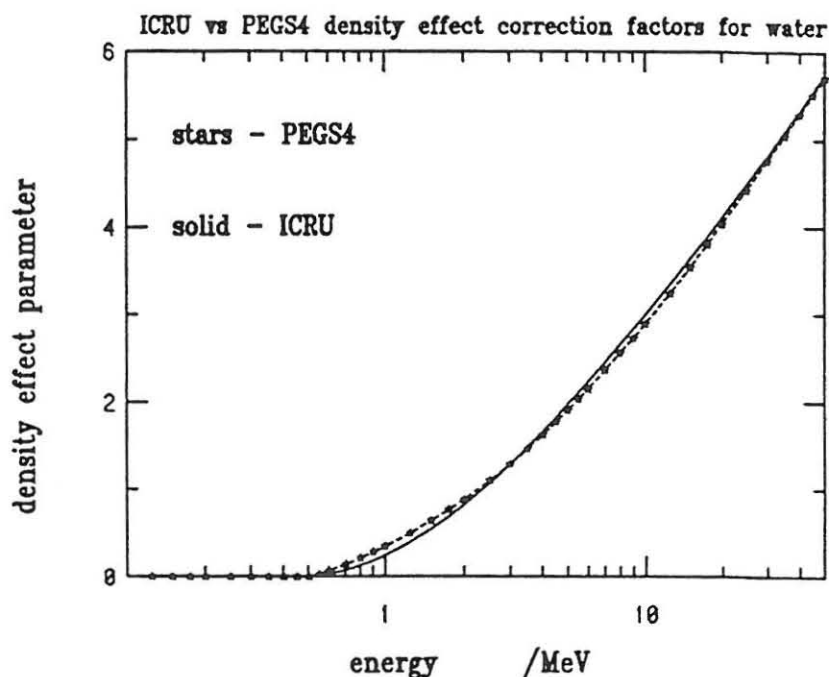


Figure 2: Comparison of the density-effect corrections for water as used in the default PEGS4 code (stars, dashed line) and as presented in ICRU Report 37 (solid curve).

2 Changes to PEGS4

All changes have been implemented so that a standard input file, as defined in the EGS4 documentation[1], will produce the same results as in the original version of PEGS4. To invoke the new option, the following must be done:

- In the user's input file, the ENER option must come before the MIXT, ELEM or COMP options (so an internal check on energy limits is valid).
- In the input file, in the ELEM, MIXT or COMP options, set a new flag called EPSTFL to have a value of 1. This instructs PEGS4 to read in a file containing the density-effect correction as a function of energy for the material being studied.
- Assign to FORTRAN unit 20, an input file for the density-effect correction which has the following format:
 - Title line (≤ 80 characters)
 - NDATA, IEV, RHO, NE, (Z(I),FW(I),I=1,NE)
 where
 - * NDATA is the number of data points to follow (≤ 150),
 - * IEV is the mean value of I in eV for the material (real format). This overrides any other value in PEGS4.
 - * RHO is the density for which these density effect corrections apply. This is forced to equal the value used in the rest of PEGS4 within 1%.
 - * NE is the number of elements in the material being input.
 - * (Z(I),FW(I)) are the atomic number and fractional weight of this element in the material being input. These must match the composition being used in the rest of PEGS4 within a 1% tolerance.
 - ENERGY(I), DELTA(I), I = 1, NDATA
 where
 - * ENERGY(I) and DELTA(I) are the energies and density-effect corrections at these energies. The energies are *kinetic* energies in MeV. The energy range spanned by the data set should exceed the values for which calculations are to be done. If the energies requested are not covered, a message is printed and the calculation carries on after setting the lower or upper energy to the minimum or maximum required in the code (i.e. one effectively extrapolates the lowest or highest energies input to those needed - this could be wrong in extreme cases!!).

- Run PEGS4

The output data file from PEGS4 will have the same format as in the original (with some minor additions on the second line which do *not* affect EGS4). The only real difference is that the density-effect correction used to calculate the collision stopping powers for electrons and positrons will be those from the input file on unit 20.

Appendix A presents a differences comparison showing all the changes made in PEGS4 to implement these changes. Note that almost all new variables have been introduced with EPST or EPS in the name.

When we input a table of density-effect correction factors from ICRU Report 37, the resulting unrestricted collision stopping powers, output by PEGS4 with the IUNRST=1 option turned on, are the same as those in ICRU Report 37 within 0.01%. Similarly, the ratio of the restricted collision stopping powers to the unrestricted collision stopping powers were checked against Table 7.1 of ICRU Report 37 and found to agree within ± 1 in the last digit.

3 Data Sets from EPSTAR/ICRU 37

In principle, the option described in this report can be used to input any arbitrary density effect for use in calculating the electron and positron collision stopping power. The data set is interpolated linearly, so that not a great deal of data is needed. However, what spurred this work was the availability of the PC-based EPSTAR/ESPA programs written by Steven Seltzer of NBS[7]. These programs can generate the entire data base available in ICRU Report 37 (they are the programs which generated the data base), or they can do *ab initio* calculations for an arbitrary material. We have run these codes for a variety of compounds and elements which appear in ICRU Report 37 and have put the density-effect correction data into two files. These data are available on a floppy disk or via bitnet. The elements/compounds included are listed below, along with the first few lines of that part of the data file which specifies the density effect for that material in the format described above. To make a file which is suitable for use as input to PEGS4 one just extracts the data of interest from the larger files.

File COMPOUNDS.DEL

A-150 TISSUE-EQUIVALENT PLASTIC

113	65.10000	1.127000	6
1	0.101327	6	0.775501
7	0.035057	8	0.052316
9	0.017422	20	0.018378

AIR, DRY (NEAR SEA LEVEL)

113	85.66600	1.2047900E-03	4
6	0.000124	7 0.755267	8 0.231781 18 0.012827

C-552 AIR-EQUIVALENT PLASTIC

113	86.79900	1.760000	5
1	0.024680	6 0.501611	8 0.004527 9 0.465209 14 0.003973

CARBON DIOXIDE

113	85.00000	1.8421200E-03	2
6	0.272916	8 0.727084	

FERROUS AMMONIUM SULFATE (STANDARD FRICKE) DOSIMETER SOLUTION

113	76.31200	1.024000	7
1	0.108366	7 0.000027	8 0.878913 11 0.000022 16 0.012582 17 0.000035
26	0.000055		

LITHIUM FLUORIDE

113	94.00000	2.635000	2
3	0.267585	9 0.732415	

NYLON, TYPE 6 AND TYPE 6/6

113	63.90000	1.140000	4
1	0.097976	6 0.636856	7 0.123779 8 0.141389

POLYETHYLENE

113	57.40000	0.9400000	2
1	0.143711	6 0.856289	

POLYMETHYL METHACRYLATE, "LUCITE", "PERSPEX", "PLEXIGLAS"

113	74.00000	1.190000	3
1	0.080538	6 0.599848	8 0.319614

POLYSTYRENE

113	68.70000	1.060000	2
1	0.077418	6 0.922582	

SODIUM IODIDE

113	452.0090	3.667000	2
11	0.153373	53 0.846627	

WATER, LIQUID

113	75.00000	1.000000	2
1	0.111894	8 0.888106	

WATER VAPOR

113	71.60000	7.5618201E-04	2
1 0.111894	8 0.888106		

File ELEMENTS.DEL

CARBON, GRAPHITE (2.265 g/cm³)

113	78.00000	2.265000	1
6 1.000000			

CARBON, GRAPHITE (1.700 g/cm³)

113	78.00000	1.700000	1
6 1.000000			

ALUMINUM

113	166.0000	2.698900	1
13 1.000000			

SILICON

113	173.0000	2.330000	1
14 1.000000			

IRON

113	286.0000	7.874000	1
26 1.000000			

COPPER

113	322.0000	8.960000	1
29 1.000000			

GERMANIUM

113	350.0000	5.323000	1
32 1.000000			

TUNGSTEN

113	727.0000	19.30000	1
74 1.000000			

GOLD

113	790.0000	19.32000	1
79 1.000000			

LEAD

113	823.0000	11.35000	1
82 1.000000			

URANIUM				
	113	889.9990	18.95000	1
92	1.000000			

4 The Distribution Files

The following files are available on a PC floppy.

PEGS4.MOR

This is the current NRC version. It therefore includes the upgrade described in PIRS177 [8] to allow ICRU 37 radiative stopping powers to be used by PEGS4. It also includes two patches: one to correct an error in calculating the density effect for gases not at NTP (i.e. for GASP non-zero: see SPINIT, error was pointed out by Prof. Kamae in Tokyo, via Hideo Hirayama); the second to correct some errors in SPTOTE(P) when IUNRST=2, 3 or 4 were used in the PLOT or CALL option.

COMPOUNDS.DEL

The file of deltas described above for a set of compounds.

ELEMENTS.DEL

The file of deltas described above for a set of elements.

5 Acknowledgements

We wish to thank Stephen Seltzer of NBS for sending a copy of his PC program EPSTAR which calculates the ICRU 37 density-effect corrections for an arbitrary material.

Appendix A

Changes Introduced into PEGS4.MOR

```

*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
  2  "PLAYED WITH AT NRC NOV 1988 TO GET DENSITY EFFECT  "
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
  2  " !COMMENTS;"
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
255  " ***EPSTAR      NRCC ADDITION, NOV 1988      "
256  "-----"
257  REPLACE {;COMIN/EPSTAR/;} WITH
258  {;INTEGER EPSTFL; CHARACTER*1 EPSTTL(80); INTEGER ZEPST;
259  COMMON/EPSTAR/EPSTEN(150), EPSTD(150), EPSTFL, EPSTTL, WEPST, IEPST,
260  NELEPS, ZEPST(20), WEPST(20), IAPRIN; }
261
262  "THIS COMMON IS USED FOR OPTION WHICH READS IN DENSITY EFFECT "
263  "CORRECTION IN SPIKIT AND CALCULATES USING IT IN SPIONB      "
264  "THE FLAG EPSTFL IS READ UNDER NAMELIST INPUT, AND DEFAULTS  "
265  " TO ZERO IN THE BLOCK DATA. SET TO UNITY TO USE THE OPTION "
266  "PEGS USES THE I-VALUE IN THE DENSITY INPUT FILE             "
267  "VARIOUS CHECKS ARE DONE TO ENSURE THE DENSITY CORRECTION   "
268  " CORRESPONDS TO THE MATERIAL DEFINITION IN PEGS            "
269  "THE ENERGY TABLE READ IN IS ASSUMED TO BE KINETIC ENERGY IN "
270  " MEV BUT IS CONVERTED TO TOTAL ENERGY BY THE CODE.         "
271  "THE ENERGY OPTION MUST BE USED IN PEGS PRIOR TO THE MIXT,COMP"
272  " OR ELEM OPTIONS TO ALLOW ALL THE CHECKS TO WORK PROPERLY.  "
273  "NELEPS IS THE NUMBER OF ELEMENTS IN THE MATERIAL            "
274  "ZEPST(I) (INTEGER), WEPST(I) ARE THE Z VALUE AND FRACTION   "
275  " BY WEIGHT OF THE I-TH ELEMENT IN THE DATA FILE.          "
276
277  "-----"
278  " *** FUNCS      "
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
247  " *** FUNCS      "
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
540  PHPAIR, PHCONS, PWLFIN, RAYLEI, RSLTS, THRESH, EPSTAR/; "MODNOV 23, 1988"
541  REAL IP(4), WASAV(20);
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
510  PHPAIR, PHCONS, PWLFIN, RAYLEI, RSLTS, THRESH/;
511  REAL IP(4), WASAV(20);
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
569  EI, ISUB, GASP, IUNRST, IRAYL, AFACT, SK, XO, XI, IEV, CBAR, ISSB, EPSTFL,
570  IAPRIN;
571  " MOD NOV 23, 1988      "
572  NAMELIST/PWLFNM/EPE, ZTHRE, ZEPE, NIPE, NALE, EPG, ZTHRG, ZEPG, NIPG, NALG,
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
539  EI, ISUB, GASP, IUNRST, IRAYL, AFACT, SK, XO, XI, IEV, CBAR, ISSB;
540  NAMELIST/PWLFNM/EPE, ZTHRE, ZEPE, NIPE, NALE, EPG, ZTHRG, ZEPG, NIPG, NALG,
*****

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File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
 940      PHPAIR,PMCONS,PWLFIN,RADLEN,RAYLEI,SPCOMM,RSPTS,THRESH,EPSTAR;/
 941      "                                MOD NOV 22 1988      *****"
 942
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
 908      PHPAIR,PMCONS,PWLFIN,RADLEN,RAYLEI,SPCOMM,RSPTS,THRESH;/
 909
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
1185
1186      "DATA FOR EPSTAR"
1187      DATA EPSTFL/0/,IEPST/1/,IAPRIH/0/;
1188
1189      END; "END OF BLOCK DATA"
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
1152      END; "END OF BLOCK DATA"
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
2256      COMIN/PMCONS,SPCOMM,DERCON,MOLVAR,MIYDAT,ELEMTB,LSPION,EPSTAR,THRESH;/
2257      "                                MOD NOV 23,1988      *****"
2258
2259      REAL IMEV;
2260      TOLN10=2.0*ALOG(10.0);IM=-100;
2261
2262      IF(EPSTFL < 0 | EPSTFL > 1) [EPSTFL = 0;"ERROR ON INPUT, IGNORE"]
2263      "ABOVE IS NRCC MOD DEC 1988"
2264
2265      IF(EPSTFL=0) ["DEFAULT TO STANDARD PEGS4 METHODS"
2266
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
2144      COMIN/PMCONS,SPCOMM,DERCON,MOLVAR,MIYDAT,ELEMTB,LSPION;/
2145      REAL IMEV;
2146      TOLN10=2.0*ALOG(10.0);
2147
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
2395      ]"END OF EPSTFL=0 BLOCK"
2396
2397      ELSE[ "EPSTFL=1 BLOCK I.E. READ IN THE INPUT FROM THE DENSITY"
2398      "INPUT FILE"
2399
2400      READ(20,:A:)EPSTTL;:A: FORMAT(80A1);
2401      READ(20,*) NEPST,IEV,EPSTRH,WELEPS,(ZEPST(I),WEPST(I),I=1,WELEPS);
2402      READ(20,*) (EPSTEN(I),EPSTD(I),I=1,NEPST);
2403
2404      IF(NEPST>150)[OUTPUT NEPST;
2405      (//' *****NEPST=',I4,' IS GREATER THAN THE 150 ALLOWED';STOP;]
2406      "CONVERT TO TOTAL ENERGIES"
2407      DO I=1,NEPST[EPSTEN(I) = EPSTEN(I) + RM;]
2408      IMEV = IEV*1.E-06;
2409
2410      "CHECK THAT WE HAVE COVERED ENERGY RANGES NEEDED"
2411      IF( AE < EPSTEN(1))[OUTPUT EPSTEN(1),AE;
2412      (//' *****LOWEST ENERGY INPUT FOR DENSITY EFFECT IS',1PE10.3/
2413      T20,'WHICH IS HIGHER THAN THE VALUE OF AE=',1PE10.3,' MEV'/
2414      ' ***IT HAS BEEN SET TO AE***'//);EPSTEN(1) = AE;]
2415      IF( UE > EPSTEN(NEPST))[ OUTPUT EPSTEN(NEPST),UE;
2416      (//' *****HIGHEST ENERGY INPUT FOR DENSITY EFFECT IS',1PE10.3/
2417      T20,'WHICH IS LOWER THAN THE VALUE OF UE=',1PE10.3,' MEV'/
2418      ' ***IT HAS BEEN SET TO UE***'//);EPSTEN(NEPST) = UE;]

```

```

2419
2420 "DO A CHECK ON THE COMPOSITION AND DENSITY TO INSURE THE RIGHT DELTA"
2421 "HAS BEEN PICKED UP. ALLOW A TOLERANCE OF 1 PERCENT ERROR ON THE"
2422 "COMPOSITION BY WEIGHT."
2423
2424 ICHECK=0; "FLAG GETS SET TO UNITY IF THE COMPOSITION DOES NOT MATCH"
2425 TLRNCE=0.01; "TOLERANCE ALLOWED ON FRACTION BY WEIGHT"
2426
2427 "FIRST CHECK THAT THE NUMBER OF ELEMENTS ARE THE SAME"
2428 IF(NELEPS.NE.NE) ICHECK=1;
2429
2430 "NOW CHECK THAT THE DENSITIES ARE THE SAME WITHIN TOLERANCE"
2431 IF( (ICHECK.EQ.0) .AND.
2432 ( (EPSTRH.LT.((1.0-TLRNCE)*RHO)) .OR. (EPSTRH.GT.((1.0+TLRNCE)*RHO))
2433 ) ) ICHECK=1; "DENSITY IS OUT OF RANGE"
2434 "WE MUST FIRST NORMALIZE THE PEGS FRACTIONS BY WEIGHT TO ENSURE THEY"
2435 "ARE NORMALIZED TO UNITY"
2436 EPSTWT = 0.0; DO I=1,NE[ EPSTWT = EPSTWT + RHOZ(I);]
2437 IF(EPSTWT=0.0)[
2438 OUTPUT;(/' *****IN SPINIT***SOMETHING WRONG, MOLECULAR WEIGHT OF',
2439 'MOLECULE IS ZERO (I.E. SUM OF RHOZ)***'//);]
2440
2441 IF(ICHECK.EQ.0)[
2442 IESPEL=0; "INITIALIZE ESP ELEMENT COUNTER"
2443 ICHECK=1; "ASSUME FAILURE"
2444 LOOP["LOOP OVER ESP COMPONENTS"
2445 IESPEL=IESPEL+1;
2446 IPEGEL=0; "INITIALIZE PEGS ELEMENT COUNTER"
2447 LOOP["LOOP OVER PEGS COMPONENTS"
2448 IPEGEL=IPEGEL+1;
2449 IF(IFIX(Z(IPEGEL)).EQ.ZEPST(IESPEL))[ICHECK=0;EXIT;]
2450 ]WHILE(IPEGEL.LT.NE);
2451 IF( (ICHECK.EQ.0) "Z OF ELEMENT MATCHES"
2452 .AND.
2453 ( (WEPST(IESPEL).LT.((1.0-TLRNCE)*RHOZ(IPEGEL)/EPSTWT))
2454 .OR. (WEPST(IESPEL).GT.((1.0+TLRNCE)*RHOZ(IPEGEL)/EPSTWT))
2455 ) ) ICHECK=1; "MATCHED ELEMENT BUT WEIGHT FRACTION WRONG"
2456 ]WHILE(IESPEL.LT.NELEPS);
2457 ] "END OF TEST FOR ICHECK = 0"
2458
2459 IF(ICHECK.EQ.1)[ "PRINT MESSAGE AND STOP"
2460 OUTPUT;
2461 (/'/'/'0*** COMPOSITION IN INPUT DENSITY FILE DOES NOT MATCH',
2462 'THAT BEING USED BY PEGS, QUITTING EARLY***'//);]
2463 STOP; " ERRORS DETECTED";
2464 ]
2465
2466
2467 ]"END OF EPSTFL=1 BLOCK"
2468
2469
2470 SPC1=2.*PI*RO**2*RH*EDEN*RLC;
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
2276 SPC1=2.*PI*RO**2*RH*EDEN*RLC;
*****
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
2478 ELSEIF(IM = -1) [OUTPUT;
2479 (' STERNHEIMER-SELTZER-BERGER DENSITY EFFECT DATA SUPPLIED BY USER');]
2480 ELSE[
2481 OUTPUT EPSTTL;(' DENSITY EFFECT READ IN DIRECTLY:'/'T10,80A1);]
2482 OUTPUT;(1X,64(' '));]
2483 OUTPUT IEV;(/' ADJUSTED MEAN IONIZATION = ',F8.2,' EV'/1X,38(' '));]
2484 IF(EPSTFL = 0) [$DUMP IEV,VPLASH,CBAR,X0,X1,SK,AFAC;]
2485 $DUMP SPC1,SPC2;

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```

2486
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
2284 ELSE [OUTPUT;
2285 (' STERNHEIMER-SELTZER-BERGER DENSITY EFFECT DATA SUPPLIED BY USER');]
2286 OUTPUT;(IX,64('-'//));
2287 OUTPUT IEV;(/' ADJUSTED MEAN IONIZATION = ',F8.2,' EV'/IX,38('-'//));
2288 $DUMP IEV,VPLASH,CBAR,XO,XI,SK,AFACT,SPC1,SPC2;
2289
*****
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
2783 %L
2784 %I4 "INDEXT MORTAN"
2785 !INDEXT F2;
2786 "*****"
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
2585 "*****"
*****
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
4326 COMIN/DERCON,LSPION,EPSTAR/; "MOD NOV 24,1988"
4327 " COMMON POINT FOR E- AND E+ ENTRIES. "
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
4079 COMIN/DERCON,LSPION/;
4080 " COMMON POINT FOR E- AND E+ ENTRIES. "
*****
*****
File SYS$SYSDEVICE: NEW_PEGS4.MOR;9
4355
4356 " NOW COMPUTE THE DENSITY CORRECTION TERM. "
4357
4358 IF(EPSTFL = 0) ["USE STANDARD PEGS4 METHOD"
4359 IF (X.LE.XO) [DELTA=0.0;]
4360 ELSEIF (X.LT.XI) [DELTA=TOLN10*X - CBAR + AFACT*(XI - X)*SK;]
4361 ELSE [DELTA=TOLN10*X - CBAR;]]
4362
4363 ELSE ["USE LINEAR INTERPOLATION OF USER SUPPLIED INPUT TABLE"
4364
4365 "IEPST IS A POINTER SUCH THAT "
4366 " EPSTEN(IEPST) <= EO < EPSTEN(IEPST+1) "
4367 " "
4368 "IEPST IS INITIALIZED IN BLOCK DATA TO 1. WE START FROM "
4369 "THE PREVIOUS VALUE OF THE POINTER SINCE WE ASSUME THAT "
4370 "THE CODE IS WORKING UP OR DOWN A GRID. "
4371 " THIS CODING IS FAR FROM OPTIMAL "
4372
4373 IF(EO >= EPSTEN(IEPST))["AT OR ABOVE PREVIOUS ENTRY"
4374 IF(EO = EPSTEN(IEPST))["FOUND ENTRY, INCLUDING THE POSSIBILITY"
4375 "THAT WE ARE AT THE TOP OF THE TABLE" GO TO :END-SEARCH;]
4376
4377 DO I= IEPST,NEPST-1 [
4378 IF(EO<EPSTEN(I+1))["WE FOUND IT" IEPST = I; GO TO :END-SEARCH;]
4379 ]
4380 "IF WE FALL THRU TO HERE, WE MUST BE AT UPPER ENERGY"
4381 IEPST = NEPST; GO TO :END-SEARCH;
4382 ]"END OF BLOCK EO>EPSTEN(IEPST)"
4383
4384 ELSE [ "EO<EPSTEN(IEPST)"
4385
4386 DO I = IEPST,2,-1 [
4387 IF(EO >= EPSTEN(I-1)) [IEPST = I-1; GO TO :END-SEARCH;]
4388 ]
4389 " IF WE GET HERE WE MUST BE IN THE FIRST REGION"

```

```

4390      IEPST = 1;]
4391
4392      :END-SEARCH:
4393
4394      "NOW JUST INTERPOLATE LINEARLY IN THE ENERGY"
4395      IF(IEPST < NEPST) [
4396          DELTA = EPSTD(IEPST) + (EO - EPSTEN(IEPST))/
4397              (EPSTEN(IEPST+1) - EPSTEN(IEPST)) * (EPSTD(IEPST+1) - EPSTD(IEPST));]
4398      ELSE [DELTA = EPSTD(NEPST);]
4399
4400      ]"END OF EPSTFL NON-ZERO BLOCK"
4401
4402      "      NOW PUT IT ALL TOGETHER                                "
*****
File SYS$SYSDEVICE: OLD_PEGS4.MOR;8
4108      "      NOW COMPUTE THE DENSITY CORRECTION TERM.                "
4109      IF (X.LE.X0) [DELTA=0.0;]
4110      ELSEIF (X.LT.X1) [DELTA=TOLN10*X - CBAR + AFACT*(X1 - X)**SK;]
4111      ELSE [DELTA=TOLN10*X - CBAR;]
4112      "      NOW PUT IT ALL TOGETHER                                "
*****

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References

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