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TITLE: DEPOS: PARAMETRIC ELECTRON-ENERGY-DEPOSITION MODULE IN SLABS

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DEPOS: Parametric Electron Energy Deposition Module in Slabs

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ABSTRACT

DEPOS is a code module that computes the energy deposition of monoenergetic fast electrons normally incident on a one dimensional slab absorber. The numerical algorithm is based on the highly accurate parametric fits of Tabata and Ito, valid for atomic number $5.3 \leq Z \leq 82$ and for kinetic energy $0.1 \text{ MeV} \leq T \leq 20 \text{ MeV}$. Empirical equations developed for the extrapolated range and backscattering of electrons are utilized and bremsstrahlung production is included in the analysis. Adjustable parameters are least squares fit to experimental and Monte Carlo results and overall agreement is excellent.

1. INTRODUCTION

Calculations of energy deposition by electron beams incident on thick absorbers can be made by analytic moments methods,^{1,2} stochastic Monte Carlo techniques,^{3,4} or deterministic S_n approaches.^{5,6} A large body of experimental measurements also exists.⁷⁻¹⁰ An analytic expression which synthesizes experimental and computational efforts is valuable because of its simplicity, range of validity, and applicability to a wide spectrum of problems. An analytic expression is also inexpensive as far as computer time and storage are concerned. For this reason Tabata and Ito¹¹ have developed a set of parametric equations to describe electron energy deposition in slab absorbers, extrapolated (effective) electron ranges, backscatter, bremsstrahlung, and secondary electron production. Adjustable parameters have been least squares fitted to existing published data for a consistent representation. DEPOS is a stand-alone or an

interface Fortran module which computes electron energy deposition in slab geometry using the Tabata and Ito equations.

Section II describes the fit equations and associated physics. Section III details the code module and I/O stream while Section IV gives some specific examples and results. Section V contains the code listing. Presently, DEPOS is structured for use on the Los Alamos Cray-1 or CDC-7600 computers, but minor revisions are anticipated for other systems. Code and documentation are available from the authors.

II. PARAMETRIC DEPOSITION FITS

The extrapolated range, R_{ex} , is not the true electron range, R , usually employed in deposition studies. The parameter R_{ex} is useful in fitting deposition profiles when energy loss straggling and multiple scattering detours are neglected.¹² Generally, $R_{ex} \leq R$. The expression used to compute R_{ex} is

$$R_{ex} = a_1 \left[(1/a_2) \ln(1 + a_2 \tau) - a_3 \tau / (1 + a_4 \tau)^{a_5} \right] (g/cm^2) \quad (1)$$

with

$$\begin{aligned} a_1 &= 0.2335 A / Z^{1.209} \\ a_2 &= 1.78 \times 10^{-4} Z \\ a_3 &= 0.9891 - 3.01 \times 10^{-4} Z \\ a_4 &= 1.468 - 1.180 \times 10^{-3} Z \\ a_5 &= 1.232 Z^{-1.09} \\ \tau &= T / 0.511 \end{aligned} \quad (2)$$

where T is the incident electron kinetic energy in MeV, A the absorber atomic mass, and Z the absorber atomic number.

The energy deposited per unit path length is denoted by $D(x)$.

$$D(x) = \frac{-d}{dx} (\eta I) \quad (\text{MeV-cm}^2/\text{g}) \quad (3)$$

where η is the fraction of the number of incident electrons deposited at depths greater than x and I is the ratio of the total kinetic energy deposited at depths greater than x to the number of electrons deposited at the same depth. Effects of backscattering from the incident surface and depths greater than x , of bremsstrahlung, and of secondary electron energy production are neglected in Eq. (3A). However, to include these tail effects, $D(x)$ is renormalized as follows:

$$\int_0^\infty D(x) dx = (1 - f_b - f_r) T = f_s T \quad (4)$$

where f_b and f_r are the average fractions of the incident energy backscattered from the surface and deposited by bremsstrahlung and secondary processes. These renormalized fractions are given by,¹²

$$f_b = \eta_b (1 - \Delta T_b / T) \quad (5)$$

$$f_r = \gamma Z \tau / (1 + \gamma Z \tau) \quad (6)$$

where

$$\gamma = 2.26 \times 10^{-4} \quad (7)$$

$$\eta_b = d_1 / (1 + d_2 \tau^{d_3}) \quad (8)$$

$$\Delta T_b / T = g_1 \tau^{g_2} + g_2 / \tau^{g_4} \quad (9)$$

and,

$$\begin{aligned}
 d_1 &= 1.15 \exp(-8.35/Z^{.525}) \\
 d_2 &= 0.0185 + 15.7/Z^{1.59} \\
 d_3 &= 1.56 - 4.42/Z \\
 g_1 &= 1.33/Z^{.385} \\
 g_2 &= 0.066 Z^{.33} \\
 g_3 &= 0.048/Z^{.35} \\
 g_4 &= 0.47 Z^{.12}
 \end{aligned} \tag{10}$$

The segmented deposition function $I(x)$ is obtained from the fit employing the extrapolated range R_{ex} ,

$$\begin{aligned}
 I(x) &= f_d W(R_{ex} - k_1 x) & k_1 x \leq k_2 R_{ex} \\
 &= f_d W[(1 - k_2) R_{ex}] \exp \left\{ - \frac{\partial W}{\partial x} [(1 + k_2) R_{ex}] / W[(1 - k_2) R_{ex}] \right\} & (11) \\
 &\quad \times (k_1 - k_2 R_{ex}) & k_1 x > k_2 R_{ex}
 \end{aligned}$$

and the following least squares parameters evaluated from experimental data,

$$\begin{aligned}
 k_1 &= h_1 / Z^{h_2} \\
 k_2 &= 0.90 \\
 h_1 &= 1.277 \pm .083 \\
 h_2 &= 0.134 \pm 0.020
 \end{aligned} \tag{12}$$

$W(x)$ is the renormalized kinetic energy of electrons at depth x obtained from the the fitted inverse range-energy curve, $F(x)$, as follows,

$$W(x) = T F(x) / F(R_{ex}) \tag{13}$$

where

$$F(x) = q_1 \exp \left\{ x [q_2 + q_3 / (1 + q_4 x^{q_5})] / q_1 \right\} - q_1 \tag{14}$$

and

$$\begin{aligned}
 q_1 &= 2.98 \times 10^3 \times .511 / Z \\
 q_2 &= 6.14 Z^{1.026} / A \\
 q_3 &= 2.57 \times 10^2 - .34 Z \\
 q_4 &= 1.47 \times 10^3 / Z^{.892} \\
 q_5 &= 0.905 / Z^{.1874}
 \end{aligned}
 \tag{15}$$

The fractional number of electrons at depth x is exponentially attenuated by the expression,

$$\eta(x) = \exp[-\xi(x/R_{es})^\beta] \quad , \tag{16}$$

with,

$$\xi = (1 - \beta^{-1})^{1-\beta} \quad , \tag{17}$$

and,

$$\begin{aligned}
 \beta &= s_1 Z^{-s_2} e^{-\tau x} \\
 \kappa &= s_3 Z^{s_4} \quad ,
 \end{aligned}
 \tag{18}$$

subject to the least squares fit to the Monte Carlo results,¹¹

$$\begin{aligned}
 s_1 &= 4.090 \pm 0.33 \\
 s_2 &= 0.280 \pm 0.027 \\
 s_3 &= 0.106 \pm 0.031 \\
 s_4 &= 0.103 \pm 0.089 \quad .
 \end{aligned}
 \tag{19}$$

Equations (4), (5), (6), (11), (13), (14), and (16) directly renormalize and fit Eq. (3) in the range $5.3 \leq Z \leq 82$, $0.1 \text{ MeV} \leq T \leq 20 \text{ MeV}$. In summary, DEPOS

computes Eq. (3) using the parametric approach described above. Distances are measured in (g/cm^2) and the energy deposition is given in $(MeV-cm^2/g)$.

Details concerning the parametric compilation and additional associated physics can be found in the Tabata and Ito and in the Tabata, Ito, and Okabe references.^{11,12}

For absorbers that are mixtures or compounds, Z and A are obtained from the weight fractions f_i of the constituent elements A_i, Z_i ¹³ as follows

$$Z = \sum_i f_i Z_i \quad (20)$$

$$A = Z \left(\sum_i f_i Z_i / A_i \right)^{-1} \quad (21)$$

III. CODE MODULE

The program DEPOS is a Fortran source code which calculates the energy deposition profiles of monoenergetic electrons normally incident on the surface of slabs, using the Cray-1 or CDC-7600 computers.

The program consists of two parts, the main routine and a subfunction. The subfunction contains the algorithm EDEPOS, which calculates the energy deposition profiles. EDEPOS needs five parameters that are supplied by the user. These parameters are T , the incident kinetic energy of the electron expressed in MeV ; Z , the atomic number of the absorber; A , the atomic weight of the absorber; D_{MAX} , the maximum penetration depth from the incident surface (cm); and RHO , the density (g/cm^3) of the absorber.

The main routine uses EDEPOS to calculate energy deposition at 22 equally spaced points. These values are dependent on the variable D_{MAX} . The depth

(g/cm^2) and the local deposition ($MeV-cm^2/g$), along with the five identifying parameters and the material designation, are written to both an external print file and a graphics metafile. The program generates one plot and one set of numbers for each material and its five parameters. The print file is OUTPUT and the graphics metafile is PLOT.

Plotting is done by a graphics package called Display Integrated Software System and Plotting Language (DISSPLA).¹⁴ Compilation and execution are controlled by the CFT and FTN utilities on the Cray-1 (CTSS) and CDC-7600 (LTSS) machines. External libraries required by the module are CFTMATH and DISCFT on the Cray-1 and FTNMATH and *DISFTN on the CDC-7600. The CGS metafile PLOT can be processed as microfilm, microfiche, electrostatic plot, or Tektronics display.

IV. SAMPLE PROBLEMS

Following compilation, loading, and execution, the program will first query you for the absorber material. The computer will provide you with a "prompt" (usually a question mark). Respond by entering the name or symbol (eight characters or less) and then hit return.

EXAMPLE 1

```
ENTER THE ABSORBER MATERIAL  
? ALUMINUM
```

The program will then ask you to enter T (incident kinetic energy of the electron), Z (the atomic number of the absorber), A (the atomic weight of the absorber), DMAX (maximum depth penetration), and RHC (density). You may enter the numbers on one line, separating them by commas. If you wish you

may also enter the data one line at a time. The computer will continue to prompt you until all the data has been entered.

EXAMPLE 2

```
ENTER T, Z, A, DMAX, AND RHO
? 0.5,13.0,26.98,0.0831,2.6989
T= 0.500 Z= 13.0000 A= 26.9800 DMAX= 0.0831
RHO= 2.6989 MAT=ALUMINIUM
```

EXAMPLE 3

```
ENTER T, Z, A, DMAX, AND RHO
? 0.5
? 13.0
? 26.98
? 0.0831
? 2.6989
T= 0.500 Z= 13.0000 A= 26.9800 DMAX= 0.0831
RHO= 2.6989 MAT=ALUMINIUM
```

After the last number (RHO) has been entered and a carriage return hit, the program prints a line of brief information that tells you what you have just entered and proceeds with the computations for the particular case entered. Upon completion of these computations, the computer will ask for a new material and a new set of input parameters. If you wish to escape the loop, simply type a space and then a return at the name/symbol prompt line, and the program will then terminate.

Another feature of the input is the self-scaling of the variable DMAX. If you enter zero for DMAX, the program will automatically give you a value based upon the computed extrapolated range $R_{1.0}$.

EXAMPLE 4

```
ENTER THE ABSORBER MATERIAL
? TITANIUM
ENTER T, Z, A, DMAX, AND RHO
? 1.,22.,47.9,0.,4.54
T= 1.000 Z= 22.0000 A= 47.9000 DMAX= 0.0789
RHO= 4.5400 MAT=TITANIUM
```

Output from the program will appear in two separate files, one labeled OUTPUT and the other labeled PLOT. The output file contains the energy deposition profiles that were generated by the program. The plot file contains packed graphics information. The OUTPUT file has the following structure and information.

EXAMPLE 5

```

1 ALUMINUM
2 T= 0.500 Z= 13.0000 A= 26.9800 DMAX= 0.0831 RHO= 2.6989 MAT=
3 DEPTH .0000E+00 .2243E-01 .4486E-01 .6728E-01 .8971E-01 .1121E+00 .1348E+00 .1570E+00 .1794E+00 .2019E+00 .2243E+00
4 DEPOSITION .2015E+01 .3481E+01 .4148E+01 .4020E+01 .3325E+01 .2388E+01 .1500E+01 .8368E+00 .2265E+00 .5644E-01 .1295E-01
5 -----
6
7
8 TITANIUM
9 T= 1.000 Z= 22.0000 A= 47.9000 DMAX= 0.0789 RHO= 4.5400 MAT=
10 DEPTH .0000E+00 .3582E-01 .7164E-01 .1075E+00 .1433E+00 .1791E+00 .2149E+00 .2507E+00 .2866E+00 .3224E+00 .3582E+00
11 DEPOSITION .1866E+01 .2722E+01 .3299E+01 .3496E+01 .3374E+01 .3020E+01 .2529E+01 .1991E+01 .1476E+01 .1031E+01 .6793E+00
12 -----
13
14
15 SILVER
16 T= 2.000 Z= 47.0000 A= 107.8700 DMAX= 0.1361 RHO= 10.5000 MAT=
17 DEPTH .0000E+00 .1429E+00 .2858E+00 .4287E+00 .5716E+00 .7145E+00 .8574E+00 .1000E+01 .1143E+01 .1286E+01 .1429E+01
18 DEPOSITION .1485E-01 .3198E-01 .2988E-01 .2076E-01 .1172E-01 .5428E-02 .1515E-02 .3209E-03 .2924E-02 .3525E-03 .3884E-04
19 -----
20
21
22 COPPER
23 T= 2.000 Z= 29.0000 A= 63.5500 DMAX= 0.1500 RHO= 8.9600 MAT=
24 DEPTH .0000E+00 .1344E+00 .2688E+00 .4032E+00 .5376E+00 .6720E+00 .8064E+00 .9408E+00 .1075E+01 .1210E+01 .1344E+01
25 DEPOSITION .1855E+01 .2871E+01 .3190E+01 .2698E+01 .1855E+01 .1047E+01 .4831E+00 .1157E+00 .1912E+01 .2818E+02 .3706E+03
26 -----
27
28
29 CARBON
30 T= 2.000 Z= 6.0000 A= 12.0100 DMAX= 0.6893 RHO= 1.6000 MAT=
31 DEPTH .0000E+00 .1103E+00 .2206E+00 .3309E+00 .4412E+00 .5514E+00 .6617E+00 .7720E+00 .8823E+00 .9926E+00 .1103E+01
32 DEPOSITION .1894E+01 .1829E+01 .2125E+01 .2439E+01 .2623E+01 .2661E+01 .2218E+01 .1664E+01 .1053E+01 .4612E+00 .1243E+00
33 -----
34

```

V. SAMPLE PLOTS

For the purposes of demonstration, Figures 1-12 depict typical deposition profiles for various materials and incident electron kinetic energies.

Fig.1. Carbon Deposition ($T=2$ MeV).

Fig. 2. Aluminum Deposition ($T=2$ MeV).

DEPOSITION

Fig. 3. Copper Deposition ($T=2$ MeV).

DEPOSITION

Fig. 4. Silver Deposition ($T=2$ MeV).

Fig. 5. Polystyrene Deposition (T=0.4 McV).

Fig. 6. Aluminum Deposition (T=0.5 McV).

Fig. 7. Copper Deposition (T=1 MeV).

Fig. 8. Lead Deposition (T=1 MeV).

DEPOSITION

Fig. 9. Water Deposition ($T=10$ MeV).

DEPOSITION

Fig. 10. Aluminum Deposition ($T=10$ MeV).

Fig. 11. Lead Deposition (T=10 MeV).

Fig. 12. Water Deposition (T=20 MeV).

VI. CODE LISTING

The following is a code listing of the Fortran program DEPOS described in the previous section. This listing includes the main routine and subfunction program that provides the parametric algorithm for energy deposition by electrons in slabs.

DEPOS

```

1 C      MAIN DRIVER ROUTINE FOR EDEPOS
2 C
3      PROGRAM DEPOS (INPUT,OUTPUT,TTY,TAPE5=INPUT,TAPE6=OUTPUT,TAPE59
4      1=TTY)
5      EXTERNAL EDEPOS
6      COMMON DMAX, RHO
7      DIMENSION X(22), D(22), FLINE(120)
8      DATA FLINE /120*'/
9      CALL GPLOT (1MU)
10     II=22
11 C      MAIN LOOP
12 C      READ INPUT DATA (MATERIAL,T,Z,A,DMAX,RHO)
13 C      10 WRITE (59,110)
14      READ (59,130) AMAT
15      IF (AMAT.EQ." ") GO TO 40
16      WRITE (59,120)
17      READ (59,*) TO,Z,A,DMAX,RHO
18      IF (DMAX.LE.0.0) DUMMY=EDEPOS(0.,TO,Z,A,1)
19      WRITE (59,50) TO,Z,A,DMAX,RHO,AMAT
20 C      COMPUTE DEPOSITION, STORE IN X, Y ARRAYS
21      DO 20 J=1,22
22      DEPTH=(DMAX/20.)*(J-1)+RHO
23      X(J)=DEPTH
24      MODE=3
25      IF (J.EQ.1) MODE=1
26      D(J)=EDEPOS(DEPTH,TO,Z,A,MODE)
27 C      20 CONTINUE
28 C      WRITE RESULTS TO OUTPUT FILE, INITIALIZE GRAPHICS
29      AMAX=0.
30      DO 30 I=1,22
31      30 IF (D(I).GT.AMAX) AMAX=D(I)
32      XMAX=DMAX*(22./20.)*RHO
33      WRITE (6,100) AMAT
34      WRITE (6,50) TO,Z,A,DMAX,RHO
35      WRITE (6,60) (X(K),K=1,21,2)
36      WRITE (6,70) (D(J),J=1,21,2)
37      WRITE (6,80) FLINE
38      WRITE (6,90)
39 C      PROCESS PLOTS USING DISSPLA
40      CALL PAGE (8,5,11.)
41      CALL NORRDR
42      CALL SETCLR ('MAGENTA')
43      CALL YTITLE ('DEPOSITION',10,"G/CM2",5,"MEV-CM2/G",9,7,.9,0)
44      CALL GRAF (0,"SCALE",XMAX,0.0,"SCALE",AMAX)
45      CALL GRACE (0,0)
46      CALL POLYB
47      CALL CURVE (X,D,11,0)
48      CALL COMPLX
49      CALL BASALF ('STANDARD')
50      CALL MESSAG (AMAT,8,5,0,8,5)
51      CALL MESSAG ('T=8',100,5,0,8,25)
52      CALL REALNO (TO,2,'ABUT','ABUT')
53      CALL MESSAG ('Z=8',100,5,0,8,0)
54      CALL REALNO (Z,2,'ABUT','ABUT')
55      CALL MESSAG ('A=8',100,5,0,7,75)
56      CALL REALNO (A,2,'ABUT','ABUT')
57      CALL MESSAG ('RHO=8',100,5,0,7,50)
58      CALL REALNO (RHO,2,'ABUT','ABUT')
59      CALL MESSAG ('DMAX=8',100,5,0,7,25)
60      CALL REALNO (DMAX,4,'ABUT','ABUT')
61      CALL RESET ('BASALF')
62      CALL RESET ('COMPLX')
63      CALL ENDPL (0)
64 C      EXIT LOOP, CLOSE PLOT METAFILE

```

```

65      GO TO 10
66      40 CALL DONEPL
67      STOP
68 C
69      50 FORMAT (1X,'T=',F6.3,' Z=',F9.4,' A=',F9.4,' DMAX=',F9.4,' RHO
70      1=',F9.4,' MAT=',A8/)
71      60 FORMAT (1X,'DEPTH',6X,11(E9.4,1X))
72      70 FORMAT (1X,'DEPOSITION',1X,11(E9.4,1X))
73      80 FORMAT (1X,12I4)
74      90 FORMAT (/)
75      100 FORMAT (1X,A8)
76      110 FORMAT (1X,'ENTER THE ABSORBER MATERIAL')
77      120 FORMAT (1X,'ENTER T, Z, A, DMAX, AND RHO')
78      130 FORMAT (A8)
79      END
80      FUNCTION EDEPOS (DEPTH,TO,Z,A,MODE)
81      COMMON DMAX, RHO
82 C
83 C      PURPOSE
84 C      CALCULATE THE ENERGY DEPOSITION OF ELECTRONS
85 C      NORMALLY INCIDENT ON THE SURFACE
86 C
87 C      USAGE
88 C      EDEP = EDEPOS(DEPTH,TO,Z,A,MODE)
89 C
90 C      DESCRIPTION OF PARAMETERS
91 C      DEPTH -DEPTH FROM THE INCIDENT SURFACE EXPRESSED IN G/CM2
92 C      TO    -INCIDENT KINETIC ENERGY OF THE ELECTRON IN MEV
93 C      Z     -ATOMIC NUMBER OF THE ABSORBER
94 C      A     -ATOMIC WEIGHT OF THE ABSORBER
95 C      MODE  -SHOULD BE SET AS FOLLOWS
96 C      =1    IN THE FIRST USAGE FOR A GIVEN SET OF
97 C            VALUES OF TO, Z, AND A
98 C            GREATER THAN 2 IN THE 2ND AND LATER USAGES FOR THE
99 C            GIVEN THE SET OF VALUES OF TO, Z, AND A
100 C      EDEPOS - ENERGY DEPOSITION IN MEV/(G/CM2)
101 C
102 C      STATEMENT FUNCTIONS FOR THE INVERSE EXTRAPOLATED RANGE -ENERGY
103 C      RELATION AND ITS DERIVATIVES
104 C
105      D1(X,Z)=1470./Z**0.692*X**C3
106      D2(X,Z)=1.+D1(X,Z)
107      D3(X,Z)=(257.-0.34*Z)/D2(X,Z)
108      D4(X,Z,A)=EXP(X*(C2+D3(X,Z)))/C1)
109      T(X,Z,A)=C1*(D4(X,Z,A)-1.)
110      DTDX(X,Z,A)=D4(X,Z,A)*(C2+D3(X,Z))*((1.-C3-D1(X,Z)/D2(X,Z)))
111 C
112 C      CALCULATE DEPTH-INDEPENDENT TERMS
113 C
114      IF (MODE-1) 10,10,50
115      10 C1=2980./Z
116      C2=6.14*Z**1.026/A
117      C3=0.905/Z**0.1874
118      CZ=0.000178*Z
119      FK1=1.277/Z**0.134
120      TAU=TO/0.511004
121      FEB=1.-1.33/Z**0.385*TAU**((0.066*Z**0.33)-0.048/Z**0.35/TAU**((0.47
122      1*Z**0.12))
123      IF (FEB) 20,20,30
124      20 FB=0.
125      GO TO 40
126      30 FB=1.15*EXP(-8.35/Z**0.525)/((1.+(0.0185+15.7/Z**1.59)*TAU**((1.56-4
127      1.42/Z)))*FEB
128      40 FRZTAU=0.000226*Z*TAU
129      REX=0.2335-A/Z**1.209*(ALOG(1.+CZ*TAU)/CZ-(0.9891-0.000301*Z)*TAU/
130      1*(1.+(1.468-0.0118*Z)*TAU**((1.232/Z**0.109)))
131      FACTOR=(1.-FB-FRZTAU/(1.+FRZTAU))*TO/T(REX,Z,A)
132      BETA=4.09/Z**0.28*TAU**((0.106*Z**0.103)
133      ALPHA=(1.-1./BETA)**(1.-BETA)
134      XRLIM=0.*REX
135      W1=T(XRLIM,Z,A)
136      A1=DTDX(XRLIM,Z,A)/W1
137      IF (DMAX.LE.0.) DMAX=REX/RHO
138 C
139 C      CALCULATE DEPTH-DEPENDENT TERMS
140 C
141      50 IF (DEPTH) 60,70,70
142      60 EDEPOS=0.
143      RETURN

```

```
144 70 XRESID=REX-FK1-DEPTH
145 XDEEP=XRLIM-XRESID
146 IF (XDEEP) 80,80,90
147 80 DWDX=DTD(XRESID,Z,A)-FK1
148 IF (DEPTH.EQ.0) GO TO 110
149 W=T(XRESID,Z,A)
150 GO TO 100
151 90 W=W1*EXP(-A1*XDEEP)
152 DWDX=A1-FK1-W
153 100 S=DEPTH/REX
154 ASB=ALPHA*S-BETA
155 EDEPOS=FACTOR*EXP(-ASB)*(ASB-BETA/S/REX+W*DWDX)
156 RETURN
157 110 EDEPOS=FACTOR*DWDX
158 RETURN
159 END
```

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