**MCDAN - A Monte Carlo
Computer Code for Calculating
the Dancoff Correction Factor
for Spheres and Rods**

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August 1979

**Prepared for the U.S. Department of Energy
under Contract EY-76-C-06-1830**

**Pacific Northwest Laboratory
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BATTELLE
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UNITED STATES DEPARTMENT OF ENERGY
Under Contract EY-76-C-06-1830

Printed in the United States of America
Available from
National Technical Information Service
United States Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

Price: Printed Copy \$____*; Microfiche \$3.00

*Pages	NTIS Selling Price
001-025	\$4.00
026-050	\$4.50
051-075	\$5.25
076-100	\$6.00
101-125	\$6.50
126-150	\$7.25
151-175	\$8.00
176-200	\$9.00
201-225	\$9.25
226-250	\$9.50
251-275	\$10.75
276-300	\$11.00

MCDAN - A MONTE CARLO COMPUTER CODE FOR
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FOR SPHERES AND RODS

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SUMMARY

MCDAN is a computer code that uses Monte Carlo techniques to calculate the Dancoff correction factor for arrays of spheres or rods. Neutrons are started from the surface of the sphere (rod) and tracked until they intersect another sphere (rod). The histories of a number of neutrons are statistically combined to give a value for the Dancoff correction factor.

MCDAN was written as a tool to verify the accuracy of an expression for the Dancoff correction factor used in a study of the reactivity effect of fuel particles in uranium-water mixtures. The accuracy of MCDAN has been verified by comparison with tabulated data for systems of two spheres (rods).

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MCDAN - A MONTE CARLO CODE FOR CALCULATING THE DANC OFF CORRECTION FACTOR FOR SPHERES AND RODS

INTRODUCTION

MCDAN is a computer code that calculates the Dancoff correction factor for cubic arrays of spheres or square arrays of rods. The Dancoff correction factor is the probability that neutrons emerging from the surface of a fuel lump with a cosine shaped angular distribution enter another fuel lump without first undergoing a moderator collision.

Neutrons are started from the surface of a sphere (rod) and tracked until they intersect another sphere (rod) or until they exceed a fixed total track length. The histories of a number of neutrons are statistically combined to give a value for the Dancoff correction factor.

Since the rod array calculation is a simplification of the more general sphere array, the following detailed description of the code will be in terms of the sphere case.

MODEL DESCRIPTION

The model consists of a cubic array of spheres in a "sea" of moderator. The entire matrix can be represented as an array of moderator cubes having a sphere located at the center of each cube. Since each cube is identical, the calculations are performed using only a single cubic cell. Whenever a neutron crosses the cell boundary, its position is reflected such that it re-enters the cube. The two-dimensional model shown in Figure I will help clarify this discussion.

In Figure I-A a neutron leaves the surface of the sphere in cube 1, misses the sphere in cube 2 and strikes the sphere in cube 3. In Figure I-B the neutron leaves the sphere and exits the cube at X_1, Y_1 . The neutron is re-positioned to

$$\begin{aligned} X2 &= X1 \\ Y2 &= Y1 - \text{lattice pitch} \end{aligned}$$

Similarly, after the next exit, the neutron is repositioned to

$$\begin{aligned} X4 &= X3 + \text{lattice pitch} \\ Y4 &= Y3 \end{aligned}$$

The path lengths traveled by the neutrons in Figures I-A and I-B are identical. Figure I-B represents a much simpler and more efficient method for tracking the neutrons.

Neutron tracking in the model consists of three basic segments: starting the neutron, determining where the neutron exits from the cube, and determining if the neutron intersects a sphere. After a neutron has hit a sphere or traveled more than a fixed number of mean free paths, typically 10, in the moderator its total distance traveled, TOTX, is used to evaluate the fractional contribution to the Dancoff correction factor as

$$C = e^{-\text{TOTX} * \Sigma}$$

where Σ is the moderator macroscopic total cross section. A large number of values of C are averaged to obtain the Dancoff correction factor.

Starting a neutron consists of two parts, choosing the starting point on the surface of the sphere and choosing the direction of the neutron. A random number generator capable of producing random numbers uniformly distributed over the interval (0,1) is used in these calculations.

The following algorithm is used to choose the starting point on the sphere's surface. Figure II shows the coordinate system.

- a. Pick an angle, θ , uniformly over the range 0 to 2π
- b. Pick an angle, ϕ , whose cosine is between 1 and -1 (Choosing ϕ over 0 to 2π biases the location of the starting point.) For the rod case $\phi = \pi/2$.

- c. Using the sphere radius, R , calculate the x , y and z coordinates of the starting point

$$x = R \sin \phi \cos \theta$$

$$y = R \sin \phi \sin \theta$$

$$z = R \cos \phi$$

When choosing the direction of the neutron path, care must be taken to assure that the distribution function of the neutron directions at the sphere's surface is cosine shaped about the radius vector through the starting point. This requirement is met if a random point is chosen inside the sphere and the neutron path given the direction cosines of the line from this interior point to the point on the sphere's surface. The following algorithm is used to pick the random point inside the sphere and determine neutron's direction cosines.

- a. Pick a radius, R_1 , over 0 to R
- b. Pick an angle, θ_1 , over 0 to 2π
- c. Pick an angle, ϕ_1 , whose cosine is between 1 and -1 (for the rod case $\phi_1 = \pi/2$)
- d. Calculate the coordinates of the interior point

$$x_1 = R_1 \sin \phi_1 \cos \theta_1$$

$$y_1 = R_1 \sin \phi_1 \sin \theta_1$$

$$z_1 = R_1 \cos \phi_1$$

- e. Calculate the direction cosines of the neutron path as

$$\alpha = \frac{x - x_1}{\sqrt{(x-x_1)^2 + (y-y_1)^2 + (z-z_1)^2}}$$

$$\beta = \frac{y - y_1}{\sqrt{(x-x_1)^2 + (y-y_1)^2 + (z-z_1)^2}}$$

$$\gamma = \frac{z - z_1}{\sqrt{(x-x_1)^2 + (y-y_1)^2 + (z-z_1)^2}}$$

The distance from the current position of the neutron (x,y,z) to the six surfaces of the cube are calculated and the closest distance, DMIN, is used to determine the exit point. Using DMIN and the direction cosines α , β and γ the exit point (x_E, y_E, z_E) is

$$x_E = x + \alpha * DMIN$$

$$y_E = y + \beta * DIMN$$

$$z_E = z + \gamma * DIMN$$

The distance DMIN is summed to generate the total track length, TOTX.

Once the exit point has been established, the neutron is repositioned so that it reenters the cube in the manner discussed earlier.

The neutron will intersect the sphere in the cube if the length of a line from the center of the sphere perpendicular to the neutron path is less than the sphere radius as shown in Figure III. The neutron is at A traveling along AC with direction cosines α , β and γ . The sphere is centered at B with radius BD. $\overline{BC}$ is perpendicular to the neutron path. ψ is the angle between the neutron path and a line from the current neutron position to the center of the sphere. If BC is less than BD, then the neutron intersects the sphere at D.

The length of line $\overline{BC}$ is

$$BC = AB \sin \psi$$

The angle between the lines $\overline{AB}$ and $\overline{AC}$, ψ , is calculated by first calculating the direction cosines of $\overline{AB}$. They are

$$\alpha_1 = \frac{-x}{\sqrt{x^2 + y^2 + z^2}}$$

$$\beta_1 = \frac{-y}{\sqrt{x^2 + y^2 + z^2}}$$

$$\gamma_1 = \frac{-z}{\sqrt{x^2 + y^2 + z^2}}$$

Then

$$\cos \psi = \alpha \alpha_1 + \beta \beta_1 + \gamma \gamma_1$$

If the neutron intersects the sphere at D, the track length AD is

$$AD = \frac{BD * \sin [2\pi - \psi - \cos^{-1}(BC/BD)]}{\sin \psi}$$

The value of AD is added to the neutron's track length to give the total track length, TOTX.

Once a neutron has intersected a sphere or exceeded the maximum allowable track length, the Dancoff correction is calculated and a new neutron is started.

CALCULATED RESULTS

The accuracy of the methods used in this code was tested by comparing the results with data given by Knight¹ for two spheres. It was necessary to modify the code to consider only two spheres but the methods described for starting and tracking the neutrons were not changed. A comparison between the two methods is shown in Table I. The results of the two methods compare very closely.

Tables II - IV give MCDAN calculated Dancoff correction factors for systems having various sphere radii, sphere volume fractions and moderator cross sections.

FIGURE I. Model Used in MCDAN

FIGURE II. Coordinate System Used in MCDAN

FIGURE III. Neutron Intersection with Sphere

TABLE I. Comparison Between MCDAN and Data Given by Knight¹

R/λ	0.1		0.3		0.5	
D/R	KNIGHT	MCDAN*	KNIGHT	MCDAN*	KNIGHT	MCDAN*
2.0	.07296	.06683 $\pm$.00155	.06813	.06370 $\pm$.00158	.06383	.06082 $\pm$.00161
3.0	.02550	.02464 $\pm$.00112	.01898	.01895 $\pm$.00087	.01417	.01460 $\pm$.00068
4.0	.01254	.01220 $\pm$.00022	.00757	.00765 $\pm$.00013	.00459	.00480 $\pm$.00009
5.0	.00715	.00733 $\pm$.00041	.00352	.00373 $\pm$.00027	.00174	.00190 $\pm$.00011
6.0	.00446	.00445 $\pm$.00059	.00179	.00186 $\pm$.00024	.00072	.00078 $\pm$.00010
7.0	.00295	.00306 $\pm$.00044	.00097	.00104 $\pm$.00016	.00032	.00036 $\pm$.00005
8.0	.00204	.00232 $\pm$.00022	.00055	.00064 $\pm$.00007	.00015	.00018 $\pm$.00002
9.0	.00145	.00154 $\pm$.00011	.00033	.00035 $\pm$.00003	.00007	.00008 $\pm$.00001

R = sphere radius

D = center-to-center separation

λ = moderator mean free path

*MCDAN modified to consider a system of two spheres

TABLE II. MCDAN Calculated Dancoff Correction Factors for Spheres, $\Sigma_m = 1.0 \text{ cm}^{-1}$

Sphere Volume Fraction	R = 0.005 cm		R = 0.02 cm		R = 0.1 cm	
	Lattice Pitch (cm)	Dancoff Correction Factor	Lattice Pitch (cm)	Dancoff Correction Factor	Lattice Pitch (cm)	Dancoff Correction Factor
0.005	0.0471	0.4292	0.1885	0.1414	0.9427	0.0218
0.010	0.0374	0.6160	0.1496	0.2621	0.7482	0.0505
0.025	0.0276	0.8132	0.1103	0.4989	0.5513	0.1312
0.050	0.0219	0.8995	0.0875	0.6781	0.4376	0.2564
0.100	0.0174	0.9492	0.0695	0.8196	0.3473	0.4469
0.200	0.0138	0.9771	0.0551	0.9136	0.2756	0.6638
0.300	0.0120	0.9866	0.0482	0.9474	0.2408	0.7766
0.400	0.0109	0.9913	0.0438	0.9662	0.2188	0.8502
0.500	0.0102	0.9941	0.0406	0.9770	0.2031	0.8942

TABLE III. MCDAN Calculated Dancoff Correction
Factor for Spheres, $\Sigma_m = 2.0 \text{ cm}^{-1}$

Sphere Volume Fraction	R = 0.005 cm		R = 0.02 cm		R = 0.1 cm	
	Lattice Pitch (cm)	Dancoff Correction Factor	Lattice Pitch (cm)	Dancoff Correction Factor	Lattice Pitch (cm)	Dancoff Correction Factor
0.005	0.0471	0.2573	0.1885	0.0683	0.9427	0.0064
0.010	0.0374	0.4365	0.1496	0.1416	0.7482	0.0170
0.025	0.0276	0.6774	0.1103	0.3098	0.5513	0.0544
0.050	0.0219	0.8145	0.0875	0.4975	0.4376	0.1313
0.100	0.0174	0.9021	0.0695	0.6863	0.3473	0.2619
0.200	0.0138	0.9550	0.0551	0.8382	0.2756	0.4771
0.300	0.0120	0.9732	0.0482	0.8996	0.2408	0.6265
0.400	0.0109	0.9828	0.0438	0.9331	0.2188	0.7339
0.500	0.0102	0.9883	0.0406	0.9547	0.2031	0.8066

TABLE IV. MCDAN Calculated Dancoff Correction
Factors for Spheres, $\Sigma_m = 3.0 \text{ cm}^{-1}$

Sphere Volume Fraction	R = 0.005 cm		R = 0.02 cm		R = 0.1 cm	
	Lattice Pitch (cm)	Dancoff Correction Factor	Lattice Pitch (cm)	Dancoff Correction Factor	Lattice Pitch (cm)	Dancoff Correction Factor
0.005	0.0471	0.1858	0.1385	0.0467	0.9427	0.0023
0.010	0.0374	0.3290	0.1496	0.0887	0.7482	0.0076
0.025	0.0276	0.5759	0.1103	0.2212	0.5513	0.0293
0.050	0.0219	0.7428	0.0875	0.3868	0.4376	0.0727
0.100	0.0174	0.8606	0.0695	0.5860	0.3473	0.1753
0.200	0.0138	0.9338	0.0551	0.7726	0.2756	0.3645
0.300	0.0120	0.9603	0.0482	0.8554	0.2408	0.5190
0.400	0.0109	0.9744	0.0438	0.9047	0.2188	0.6433
0.500	0.0102	0.9828	0.0406	0.9331	0.2031	0.7323

REFERENCES

1. "SUPERDAN: Computer Programs for Calculating the Dancoff Factor of Spheres, Cylinders and Slabs," J. R. Knight, ORNL/NUREG/CSD/TM-2, March 1979.

APPENDIX A

Input to MCDAN

Input to MCDAN is straightforward and can be easily modified by the user to suit his own needs. The version of the code as listed in Appendix B requires the following input.

<u>CARD #</u>	<u>FORMAT</u>	<u>VARIABLE</u>	<u>DESCRIPTION</u>
1	A1	ISC	ISC=S to calculate the Dancoff correction for an array of spheres. ISC=R to calculate the Dancoff Correction for an array of rods.
2	List Directed	R, SIG, VF	R = sphere or rod radius in centimeters SIG - moderator macroscopic total cross section, cm^{-1} VF - sphere volume fraction or rod lattice pitch.

Control returns to Card 2. To terminate execution input R, SIG and VF as 0.0.

APPENDIX B

Listing of MCDAN

```

C A MONTE CARLO CODE FOR CALCULATING THE DANCUFF CORRECTION
C FOR CUBIC ARRAY OF SPHERES OR SQUARE ARRAY OF RODS
C WRITTEN BY J.P. MCNEECE
C
C      BATTELLE
C      PACIFIC NORTHWEST LAB
C      PO BOX 999
C      RICHLAND, WASHINGTON 99352
C R=SPHERE OR ROD RADIUS (CM)
C SIG=MODERATOR MACRO XSECT (CM-1)
C XMAX=MAX NUMBER MFP N WILL BE TRACKED (MFP)
C VF=VOLUME FRACTION OF SPHERES = LATTICE PITCH FOR RODS(CM)
C NB=NUMBER OF NEUTRON BATCHES
C NPB=NUMBER OF NEUTRONS PER BATCH
C ISO=FLAG FOR SELECTING N DISTRIBUTION
C ISC='S' FOR SPHERE='R' FOR RODS
C RANF(DUM)=RANDOM NUMBER OVER 0-1
C ISO MUST BE SET TO 1 TO GIVE CORRECT N DISTRIBUTION
      ISO=1
C XMAX CAN BE ANY VALUE. SHOULD BE AT LEAST 10
      XMAX=10.
C NPB SHOULD BE 3000 TO 5000
      NPB=5000
C NB CAN BE ANY NUMBER . AT LEAST 3
      NB=3
      PI=3.14159
      PI2=PI/2.
      TPI=2.*PI
C READ LUMP GEOMETRY INDICATOR
      READ(5,98)ISC
98      FORMAT(A1)
99      CONTINUE
      READ(5,101)R,SIG,VF
      IF(R.LE.0.0)GO TO 999
101     FORMAT()
C CALCULATE LATTICE PITCH
      PITCH=R*(4.*PI/(3.*VF))**.5
      IF(ISC.EQ.'R')PITCH=VF
      P2=PITCH/2.
C CONVERT XMAX TO CM
      XMAX=XMAX/SIG
      WRITE(6,104)R,SIG,XMAX,VF,PITCH,NB,NPB
104     FORMAT(' R=',1PE12.5,' SIG=',E12.5,' XMAX=',E12.5,
+/' VF=',E12.5,' PITCH=',E12.5,
+/' NUMBER OF BATCHES=',13,' NEUTS/BATCH=',16)
      WRITE(6,105)
105     FORMAT(' BATCH          C          AVG C          STD          AVG X
+NHITS')
      SUM1=0.0
      SUM2=0.0
      DO 1 I=1,NB
      NHITS=0
      X=0.0
      SUM3=0.0
      STD=0.0
      DO 2 J=1,NPB
      TOTX=0.0
C CALL ROUTINE FOR STARTING NEUTRON
      CALL START(X,Y,Z,XP,YP,ZP,P2,DC4,DC6,DC6,PI,TPI,PI2,R,ISO,TOTX
+ ,ISC)
10      XDIS=0.0
15
C SEE IF NEUTRON HITS SPHERE IN BOX

```

```

      CALL HIT(XDIS,IT,DCA,DCB,DCG,X,Y,Z,R,PI2)
C IF NO HIT THEN WHERE DOES N EXIT BOX
      IF(IT.EQ.'NO')CALL INSECT(XDIS,X,Y,Z,XP,YP,ZP,DCA,DCB,DCG,P2)
C CALCULATE TOTAL DISTANCE NEUTRON HAS TRAVELED
      TOTX=TOTX+XDIS
      IF(TOTX.LT.XMAX.AND.IT.EQ.'NO')GO TO 10
      IF(IT.EQ.'YES')NHITS=NHITS+1
      W=W*EXP(-SIG*TOTX)
      SUM3=SUM3+TOTX
2     CONTINUE
      W=W/FLOAT(NPH)
      AVGX=SUM3/FLOAT(NPH)
      SUM1=SUM1+W
      SUM2=SUM2+W*W
      AVGW=SUM1/FLOAT(I)
      IF(I.EQ.1)GO TO 11
      ARG=SUM2/FLOAT(I-1)-AVGW*AVGW*FLOAT(1)/FLOAT(I-1)
      IF(ARG.LT.0.0)ARG=0.0
      STD=SQRT(ARG)
11    WRITE(6,103)I,W,AVGW,STD,AVGX,NHITS
103   FORMAT(1H,14,1P4E12.5,110)
1     CONTINUE
      GO TO 99
999   STOP
      END
C SUBROUTINE FOR STARTING NEUTRON
      SUBROUTINE START(X1,Y1,Z1,XP,YP,ZP,P2,DCA,DCB,DCG,PI,PI1,PI2,R
      +,ISO,XDIS,ISC)
C PICK A POINT ON SURFACE OF SPHERE OR ROD
      T0=R*ANF(DUM)+PI1
      P0=ACOS(2.*RANF(DUM)-1.0)
      IF(ISC.EQ.'R')P0=PI2
      T1=R*SIN(P0)
      X1=T1*COS(T0)
      Y1=T1*SIN(T0)
      Z1=R*COS(P0)
C PICK AN INTERIOR POINT
C IF ISO=0, N DISTRIBUTION AT SURFACE OF SPHERE WILL BE ISOTROPIC
C IF ISO=1 N DISTRIBUTION AT SURFACE OF SPHERE WILL BE COGNE
C IF ISO=2 N PATH WILL BE ALONG RADIUS VECTOR( USED FOR DEBUG)
C ISO=1 IS THE CORRECT CHOICE
      IF(ISO.EQ.0)R1=R
      IF(ISO.EQ.1)R1=R+RANF(DUM)
      IF(ISO.EQ.2)R1=0.0
      T2=RANF(DUM)+PI1
      P3=ACOS(2.*RANF(DUM)-1.0)
      IF(ISC.EQ.'R')P3=PI2
      T1=R1*SIN(P3)
      X2=T1*COS(T2)
      Y2=T1*SIN(T2)
      Z2=R1*COS(P3)
C CALCULATE DIRECTION COSINES
      A=X1-X2
      B=Y1-Y2
      C=Z1-Z2
      D=SQRT(A*A+B*B+C*C)
      DCA=A/D
      DCB=B/D
      DCG=C/D
C WHICH 3 PLANE CAN N HIT
      XP=DCA+P2/ABS(DCA)

```

```

      YP=DCB*P2/ABS(DCB)
      ZP=DCG*P2/ABS(DCG)
C WHERE DOES N INTERSECT BOX
      CALL INSECT(XDIS,X1,Y1,Z1,XP,YP,ZP,DCA,DCB,DCG,P2)
      RETURN
      END
C SUBROUTINE FOR DETERMINING IF NEUTRON HITS SPHERE IN BOX
      SUBROUTINE HIT(XDIS,IT,DCA,DCB,DCG,X,Y,Z,R,PI2)
      IT='NO'
C CALCULATE DIRECTION COSINES OF LINE FROM X,Y,Z TO CENTER OF
C SPHERE IN BOX( SPHERE IS AT 0,0,0)
      D=SQRT(X*X+Y*Y+Z*Z)
      DCA1=-X/D
      DCB1=-Y/D
      DCG1=-Z/D
C CALCULATE COSINE OF ANGLE BETWEEN N PATH AND LINE TO CENTER OF SPHERE
      A1=DCA*DCA1+DCB*DCB1+DCG*DCG1
C IF A1 LE 0.0 THEN N SURELY CANT HIT SPHERE
      IF(A1.LE.0.0)RETURN
      ABTL=ACOS(A1)
      A2=5(IN(ABTL))
C CALCULATE LENGTH OF NORMAL TO N PATH AND CENTER OF SPHERE
      A=D*A2
      IF(A.GT.R)RETURN
      IT='YES'
C CALCULATE DISTANCE TO WHERE N HITS SURFACE OF SPHERE
      XDIS=R*SIN(PI2-ABTL-ACOS(A/R))/A2
      RETURN
      END
C SUBROUTINE FOR DETERMINING INTERSECTION OF N AND BOX BOUNDARY
      SUBROUTINE INSECT(XDIS,X,Y,Z,XP,YP,ZP,DCA,DCB,DCG,P2)
      DIMENSION D(3)
      D(1)=999.
      D(2)=999.
      D(3)=999.
C CALCULATE DISTANCES N MUST TRAVEL TO INTERSECT THE 3 POSSIBLE PLANES
      IF(DCA.NE.0.0)D(1)=(XP-X)/DCA
      IF(DCB.NE.0.0)D(2)=(YP-Y)/DCB
      IF(DCG.NE.0.0)D(3)=(ZP-Z)/DCG
C DETERMINE WHICH IS SHORTEST
      IS=1
      IF(D(2).LT.D(1))IS=2
      IF(D(3).LT.D(IS))IS=3
      XDIS=D(IS)
C CALCULATE X,Y,Z COORDINATES OF INTERSECTION POINT
      X=X+D(IS)*DCA
      Y=Y+D(IS)*DCB
      Z=Z+D(IS)*DCG
C MOVE N POSITION SO IT REENTERS BOX CORRECTLY
      GO TO (1,2,3),IS
1      X=X-2.*XP
C CHECK FOR INTERSECTION AT CORNERS AND EDGES
      IF(D(2).EQ.D(1))Y=Y-2.*YP
      IF(D(3).EQ.D(1))Z=Z-2.*ZP
      RETURN
2      Y=Y-2.*YP
      IF(D(3).EQ.D(2))Z=Z-2.*ZP
      RETURN
3      Z=Z-2.*ZP
      RETURN
      END

```

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