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DETERMINATION OF INTERSECTION OF PARTICLE FLIGHT PATH WITH SURFACE OF HELICAL TUBULAR VOID REGION

by Millard L. Wohl and Carl D. Bogart

Lewis Research Center
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SUMMARY

A method for determining the intersections of a nuclear particle flight path and the wall of a helical tubular duct is presented. FORTRAN listings of computer subroutines which perform the numerical analysis involved are included. The subroutines are useful in any Monte Carlo transport analysis where complex void configurations of helical or pseudohelical geometry are involved. Their immediate purpose in this work is to serve as geometry subroutines to be used in conjunction with 05-R, a Monte Carlo transport code developed at Oak Ridge National Laboratory.

INTRODUCTION

In many reactor and shield analyses which involve the transport of neutrons and gamma rays, it is necessary for high accuracy in local and emergent particle flux or current calculations to include the actual geometry of such system components as voids and coolant flow passages. An example of a coolant flow passage of complex geometry is a helical tubular duct. In performing a reactor-shield Monte Carlo transport analysis to determine the effects of such complex ducting on overall shield performance, individual neutron and gamma-ray histories are simulated on the digital computer. In the computation of distances between successive particle collisions, it must be determined whether a void traversal occurs. If so, the points of intersection of the particle path and void surface must be determined, and the between-collisions path length in the material must be incremented by the in-void path length before a subsequent collision point is determined. It is possible to track correctly without incrementing path lengths by appropriate void-crossing distances. However, the method employed herein allows the determination of in-void fluxes, while the latter method does not.

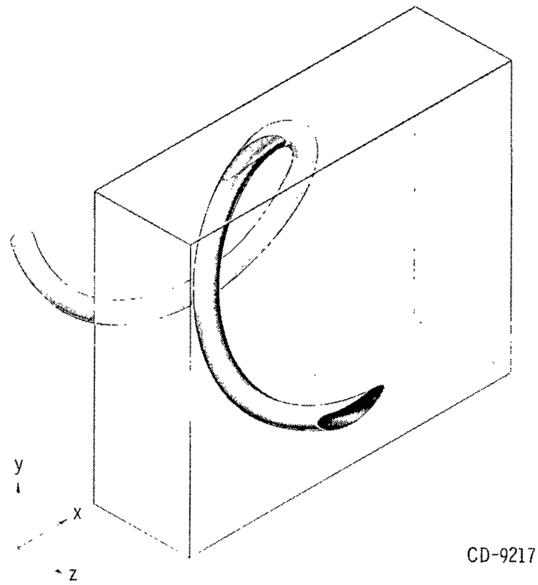


Figure 1. - One turn of helical tube penetrating slab of finite thickness.

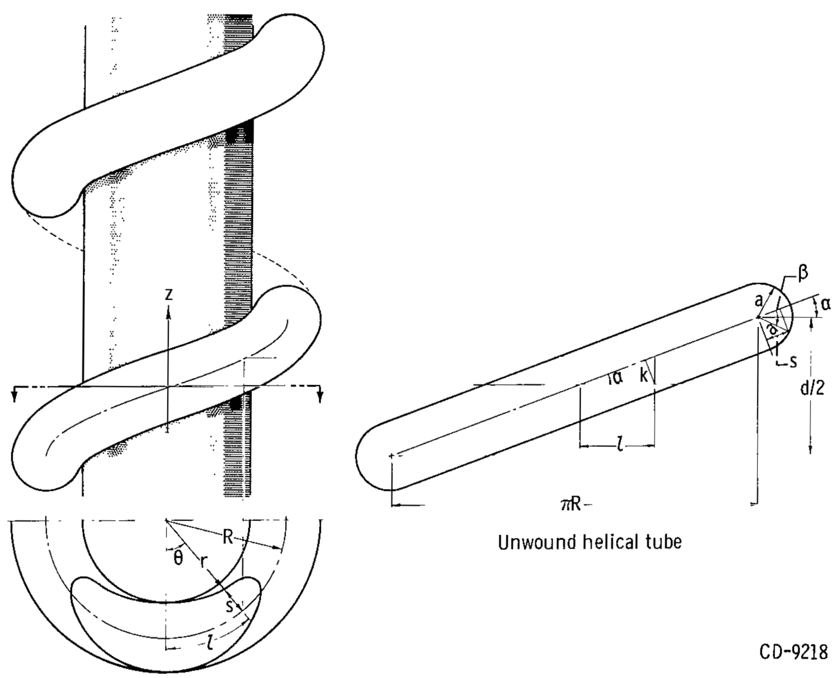


Figure 2. - Projections of half-turn helical duct.

PHYSICAL MODEL

The physical model is shown in figure 1. A slab of homogeneous shield material is penetrated by a helical duct. When the principles of descriptive geometry (ref. 1) are used, projections of the helical duct may be obtained, as shown in figure 2 where $r = R \pm s$, $\sin \alpha = k/l$, and $l = R\theta$. This is also shown by the following equations:

$$\frac{(r - R)^2}{a^2} + \left(\frac{R^2}{a^2} \sin^2\alpha\right)\theta^2 = 1$$

or

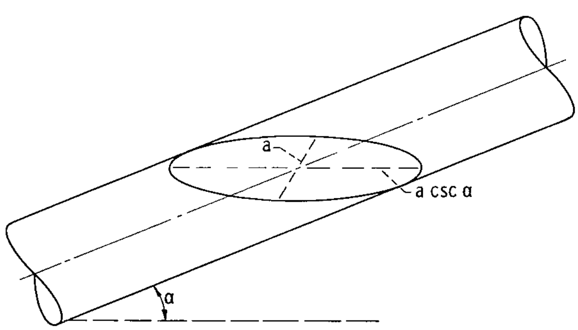
$$\frac{r}{R} = 1 \pm \sqrt{\left(\frac{a}{R}\right)^2 - (\sin^2\alpha)\theta^2}$$

(All symbols are defined in the appendix.) The coordinates of the projection of the center of the duct on a plane perpendicular to the axis of the cylinder about which the duct is wound (x, y-plane) are given by

$$x = R \cos \omega z \tag{1a}$$

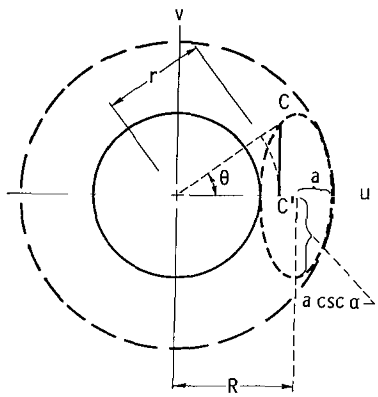
$$y = R \sin \omega z \tag{1b}$$

where $\omega = 2\pi/d$ and d is the helical pitch. Consider an unwound (inclined cylindrical) section of the helical tube cut by a plane normal to the axis of the cylinder about which the tube is wound. The elliptical intersection of the plane and inclined cylinder is shown in sketch (a).



(a)

This elliptical intersection is shown in an end view in sketch (b).



(b)

The equation of the ellipse in the u, v-coordinate system is

$$\frac{(u - R)^2}{a^2} + \frac{v^2}{a^2 \csc^2 \alpha} = 1 \tag{2a}$$

or

$$(u - R)^2 + v^2 \sin^2 \alpha = a^2 \tag{2b}$$

Consider, now, winding the inclined cylinder about an inner cylinder, as shown in figure 2. As the tube is wound around the cylinder, vertical chords CC' of the ellipse (sketch (b)) transform into arcs of circles of radius r. Thus, the "winding transformation" is represented by

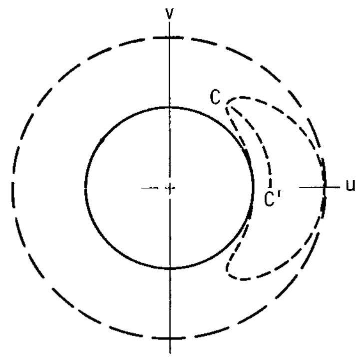
$$u \longrightarrow r \tag{3a}$$

$$v \longrightarrow r\theta \tag{3b}$$

Equation (2b) now becomes

$$(r - R)^2 + r^2\theta^2 \sin^2 \alpha = a^2 \tag{4}$$

which is the equation of the transformed elliptical, or bean-shaped, intersection shown in sketch (c).



(c)

where θ is the angular displacement of points on the periphery of the "bean" from the semiminer axis of the unwrapped ellipse. Equation (4) describes the intersection of the helical duct surface with the x, y-plane. The shape of the intersection with any plane of constant z is invariant, and its position on an arbitary plane is determined by an angular displacement of ωz. Equation (4) may thus be generalized for an arbitrary plane of constant z as follows:

$$(r - R)^2 + R^2 \sin^2\alpha(\theta - \omega z)^2 = a^2 \tag{5}$$

Next, the intersection of the particle track and the helical duct must be considered. The equation of the straight line specifying the particle track may be written in parametric form as follows (ref. 2):

$$x = x_1 + (x_2 - x_1)t \tag{6a}$$

$$y = y_1 + (y_2 - y_1)t \tag{6b}$$

$$z = z_1 + (z_2 - z_1)t \tag{6c}$$

where $0 \le t \le 1$. The starting point of a particle track is at x_1, y_1, z_1 and the termination point is at x_2, y_2, z_2. For simplicity of notation, let

$$\Delta x = x_2 - x_1 \tag{7a}$$

$$\Delta y = y_2 - y_1 \tag{7b}$$

$$\Delta z = z_2 - z_1 \tag{7c}$$

The transformation equations from x, y to r, θ coordinates are

$$r^2 = x^2 + y^2 \tag{8a}$$

$$\theta = \tan^{-1}\left(\frac{y}{x}\right) \tag{8b}$$

Substituting equations (6) modified by equations (7) into equations (8) yields

$$r^2 = (x_1 + t\,\Delta x)^2 + (y_1 + t\,\Delta y)^2 \tag{9a}$$

$$\theta = \tan^{-1}\left(\frac{y_1 + t\,\Delta y}{x_1 + t\,\Delta x}\right) \tag{9b}$$

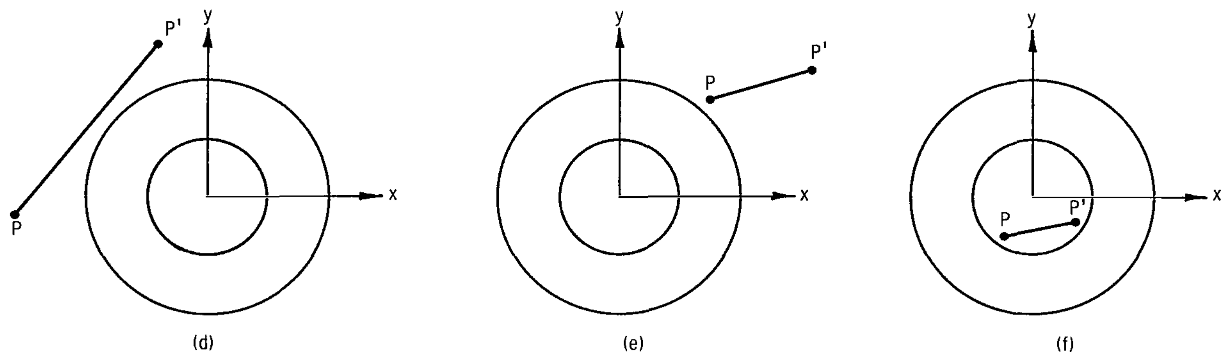
Substitution of equations (9) into equation (5) yields

$$\left\{\left[(x_1 + t\,\Delta x)^2 + (y_1 + t\,\Delta y)^2\right]^{1/2} - R\right\}^2 + R^2 \sin^2\alpha \left[\tan^{-1}\left(\frac{y_1 + t\,\Delta y}{x_1 + t\,\Delta x}\right) - \omega(z_1 + t\,\Delta z)\right]^2 = a^2 \tag{10}$$

The intersections of the helical tubular surface and the straight-line particle track are determined by solving equation (10) for those values of t which satisfy $0 \leq t \leq 1$.

NUMERICAL ANALYSIS

Before directly attempting to solve equation (10), certain special cases may be eliminated. Consider the cases illustrated in sketches (a), (b), and (c), where P and P' are the projections of initial and final collision points defining a particle track on a plane normal to the axis of the cylindrical shell containing the duct.



The annular region shown in sketches (d) to (f) is the projection of the cylindrical shell containing the helical duct on a plane normal to the axis of the shell. In all three cases, no intersection of the particle track and the helical duct can occur.

The equation of the outer circle of these annular projections is

$$x^2 + y^2 = (R + a)^2 \tag{11a}$$

and the equation of the inner circle is

$$x^2 + y^2 = (R - a)^2 \tag{11b}$$

When the values given in equations (6) and (7) are substituted into equation (11a), the intersection of the projected particle track and the larger circle is given by

$$(x_1 + t\,\Delta x)^2 + (y_1 + t\,\Delta y)^2 = (R + a)^2 \tag{12a}$$

Performing the operations indicated in equation (12a) yields

$$t^2\left[(\Delta x)^2 + (\Delta y)^2\right] + 2t(x_1\,\Delta x + y_1\,\Delta y) + x_1^2 + y_1^2 - (R + a)^2 = 0 \tag{12b}$$

Let

$$A = (\Delta x)^2 + (\Delta y)^2 \tag{13a}$$

$$B = 2(x_1\,\Delta x + y_1\,\Delta y) \tag{13b}$$

$$C = x_1^2 + y_1^2 - (R + a)^2 \tag{13c}$$

The discriminant of equation (12b) is thus given as

$$D = B^2 - 4AC \tag{14}$$

If $D \leq 0$, the situation is as depicted in sketch (a). For $D > 0$, consider

$$t_1 = \frac{-0.5(B + D^{1/2})}{A} \tag{15a}$$

and

$$t_2 = \frac{-0.5(B - D^{1/2})}{A} \tag{15b}$$

Let

$$t_{low} = \mathrm{MAX}(0, t_1) \tag{16a}$$

$$t_{up} = \mathrm{MIN}(1, t_2) \tag{16b}$$

If $t_{low} > t_{up}$, the situation is that of sketch (b). Let

$$f(t) = At^2 + Bt + \left[x_1^2 + y_1^2 - (R - a)^2\right] \tag{17}$$

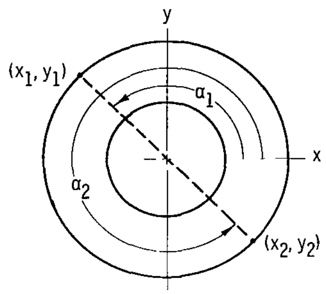
(The quantity in brackets is the equation of the inner circle.) If $f(t_{low}) \leq 0$ and $f(t_{up}) \leq 0$, the situation is as depicted in sketch (c).

Consider the solution of equation (10). If the particle path length in the material is such that it would normally have its path terminated within the helical void, the upper value of t must be reset. Define $g(t)$ as

$$g(t) = \frac{\left\{\left[(x_1 + t\,\Delta x)^2 + (y_1 + t\,\Delta y)^2\right]^{1/2} - R\right\}^2}{a^2} + \frac{\left[\tan^{-1}\left(\dfrac{y_1 + t\,\Delta y}{x_1 + t\,\Delta x}\right) - \omega(z_1 + t\,\Delta z)\right]^2}{\left(\dfrac{a}{R \sin \alpha}\right)^2} - 1 \tag{18}$$

If $g(t_{up}) < 0$, set $t_{up} = t_2$. The limiting solutions of equation (10) or, alternatively, equation (18) for $g(t) = 0$ are t_{low} and t_{up}.

It is necessary to determine the relative orientations of the flight path and helical void to see whether intersection actually occurs. For the values of t_{low} and t_{up}, there are corresponding values of z (eq. (6c)). From $x(t_{up})$, $x(t_{low})$, $y(t_{up})$, and $y(t_{low})$, two angles may be computed to determine whether the particle flight path penetrates the void. Consider the following projection of flight path and void-containing shell in the x, y-plane:



(g)

where x_1, y_1 and x_2, y_2 are the coordinates of the points of intersection of the projected flight path and outer radius of the shell projection. Let

$$\alpha_1 = \tan^{-1}\left(\frac{y_1 + t_{low}\,\Delta y}{x_1 + t_{low}\,\Delta x}\right) \tag{19a}$$

$$\alpha_2 = \tan^{-1}\left(\frac{y_1 + t_{up}\,\Delta y}{x_1 + t_{up}\,\Delta x}\right) \tag{19b}$$

The angles α_1 and α_2 correspond to values of ωz or to different z-coordinates of the intersection point of the path and void. Values of the z-coordinate in a certain specified range of z-values (i.e., $z(t_{low}) \rightarrow z(t_{up})$) correspond to real intersections and necessitate the solution of equation (10); others do not correspond to real intersections.

The following values of z must be tested for a helical tube of $1\frac{1}{2}$ turns:

$$z_1 = \frac{\alpha_1}{\omega} + \frac{a}{R \sin \alpha} \tag{20a}$$

$$z_2 = \frac{\alpha_1}{\omega} - \frac{a}{R \sin \alpha} \tag{20b}$$

$$z_3 = z_1 + 2\pi \tag{20c}$$

$$z_4 = z_2 + 2\pi \tag{20d}$$

$$z_5 = \frac{\alpha_2}{\omega} + \frac{a}{R \sin \alpha} \tag{20e}$$

$$z_6 = \frac{\alpha_2}{\omega} - \frac{a}{R \sin \alpha} \tag{20f}$$

$$z_7 = z_5 + 2\pi \tag{20g}$$

$$z_8 = z_6 + 2\pi \tag{20h}$$

$$z_9 = z_1 - 2\pi \tag{20i}$$

$$z_{10} = z_2 - 2\pi \tag{20j}$$

$$z_{11} = z_5 - 2\pi \tag{20k}$$

$$z_{12} = z_6 - 2\pi \tag{20l}$$

It is not necessary to test the z-values which are not in the range $0 \leq z \leq d$ to see if they lie between $z(t_{low})$ and $z(t_{up})$.

SEQUENCING OF COMPUTER PROGRAMS AND SUBROUTINES

When, in the sequence of computing in the controlling program (such as 05-R), a collision is about to occur, the effect of the presence of the helical duct must be determined. The controlling program must have a geometry subroutine, GEOM, which implements the mathematics discussed herein. GEOM calls for subroutine TRSOL, which determines the roots (values of t) of equation (18). (This equation is equivalent to equation (10).) TRSOL calls for subroutine ITER, which refines these roots. When the collision point has been determined, return is executed through TRSOL and GEOM to the main program. Function subprograms DES and GOFT, respectively, generate D of equation (14) and g(t) of equation (18). LOOKZ is a utility function subprogram required by 05-R, the main program. Figures 3 and 4 represent the logical flow of the subroutines. (All symbols are defined in the appendix.)

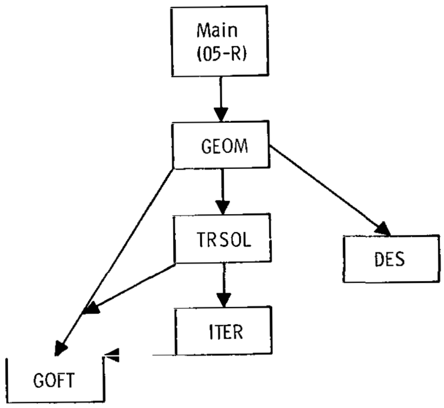
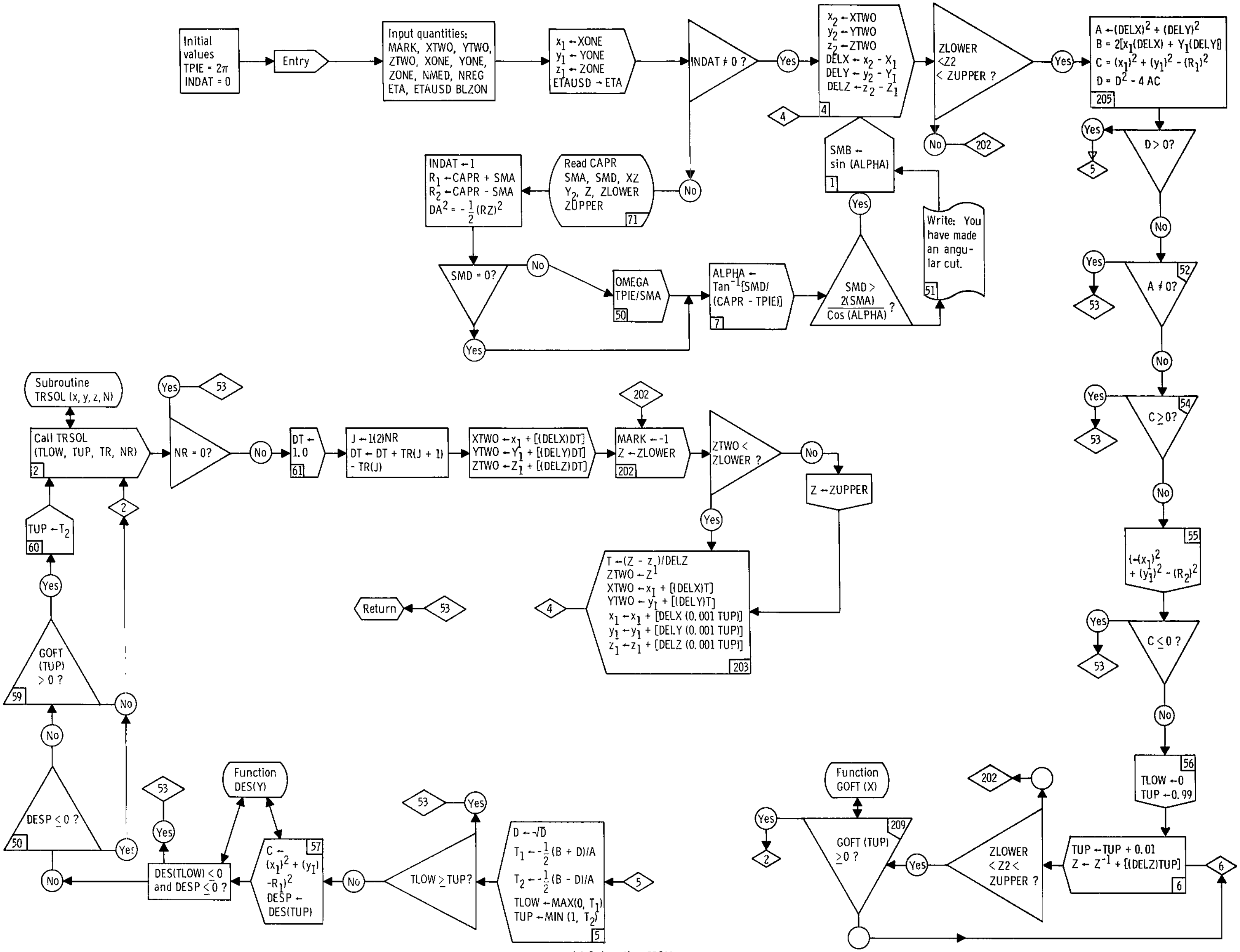
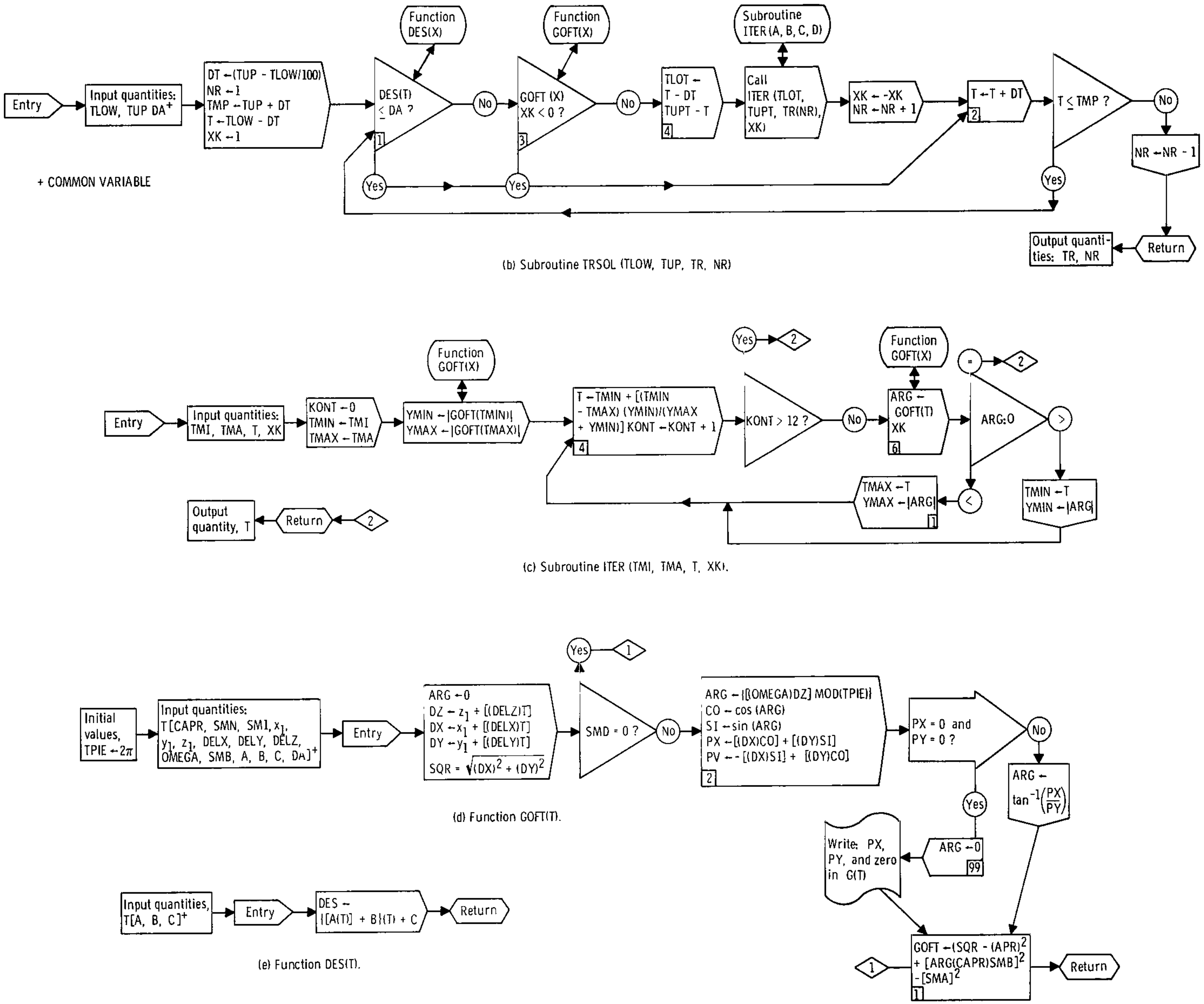


Figure 3. - Fortran programs used in 05-R code.



(a) Subroutine GEOM

Figure 4. - Flow diagrams for subroutines and functions.



(b) Subroutine TRSOL (TLOW, TUP, TR, NR)

(c) Subroutine ITER (TMI, TMA, T, XK).

(d) Function GOFT(T).

(e) Function DES(T).

Figure 4. - Concluded.

FORTRAN IV Listings of Computer Subprograms

```
$IBFTC GEOMAA  REF,DD,FULIST,NODECK
      SUBROUTINE GEOM
      DATA TPIE/ 6.2831853/
      DATA INDAT/ 0/
      COMMON/ GEOMC  / MARK, XTWO, YTWO, ZTWO, XONE, YONE,
     1ZONE,NMED,NREG,ETA,ETAUSD,BLZON
      COMMON/ CARL  / CAPR, SMA, SMD, X1, Y1, Z1, DELX,
     1DELY,DELZ,OMEGA,SMB,A,B,C,DA
      DIMENSION X(2),Y(2),Z(2),TR(10)
      EXTERNAL DES
      EXTERNAL GOFT
      FZIT(DDD,EEE,FFF)=EEE+FFF+DDD
      SIGNT(GGG,HHH,PPP)=(GGG-PPP)*(HHH-PPP)
      X1=XONE
      Y1=YONE
      Z1=ZONE
      ETAUSD=ETA
      IF(INDAT.NE.0) GO TO 4
   71 READ( 5,200)CAPR,SMA,SMD,XZ,YZ,ZZ,ZLOWER,ZUPPER
  200 FORMAT(8F10.5)
      INDAT=1
      R1=CAPR+SMA
      R2=CAPR-SMA
      DA=-.5*(R2)**2
      IF(SMD.EQ.0.0)GO TO 7
   50 OMEGA=TPIE/SMD
    7 ALPHA=ATAN (SMD/(TPIE*CAPR))
```

```
C       CHECK FOR TORUS
        IF(SMD.GT.(2.*SMA/COS (ALPHA))) GO TO 1
   51 WRITE(6, 100)
  100 FORMAT(30HOYOU HAVE MADE AN ANNULAR CUT     )
    1 SMB=SIN (ALPHA)
    4 X2=XTWO
      Y2=YTWO
      Z2=ZTWO
      DELX=X2-X1
      DELY=Y2-Y1
      DELZ=Z2-Z1
      IF(SIGNT(ZLOWER,ZUPPER,Z2))205,202,202
  205 CONTINUE
      A=DELX**2+DELY**2
      B=2.*(X1*DELX+Y1*DELY)
      C=X1**2+Y1**2-R1**2
      D=B*B-4.*A*C
      IF(D.GT.0.0)   GO TO 5
   52 IF(A.NE.0.0) GO TO 53
C       A VERTICAL TRAJECTORY
   54 IF(C.GE.0.0) GO TO 53
   55 CONTINUE
      C=X1**2+Y1**2-R2**2
      IF(C.LE.0.0) GO TO 53
C       IT MIGHT HIT
   56 TLOW=0.0
      TUP=.99
    6 TUP=TUP+.01
      Z=Z1+DELZ*TUP
      IF(SIGNT(ZLOWER,ZUPPER,Z)) 209,202,202
```

```
  209 CONTINUE
      IF(GOFT(TUP)) 6,2,2
    5 D=SQRT (D)
      T1=-.5*(B+D)/A
      T2=-.5*(B-D)/A
      TLOW=MAX1 (0.0,T1)
      TUP=MIN1 (1.,T2)
      IF(TLOW.GE.TUP) GO TO 53
  101  FORMAT( 1H0, 6E12.3 )
   57 CONTINUE
      C=X1**2+Y1**2-R2**2
      DESP=DES(TUP)
      IF((DES(TLOW).LE.0.).AND.(DESP.LE.0.)) GO TO 53
   58 IF(DESP      .LE.0.) GO TO 2
   59 IF(GOFT(TUP).GE.0.) GO TO 60
      GO TO 2
   60 TUP=T2
C     LIMITS ARE NOW TUP,TLOW
C     MUST NOW SOLVE EQN 17
    2 CALL TRSOL(TLOW,TUP,TR,NR)
C     NOW HAVE ALL THE ROOTS
  102 FORMAT(I5)
      IF(NR.EQ.0) GO TO 53
   61 DT=1.0
      DO 3 J=1,NR,2
    3 DT=DT+TR(J+1)-TR(J)
      XTWO=X1+DELX*DT
      YTWO=Y1*DELY*DT
      ZTWO=Z1+DELZ*DT
```

```
202 MARK=-1
    Z=ZLOWER
    IF(ZTWO.LE.ZLOWER) GO TO 203
204 Z=ZUPPER
203 T=(Z-Z1)/DELZ
    ZTWO=Z
    XTWO=X1+DELX*T
    YTWO=Y1+DELY*T
    X1=X1+DELX*(TUP+1.E-3)
    Y1=Y1+DELY*(TUP+1.E-3)
    Z1=Z1+DELZ*(TUP+1.E-3)
    GO TO 4
 53 RETURN
    END
```

```
$IBFTC TRSOLS  REF,DD,FULIST,NODECK
      SUBROUTINE TRSOL(TLOW,TUP,TR,NR)

C   UTILITY SR USED BY BOGART/WOHL VERSION OF 05R SR# GEOM (GEOMAA)

      DIMENSION TR(10)

      COMMON/CARL/CAPR,SMA,SMD,X1,Y1,Z1,DELX,

     1DELY,DELZ,OMEGA,SMB,A,B,C,DA

      EXTERNAL DES

      EXTERNAL GOFT

      DT=(TUP-TLOW)/100.

      NR=1

      TMP=TUP+DT

      T=TLOW-DT

      XK=1.

    1 CONTINUE

C     CHECK IF NEAR ORIGIN

      IF(DES(T).LE.DA) GO TO 2

    3 IF((GOFT(T)*XK).GT.0.0) GO TO 2

C     MUST HAVE PASSED A ROOT

    4 TLOT=T-DT

      TUPT=T

      CALL ITER(TLOT,TUPT,TR(NR),XK)

      XK=-XK

      NR=NR+1

    2 T=T+DT

      IF(T.LE.TMP) GO TO 1

    5 NR=NR-1

      RETURN

      END
```

```
$IBFTC ITERA    REF,DD,FULIST,NODECK
      SUBROUTINE ITER(TM1,TMA,T,XK)
C  UTILITY SR USED BY BOGART/WOHL VERSION OF 05R SR# GEOM (GEOMAA)
      EXTERNAL GOFT
      KONT=0
      TMIN=TMI
      TMAX = TMA
C     METHOD OF REGULA FALSI
      YMIN=ABS (GOFT(TMIN))
      YMAX=ABS (GOFT(TMAX))
    4 T=TMIN+(TMAX-TMIN)*YMIN/(YMAX+YMIN)
      KONT=KONT+1
      IF(KONT.GT.12) GO TO 2
    6 ARG=GOFT(T)*XK
      IF(ABS (ARG).LT.1.E-6) GO TO 2
    5 IF(ARG)1,2,3
    3 TMIN=T
      YMIN=ABS (ARG)
      GO TO 4
    1 TMAX=T
      YMAX=ABS (ARG)
      GO TO 4
    2 CONTINUE
  103 FORMAT(1H0,I5,3E12.3)
      RETURN
      END
```

```
$IBFTC GOFT     REF,DD,FULIST,NODECK
      FUNCTION GOFT(T)
C  UTILITY FUNCTION USED BY BOGART/WOHL VERSION OF 05R SR+ GEOM (GEOMAA)
      COMMON/CARL/CAPR,SMA,SMD,X1,Y1,Z1,DELX,
     1DELY,DELZ,OMEGA,SMB,A,B,C,DA
      DATA TPIE / 6.2831853/
      ARG=0.
      DZ=Z1+DELZ*T
      DX=X1+DELX*T
      DY=Y1+DELY*T
      SQR=SQRT (DX**2+DY**2)
C     SMD=0 IMPLIES OMEGA=INFINITY
      IF(SMD.EQ.0.0) GO TO 1
    2 ARG=AMOD (OMEGA*DZ,TPIE)
      CO=COS (ARG)
      SI=SIN (ARG)
      PX=DX*CO+DY*SI
      PY=-DX*SI+DY*CO
      IF ( ( PY .EQ. 0.0) .AND. ( PX .EQ. 0.0 ) ) GO TO 99
      ARG=ATAN2(PY,PX)
      GO TO 1
   99 ARG = 0.0
      WRITE( 6, 555)
  555 FORMAT( 21H PX, PY, ZERO IN G(T)     )
    1 GOFT= (SQR-CAPR)     **2+(ARG*CAPR*SMB)**2-SMA*SMA
      RETURN
      END
```

```
$IBFTC DES      REF,DD,FULIST,NODECK
      FUNCTION DES(T)

C   UTILITY FUNCTION USED BY BOGART/WOHL VERSION OF 05R SR+ GEOM (GEOMAA)

      COMMON/CARL/CAPR,SMA,SMD,X1,Y1,Z1,DELX,

     1DELY,DELZ,OMEGA,SMB,A,B,C,DA

      DES=(A*T+B)*T+C

      RETURN

      END

$IBFTC LOOKZ    REF,DD,FULIST,NODECK
      SUBROUTINE LOOKZ( X, Y, Z )

C   UTILITY FUNCTION USED BY BOGART/WOHL VERSION OF 05R SR+ GEOM (GEOMAA)

       NMED = 1

       NREG = 1

      BLZON=0.0

      RETURN

      END

$IBFTC JOMIN    REF,DD,FULIST,NODECK

      SUBROUTINE JOMIN( NADD )

C   UTILITY FUNCTION USED BY BOGART/WOHL VERSION OF 05R SR+ GEOM (GEOMAA)

      COMMON/GEOM/MARK,XTWO,YTWO,ZTWO,XONE,YONE,

     1ZONE,NMED,NREG,ETA,ETAUSD,BLZON

      NADD=0

      RETURN

      END
```

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, October 19, 1967,
126-15-01-03-22.

APPENDIX - SYMBOLS

Mathematical symbol	FORTRAN variable	Description
a	SMA	Internal radius of ducts, cm
D	DES	Discriminant of eq. (12b)
d	SMD	Pitch of helical duct, cm
$g(t)$	GOFT	$g(t)$
k		See fig. 2
l		See fig. 2
R	CAPR	Radius of cylinder around which internal duct is wound, cm
r		See fig. 2
s		See fig. 2
t		Particle track parameter
t_{low}	TLOW	Lower particle track parameter (inner circle)
t_{up}	TUP	Upper particle track parameter (outer circle, sketch (b))
x_1, y_1, z_1		Coordinates of starting point of particle path
x_2, y_2, z_2		Coordinates of termination point of particle path
Δx	DELX	Δx
Δy	DELY	Δy
Δz	DELZ	Δz
α	ALPHA	Pitch angle of helical duct, deg
β		See fig. 2
θ		See fig. 2

ω	OMEGA	Parameter specifying position of intersection of helical tube and x, y-plane
	ZLOWER	Lower-boundary z-coordinate of slab of material penetrated by void with axis of revolution in z-direction
	ZUPPER	Upper-boundary z-coordinate of slab

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