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Cavity Inventory Relationships

by

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PACER PROCESSING: CAVITY INVENTORY RELATIONSHIPS

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R. J. Dietz and L. A. Gritzo

ABSTRACT

The Pacer cavity and its associated primary power loop comprise a recirculating system in which materials are introduced by a series of thermonuclear explosions while debris is continuously removed by radioactive decay, sorption phenomena, and deliberate processing. Safe, reliable, and economical realization of the Pacer concept depends on the removal and control of both noxious and valuable by-products of the fusion reaction. In this paper, mathematical relationships are developed that describe the quantities of materials that are introduced into the Pacer cavity by a series of discrete events and are removed continuously by processing and decay. An iterative computer program based on these relationships is developed that allows both the total cavity inventory and the amounts of important individual species to be determined at any time during the lifetime of the cavity in order to establish the effects of the thermonuclear event, the cavity, the flow, and various processing parameters on Pacer design requirements.

I. INTRODUCTION

Pacer is a concept to exploit existing thermonuclear technology by utilizing the fusion energy and the neutrons produced by repetitive detonations of thermonuclear devices in a large decoupling cavity located more than a kilometer underground. The ultimate objective of the Pacer concept is to produce electrical power on a national scale, directly, by using fusion energy to drive a steam turbine power plant, as well as indirectly, by using excess fusion neutrons to produce fissile fuel for conventional nuclear power plants.

The Pacer cavity would be cooled by a working fluid, presently considered to be a high-pressure condensable gas. Circulation of this working fluid will transport materials from the cavity to cooler portions of the circulation loop where some materials will precipitate from the coolant gas. Depending on their physical and chemical properties, these precipitated materials may produce corrosive and/or erosive effects, inhibit heat transfer, and otherwise prove generally troublesome, just as they do in conventional (combustion-fired) power plants. These considerations suggest that the Pacer working fluid be confined in a primary loop to simplify the initial Pacer design and to allow conventional steam power plant components to be purchased for the secondary generating loop.

While pure-fusion devices and other advanced thermonuclear concepts now under study may eventually provide Pacer with more economical energy sources, our

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commitment to existing technology dictates that we consider fission-ignited thermonuclear devices of current design as the best source of Pacer power presently available. Safe containment of relatively high-yield, cost-effective devices of this type (approximately 20-50 kilotons) will require underground cavities comparable in size to the largest ever mined for the storage of petroleum products. Cavities of this magnitude require enormous volumes of working fluid. For example, a typical 300-m-diam Pacer cavity could contain nearly a million tonnes of dry steam at approximately 800°K and 200 atmospheres pressure.

II. PACER PROCESSING REQUIREMENTS

The debris introduced by the thermonuclear device can be controlled, within limits, by the device design, and the device debris will represent a very small fraction of the cavity volume, even if it is allowed to accumulate. There is no fundamental physical reason for removing fission products or other neutron poisons from Pacer as there is in a conventional nuclear reactor; however, operational considerations may require the removal of device debris from the Pacer power loop. Foremost among these is the probability that some debris may be carried by the working fluid as an abrasive aerosol. Additionally, the intrinsic value of the fertile and fissile debris may make their efficient recovery from the cavity essential to the economic success of Pacer.

In general, all components of the thermonuclear device will be vaporized in the exploding fireball. Extremely fine particles of mixed oxides may remain entrained in the working fluid, may agglomerate into larger particles and settle to the bottom of the cavity, or may adhere to the cavity walls. Some debris will be dissolved in the working fluid along with soluble cavity materials. Gaseous products of combustion, fission product gases, unburned deuterium and by-product tritium will exchange and mix with the working fluid and will also be carried to the surface.

In view of the complexity of the Pacer primary loop and the variety of the products it might contain, it is essential to develop the capability for determining the net inventory of contaminants introduced into the cavity by a repetitive series of Pacer events as they are simultaneously and continuously removed by both deliberate and incidental processes. The following treatment presents a preliminary solution for the problem and one that will serve as the basis for additional refinements as they are developed. This treatment has already been programmed for routine computer calculation in a manner described in the Appendix to this report.

III. PACER CAVITY RELATIONSHIPS

A number of atoms, N_o, of a species of interest is generated instantaneously by the explosion of each of a series of Pacer devices detonated at regular intervals, T_I. This material is generally removed by two first order processes: radioactive decay and the continuous recirculation and processing of a large mass of working fluid, M_o. The working fluid is a diluent for the accumulated quantity N of a particular species, which is partially removed by a natural or induced process having an efficiency for removal, ε.

At the beginning of each shot interval of duration T_I, N_o of new material is introduced (instantaneously), and the subsequent rate of removal is:

$$\left(\frac{dN}{dt}\right) = -\lambda N \qquad (1)$$

where the total first-order removal constant, λ, is the sum of the first-order decay constant λ_D and the processing constant λ_P.

$$\lambda = \lambda_D + \lambda_P \ . \tag{2}$$

In general, and for a particular fission product, λ_D should include the effects of its radioactive decay as well as its formation as the daughter product in a chain of precursor decay products. Similarly, λ_P should include all the first-order removal processes, both deliberate and incidental, that involve the species of interest. However, for simplicity, this treatment is restricted to primary formation and removal processes. The more general case will be treated in a subsequent report.

IV. THE PACER SHOT SERIES

A typical plot of the cavity inventory during a series of Pacer events is shown in Fig. 1, which also serves to establish our nomenclature for an infinite series of Pacer events. Note that after a large number of events, the Pacer inventory begins to "rachet" just below an equilibrium value, N(eq). This occurs when the amount of new material introduced by each shot, N_o, is equal to that removed during the interval between each shot, or when N is sufficiently large so that C approaches 1 in the equation:

$$N_1(n) - N_2(n) = CN_o \qquad \lim_{n\to\infty} C=1 \ . \tag{3}$$

C is the convergence factor: a measure of the extent to which $N_1(n)$ approximates the equilibrium value.

The amount of material introduced by the initial shot, and every subsequent shot, is N_o. Before the end of the first interval, T_I, and prior to the next shot:

$$N(t) = N_o e^{-\lambda t} \qquad (0<t<T_I) \tag{4}$$

which reduces, at the end of this interval, and just before the next shot, to:

$$N_2(0) = N_o e^{-\lambda T_I} \qquad (t=T_I) \ . \tag{5}$$

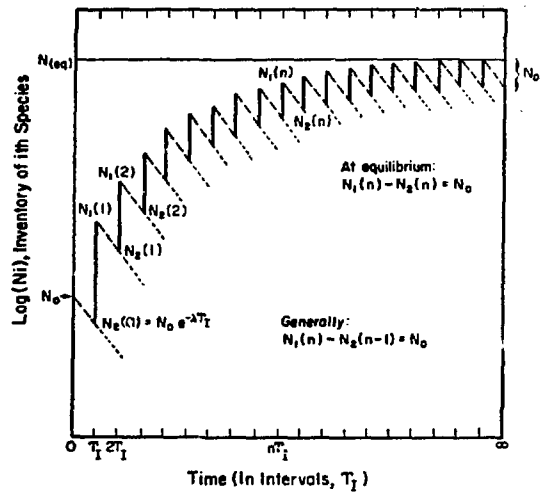


Fig. 1. Cavity inventory of a material produced by a series of Pacer events.

Similarly, in the next interval,

$$N(t) = \left(N_2(0) + N_o\right) e^{-\lambda(t-T_I)} \ , \tag{6}$$

valid over the interval $(T_I<t<2T_I)$ and

which reduces to:

$$N(t) = N_o e^{-\lambda t}\left(1 + e^{\lambda T_I}\right), \tag{7}$$

and after the nth shot to:

$$N(t) = N_o e^{-\lambda t} \sum_{n=o}^{n=j} e^{n\lambda T_I}, \tag{8}$$

valid over the interval $(jT_I<t<(j+1)T_I)$.

This general series expression is readily amenable to computer solution by the iterative techniques described in the Appendix; however, manual calculations are more conveniently performed with the equivalent equation, in closed form:

$$N(t) = N_o e^{-\lambda t}\left(\frac{1-e^{(j+1)\lambda T_I}}{1-e^{\lambda T_I}}\right) \tag{8a}$$

valid over the interval $\left(jT_I < t < (j+1)T_I\right)$.

As $n \to \infty$, $N(n) - N(n-1)$ reduces to the quasi-steady state value in Equation 3,

$$N_1(eq) - N_2(eq) = N_o \tag{3a}$$

$$N_1(eq) - N_1(eq)e^{-\lambda T_I} = N_o \quad \text{and} \tag{9}$$

$$N_1(eq) = \frac{N_o}{1 - e^{-\lambda T_I}} \tag{10}$$

The amount, N_o, of a particular material, i, introduced by each fusion event will generally be a function of the yield of the device. In the simplest case, that for an individual fission product,

$$N_{oi} = cf_iY, \tag{11}$$

where f_i is the fission fraction for the ith species, Y the fission yield of the device in kilotons (kt), and the constant c has the approximate value of 1.45×10^{23} fissions/kt. A typical example of this method of defining N_o is given in the Appendix.

V. EQUILIBRIUM APPROXIMATIONS

Equation (10) is the analytical solution for the equilibrium value for the species of interest. In fact, this value is approached asymptotically, and, for real systems of interest, very slowly. For our purposes, it has been convenient to define an arbitrary "equilibrium time" by terminating the series solution at $C \geq 0.99$. This "equilibrium" value is compared with the analytical solution of Equation (10) as a check.

For small values of λT_I, Equation (10) approaches as a limit:

$$N_1(eq) = \frac{N_o}{\lambda T_I}, \tag{12}$$

but this approximation applies to long-lived species and extremely inefficient processing -- conditions of minimal interest to the Pacer program. When $T_I \to 0$, the incremental Pacer relationships approach the value for equilibrium under continuous production conditions, described by the equilibrium expression:

$$\frac{dN(eq)}{dt} = \frac{N_o}{T_I} - \lambda N(eq) = 0 . \tag{13}$$

This solution is also a trivial one because it fails to consider the basic incremental nature of species production in Pacer and "synthesizes" an average equilibrium value that differs from the true maximum inventory possible in the Pacer cavity. The true equilibrium values will always be given by Equations (10) and (3), as illustrated in Fig. 1.

VI. THE RATE CONSTANT λ

In general, the first-order rate constant, λ, of a given species, is the sum of all first-order processes operating on that species.

$$\lambda = \sum_P \lambda_P . \tag{14}$$

In practice, however, we are mainly interested in two major depletion processes in Pacer, radioactive decay and the deliberate, or incidental, processing of continuously-circulating working fluid:

$$\lambda = \lambda_D + \lambda_P + \cdots\cdots \tag{15}$$

where the decay constant,

$$\lambda_D = -\frac{1}{N}\left(\frac{dN}{dt}\right)_D = \frac{\ln 2}{T_{\frac{1}{2}}} \tag{16}$$

for radioactive decay, and

$$\lambda_P = -\frac{1}{N}\left(\frac{dN}{dt}\right)_P \tag{17}$$

for removal by some other continuous process.

The processing efficiency, ε_i, for a continuous flow system is defined for the

ith species as the ratio of the rate of processing removal, R_p, to the rate of recirculation, R_F.

$$\epsilon_i = \frac{R_p}{R_F} = - \frac{\left(\frac{dN_i}{dt}\right)_p}{\left(\frac{dN_i}{dt}\right)_F} \tag{18}$$

$$\left(\frac{dN_i}{dt}\right)_F = F_m \cdot C_i \tag{19}$$

where F_m is the mass flow rate of the cavity contents and C_i the concentration of species i in the cavity:

$$F_m = \frac{M_o}{T_p}, \text{ and } C_i = \frac{N_i}{M_o}, \text{ where} \tag{20}$$

M_o is the mass of the cavity working fluid and T_p the processing "turn-around time": the time required to re-fill the cavity at a flow rate F_m. Substitution in Equations (17), (18), and (19) gives:

$$\left(\frac{dN_i}{dt}\right)_p = - \frac{\epsilon_i N_i}{T_p} = -\lambda_p N_i \quad \text{....and} \tag{21}$$

$$\lambda_p = \frac{\epsilon_i}{T_p} \quad . \tag{22}$$

Note that, under these conditions of recirculating flow, the removal of N_i is inherently a first-order process, regardless of the actual mechanism involved, verifying the assumptions implicit in Equations (1) ff. Generally, then

$$\lambda_i = \lambda_{D_i} + \lambda_{P_i} = \frac{\ln 2}{t_{\frac{1}{2}}} + \frac{\epsilon_i}{T_p} \quad . \tag{23}$$

Clearly, short half-lives, short processing times, and high processing efficiencies will dominate Equation (8) and its equilibrium variants. For processing times of the order of one day and processing efficiencies greater than 10%, the radioactive decay of species with half-lives greater than a few months does not contribute significantly to their removal. At the highest processing efficiencies, $\epsilon \to 100\%$, and the radioactive decay of species with half-lives longer than a week or so is equally unimportant. Such high processing efficiencies would not be generally typical of Pacer because of its characteristically enormous flow rates, low concentrations, and huge volumes, but they might be approached in the simplest of separations, such as the removal of non-condensable gases from the primary loop.

Conversely, for short-lived radioactive species, the processing efficiency must roughly exceed the reciprocal of the half-life, in days, before removal by processing becomes dominant. This consideration would lead the designer to conclude that short-lived materials and those difficult to process would best be left alone, unless their partial removal results in some direct economic benefit.

While the equilibrium values calculated here, as well as some of the approximate relationships derived from these equations, may satisfy some of the Pacer design requirements, accurate Pacer inventories, as a function of time and the number of events are best studied by the solution of Equation (8). Accordingly, we have incorporated this relationship in the PACE computer program, which follows immediately. The PACE program is currently stored in the LASL Central Computer Facility.

APPENDIX

PACE FORTRAN PROGRAM

The PACE program is written in the FORTRAN programming language for operation with the KRONOS time-sharing system. Computations were performed on a LASL CDC-6600 computer, with access via a Texas Instruments Silent 700 ASR Electronic Data Terminal.

Most of PACE is concerned with input/output, including interactive pauses, and with a print-plot subroutine (PPLOT) for graphic display of the computed results. The actual computation loop involves only the addition of the number of atoms of the particular species generated per cycle to that previously present, and the subsequent decay in the number of atoms over the time span of one cycle.

The program listed in Table A-1 is constructed in several sections:

1. An instruction section specifies how to enter new input data;
2. An initialization section derives certain quantities from the input data for future use;
3. An interactive section allows a printout of the starting variable values and the specification of the operation mode (i.e., all cycles or selected cycles for printout);
4. A computation section; and
5. A print-plot subroutine.

The input data required prior to execution of the program are given in Table A-2. These data are part of the FORTRAN program and must be present in the FORTRAN program file prior to issuance of the "RUN" command. Data derived from the input data prior to the sequential computation are given in Table A-3.

TABLE A-1

PACE FORTRAN LISTING

LASL Identification No. LP-0572

```
00100 PROGRAM PACE(INPUT,OUTPUT)
00110 DIMENSION XXX(100),YYY(100)
00120 DIMENSION ZZZ(100),TIT(5)
00122*
00124*  L. GRITZO, LASL GROUP TD-7, (505) 667-6922*
00126*
00130 PRINT,*      SEQUENTIAL COMPUTATION FOR PACER INVENTORY*
00140 PRINT 100
00142 PRINT,*                +++++ VERSION 2 ++++++
00144 PRINT 100
00150 PRINT,* ++++ WANT INSTRUCTIONS?  Y=YES, N=NO +++++
00160 READ,IT
00170 IF (IT.NE.1HY) GO TO 44
00175 PRINT 100
00180 PRINT,* IN ORDER TO CHANGE THE VALUE OF A VARIABLE FROM ITS*
00190 PRINT,* STANDARD VALUE, TYPE IN ONE OF MORE OF THE FOLLOWING:*
00200 PRINT 100
00210 PRINT,*          350 Y=(  NEW VALUE  )*
00220 PRINT,*          360 FF=       "*
00230 PRINT,*          370 THALF=    "*
00240 PRINT,*          380 EPSI=     "*
00250 PRINT,*          390 FLOW=     "*
00260 PRINT,*          400 EMZERO=   "*
00270 PRINT,*          410 BIGT=     "*
00280 PRINT,*          420 NINT=     "*
00290 PRINT,*          430 CONV=     "*
```

TABLE A-1 (cont)

```
00200 PRINT 100
00210 PRINT,* THEN TYPE "RUN".*
00320 PRINT 100
00330 STOP
00340 44 CONTINUE
00350 Y=0.0
00360 FF=0.0
00370 THALF=0.0
00380 EPS1=0.0
00390 FLOW=1.0E6
00400 EMZERO=1.0E6
00410 BIGT=1.0
00420 NINT=10
00430 CONV=0.99
00440 CTEST=1.E10
00450 PRINT 100
00460 100 FORMAT(1H )
00470 50 CONTINUE
00480 PRINT,* ++++ INPUT NAME OF SPECIES. +++++*
00490 READ,TIT(1)
00500 PRINT 100
00510 ENZERO=(1.45E23)*FF*Y
00520 CONSTD=0.693/THALF
00530 CONSTP=EPS1*FLOW/EMZERO
00540 CONS=CONSTD+CONSTP
00545 ENEQ=ENZERO/(1.-EXP(-CONS*BIGT))
00550 PRINT,* ++++ WANT OUTPUT OF STARTING VALUES?  Y=YES, N=NO +++++*
00560 READ,IT
00570 IF(IT.NE.1HY) GO TO 27
00580 PRINT 100
00590 PRINT 107
00600 107 FORMAT(20X,*INPUT PARAMETERS*)
00610 PRINT 108,Y,FF
00620 108 FORMAT(1X,*YIELD =*,F7.3,* ,T*,10X,*F. F. =*,F7.5)
00630 PRINT 109,THALF,EPS1
00640 109 FORMAT(1X,*T 1/2 =*,1PE13.5,* DAYS*,10X,*EFF. =*,0PF7.5)
00650 PRINT 110,FLOW,EMZERO
00660 110 FORMAT(1X,*FLOW =*,1PE13.5,* TONS/DAY*,10X,
00661+*EMZERO =*,E13.5,* TONS*)
00670 PRINT 111,BIGT
00680 111 FORMAT(1X,*INTERVAL TIME =*,F7.4,* DAYS*)
00690 PRINT 112,NINT
00700 112 FORMAT(1X,*MAX. NO. OF CYCLES = *,I6)
00710 PRINT 113,CONV
00720 113 FORMAT(1X,*CONVERGENCE CRITERION = *,F8.6)
00730 PRINT 100
00740 PRINT 114
00750 114 FORMAT(20X,*DERIVED QUANTITIES*)
00760 PRINT 100
00770 PRINT 115, CONSTD
00780 115 FORMAT(1X,*LAMBDA D =*,1PE14.6,* PER DAY*)
00782 PRINT 128, CONSTP
00784 128 FORMAT(1X,*LAMBDA P =*,1PE14.6,* PER DAY*)
00786 PRINT 129, CONS
00788 129 FORMAT(1X,*TOTAL LAMBDA =*,1PE14.6,* PER DAY*)
00810 PRINT 117, EMZERO
00820 117 FORMAT(1X,*EMZERO = *,1PE12.4)
00822 TAUP=EMZERO/FLOW
00824 PRINT 132,TAUP
00826 132 FORMAT(1X,*PROC. TURNOVER TIME =*,F10.4,* DAYS*)
00830 PRINT 127, ENEQ
00835 127 FORMAT(1X,*THEORETICAL EQUIL. =*,1PE14.6)
00838 PRINT 100
00840 27 CONTINUE
00850 PRINT,* ++++ WANT SPECIFIC ITERATIONS OR ALL ITERATIONS?*
00860 PRINT,*       S=SPECIFIC, A=ALL +++++*
00870 READ, ITER
00880 IF(ITER.EQ.1HA) GO TO 28
```

```
00890 PRINT,*INPUT ITERATION NUMBER DESIRED.*
00900 READ,ITNO
00910 28 CONTINUE
00920 PRINT 104
00930 104 FORMAT(//,4X,*CYCLE*,9X,*N1*,15X,*N2*,13X,*CURIES*)
00940 DIM=EXP(-CONS*BIGT)
00950 NCT=1
00960 NOT=NINT
00970 KNT=0
00980 ENR=0.0
00990 42 CONTINUE
01000 33 CONTINUE
01010 KNT=KNT+1
01020 ICT=0
01030 ENL=ENR+ENZERO
01040 ENR=ENL*DIM
01050 IF(KNT.GT.100) GO TO 36
01060 ZZZ(KNT)=ENL
01070 XXX(KNT)=KNT
01080 YYY(KNT)=ENR
01090 36 CONTINUE
01095 DECAY=CONSTD*ENR/(3.7E10*3600.*24.)
01100 DELTA=ABS(ENL-ENR)/ENZERO
01120 IF((DELTA.GE.CONV).AND.(KNT.NE.1)) ICT=1
01130 IF(ICT.EQ.1) GO TO 22
01140 CTEST=ENR
01150 IF(ITER.EQ.1HS) GO TO 31
01160 PRINT 105,KNT,ENL,ENR,DECAY
01170 105 FORMAT(2X,I5,3X,3(1PE14.5,3X))
01180 GO TO 20
01190 31 IF(KNT.EQ.ITNO) PRINT 105,KNT,ENL,ENR,DECAY
01191 DIFF=ENL-ENR
01192 IF(KNT.EQ.ITNO) PRINT 141,DIFF,DELTA
01193 141 FORMAT(10X,*N1-N2=*,1PE15.7,5X,*DELTA=*,0PF8.6)
01200 IF(KNT.NE.ITNO) GO TO 33
01210 PRINT 100
01220 PRINT,*SELECT ANOTHER ITERATION NO.*
01230 READ,ITNO
01240 IF(ITNO.EQ.0) STOP
01250 NST=KNT
01260 NOT=ITNO
01270 GO TO 33
01280 20 IF(KNT.LT.NOT) GO TO 33
01290 22 CONTINUE
01300 PRINT 100
01310 IF(ICT.NE.1) GO TO 24
01320 PRINT 106
01330 106 FORMAT(1H 5(1H+),* CONVERGENCE CRITERION MET *,5(1H+))
01335 DIFF=ENL-ENR
01340 PRINT 118,KNT,ENL,ENR
01350 118 FORMAT(1X,*CYCLE = *,I5,5X,*N1 = *,1PE12.4,6X,*N2 = *,E12.4)
01352 RESID=CONSTD*ENR/(3.7E10*3600.*24.)
01360 PRINT 100
01362 PRINT 141,DIFF,DELTA
01364 PRINT 147,RESID
01366 147 FORMAT(/,10X,*RESIDUAL ACTIVITY =*,1PE12.4,* CURIES*)
01367 ENEOCA=ENL/CONV
01368 PRINT 163
01369 163 FORMAT(/,*CONVERGENCE CHECK*,/)
01370 PRINT 164,ENEO
01371 164 FORMAT(10X,*THEO. EQ. NUMBER =*,1PE12.5)
01372 PRINT 165,ENEOCA
01373 165 FORMAT(10X,*CALC. EQ. NUMBER =*,1PE13.5)
01374 PRINT 100
01375 PRINT,* ++++ WANT A PLOT?   Y=YES, N=NO.*
01380 READ,IP
01390 IF(IP.NE.1HY) STOP
01400 CALL PPLOT(XXX,YYY,ZZZ,KNT,TIT)
01410 STOP
01420 24 CONTINUE
```

TABLE A-1 (cont)

```
01430 PRINT 100
01440 PRINT,*INPUT NUMBER OF ADDITIONAL INTERVALS DESIRED*
01450 PRINT,*    (ENTER 0 FOR STOP) *
01460 READ,NADD
01470 IF(NADD.EQ.0)STOP
01480 NOT=NOT+1
01490 NOT=NOT+NADD
01500 GO TO 42
01510 END
```

```
1520 SUBROUTINE PPLOT(X,Y,Z,N,TIT)
01530 DIMENSION X(1),Y(1),YP(52),YCAL(52)
01540 DIMENSION Z(1)
01550 DIMENSION TIT(1)
01560 IF(N.GT.100) N=100
01570 PRINT 100
01580 100 FORMAT(/,*SUBROUTINE PPLOT CALLED*,/)
01590 PRINT 142
01600 142 FORMAT(//,33X,*ACCUMULATION CURVE*)
01610 XMAX=-1.E10
01620 XMIN=1.0E35
01630 YMAX=XMAX
01640 YMIN=XMIN
01650 DO 10 I=1,N
01660 XMAX=AMAX1(XMAX,X(I))
01670 YMAX=AMAX1(YMAX,Y(I),Z(I))
01680 XMIN=AMIN1(XMIN,X(I))
01690 10 YMIN=AMIN1(YMIN,Y(I),Z(I))
01692 XMIN=AMIN1(XMIN,0.0)
01694 YMIN=AMIN1(YMIN,0.0)
01700 YAVE=0.5*(YMAX+YMIN)
01710 XAVE=0.5*(XMAX+XMIN)
01720 EN=AMAX0(N,100)
01730 XINT=(XMAX-XMIN)/EN
01740 YINT=(YMAX-YMIN)/50.0
01750 J=1
01760 DO 40 I=1,N
01770 40 IF(X(I).EQ.XMIN) J=I
01780 XSV=X(1)
01790 YSV=Y(1)
01800 ZSV=Z(1)
01810 X(1)=X(J)
01820 Y(1)=Y(J)
01830 Z(1)=Z(J)
01840 X(J)=XSV
01850 Y(J)=YSV
01860 Z(J)=ZSV
01870 45 KT=0
01880 DO 50 I=2,N
01890 IF(X(I).GE.X(I-1)) GO TO 49
01900 XSV=X(I-1)
01910 YSV=Y(I-1)
01920 ZSV=Z(I-1)
01930 X(I-1)=X(I)
01940 Y(I-1)=Y(I)
01950 Z(I-1)=Z(I)
01960 X(I)=XSV
01970 Y(I)=YSV
01980 Z(I)=ZSV
01990 KT=1
02000 49 CONTINUE
02010 50 CONTINUE
02020 IF(KT.NE.0) GO TO 45
02030 DO 60 I=1,51
```

TABLE A-1 (cont)

```
02040 60 YP(I)=1H+
02050 DO 61 I=1,51,5
02060 61 YP(I)=1HI
02070 PRINT 140, TIT(1)
02072 140 FORMAT(//,10X,*ORDINATE: NUMBER OF ATOMS OF *,
02073+A10,* PRESENT*)
02074 PRINT 143
02076 143 FORMAT(10X,*ABCISSA: CYCLE NUMBER*,//)
02090 PRINT 150, YMIN,YAVE,YMAX
02100 150 FORMAT(10X,1PE10.3,15X,E10.3,15X,E10.3)
02110 PRINT 110,XMIN,(YP(I),I=1,51)
02120 110 FORMAT(/,2X,1PE10.3,4X,51A1)
02130 NN=EN
02140 NN2=EN/2.0
02150 DO 62 I=1,51
02160 62 YCAL(I)=YMIN+FLOAT(I-1)*YINT
02170 DO 75 I=1,NN
02180 DO 64 L=1,51
02190 64 YP(L)=1H
02200 YP(1)=1H.
02210 KTEST=MOD(I,5)
02220 IF(KTEST.EQ.0) YP(1)=1H-
02230 XDN=XMIN+FLOAT(I-1)*XINT
02240 XUP=XDN+XINT
02250 DO 70 J=1,N
02255 IF((X(J).LE.XDN).OR.(X(J).GT.XUP)) GO TO 69
02260 DO 68 K=2,51
02265 YDN=YCAL(K-1)
02270 YUP=YCAL(K)
02275 PQ1=0
02280 PQ2=0
02285 IF((Y(J).GE.YDN).AND.(Y(J).LT.YUP)) PQ1=1
02290 IF((Z(J).GE.YDN).AND.(Z(J).LT.YUP)) PQ2=1
02300 IF(PQ1.EQ.1) YP(K)=1H+
02302 IF(PQ2.EQ.1) YP(K)=1H*
02304 IF((PQ1.EQ.1).AND.(PQ2.EQ.1)) YP(K)=1HP
02310 68 CONTINUE
02320 69 CONTINUE
02330 70 CONTINUE
02340 IF(I.NE.NN2) GO TO 85
02350 PRINT 170,XAVE,(YP(L),L=1,51)
02360 170 FORMAT(1X,1PE10.3,4X,51A1)
02370 GO TO 74
02380 85 IF(I.NE.NN) GO TO 73
02390 PRINT 160,XMAX,(YP(L),L=1,51)
02400 160 FORMAT(1X,1PE10.3,4X,51A1)
02410 GO TO 74
02420 73 CONTINUE
02430 PRINT 120,(YP(L),L=1,51)
02440 120 FORMAT(15X,51A1)
02450 74 CONTINUE
02460 75 CONTINUE
02470 DO 88 I=1,51
02480 YP(I)=1H+
02490 88 IF(MOD(I,5).EQ.1) YP(I)=1HI
02500 PRINT 175,(YP(L),L=1,51)
02510 175 FORMAT(16X,51A1)
02520 PRINT 130
02530 130 FORMAT(//,*EXECUTION OF PPLOT COMPLETE*,///)
02540 RETURN
02550 END
```

TABLE A-2

INPUT VARIABLES

Symbol	FORTRAN Variable Name	Explanation
Y	Y	Yield of source device (kt)
f	FF	Fractional fission yield of isotope
$t_{1/2}$	THALF	Half-life of isotope (days)
ε	EPSI	Processing efficiency
F_M	FLOW	Processing flow rate (tons/day)
M_o	EMZERO	Cavity fluid mass (tons)
T_I	BIGT	Source reloading time (days)
n	NINT	Number of cycles desired in "print all" mode before Pause occurs (usually 100)
C	CONV	Convergence criterion (see text, usually 0.99-0.999)

TABLE A-3

DERIVED QUANTITIES

Symbol	FORTRAN Variable Name	Explanation
λ_D	CONSTD	Decay constant (per day)
λ_P	CONSTP	Decay-equivalent of processing rate, $\lambda P = \varepsilon F/M_o$ (per day)
λ	CONS	Total effective decay constant, $\lambda = \lambda_D + \lambda_P$ (per day)
N_o	ENZERO	Number of atoms added per cycle, $N_o = 1.45 \times 10^{23}\ fY$
T_P	TAUP	Processing turnover time, $T_P = M_o/F_M$ (days)
$N(eq)$	ENEQ	Theoretical equilibrium no. of atoms, $N_1(eq) = \dfrac{N_o}{1 - e^{-\lambda T_I}}$

For the purpose of illustration, an arbitrary test problem is included here for which the assumed input data are:

$Y = 5$ kt

$f = 0.065$

$t_{1/2} = 3000$ days

$\varepsilon = 0.1$

$F_M = 10^6$ tons/day

$M_o = 10^6$ tons

$T_I = 1$ day

$n = 10$

$C = 0.99$

The species name is FAKE-303. Output listings are given in Tables A-4 and A-5. Table A-4 contains the output for the case where instructions, specific iterations, and a plot are requested. Table A-5 contains the output for the case where only a printout of each iteration (leading to convergence) is requested. In both tables, the items underlined are those supplied by the user.

The central processer (CP) time used by PACE is minimal; the examples of Tables A-4 and A-5 used less than 3.5 seconds total, including two compilations and assemblies. Fairly long sessions, with many executions of the program, may consume half a minute of CP time.

TABLE A-4

OUTPUT OF PACE
Case 1

```
FOR.OLD.JACK
READY.

RUN

 75/05/05. 15.05.33.
PROGRAM   JACK

     SEQUENTIAL COMPUTATION FOR PACER INVENTORY

                +++++ VERSION 2 +++++

 ++++ WANT INSTRUCTIONS?  Y=YES, N=NO ++++
? Y

 IN ORDER TO CHANGE THE VALUE OF A VARIABLE FROM ITS
 STANDARD VALUE, TYPE IN ONE OF MORE OF THE FOLLOWING:

          350 Y=   NEW VALUE
          360 FF=        "
          370 THALF=     "
          380 EPSI=      "
          390 FLOW=      "
          400 EMZERO=    "
          410 BIGT=      "
          420 NINT=      "
          430 CONV=      "

 THEN TYPE "RUN".

    STOP

CP        1.618 SECS.

RUN COMPLETE.

350 Y=5.0
360 FF=0.065
370 THALF=3000.0
380 EPSI=0.1
390 FLOW=1.E6
400 EMZERO=1.E6
410 BIGT=1.0
420 NINT=10
430 CONV=0.99
RUN

 75/05/05. 15.08.13.
PROGRAM   JACK

     SEQUENTIAL COMPUTATION FOR PACER INVENTORY

                +++++ VERSION 2 +++++

 ++++ WANT INSTRUCTIONS?  Y=YES, N=NO ++++
? N

 ++++ INPUT NAME OF SPECIES. ++++
? FAKE-303

 ++++ WANT OUTPUT OF STARTING VALUES?  Y=YES, N=NO ++++
? Y
```

TABLE A-4

OUTPUT OF PACE
Case 1 (cont)

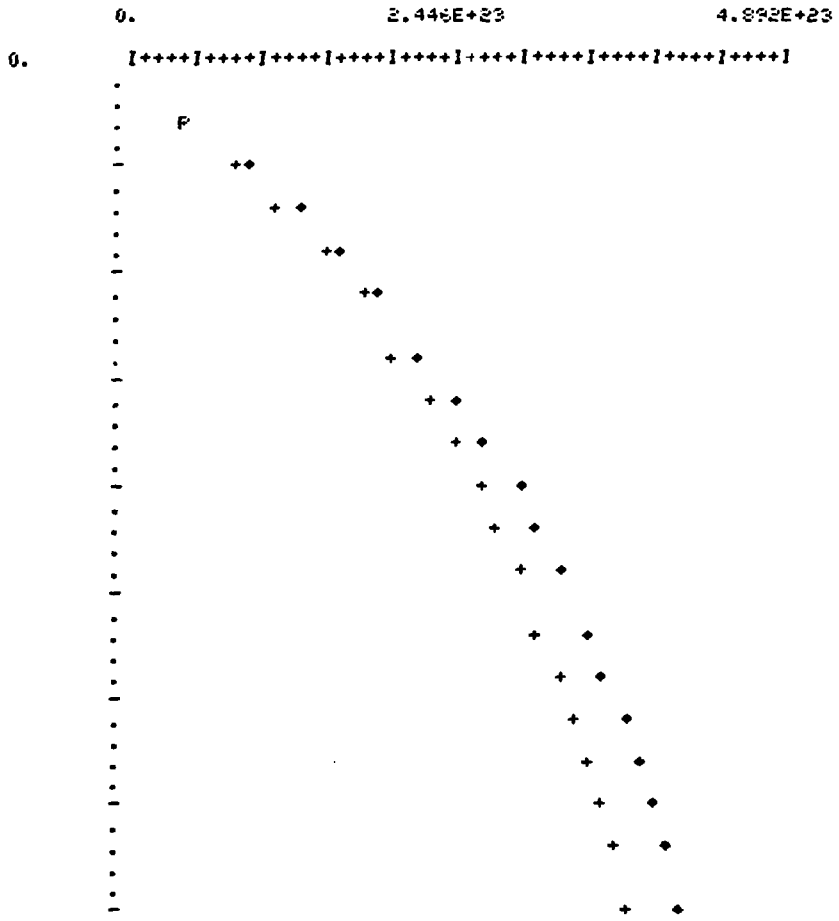
```
                    INPUT PARAMETERS
 YIELD =  5.000 KT            F. F. = .06500
 T 1/2 =  3.00000E+03 DAYS          EFF. = .10000
 FLOW =  1.00000E+06 TONS/DAY          ENZERO =  1.00000E+06 TONS
 INTERVAL TIME = 1.0000 DAYS
 MAX. NO. OF CYCLES =     10
 CONVERGENCE CRITERION =  .990000

                    DERIVED QUANTITIES

 LAMBDA D =  2.310000E-04 PER DAY
 LAMBDA P =  1.000000E-01 PER DAY
 TOTAL LAMBDA =  1.002310E-01 PER DAY
 ENZERO =   4.7125E+22
 PROC. TURNOVER TIME =    1.0000 DAYS
 THEORETICAL EQUIL. =  4.941200E+23

 ++++ WANT SPECIFIC ITERATIONS OR ALL ITERATIONS?
      I=SPECIFIC, A=ALL ++++
? I
INPUT ITERATION NUMBER DESIRED.
? 1

    CYCLE          N1                N2              CURIES
      1       4.71250E+22       4.26306E+22       3.08048E+03
          N1-N2=  4.4943855E+21      DELTA= .095372

SELECT ANOTHER ITERATION NO.
? 7
      7       2.49144E+23       2.25382E+23       1.62861E+04
          N1-N2=  2.3761227E+22      DELTA= .504217

SELECT ANOTHER ITERATION NO.
? 30
     30       4.69689E+23       4.24894E+23       3.07027E+04
          N1-N2=  4.4794987E+22      DELTA= .950557

SELECT ANOTHER ITERATION NO.
? 90

 +++++ CONVERGENCE CRITERION MET +++++
 CYCLE =    46      N1 =   4.8921E+23       N2 =   4.4255E+23

          N1-N2=  4.6656314E+22      DELTA= .990054

          RESIDUAL ACTIVITY =  3.1979E+04 CURIES

CONVERGENCE CHECK

          THEO. EQ. NUMBER =  4.94120E+23
          CALC. EQ. NUMBER =  4.94147E+23

 ++++ WANT A PLOT?   Y=YES, N=NO.
? Y

SUBROUTINE PPLOT CALLED
```

TABLE A-4

OUTPUT OF PACE
Case 1 (cont)

ACCUMULATION CURVE

ORDINATE: NUMBER OF ATOMS OF FAKE-303 PRESENT
ABCISSA: CYCLE NUMBER



(Plot Terminated)

TABLE A-5

OUTPUT OF PACE
Case 2

```
RUN

 75/05/05. 15.15.47.
PROGRAM   JACK

     SEQUENTIAL COMPUTATION FOR PACEP INVENTORY

                +++++ VERSION 2 +++++

 ++++ WANT INSTRUCTIONS?  Y=YES, N=NO ++++
? N

 ++++ INPUT NAME OF SPECIES. ++++
? FAKE-303

 ++++ WANT OUTPUT OF STARTING VALUES?  Y=YES, N=NO ++++
? N
 ++++ WANT SPECIFIC ITERATIONS OR ALL ITERATIONS?
      S=SPECIFIC, A=ALL ++++
? A
```

CYCLE	N1	N2	CURIES
1	4.71250E+22	4.26306E+22	3.08048E+03
2	8.97556E+22	8.11955E+22	5.86717E+03
3	1.28320E+23	1.16082E+23	8.38808E+03
4	1.63207E+23	1.47642E+23	1.06686E+04
5	1.94767E+23	1.76192E+23	1.27316E+04
6	2.23317E+23	2.02019E+23	1.45978E+04
7	2.49144E+23	2.25382E+23	1.62861E+04
8	2.72507E+23	2.46518E+23	1.78133E+04
9	2.93643E+23	2.65638E+23	1.91949E+04
10	3.12763E+23	2.82934E+23	2.04448E+04

```
INPUT NUMBER OF ADDITIONAL INTERVALS DESIRED
   (ENTER 0 FOR STOP)
? 20
```

11	3.30059E+23	2.98581E+23	2.15754E+04
12	3.45706E+23	3.12735E+23	2.25982E+04
13	3.59860E+23	3.25540E+23	2.35234E+04
14	3.72665E+23	3.37123E+23	2.43604E+04
15	3.84248E+23	3.47602E+23	2.51176E+04
16	3.94727E+23	3.57081E+23	2.58026E+04
17	4.04206E+23	3.65656E+23	2.64222E+04
18	4.12781E+23	3.73414E+23	2.69828E+04
19	4.20539E+23	3.80431E+23	2.74899E+04
20	4.27556E+23	3.86780E+23	2.79486E+04
21	4.33905E+23	3.92522E+23	2.83636E+04
22	4.39647E+23	3.97718E+23	2.87390E+04
23	4.44843E+23	4.02417E+23	2.90786E+04
24	4.49542E+23	4.06669E+23	2.93858E+04
25	4.53794E+23	4.10515E+23	2.96637E+04
26	4.57640E+23	4.13994E+23	2.99151E+04
27	4.61119E+23	4.17141E+23	3.01425E+04
28	4.64266E+23	4.19988E+23	3.03483E+04
29	4.67113E+23	4.22564E+23	3.05344E+04
30	4.69689E+23	4.24894E+23	3.07027E+04

TABLE A-5

OUTPUT OF PACE
Case 2 (cont)

```
INPUT NUMBER OF ADDITIONAL INTERVALS DESIRED
   (ENTER 0 FOR STOP)
? 20
     31      4.72019E+23      4.27002E+23      3.08551E+04
     32      4.74127E+23      4.28909E+23      3.09928E+04
     33      4.76034E+23      4.30634E+23      3.11175E+04
     34      4.77759E+23      4.32194E+23      3.12302E+04
     35      4.79319E+23      4.33606E+23      3.13322E+04
     36      4.80731E+23      4.34883E+23      3.14245E+04
     37      4.82008E+23      4.36038E+23      3.15080E+04
     38      4.83163E+23      4.37083E+23      3.15835E+04
     39      4.84208E+23      4.38028E+23      3.16518E+04
     40      4.85153E+23      4.38883E+23      3.17136E+04
     41      4.86008E+23      4.39657E+23      3.17695E+04
     42      4.86782E+23      4.40357E+23      3.18201E+04
     43      4.87482E+23      4.40990E+23      3.18658E+04
     44      4.88115E+23      4.41563E+23      3.19072E+04
     45      4.88688E+23      4.42081E+23      3.19446E+04

 +++++ CONVERGENCE CRITERION MET +++++
 CYCLE =    46      N1 =   4.3921E+23      N2 =   4.4255E+23

          N1-N2=  4.6656314E+22      DELTA= .990054

          RESIDUAL ACTIVITY =  3.1979E+04 CURIES

CONVERGENCE CHECK

          THEO. EQ. NUMBER =  4.94120E+23
          CALC. EQ. NUMBER =  4.94147E+23

 ++++ WANT A PLOT?   Y=YES, N=NO.
? N
   STOP

CP        1.839 SECS.

RUN COMPLETE.
```