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Abstract

A computer code, RAPTOR, has been developed to estimate the transport of activated material throughout a fusion reactor heat transfer and/or tritium breeding material loop. A method is devised which treats the components of the heat transfer/tritium breeding loop separately and determines the source rates, deposition and erosion rates, decay rates, and purification rates. A matrix operator method is employed to solve the resulting coupled linear differential equations as a function of time. A user's guide is also supplied.

I. Introduction

The calculation of the transport of radioactive materials throughout the heat transfer/tritium breeding medium of fusion reactors is important for a number of applications. Health physics considerations are likely to determine the accessibility of major reactor components for maintenance and repair operations. If the radiation fields around these components reach levels which preclude direct personnel involvement, then remote handling and maintenance techniques must be devised. Also, the amount of radioactive material entrained in the heat transfer/tritium breeding fluid and distributed throughout the system will be important in the event that this fluid ever is released during an abnormal event or accident. These calculations should also determine some of the waste handling capabilities which will be required during operation.

The RAPTOR computer code was written to assess the transport of activation products throughout the tritium breeding/heat transfer system of fusion reactors.[1] It is able to calculate the time dependent buildup and decay of 9 radioactive isotopes through 15 different nuclear reactions. This report is written to describe the code in its present form, and to provide a user's guide of the input files and parameters necessary for its use.

RAPTOR is written in FORTRAN and runs on the CRAY-1 machines in use by the National Magnetic Fusion Energy Computer Center (NMFECC) based in Livermore, California. It is entirely selfcontained, except for the use of the DISSPLA graphics package in use at NMFECC [2]. The built-in differential equation solution routine used is that of Lee *et al*. [3].

II. Transport Modeling

II.A. Activation Product Transport Model

A general description of the theory of corrosion product generation, dispersion, and transport was proposed by Bartlett [4], and others have applied this to a number of fission reactor systems [5-7]. The present work takes similar ideas and formulates them in terms applicable to a fusion reactor system. A more complete treatment of the problem can be seen in reference 1.

Before listing the equations used to describe the model it is important to state some of the assumptions on which it is based. First, it is assumed that the coolant is completely mixed and that variations in the concentration of the activation products in the loop are small. Second, the assumption is made that the concentrations are so small as to have no effect on fluid flow characteristics, neutron fluxes, or the heat transfer properties of the system. Also, it can be assumed that the nuclear reactions occur in the form of simple pairs, such that

$$\begin{matrix}\text{stable}\\ \text{isotope}\end{matrix}\quad (n,\text{reaction})\quad \begin{matrix}\text{active}\\ \text{isotope}\end{matrix}\quad \xrightarrow[\text{decay}]{}$$

In this way, production reactions are modeled individually, necessitating the calculation of each one of the important reactions independently. Table 1 lists the reactions currently considered.

It is possible, then, to construct a model of the plant system which will account for the mass transport of the stable and radioactive corrosion and sputtering products throughout the coolant/tritium

TABLE 1

Activation Products Considered by RAPTOR

Formation Reaction	Activation Product	Half-life	Gamma Energies (MeV)
^{59}Co(n,γ) ^{60}Ni(n,p)	^{60}Co	5.26 y	1.173, 1.332
^{58}Ni(n,p) ^{59}Co(n,2n)	^{58}Co	71.3 d	0.511, 0.81, 0.865, 1.67
^{54}Fe(n,P) ^{55}Mn(n,2n)	^{54}Mn	303 d	0.835
^{50}Cr(n,γ) ^{52}Cr(n,2n) ^{54}Fe(n,α)	^{51}Cr	27.8 d	0.32
^{55}Mn(n,γ)	^{56}Mn	2.6 h	0.847, 1.811, 2.11
^{58}Fe(n,γ) ^{59}Co(n,p)	^{59}Fe	45.6 d	0.143, 0.192, 1.095, 1.292
^{64}Ni(n,γ)	^{65}Ni	2.6 h	0.368, 1.115, 1.481
^{92}Mo(n,γ)	^{93}Mo	6.9 h	0.264, 0.685, 1.479
^{98}Mo(n,γ)	^{99}Mo	66.7 h	0.181, 0.372, 0.74, 0.78

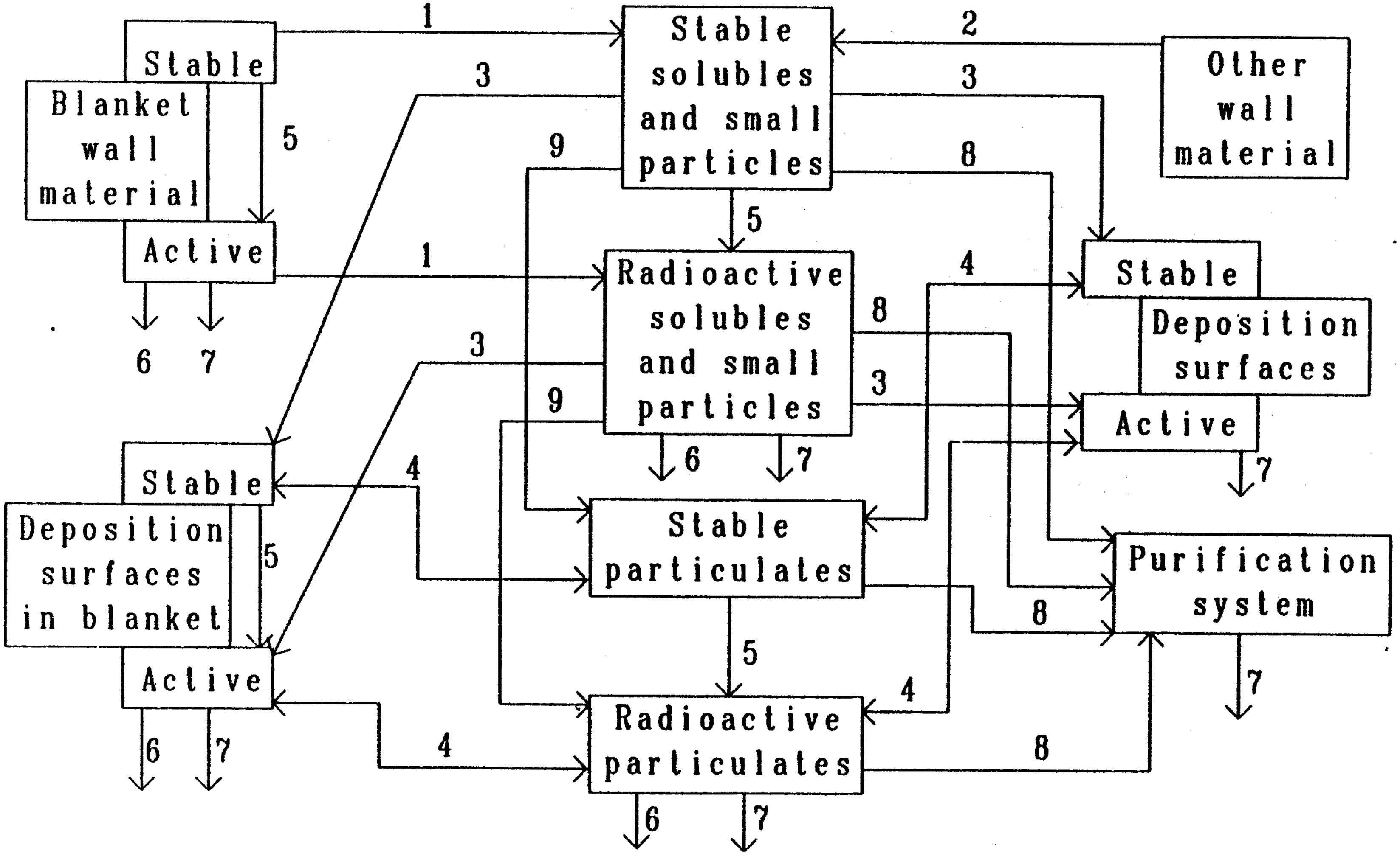
breeding loop. It is necessary to model the many different transport phenomena so that an understanding of the problem can be obtained. The sources of stable and radioactive materials must be included as well as the mechanisms for removal of the activation products from the coolant stream by deposition on component surfaces and by the cleanup and purification system. The erosion of the deposited material by the heat transfer fluid must also be considered. By including nuclear reactions and radioactive decay the activation product transport model can take the form of figure 1. It is important to note from this figure that the in-coolant corrosion and activation products are assumed to exist in two components:

(1) dissolved material and small particles (on the order of a few atoms in diameter), or

(2) agglomerations of the smaller species into large particles (about 0.01 to 10 μm in diameter).

Once material is released from the plant components into the coolant/tritium breeding fluid it is subject to a number of transport processes. These include each species in the fluid depositing on component surfaces throughout the loop, forming agglomerates with other particles, or being removed by the purification system. Stable isotopes in the blanket walls, flowing through the blanket in the fluid, or deposited in the blanket region can undergo a nuclear reaction and become radioactive. Radioactive isotopes throughout the system will decay and then no longer be considered by the model.

Once all of these processes are described, and the mechanisms of transport are defined, mass balance equations of the concentrations



ACTIVATION PRODUCT TRANSPORT MODEL

Figure 1. Activation product transport model.

LEGEND

Figure 1

1. Corrosion, erosion, and neutron sputtering
2. Corrosion and erosion
3. Deposition
4. Deposition and erosion
5. Activation
6. Removal
7. Decay
8. Cleanup removal
9. Agglomeration

of material in the fluid and deposited on the system surfaces can be written. The deposits on each plant component are treated separately and each nuclear reaction requires individual attention. The amounts of material deposited and the concentrations of both stable and radioactive isotopes in the coolant/tritium breeding system are considered as a function of time.

For the stable solubles and small particles in the fluid

$$\begin{aligned}\frac{\partial C_{SS}}{\partial t} = {} & \sum_{i=1}^{I} S_{SS}^{i}(t) - \sum_{i=1}^{I} k_{Si} \frac{A_i}{V} C_{SS} \\ & - \sum_{i_f=1}^{I_f} \sum_{n=1}^{NG} f_{i_f} \sigma_{nt}^{i_f} \phi_n^{i_f} C_{SS} - b_c \frac{A_c}{V} C_{SS} \\ & - \sum_{i=1}^{I} g_i C_{SS}\end{aligned} \tag{1}$$

For the radioactive solubles and small particles in the fluid

$$\begin{aligned}\frac{\partial C_{AS}}{\partial t} = {} & \sum_{i=1}^{I} S_{AS}^{i}(t) - \sum_{i=1}^{I} k_{Si} \frac{A_i}{V} C_{AS} - \sum_{i_f=1}^{I_f} \sum_{n=1}^{NG} f_{i_f} \sigma_{nt}^{i_f} \phi_n^{i_f} C_{AS} - \lambda C_{AS} \\ & + \sum_{i_f=1}^{I_f} P_A^{i_f} N_A + \sum_{i_f=1}^{I_f} \sum_{n=1}^{NG} f_{i_f} \sigma_{nr}^{i_f} \phi_n^{i_f} C_{SS} - \sum_{i=1}^{I} g_i C_{AS} - b_c \frac{A_c}{V} C_{AS}\end{aligned} \tag{2}$$

For the stable agglomerates in the fluid

$$\frac{\partial C_{SP}}{\partial t} = \sum_{i=1}^{I} g_i C_{SS} + \sum_{i=1}^{I} e_i \frac{A_i}{V} W_{Si} - \sum_{i=1}^{I} k_{Pi} \frac{A_i}{V} C_{SP}$$

$$- b_c \frac{A_c}{V} C_{SP} - \sum_{i_f=1}^{I_f} \sum_{n=1}^{NG} f_{i_f} \sigma_{nt}^{i_f} \phi_n^{i_f} C_{SP} \qquad (3)$$

For the radioactive agglomerates in the fluid

$$\frac{\partial C_{AP}}{\partial t} = \sum_{i=1} g_i C_{AS} + \sum_{i=1}^{I} e_i \frac{A_i}{V} W_{Si} - \sum_{i=1}^{I} k_{pi} \frac{A_i}{V} C_{AP}$$

$$- b_c \frac{A_c}{V} C_{AP} - \sum_{i_f=1}^{I_f} \sum_{n=1}^{NG} f_{i_f} \sigma_{nt}^{i_f} \phi_n^{i_f} C_{AP} \qquad (4)$$

$$+ \sum_{i_f=1}^{I_f} \sum_{n=1}^{NG} f_{i_f} \sigma_{nr}^{i_f} \phi_n^{i_f} C_{SP} - \lambda C_{AP}$$

For stable deposits, for each reactor system node i in the reactor blanket

$$\frac{\partial W_{Ai}}{\partial t} = k_{Si_f} C_{SS} + k_{Pi_f} C_{SP} - e_{i_f} W_{Si}^{f}$$

$$- \sum_{n=1}^{NG} f_{i_f} \sigma_{nt}^{f} \phi_n^{i_f} W_{Si}^{f} \qquad (5)$$

For radioactive deposits, for each reactor system node i in the reactor blanket

$$\frac{\partial W_{Ai}^{f}}{\partial t} = k_{Si_f} C_{AS} + k_{Pi_f} C_{AP} - e_{i_f} W_{Ai}^{f} - \lambda W_{Ai}^{f}$$

$$+ \sum_{n=i}^{NG} \sigma_{nr}^{i_f} \phi_n^{i_f} W_{Si}^{f} - \sum_{n=1}^{NG} \sigma_{nt}^{i_f} \phi_n^{i_f} W_{Ai}^{f} \qquad (6)$$

For stable deposits, for each reactor system node i out of the reactor blanket

$$\frac{\partial W_{Si}}{\partial t} = k_{Si} C_{SS} + k_{Pi} C_{SP} - e_i W_{Si} \qquad (7)$$

For radioactive deposits, for each reactor system node i out of the reactor blanket

$$\frac{\partial W_{Ai}}{\partial t} = k_{Si} C_{AS} + k_{Pi} C_{AP} - e_i W_{Ai} - \lambda W_{Ai} \qquad (8)$$

For stable isotopes in the cleanup and purification system

$$\frac{\partial W_{SC}}{\partial t} = b_c (C_{SS} + C_{SP}) \qquad (9)$$

For radioactive isotopes in the cleanup and purification system

$$\frac{\partial W_{AC}}{\partial t} = b_c (C_{AS} + C_{AP}) - \lambda W_{AC} \qquad (10)$$

Where the notation used is summarized in Table 2.

Additionally, there is the activation of the base metal prior to release into the coolant stream. Over the lifetime of

TABLE 2

Summary of the Notation Used in Equations 1-11

C_{SS} - Concentration of stable solubles and small particles in fluid, atoms/cm^3.

C_{AS} - Concentration of radioactive solubles and small particles in the fluid, atoms/cm^3.

C_{SP} - Concentration of stable agglomerates in the fluid, atoms/cm^3.

C_{AP} - C_{AP} concentration of radioactive agglomerates in the fluid, atoms/cm^3.

W_{Si} - stable deposits for each system node i, atoms/cm^2.

W_{Ai} - radioactive deposits for each system node i, atoms/cm^2.

W_{Sc} - concentration of stable deposits in the cleanup and purification system, atoms/cm^2.

W_{Ac} - concentration of radioactive deposits in the cleanup and purification system, atoms/cm^2.

W_{Si}^{f} - stable deposits for each reactor system node i_f in the neutron flux, atoms/cm^2.

W_{Ai}^{f} - radioactive deposits for each reactor system node i_f in the neutron flux, atoms/cm^2.

N_{Ai} - concentration of radioactive nuclides in the blanket wall material for node i, atoms/cm^3.

$S_{SS}^{i}(t)$ - source rate of stable solubles and small particles from the surface of node i due to corrosion, wear, and neutron

TABLE 2 (continued)

Summary of the Notation Used in Equations 1-11

sputtering, atoms/cm^3 sec.

k_{Si} - deposition coefficient for the solubles and small particles in node i, cm/sec.

k_{pi} - deposition for agglomerates in node i, cm/sec.

e_i - erosion coefficient for node i, sec^{-1}.

g_i - agglomeration coefficient in node i, sec^{-1}.

b_c - cleanup removal coefficient, sec^{-1}.

λ - decay constant for the radioactive isotope, sec^{-1}.

$P_A^{i_f}$ - release coefficient for the radioactive wall material into the fluid, sec^{-1}.

$\phi_n^{i_f}$ - neutron flux in energy group n, in blanket node i_f, cm^2.

$\sigma_{nt}^{i_f}$ - total reaction cross section in blanket node i_f for neutron energy group n, cm^2.

$\sigma_{nr}^{i_f}$ - formation reaction cross section for node i_f in neutron energy group n, cm^2.

f_{i_f} - fraction of the total coolant flow which passes through blanket node i_f.

A_i - surface area of node i exposed to fluid, cm^2.

V_i - volume of node i, cm^3.

V - total system volume, cm^3.

TABLE 2 (continued)

Summary of the Notation Used in Equations 1-11

NG - total number of neutron groups.

l - total number of system nodes.

l_f - total number of blanket nodes.

a typical reactor blanket this provides a significant source of radioactive corrosion and sputtering products into the heat transfer/breeding system. For each system node that is in the neutron flux the concentration of active nuclides in the wall material is

$$\frac{\partial N_A}{\partial t} = \sum_{n=1}^{NG} \sigma_{nr}^{i_f} \phi_n^{i_f} N_S - \lambda N_A - P_A^{i_f} N_A \qquad (11)$$

The set of equations above provides a general treatment of the activation product transport problem in terms of the layout of the plant heat transfer/tritium breeding system as long as the transfer coefficients can be determined. In most cases, and especially during steady state power operation, the coefficients will be independent of time. In general the equations can be combined into a matrix notation of the form

$$\frac{\partial \vec{M}(t)}{\partial t} = \underset{\sim}{A}(t)\vec{M}(t) + \vec{S}(t) \qquad (12)$$

where the concentration and wall deposit vector is defined as

$$\vec{M}(t) = \left\{ \begin{matrix} C_{SS} \\ C_{AS} \\ C_{SP} \\ C_{AP} \\ W_{Si} \\ W_{Ai} \end{matrix} \right\}$$

The source vector is defined as

$$S(t) = \begin{Bmatrix} S_{SS}^{i}(t) \\ S_{AS}^{i}(t) \\ 0 \end{Bmatrix}$$

and the transfer matrix $\underset{\sim}{A}$ is a square matrix including the various transfer coefficients. Note that since direct transfer is not possible between the deposits of one node and the deposits of any other nodes the transfer matrix will be relatively sparse. This system of first order differential equations will be solved using the matrix operator method described by Lee et. al. [3].

As indicated by this description of the activation product transport model, the process of corrosion and release of the base metal into the coolant/tritium breeding fluid is treated as a source term in the equations. Experimentally determined release rates have been used to provide for the introduction of material into the system. No attempt has been made to include the mechanisms of corrosion product release in the model. Rather, it has been assumed here that material is constantly added to the system through corrosion, wear, and neutron sputtering, and that particle formation and transport are the dominant mechanisms of mass transfer. Such assumptions have proven useful in a number of studies involving activation product transport in fission reactors [5-7]. If, for a particular reactor system, other processes are found to be the dominant mass transfer mechanisms, then the transfer coefficients could be modified to accurately reflect this change.

II.B. Determination of Transport Equation Terms

Inherent in the modeling of the activation product transport is the determination of the various coefficients in the transfer matrix as well as the sources of both stable and radioactive isotopes into the coolant/tritium breeding fluid. The two ways corrosion and activation products enter the coolant stream are corrosion or wear, and neutron sputtering. Various system parameters have a strong effect upon the introduction rates, including coolant type and chemistry, base material type, temperature, coolant flow rate, neutron flux, and the coolant velocity.

The corrosion release rate expressions used in RAPTOR have been developed using data from a number of sources. Recent data from Argonne and Oak Ridge for the corrosion weight loss by stainless steels in LiPb have been very helpful [8-10]. For the interactions of water with reactor structural materials, data from Berry [11] and from Cohen [12] have been useful. This data has been organized so that temperature dependent release rate expressions can be used in RAPTOR. Most of the weight loss data shows a linear dependence with time, so that the release rate can be taken as a constant. However, a parabolic time dependence has been seen in the weight loss data for 316 stainless steel in contact with LiPb. This has been treated by breaking the time dependence into three segments (i.e., 0 to 1 month, 1 to 5 months, and 5 months on) and then determining a characteristic constant release rate expression over these time intervals. The resulting release rate expressions in water are:

for 316 SS, 304 SS, HT-9, and PCA

$$1.59 \times 10^{-14} \exp(0.0046\ T(^\circ K))\ \text{cm/sec},$$

for Inconel 600 (steam generators and heat exchangers)

$0.62 \times 10^{-10} \exp(-0.0096\ T(°K))$ cm/sec,

for Haynes-Stellite 25 (pump seals and bearings)

9.0×10^{-12} cm/sec.

Note that the Haynes-Stellite 25 release rate was assumed to be constant because little data was found, and the assumed release rate for the zirconium alloys used for fission reactor fuel rods was zero. The release rate expressions used for LiPb are:

for 316 SS, 304 SS, and PCA -- from 0 to 1 month

$1.6 \times 10^{-21} \exp(0.037\ T(°K))$ cm/sec

-- from 1 to 5 months

$2.02 \times 10^{-21} \exp(0.0345\ T(°K))$ cm/sec

-- from 5 months on

$1.05 \times 10^{-13} \exp(0.0075\ T(°K))$ cm/sec

for HT-9 at all times

$2.99 \times 10^{-16} \exp(0.0158\ T(°K))$ cm/sec

Note that no data was available for any other materials, i.e., Zircalloy or Inconel 600; however, their use with LiPb is not planned at present. As better data becomes available these expressions can be altered. Note also that the rate expressions will yield values with the dimensions cm/sec. This can be looked at as the uniform material wastage rate across a given exposed surface area, thus releasing material into the coolant/tritium breeding fluid proportional to its content in the base material. If selective leaching is observed in future weight loss experiments, then these processes could be modeled in RAPTOR.

Neutron sputtering provides another source term in the calculation of the activation product transport. This mechanism is the primary source for helium cooled fusion reactor designs [13,14]. Also, Johnson and Vogelsang have estimated that around 10% of the activation products in a liquid lithium system can be due to sputtering processes [15,16].

For a helium cooled reference design, the neutron sputtering source was examined in detail by Bickford [17]. Here he considers two sputtering processes: fast neutron induced recoil sputtering of radioactive daughter nuclei and lattice dynamic neutron sputtering (also called bulk sputtering). The former involves the ejection of daughter nuclides from (n,α), (n,p), (n,2n) and other reactions from the metal surface, while the latter results in the ejection of atoms from the surface due to cascades of atomic collisions initiated by the incoming neutrons.

Other work has been performed to calculate and measure the neutron sputtering yields of different materials [18-27]. Tables 3 and 4 contain some of the results of these studies. The most significant features of these measurements are that the bulk neutron sputtering yields are on the order of 1 to 7 x 10^{-5} atoms per neutron in both the forward and backward directions for all materials tested, and the recoil neutron sputtering yields for most reactions can be calculated with reasonable accuracy. Also from Table 4 it is evident that backward recoil sputtering is 20 to 100 times less than recoil

TABLE 3

Bulk Neutron Sputtering Yields [18-25]

Target	Neutron Source	Theory (T) Experiment (E)	Yield (atoms/neutron)	Forward (F) Backward (B)
Gold	DT	E	1.9-5 1.3-5	F B
	d,B	E	1.9-6 to 2.0-5 1.8-6 to 2.8-5	F B
	DT	T	4.0-5	F
	U235	T	1.1-5	F
	d,Be	T	2.2-5	F
Niobium	DT	E	1.1-5 1.5-5	F B
	d,Be	E	2.5-5 to 4.5-5 2.9-5 to 4.1-5	F B
	DT	T	6.1-6 to 2.7-5 6.33-6	F B
	U235	T	0.89-5	F
	d,Be	T	1.2-5	F
Cobalt	d,Be	E T	1.6-5 2.7-5	B F
Aluminum	DT	T	4.2-5	F
	U235	T	2.4-5	F
Copper	DT	T	6.0-5	F
	U235	T	1.9-5	F

TABLE 4

Recoil Neutron Sputtering Yields [19,26,27]

Target		Forward Sputtering Ratio* Experimental	Forward Sputtering Ratio* Calculated	Backward Ratio Experimental
Nb	^{93}Nb(n,2n)^{92}Nb	10.6	10.6	0.076
Mo	^{100}Mo(n,2n)^{99}Mo	2.85	3.63	0.016
	^{96}Mo(n,p)^{96}Nb	0.82	0.08	-
	^{92}Mo(n,p)^{92m}Nb	0.24	0.24	0.005
	^{95}Mo(n,p)^{95}Nb	0.16	0.15	0.006
V	^{51}V(n,α)^{48}Sc	2.85	4.27	0.169
Fe	^{54}Fe(n,α)^{51}Cr	1.19	1.06	0.081
	^{54}Fe(n,p)^{54}Mn	1.79	1.84	0.074
Ni	^{58}Ni(n,p)^{58}Co	17.0	19.2	0.23
	^{60}Ni(n,p)^{60}Co	2.78	2.94	-
	^{62}Ni(n,α)^{59}Fe	0.11	0.12	0.018
Cr	^{52}Cr(n,2n)^{51}Cr	31.2	24.6	0.043
Ti	^{48}Ti(n,p)^{48}Sc	4.28	6.53	0.034
	^{46}Ti(n,p)^{46}Sc	2.48	3.37	0.026
	^{50}Ti(n,α)^{47}Ca	0.10	0.12	0.010
Au	^{197}Au(n,2n)^{196}Au	10.5	12.1	0.283
Cu	^{63}Cu(n,α)^{60}Co	4.2	4.5	0.289
316 SS	^{58}Ni(n,p)^{58}Co	1.99	2.65	0.021
	^{54}Fe(n,p)			
	^{54}Mn	2.32	2.65	0.021
	^{55}Mn(n,2n)			
	^{52}Cr(n,2n)			
	^{51}Cr	8.10	4.38	0.061
	^{54}Fe(n,α)			
	^{58}Ni(n,d)^{57}Co	5.0	8.35	0.023
	^{60}Ni(n,p)^{60}Co	0.29	0.41	0.051

*Sputtering ratios are listed as atoms per 10^8 DT neutrons.

sputtering in the forward direction.

Once the corrosion and activation products have found their way into the heat transfer/breeding loop, it becomes important to determine where they will deposit out of the fluid. The calculation of the deposition coefficients in the set of equations in the previous section and thus the determination of the mass flux to the walls of the different components becomes the primary task.

The deposition coefficients used by RAPTOR are determined using the methodology developed by Beal [28]. The deposition coefficient is defined as

$$K_D = \frac{N_W}{C_{avg}} = \frac{Kpv}{K + pv} \tag{13}$$

where N_W is the particle flux depositing on the wall, C_{avg} is the average (bulk) particle concentration, K is the transport coefficient (determined below), p is the particle sticking probability, and v is the radial velocity of a particle. The transport coefficients are found to be

$0 \leq S^+ < 5$

$$\begin{aligned} K = \bar{U}\sqrt{f/2}\ \{&\frac{14.5}{3}\left(\frac{\nu}{D}\right)^{2/3} F\left(\frac{\nu}{D}, S^+\right) - \frac{(14.5)^2}{1.5\ h^+}\left(\frac{\nu}{D}\right)^{1/3} G\left(\frac{\nu}{D}, S^+\right) \\ &+ \left[5 + \frac{50}{\nu h^+}(D - 0.959\ \nu)\right] \ln\left(\frac{D + 5.04\ \nu}{D + 0.04\ \nu}\right) \\ &- \frac{250}{h^+} + \frac{1 - 13.73\sqrt{f/2}}{\sqrt{f/2}}\}^{-1} \end{aligned} \tag{14}$$

$5 \leq S^{+} < 30$

$$K = \frac{\bar{U}\sqrt{f/2}}{5}\left\{\{[1 + \frac{10}{\nu h^{+}}(D - 0.959\ \nu)]\ \ln[\frac{D + 5.04\ \nu}{D + \nu(\frac{S^{+}}{5} - 0.959)}] - \frac{10}{h^{+}}(6 - \frac{S^{+}}{5})\} + \frac{1 - 13.73\sqrt{f/2}}{\sqrt{f/2}}\right\}^{-1} \qquad (15)$$

$S^{+} > 30$

$$K = \frac{\bar{U}\ f/2}{(1 - 13.73\sqrt{f/2})} \qquad (16)$$

where

D = Brownian diffusion coefficient, $D = (K_B\ T)/(3\pi d\mu)$

d = particle diameter

f = Fanning friction factor (= 1/4 Moody friction factor)

h^{+} = dimensionless channel spacing or pipe diameter, $h^{+} = (h\bar{U}\sqrt{f/2})/\nu$

K_B = Boltzmann constant

S = stopping distance

$$S = \frac{\rho_p\ d^2 v}{18\mu} + \frac{d}{2} = \frac{0.05\ \bar{U}\ d^2\ \rho_p\sqrt{f/2}}{\mu} + \frac{d}{2}$$

S^{+} = dimensionless stopping distance, $S^{+} = (S\bar{U}\sqrt{f/2})/\nu$

T = absolute temperature

ν = kinematic viscosity

μ = dynamic viscosity

ρ_p = particle specific gravity

The functions $F(\frac{\nu}{D}, S^+)$ and $G(\frac{\nu}{D}, S^+)$ are defined in reference 28.

In addition to the deposition coefficients, the sticking probabilities and the erosion coefficients of particles which are stuck to the walls of each component are needed. Beal has provided preliminary correlations in these areas [29] and these have been included in RAPTOR. The code also considers the decay of the radioactive nuclides and the purification of the coolant/tritium breeding material as removal mechanisms.

After all of the transfer coefficients are determined and appropriately included in the A matrix, the set of differential equations is solved as a function of time using the matrix operator technique of Lee [3]. Section III of this report describes the computer implementation of the RAPTOR code.

II.C. Sensitivity Analysis

Once the transport of the activation products is determined, it becomes interesting to determine the sensitivity of the results to uncertainties in the coefficients of the transfer matrix. In the case of fusion reactors, where parameters are very indeterminate, sensitivity analysis can provide very useful information and can help lead to a greater understanding of the problem. In the previously described transport model, it is possible to determine the effects of changes to various parameters, including the deposition and release coefficients.

In principle, sensitivity analysis for the set of the coupled linear equations discussed earlier is easily done. If the set of equations is defined by

$$\frac{\partial M(t)}{\partial t} = \underset{\sim}{A}\vec{M}(t) + \vec{S} \tag{31}$$

where $\vec{M}(t)$ = the concentration/deposit vector (n elements)

$\underset{\sim}{A}$ = the transition matrix (nxn)

$\vec{S}$ = the cource rate vector (n)

then merely differentiating equation (31) by the coefficient of interest gives

$$\frac{\partial}{\partial k_i}\frac{\partial \vec{M}}{\partial t} = \frac{\partial}{\partial k_i}(\underset{\sim}{A}\vec{M} + \vec{S}) \tag{32}$$

and

$$\frac{\partial}{\partial t}\frac{\partial \vec{M}}{\partial k_i} = A\frac{\partial \vec{M}}{\partial k_i} + M\frac{\partial \underset{\sim}{A}}{\partial k_i} + \frac{\partial \vec{S}}{\partial k_i} \tag{33}$$

Now, knowing that the source rate is not affected at all by a change in any coefficient, and that the coefficients in the transfer matrix are independent of each other, equation (32) becomes

$$\frac{\partial}{\partial t}\frac{\partial \vec{M}(t)}{\partial k_i} = \underset{\sim}{A}\frac{\partial \vec{M}(t)}{\partial k_i} + \delta_{ij}\,\vec{M}(t) \qquad (34)$$

where

$\delta_{ij} \neq 0$ if $i = j$

$\delta_{ij} = 0$ otherwise.

That is, if any matrix element in A involves the coefficient of interest, then its concentration/deposit vector is non-zero. If a row of $\underset{\sim}{A}$ does not contain k_i, then its concentration/deposit vector is set to zero. Because of the nature of this particular system of equations, the δ_{ij} term is not the same as the usually recognized delta function. Since concentrations and deposits are recorded in different units, there are conversion factors that are needed to multiply particular coefficients so that the dimensions are correct in the transfer matrix. For example, the particle flux to the wall (in atoms per cm^2 per second) is equal to the deposition coefficient (cm per second) times the concentration of particles in the fluid (atoms per cm^3). However, to get the loss rate of particles from the coolant (in atoms per cm^3 per second) it is necessary to multiply the deposition coefficient by the ratio of the surface area of the node to the total liquid volume of the system before multiplying by the concentration of particles in the fluid. The ratio must be included with the δ_{ij} in the above equations so that the correct amount of material transfer is obtained. However, once this is understood it should cause little ambiguity.

Unfortunately, equation (36) is difficult to solve using the solution method described previously, since the second term on the right hand side of equation (36) is not constant. In principle, the equation could be solved if the details of $\vec{M}(t)$ were known, but this would require very time consuming equations. However, if equations (35) and (36) are linked together, then it is possible to calculate the deposits, concentrations, and the effects of changes to the individual coefficients at the same time.

To accomplish this, look at equations (35) and (36) again;

$$\frac{\partial \vec{M}(t)}{\partial t} = \underset{\sim}{A}\vec{M}(t) + \vec{S} \tag{35}$$

$$\frac{\partial}{\partial t}\frac{\partial \vec{M}(t)}{\partial k_i} = \underset{\sim}{A}\frac{\partial \vec{M}(t)}{\partial k_i} + \delta_{ij}\vec{M}(t) \tag{36}$$

These can be combined into a single matrix equation as

$$\frac{\vec{W}(t)}{\partial t} = \underset{\sim}{B}\vec{W}(t) + \vec{R} \tag{37}$$

where

$$\vec{W}(t) = \begin{pmatrix} \vec{M}(t) \\ \\ \frac{\partial \vec{M}(t)}{\partial k_i} \end{pmatrix}, \quad \vec{R} = \begin{pmatrix} \vec{S} \\ \\ 0 \end{pmatrix}, \quad \underset{\sim}{B} = \begin{pmatrix} \underset{\sim}{A} & 0 \\ \\ \delta_{ij} & \underset{\sim}{A} \end{pmatrix}$$

which can be solved using the previously defined matrix operator solution method since $\vec{R}$ is constant. This doubles the size of the matrix which is being manipulated and will dramatically increase the amount of time required for computation to run each case. Also, this doubled size calculation must be done for each coefficient and for each isotope of interest. For this reason, the user should be very selective about which coefficients and isotopes are chosen for sensitivity study.

In most cases it is not necessary to check the sensitivity of the results to changes in every coefficient. Certain components and reactor parts are usually of interest, so that sensitivity analysis need only be done in relation to them. It is possible to test the global trends by checking certain isotopes and only the particular coefficients of interest. This will greatly decrease the number of sensitivity calculations that need to be performed.

III. Computer Implementation

The theory and transport mechanisms described in Chapter III are implemented into the computer code RAPTOR. This code calculates the mass transfer rates, the amounts of radioactive materials in the coolant/breeding material and the amounts deposited throughout the system. This section describes this application and the methods used for these calculations.

The system of equations defined by equations (1) through (11), and compacted into matrix form in equation (12) are solved by the matrix operator method of Lee [3]. The source rate vectors are assumed to be constant over each broad time interval and can be changed for different operating conditions; likewise for the coefficients in the transfer matrix $\underset{\sim}{A}$. RAPTOR provides for the time dependent behavior of the corrosion rate by inserting additional time steps as necessary. In this way the corrosion rate is changed over these new time intervals. Initial values for the calculations can either be set to zero, or read in and thus calculations can be continued if desired.

The various transfer coefficients and sources are determined using data and theories described in the previous chapter. The reaction cross sections are taken from the decay chain data library used in the fusion reactor activation code DKR [30,31], and the decay data is from Lederer [32]. Information about the heat transfer/breeding materials is taken from a variety of sources. In this respect, the Sze, Clemmer, and Cheng paper on lithium-lead compounds [37] and the CRC Handbook of Tables for Applied Engineering Science [34] .

have been extremely useful. Other problem specific information needs to be supplied by the user.

The basic calculational scheme to determine the dose rates due to activation products in the coolant/tritium breeding loop is seen in Figure 2. To go along with the corrosion rate, sputtering rate, decay, and other data included in the RAPTOR code, it is necessary to completely describe the reactor system by separating the various components into nodes, detail the reactor operating history to be modeled, and determine the neutron flux levels corresponding to the operating history. At present, the neutron flux spectrum must be put into a 25 group structure, as seen in Table 5. With this input RAPTOR will determine the active and stable concentrations in the fluid and the deposits in all system modes as a function of time based upon the operating history, and system description. On occasion, only the amounts of deposits are of interest in certain plant components. RAPTOR allows such a choice in subroutine USEFUL and will only write out the information for the requested components.

Once the concentrations and deposits are known, the routine REDF can be used to determine the specific gamma radiations emitted from the system at each particular point of interest. These are then input into the MCNP, Monte Carlo neutron/photon transport code [35], along with the details of the component geometry to determine the photon fluxes, and using photon flux to dose conversion factors, the dose rates at points around the reactor system can be determined.

A flow chart of the operation of RAPTOR is included as Figure 3.

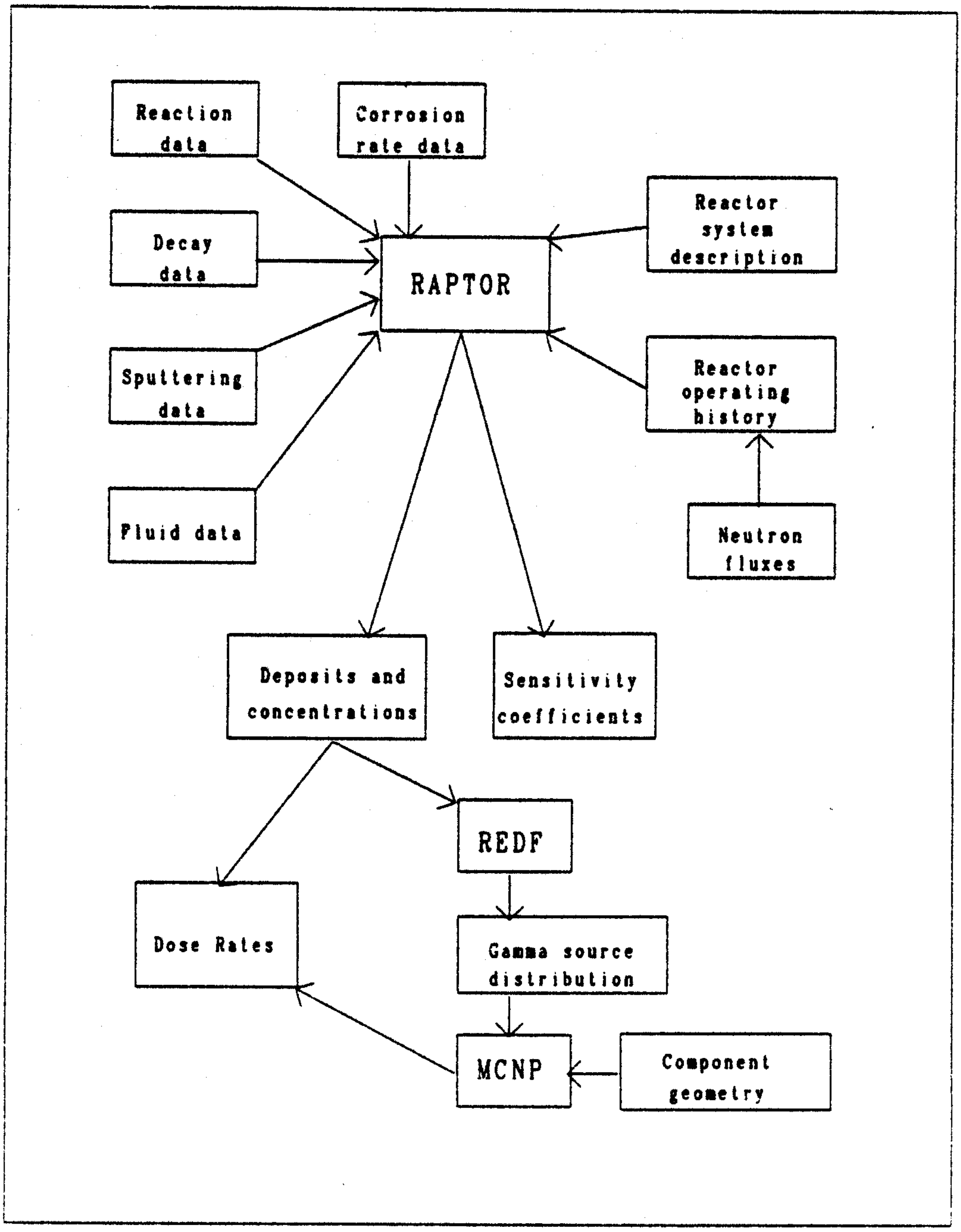


Figure 2. Basic calculational scheme for determining activation product transport and radiation fields.

TABLE 5

Neutron 25 Energy Group Structure in eV Group Limits

Group	E(Top)	E(Low)	E(Midpoint)
1	1.4918 (+7)*	1.3499 (+7)	1.4208 (+7)
2	1.3499 (+7)	1.2214 (+7)	1.2856 (+7)
3	1.2214 (+7)	1.1052 (+7)	1.1633 (+7)
4	1.1052 (+7)	1.0000 (+7)	1.0526 (+7)
5	1.0000 (+7)	9.0484 (+6)	9.5242 (+6)
6	9.0484 (+6)	8.1873 (+6)	8.6178 (+6)
7	8.1873 (+6)	7.4082 (+6)	7.7979 (+6)
8	7.4082 (+6)	6.7032 (+6)	7.0557 (+6)
9	6.7032 (+6)	6.0653 (+6)	6.3843 (+6)
10	6.0653 (+6)	5.4881 (+6)	5.7787 (+6)
11	5.4881 (+6)	4.4933 (+6)	4.9907 (+6)
12	4.4933 (+6)	3.6788 (+6)	4.0860 (+6)
13	3.6788 (+6)	3.0119 (+6)	3.3453 (+6)
14	3.0119 (+6)	2.4660 (+6)	2.7390 (+6)
15	2.4660 (+6)	1.3534 (+6)	1.9097 (+6)
16	1.3534 (+6)	7.4274 (+5)	1.0481 (+6)

---

*Read as 1.4918 x 10^7 eV

TABLE 5 (continued)

Neutron 25 Energy Group Structure in eV Group Limits

Group	E(Top)	E(Low)	E(Midpoint)
17	7.4274 (+5)	4.0762 (+5)	5.7518 (+5)
18	4.0762 (+5)	1.6573 (+5)	2.8667 (+5)
19	1.6573 (+5)	3.1828 (+4)	9.8779 (+4)
20	3.1828 (+4)	3.3546 (+3)	1.7591 (+4)
21	3.3546 (+3)	3.5358 (+2)	1.8541 (+3)
22	3.5358 (+2)	3.7267 (+1)	1.9542 (+2)
23	3.7267 (+1)	3.9279 (+0)	2.0597 (+1)
24	3.9279 (+0)	4.1339 (-1)	2.1718 (+1)

---

*Read as 1.4918×10^7 eV

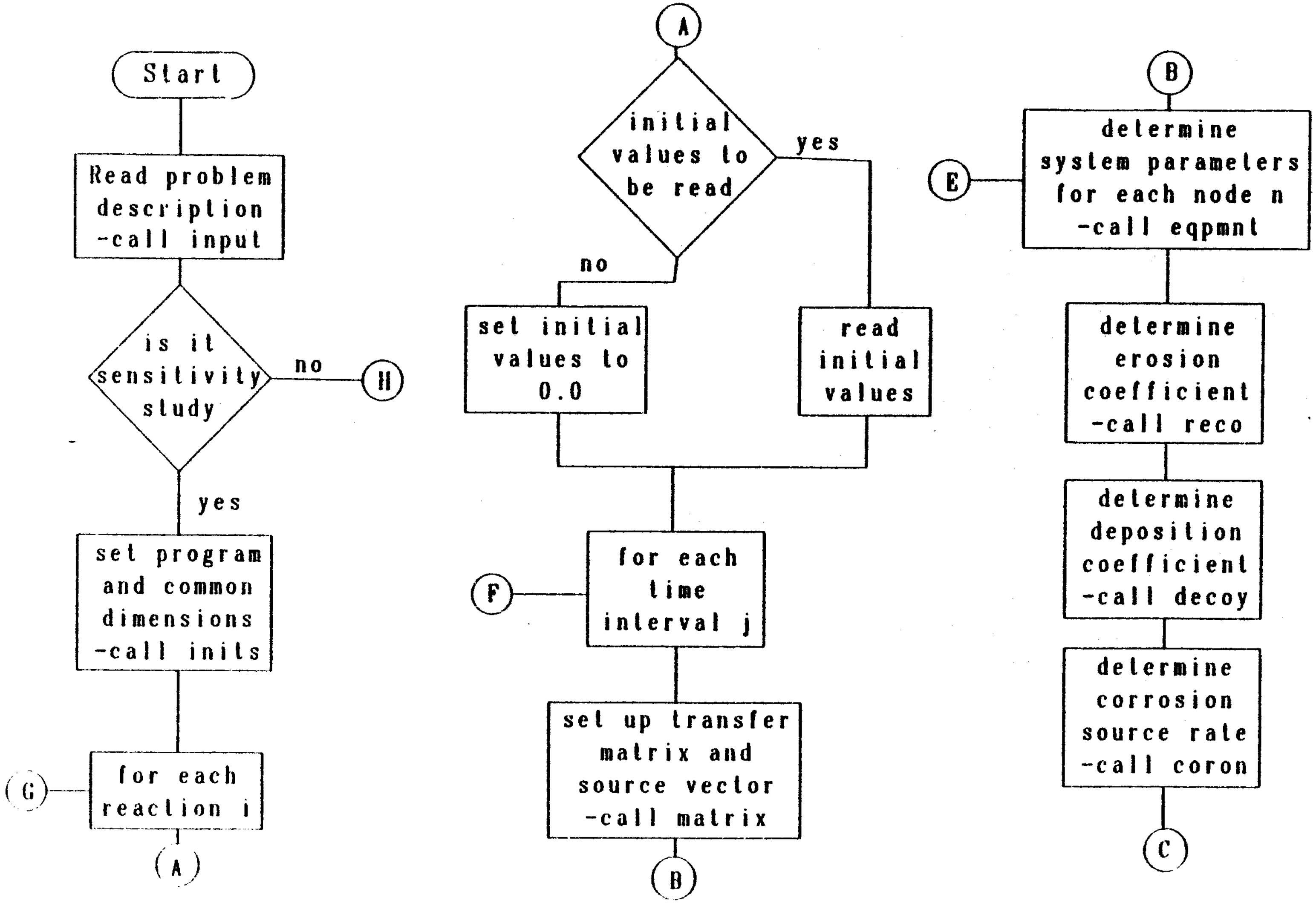


Figure 3. Functional flow chart of RAPTOR calculations.

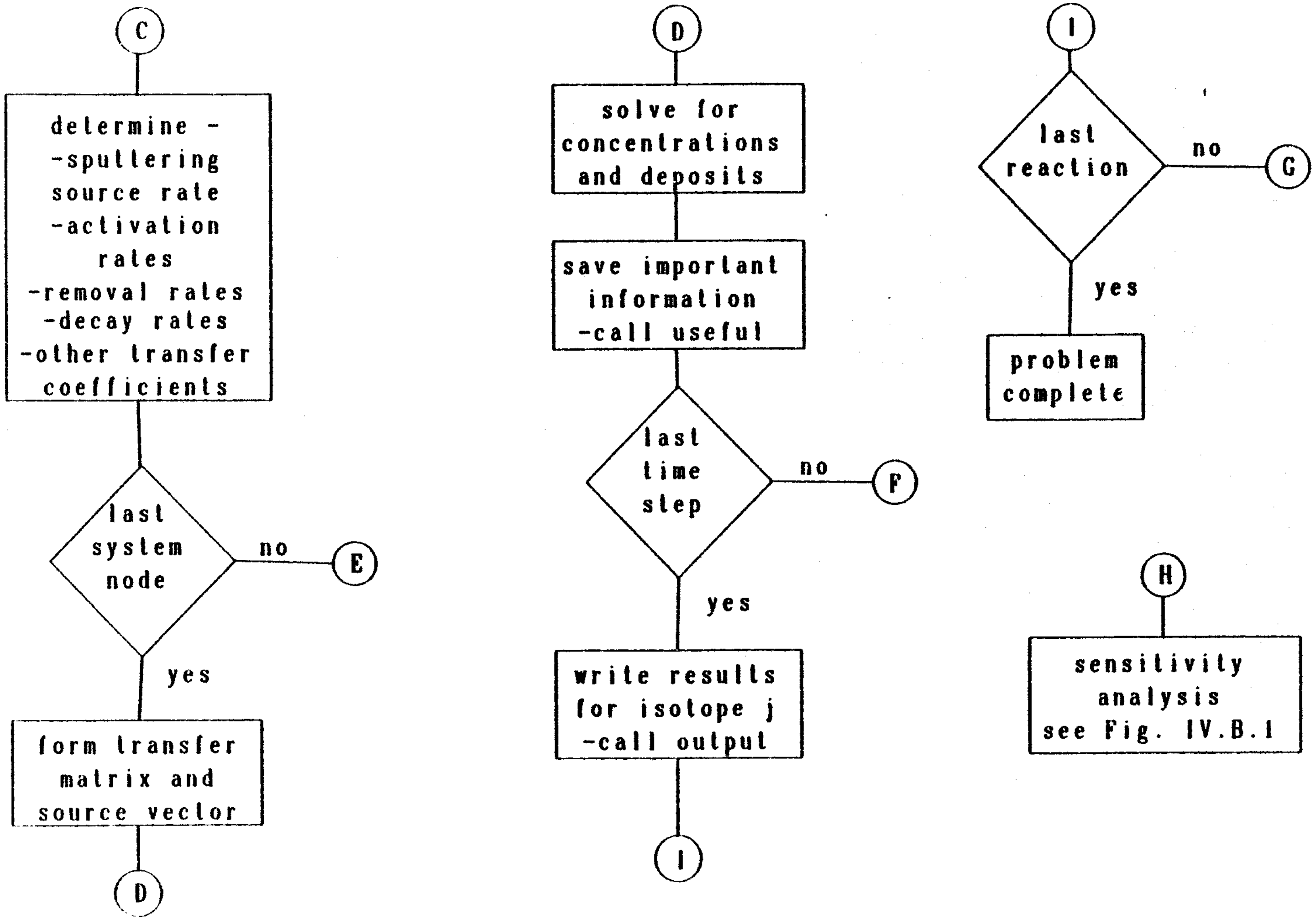


Figure 3 (continued). Functional flow chart of RAPTOR calculations.

This illustrates the operations performed by RAPTOR and the important subroutines that are called. A more complete code description and user's manual is supplied in the next section. This diagram is relatively straightforward, except for the sensitivity analysis portion of the program. The calculation of sensitivity coefficients follows a similar flow path as in Figure 3, allowing for the necessary changes.

In the general program flow, it is seen that after the problem description and the program dimensions are set the calculation is broken into three loops, one inside the other. The interior loop calculates the transfer matrix and source vector for each isotope/ reaction, and writes the concentrations and the deposits throughout the reactor system into an output file. The outer loop is used for each isotope/reaction, and when completed successfully the program ends. Along the way, the various source terms and transfer coefficients are determined, and placed in the transfer matrix.

The solution method, employed in the subroutine SOLV, is an extension of the Volterra calculus as described by Lee [3]. This routine solves the coupled linear differential equation efficiently and gives adequate results. For the details of this routine, the reader is encouraged to consult reference 3.

IV. Code Description

The RAPTOR code is presently (9/83) operational on the CRAY machine at the National Magnetic Fusion Energy Computer Center (NMFECC) and is entirely self contained, except for the use of the DISSPLA graphics routines [2]. It is written in FORTRAN and is able to calculate the time dependent buildup and decay of 9 radioactive isotopes being formed through 15 independent nuclear reactions.

Figure 4 shows the structure of RAPTOR and the names of the various subroutines that are called. The MAIN routine calculates the correct array dimensions and calls INITS, CONTR, and initializes the DISSPLA plotting routines if the time dependence of the specific activities of the various isotopes in the important reactor nodes are to be plotted. A description of the other subroutines follows.

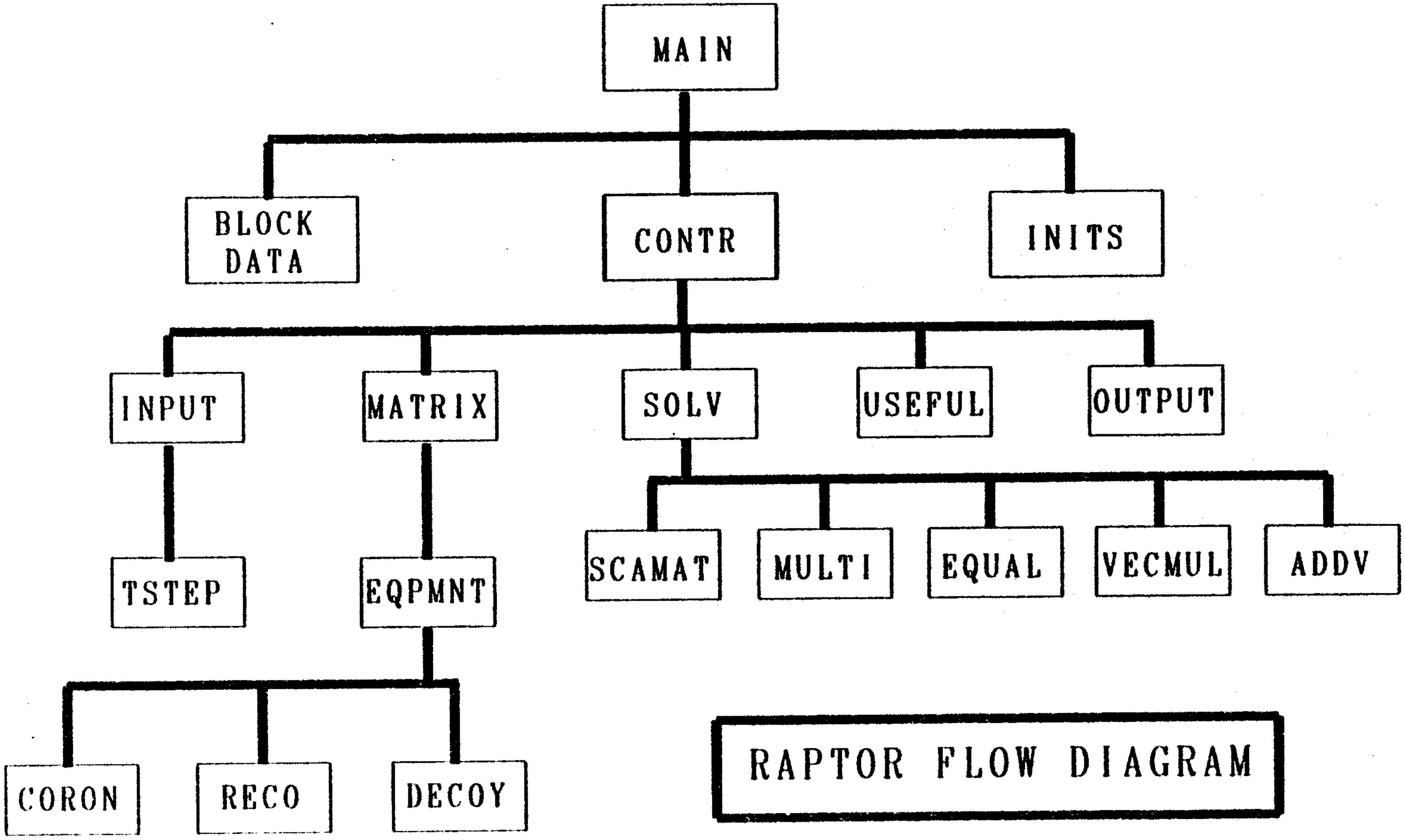


Figure 4. Schematic flow diagram for RAPTOR.

CONTR

Subroutine CONTR actually controls all of the program functions and calls other subroutines as necessary for the particular problem. Subroutines called by CONTR are INPUT, MATRIX, SOLV, USEFUL, and OUTPUT, and the total system activity for each node is plotted if requested. CONTR also controls the calculations and subroutine calls if a sensitivity analysis problem is to be run. The problem is completed successfully when a STOP 999 command is reached.

INITS

Subroutine INITS initializes the array dimensions and common block lengths, and is called by the MAIN routine.

BLOCK DATA

BLOCK DATA sets the value of a number of variables used by RAPTOR. Included in BLOCK DATA are the component and reaction names, stable wall material number densities, decay constants, fluid parameters, reaction cross sections, and sputtering coefficients. This data is used by many of the RAPTOR subroutines.

INPUT

INPUT is called by CONTR and reads the two input files INP5 and INP10 that describe the problem to be run. These parameters are described later. INPUT also writes a description of the reactor nodes in the output file and calls one subroutine, TSTEP.

TSTEP

Subroutine TSTEP adds extra time steps to the calculation to model the time dependence of the release rates of corrosion products. It keeps track of the operational history and blanket changeouts.

MATRIX

Subroutine MATRIX assembles all of the data and transfer coefficients into the transfer matrix and also determines the source vector. It is called by CONTR and calls EQPMNT. It also writes the non-zero transfer coefficients and source vector into an output file.

EQPMNT

Subroutine EQPMNT determines the node specific parameters which are used in the transfer matrix and source vector. It is called once for each system node by MATRIX, and calls RECO, DECOY, and CORON. It also calculates the neutron reaction rates and sputtering rates given the neutron flux and the reaction cross sections and sputtering coefficients.

RECO

RECO determines the node specific erosion coefficients and is called by EQPMNT.

DECOY

DECOY calculates the deposition coefficient for each node depending upon the particle size and the system parameters according to the equations of Beal [28]. It is called by EQPMNT.

CORON

Subroutine CORON is called to calculate the release rate of base metal into the coolant/tritium breeding fluid for each node. It is called by EQPMNT.

SOLV

Subroutine SOLV is the routine which solves the matrix equation for each major time step using the previously described solution method [3]. It is called by CONTR for each time step and calls subroutines, SCAMAT, MULTI, EQUAL, VECMUL, and ADDV.

SCAMAT

SCAMAT multiplies a scalar times a matrix and is called by SOLV.

MULTI

Subroutine MULTI multiplies one matrix by another and is called by SOLV.

EQUAL

Subroutine EQUAL simply sets one matrix equal to another and is called by SOLV.

VECMUL

VECMUL multiplies a matrix by a vector and is called by SOLV.

ADDV

Subroutine ADDV is called by SOLV to add two vectors together.

USEFUL

Subroutine USEFUL saves only the important information from specified nodes before the calculation continues onto the next time step. This reduces the amount of computer memory needed for the problem as well as output. It is called by CONTR.

OUTPUT

Subroutine OUTPUT writes the results into an output file and plots the specific activities as a function of time, if requested. It is called by CONTR.

RAPTOR Input Parameters

The RAPTOR code requires many input parameters for its operation. In addition to problem description flags, the reactor system to be modeled must be well defined. Various quantities must be known for each node including surface area, volumes, material type, flow rates, flow velocities, to name a few. This section describes the RAPTOR input and its format. There are a number of card image types which must be included, and it will be noted when more than one card image of a certain type is needed.

The basic RAPTOR run requires two input files to be supplied by the user. INP5 is read on unit 5 and contains the general problem description, and system information which does not change for varying system conditions. INP10 is read on unit 10 and contains the system information necessary for each time step.

INP5 Input Description

Card 1 -- Title (18a4)

Title -- may be anything to describe the problem run, up to 72 characters.

Card 2 -- iid, iact, its, node, iref, iflux, nimp, ifl, jflm, init, mkl, nsen (12i5)

iid -- problem identification number

$0 \leq$ iid < 5 -- calculates deposits and concentrations

$5 < iid < 9$ -- continues a sensitivity analysis run.

$9 < iid$ -- performs sensitivity analysis.

iact -- number of isotopes

its -- number of time steps

node -- number of nodes

iref -- print and plot flag

iflux -- number of flux containing nodes

nimp -- number of important nodes

ifl -- circulating fluid type

ifl = 1 -LiPb

= 2 -H_2O

jflm -- node number of the main flow

init -- continuation run flag ($iid < 5$)

init > 0 -- initial values must be read from unit 18

= 0 - initial values set to 0

mkl -- number of different flow/flux description sets on unit 10.

nsen -- number of coefficients on which sensitivity analysis is performed.

Card 3 -- (import (i), i = 1, nimp) (12i5)

import(i) -- node numbers of the important nodes on which dose calculations and concentrations are printed

Cards 4 & 5 -- System information cards, one set for each node (n).

4. kj, nout(n), ieqp(n), nmat(n), mhot(n), (ncon(n,i), i = 1, nout(n)) (12i5)

kj -- node number, must be in order

nout(n) -- number of nodes the outlet of n connect to.

ieqp(n) -- node type number, see Table 6.

nmat(n) -- node wall material composition

nmat(n)	Material
1	316 Stainless Steel
2	Ferritic Steel HT-9
3	304 Stainless Steel
4	Zircaloy-2
5	PCA-Titanium modified 316 SS
6	Inconel 600
7	Haynes-Stellite 25

mhot(n) -- hot/cold section flag

mhot(n) = 0 cold system node-particles formed

$\geq$ 2 hot system node-no particle formation

ncon(n,i) -- nodes that node n is connected to

TABLE 6

Equipment Type Names

ieqp(n)	Equipment Name
1	first wall
2	blanket section
3	reflector
4	blanket, forced laminar flow
5	header
6	outlet plenum
7	hot leg pipe
8	steam generator
9	cross over pipe
10	pump
11	cold leg pipe
12	inlet plenum
13	letdown line
14	tritium letdown line
15	tritium removal system
16	cleanup return line
17	tritium return line
18	connecting pipe
19	cleanup system

5. (equp(n,i), i = 1,6) (6f12.3)

equp(n,i) -- node description parameters

equp(n,1) -- pipe diameter, cm

(n,2) -- node surface area, cm^2

(n,3) -- node volume, cm^3

(n,4) -- node corrosion fraction

-- cleanup system removal fraction

(n,5) -- enhanced deposition factor (normally 0.0)

(n,6) -- enhanced release factor (normally 0.0)

Card 6 -- xps, rhop, xsl (6f12.3)

xps -- agglomerate diameter in cm

rhop -- particle density; g/cm^3

xsl -- soluble ion species diameter, cm

Card 7 -- (times (j), j = 1, itts) (6f12.3)

itts = its +1

times(j) -- times at which calculations are performed, including the initial time.

Card 8 -- (ichg(j), j = 1, its) (12i5)

ichg(j) -- system time step variability flag. For each time step, ichg(j) is the number of the flux/flow description set to be used.

Card 9 -- (kbcg(j), j = 1, its) (12i5)

kbcg(j) -- blanket change out flag for time step j

= 0 -- no change

> 0 -- blanket sections removed and activation and corrosion rates set to time equals zero

Note: first time step must have kbcg(1) greater than 1, unless it is a continuation run.

Card 10 -- (iso(j), j = 1, iact) (12i5)

iso(j) -- isotope designation numbers

Card 11 -- (nodflx(j), j = 1, jflux) (12i5)

nodflx(j) -- numbers of the nodes that have fluxes.

Card 12 -- (imsen(i), i - 1, nsen)

imsen(i) -- node numbers of the sensitivity analysis.

Card 13 -- (ks(i), i = 2, nsen)

ks(i) -- coefficient type number for sensitivity analysis

ks(i)	Coefficient type
1	deposition coefficient -- agglomerates
2	release coefficient from walls
3	deposition coefficient -- solubles
4	agglomeration coefficient

Card 14 -- nper, (xper(i), i = 1, nper) (i5,5f12.3)

nper -- number of fractional changes to the sensitivity coefficients to be calculated

xper(i) -- the percentage change of the coefficients for which the sensitivity analysis is performed

<u>Note</u>: card images 12-14 may be omitted if sensitivity analysis is not to be done (iid $<$5.)

INP10 Input Description

Each system description set is divided into two sections. The first describes the node parameters, and the second describes the fluxes to be used for those nodes that contain neutron fluxes. Two card images (cards A & B) are required for each node in the system and a 25 neutron group flux (Card C) is needed for each flux containing node.

Card A -- fvel(n), abst(n) (6f12.3)

Card B -- fr(n), (fcon(n,i), i = 1, nout(n)) (6f12.3)

fvel(n) -- node flow velocity, cm/sec

abst(n) -- node temperature, °C

fr(n) -- node flow rate, kg/hr

fcon(n,i) -- fraction of the flow rate that goes from the $n^{\underline{th}}$ node to the $i^{\underline{th}}$ node

Card C -- flux(it,ng)   (6f12.3)

flux(it,ng) -- 25 group neutron flux for each node that has a flux (in order as nodflx)

If the case to be run is a continuation run (init > 0), the initial values from the preceding calculations are read in from unit 18, file INVAL. The format for INVAL is 6f12.3 and the initial values for each isotope must be present.

RAPTOR Output Files

A number of output files are generated by RAPTOR. Not all are generated on each run, i.e. a sensitivity calculation will generate a larger number of files, and Table 7 lists the names of these files and what they contain.

Acknowledgment

Support for this work has been provided by the U.S. Department of Energy and by the Wisconsin Electric Utilities Research Foundation (WEURF).

TABLE 7

RAPTOR Output Files

Unit	File name	Purpose
6	out1 → out9 outa → outk	general output file, contains input information, important node deposition and concentration information.
7	ovv66	non-zero matrix coefficients and source vectors.
20	outall	complete output file including all nodes and concentrations.
17	sencof	sensitivity coefficients, rate of change of slope due to changes in the matrix coefficients as a function of time.
19	outps	general SA output file, contains percentage changes to slopes as a function of time due to prescribed changes in the matrix coefficients.

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