Summary Report for ITER Design Task D10:
Updating the Activation Code RACC for
ITER Design Analysis

Qingming Wang and D.L. Henderson

January 1995
(revised April 1995)

UWFDM-977
DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
Summary Report for ITER Design Task D10:
Updating the Activation Code RACC for ITER Design Analysis

Qingming Wang and D. L. Henderson

University of Wisconsin-Madison
Nuclear Engineering and Engineering Physics Department
1500 Johnson Drive
Madison, WI 53706

January 1995

UWFDM-977

## Contents

1 Executive Summary ........................................... 1

2 Introduction .................................................. 2

3 Theory ......................................................... 2
  3.1 Mathematical Formulation ................................ 2
     3.1.1 The Pulsed/Intermittent Activation Problem .......... 4
  3.2 Matrix Solution Method .................................. 5
     3.2.1 Scaling and Squaring Technique ....................... 7
     3.2.2 Schür Decomposition .................................. 7
     3.2.3 Matrix Raised to a Power ............................. 7
  3.3 Pulsing Scheme .......................................... 8

4 Results and Discussion ...................................... 8
  4.1 Implications for ITER ................................. 13

5 Conclusion and Discussion ................................ 13

References ..................................................... 15

Appendix ......................................................... 17
  A. Pulsed History Operation ................................. 17
  B. Input to the RACC-Pulse Code ......................... 19
1 Executive Summary

The computational capability of the RACC radioactivity code (now termed RACC-Pulse) has been extended by the addition of routines for the calculation of pulsed/intermittent histories. These routines allow for an accurate treatment of the pulsed irradiation history of the International Thermonuclear Experimental Reactor (ITER) facility. The transmutation of stable and radioactive nuclides and the decay of the radioactive nuclides are accounted for during each pulse and decay period. The code now has the capability to model varying flux levels, pulse widths and dwell periods, varying pulsing schedules and maintenance periods. This flexibility allows the user to model virtually any irradiation history that may be encountered during the operation of ITER. In addition, a small auxiliary program has been written to interface with the ONEDANT/TWODANT neutral particle transport codes. This allows RACC-Pulse to utilize the same spatial mesh, geometric model and spatial neutron flux as in the transport codes.

Though the RACC-Pulse code is quite flexible in its modeling of irradiation histories, the user of the code should be cautioned that the run time (CPU time) of the code can be quite excessive for a realistic, full size computational model of the facility. The CPU time is a function of the number of zones modeled and the number of transmutation generations treated. Indications are that run times on the order of hours can be expected when performing a detailed 1-D calculation having many zones, several hundred mesh intervals, and treating 3 transmutation generations. There are several reasons for this: (1) the basic calculational philosophy (transmutation-decay scheme and problem setup) of the code, (2) the complexity of the pulsing structure, and (3) the version of the code provided to our group for modification which is an older version that has been optimized for IBM computers of the late 70’s. A reduction in CPU time can, in part, be obtained by code optimization changes in the calculational philosophy within the nonpulsing parts of the code which is beyond the scope of this work. Based on the above observation, though the results are accurate, the use of the RACC-Pulse code for routine design calculations should be reconsidered.
2 Introduction

Based on current plasma physics considerations, the proposed operation mode of the International Thermonuclear Experimental Reactor (ITER) is projected to be intermittent with nonuniform pulsed irradiation histories and maintenance periods scheduled throughout the facility’s useful experimental lifetime. During the conceptual design and engineering design activity (EDA) phases of the ITER study [1] it became apparent that the activation analysis codes chosen as the base calculational tools for the activation calculations were incapable of accurately modeling the pulsed/intermittent irradiation history of the ITER device. It has been shown that steady state approximations to the pulsed irradiation history yielded poor results with answers being off by as much as the duty factor [2,3]. This posed problems for the shield and blanket designers performing radioactivity, afterheat, and biological dose rate analyses. Design recommendations, changes and facility economics depend, to a large extent, on reliable and accurate results. It was conveyed to the Joint Central Team that the activation code(s) chosen would need to be modified to perform pulsed/intermittent irradiation calculations. The two codes chosen by the JCT for the radioactivity, decay heat and safety analyses were the RACC [4] and FISPACT [5] codes. Both codes yield accurate results for the steady state case but lacked the capability to model pulsed/intermittent histories. Hence the JCT initiated Task D10, one subtask of which is the improvement and modification of the RACC radioactivity code for pulsed operation. The D10 statement of work is presented in Table 1.

A description of the computational methods implemented in the RACC code for the treatment of pulsed/intermittent activation are contained in Section 2. A discussion of the benchmark problem, CPU time and code improvements can be found in Section 3. This is followed by a conclusion in Section 4 which discusses implications to the ITER design. The Appendix contains the input instructions to RACC-Pulse and a detailed discussion of the pulsing scheme.

3 Theory

3.1 Mathematical Formulation

The transmutation and radioactive decay of a nuclide are quite well understood physical processes which are governed by a simple first order linear differential equation,

\[
\frac{dN}{dt} = -\sigma \phi N(t) \quad \text{or} \quad \frac{dN}{dt} = -\lambda N(t)
\]
Table 1: JCT Task: D10

Task Objectives

Update the existing activation code RACC for conducting ITER design analysis.

Technical Description

Modifications of the RACC activation code will be performed to provide the most important and timely of the following capabilities and features:

- Analysis of pulsed operating modes for continuous destruction and production of nuclides exposed to the irradiation field.
- Utilization of the same spatial mesh and geometrical model as employed in one-, two- and three-dimensional transport calculations.
- Calculation of space- and time-dependent activation parameters over the same mesh as the transport geometrical model.
- Utilization of spatial distribution of the neutron flux.

The pulsing algorithm should be able to treat varying flux levels, pulsing schedules and maintenance periods.

Deliverables

Deliver to the JCT the updated version of the RACC activation code including support documentation at the conclusion of the contract period.

the solution of which is

\[ N(t) = N(0)e^{-dt} \]  \hspace{1cm} (1)

where \( d \) is \( \sigma \phi \) for transmutation or \( \lambda \) for radioactive decay. Quite often a radioactive nuclide may also undergo neutron transmutation interactions. In this instance both processes compete against each other and \( d \) becomes \( (\lambda + \sigma \phi) \), i.e., the total destruction rate. The transmutation process of an isotope exposed to a neutron flux and its many generations of stable and radioactive nuclides or the radioactive decay generations of a radioactive isotope
can be described by a system of coupled differential equations which, as in the case of a single isotope, are first order linear equations (for constant cross-sections and decay constants). These coupled equations can be cast in general matrix form [4,6]:

$$\frac{d\mathbf{N}}{dt} = \mathbf{A} \mathbf{N}(t).$$

(2)

The formal mathematical solution of the above matrix equation is analogous to the single isotope case (Eq. 1):

$$\mathbf{N}(t) = e^{\mathbf{A}t} \times \mathbf{N}(0)$$

(3)

where $e^{\mathbf{A}t}$ is called the matrix exponential. The matrix $\mathbf{A}$ contains both the total destruction rates $d = (\lambda_i + \sigma \phi)$ which define the diagonal elements of matrix $\mathbf{A}(a_{ii} = -d_i)$ and the production rates ($\sigma \phi$ and $\lambda$) which define the off diagonal elements $(a_{ij})$. Matrix $\mathbf{A}$ is quite sparse.

Various numerical algorithms have been developed for the solution of these large matrix systems using the differential representation (Eq. 2) of these large matrix systems [7-9]. Though these methods produce accurate results, they do not lend themselves to nor are a suitable basis for the development of efficient pulsed/intermittent activation routines. The matrix exponential form of the solution (Eq. 3), on the other hand, allows for a mathematically explicit and concise form of the pulsed activation problem.

### 3.1.1 The Pulsed/Intermittent Activation Problem

The following derivation of the pulsed/intermittent matrix solution method is presented in its entirety in Reference 6. The essential features of the derivation are reproduced here for completeness.

For simplicity in the derivation consider a uniform series of pulses having a pulse width of $\Delta t_1$ and a dwell time of $\Delta t_2$ (see Figure 1). Using Eq. 3, the solution after the first pulse is

$$\mathbf{N}(\Delta t_1) = e^{\mathbf{A}\Delta t_1} \times \mathbf{N}(0)$$

(4)

where $\mathbf{A}$ contains the transmutation and decay rates for the pulse period. The solution after the first decay period is

$$\mathbf{N}(\Delta t_1 + \Delta t_2) = e^{\mathbf{B}\Delta t_2} \times \mathbf{N}(\Delta t_1)$$

$$= e^{\mathbf{B}\Delta t_2} \times e^{\mathbf{A}\Delta t_1} \times \mathbf{N}(0)$$

(5)
where $B$ is the decay matrix for the dwell period. It can be easily shown that after the $n$'th pulse period the solution is given by

$$N(n \Delta t_1 + (n-1) \Delta t_2) = e^{A \Delta t_1} \times \left( e^{B \Delta t_2} \times e^{A \Delta t_1} \right)^{(n-1)} \times N(0).$$  \hspace{1cm} (6)

The above represents an accurate description of the pulsed activation process which accounts for continuous burnup (transmutation) during the pulse periods and decay during the dwell periods. For the uniform pulse case discussed above, the solution involves raising a matrix to a power, one matrix and 2 vector multiplications. The above result can be easily extended to more complex operation histories (Appendix A). In general, the number of matrix and vector multiplications depends on the complexity of the pulsed operation history. Increased nonuniformity of the pulse structure results in an increased number of matrix and vector multiplications which increases the computational time.

Once the solution to the operation period is obtained the calculation proceeds to the after shutdown time. The only nuclear process occurring after shutdown is decay and the general solution at a time $t$ after shutdown is

$$\overline{N}(t) = e^{Bt} \times \overline{N}(n \Delta t_1 + (n-1) \Delta t_2)$$

where $B$ is the decay matrix for the dwell period.

### 3.2 Matrix Solution Method

Before solution methods for the evaluation of the matrix exponential are presented, a brief summary of the calculational method employed in the original RACC code is given. A discussion of the solution method for pulse and dwell periods follows.
The solution method implemented in the original RACC code [4] was the GEAR ODE (Ordinary Differential Equation) solver. GEAR solves a system of stiff first order differential equations employing a time step approach to advance the solution to the requested operation time [10-12]. However, the implementation of the time step approach makes the GEAR solver unsuitable for the above matrix solution of the pulsed/intermittent problem. Hence the GEAR solution package was replaced with a matrix solver which evaluates the matrix exponential and is compatible with the pulsing algorithms.

As noted in the preceding subsection, the formal solution to the pulsed/intermittent activation problem involves evaluations of the matrix exponential for the pulse period, dwell period and after shutdown times. For complex pulse histories additional matrix exponential evaluations are performed for each level and period. In addition the solution involves raising a matrix to a power.

The evaluation of the matrix exponential for a given general matrix $C$ is unfortunately not a trivial task. Fortunately, the numerical evaluation of the matrix exponential has, for the general case, been investigated in some detail in a review paper by Moler and Van Loan [13]. This paper discusses 19 methods which have been employed to evaluate the matrix exponential, all termed “dubious”. Recommended methods for the evaluation of the matrix exponential are the Păde approximation, Schur matrix decomposition and the scaling and squaring technique. The latter two options have been implemented in the code. If matrices $A$ and $B$ are upper- or lower- triangular matrices, the evaluation of the matrix is performed using an algorithm developed by Parlett [14,15].

Due to the occurrence of $(n, 2n)$ and $(n, p)$ neutron transmutation reactions during the pulse on periods, neutron reaction/decay chain loops occur in the transmutation/decay scheme of a stable input isotope. Loops occur when a radioactive isotope decays to a preceding nuclide in its reaction-decay pathway. The occurrences of loops complicate the structure of the matrix $A$ by introducing entries in the upper triangular half of the matrix. When this is the case, the evaluation of the matrix exponential proceeds using the Schur decomposition or the scaling and squaring technique general matrix exponential solvers. If matrix $A$ is lower- or upper- triangular the evaluation is performed using Parlett’s algorithm.

During the dwell periods and after shutdown times, the only nuclear process occurring for transmutation induced nuclides of interest in fusion calculations is nuclear decay by $\beta^-, \beta^+, \epsilon$ (electron capture), and $\alpha$-decay. If the nuclide entries in matrices $A$ and $B$ are stored in increasing $Z$ (atomic number) and $A$ (atomic number) order, then matrix $B$, the matrix for the dwell period is nearly lower triangular with a few entries in the upper-triangular part due to $\beta^+, \epsilon$ and $\alpha$ decays. If there is no coupling between the lower- and upper- triangular parts (which is usually the case) of matrix $B$, both triangular parts of the matrix can be evaluated using Parlett’s algorithm.
3.2.1 Scaling and Squaring Technique

This technique uses a Taylor series expansion of matrix $A$ combined with scaling and squaring to compute $e^{At}$ as follows:

$$B = (e^{\frac{At}{2n}})^{2n} = (e^{C})^{2n}$$

$$e^C = I + C + \frac{C^2}{2!} + \ldots + \frac{C^k}{k!} + \ldots .$$

The truncation criteria for the Taylor series is:

$$||C^k/k|| < \epsilon \max(ab(c_{ij}))$$

$$||C^k/k|| := \sum(ab(c_{ij})).$$

This technique, with proper diagnostics can be quite efficient.

3.2.2 Schür Decomposition

The Schür decomposition of a matrix is the following:

$$A = QTQ^T$$

where $T$ is an upper-triangular matrix. Details on the decomposition can be found in most linear algebra texts. Once matrix $A$ has been decomposed, the matrix exponential is evaluated from the expression:

$$e^{At} = Qe^{Tt}Q^T.$$ 

LAPACK routines [16] are used to perform the Schür decomposition. The evaluation of the matrix exponential is performed using Parlett’s algorithm.

3.2.3 Matrix Raised to a Power

The formal solution of the pulsed/intermittent irradiation history problem involves raising a matrix to a power (note Eq. 6). There are several methods that can be employed to raise a matrix to a power (of which a subset are): (1) the direct multiplication of the matrix with itself repeated $n$ times, (2) the eigenvalue decomposition method briefly described in Ref. 6, and (3) a log$_2$ based algorithm which utilizes repeated squaring and multiplication of the matrix. Of the three methods indicated above method 3 is computationally the most efficient and the method implemented in RACC-Pulse.
3.3 Pulsing Scheme

RACC-Pulse subdivides the whole operation history into different “periods”. Each period has the same flux level (power level) and many pulse levels. Each level is a grouping of pulses having the same pulse width and dwell times. Pulses in different periods can have different pulse structures and power levels. This scheme allows the user considerable flexibility in modeling regular and irregular irradiation histories. Varying pulse width, dwell times, maintenance periods and power levels can all be modeled. This flexibility has its costs, increasing complexity in the irradiation structure results in an increase in the run time. A detailed explanation of the pulsing options and its input is provided in Appendix A.

4 Results and Discussion

The water-cooled SS316 nonbreeding blanket/shield design considered during the ITER (EDA) blanket option trade-off study (BOTS) [1] served as our benchmark problem. Details of the neutronics calculations are provided in Ref. 17. The radial build used for this blanket option is shown in Figure 2. The transmutation cross section library utilized for the analyses is the USACT93 [18] and is based on isotopic radioactive decay and neutron transmutation cross section data from the ENDF/B-VI and EAF3 [19] basic data libraries.

The purpose of the comparison is threefold: to validate the computational method by comparison to the original GEAR method, to display the pulse level features of the code and to compare and discuss the calculational run times (CPU time) of the code.

Table 2 presents a comparison of the total activity of the SS316/H₂O blanket for three
cases, the original RACC code with the GEAR package and the RACC-Pulse code performing steady state and uniform pulse scenario calculations. The uniform pulse scenario and the parameters for the pulse width, dwell time and total operating time are depicted in Figure 3. These parameters are consistent with the originally proposed ITER design parameters: a nominal fusion power of \( 3.0 \text{ GW} \), an average wall loading of \( 2.0 \text{ MW/m}^2 \), \( 10^5 \) cycles with a power of \( 1.5 \text{ GW} \), a pulsed duration of 1000 seconds and a maximum duty cycle of 50\% \([1]\). We note that the steady state calculations for both RACC versions agree as is expected. The effect of pulsing on the activity results is noted by the comparison of the steady state results to the pulsed results and is consistent with other calculations of similar nature.

Table 2 also contains results computed by the DKR-Pulsar code. The results can only be compared on order of magnitude basis, however, because: (1) both codes use a different decay scheme truncation criterion, (2) the transmutation cross section library employed in the RACC-Pulse calculations contains only a subset of the reaction types considered in the library utilized in the DKR-Pulsar computations and, (3) due to memory allocation limitations on the workstation, the RACC-Pulse code was limited to only one transmutation generation. Hence the DKR-Pulsar calculations are considered to be more complete. Given the differences mentioned above, the agreement is quite good indicating that RACC-Pulse is performing well.

An indication of the run time of the RACC-Pulse code is given in Table 3 for various pulsing histories. A brief explanation is required at this point before beginning our discussion. The computer on which these calculations were performed is a DECstation 5000/200 workstation. To obtain an estimate of the CPU time required on the Cray-2 at Livermore (C-machine) or on an HP735/99MHz, the numbers in the table should be reduced by a factor of 5 to 5.5. As one surveys the results in the table, one notes that the original RACC code with the GEAR package is the most computer intensive. The computational time is a result of the low tolerance limit required to achieve the same level of accuracy as that obtained with RACC-Pulse code. The implementation of the matrix solver routine has thus improved the computational run time of the original code. Concerning the designations under the Operation Mode heading for the pulsed history cases, the descriptor “period” refers to a given operation history having the same flux level. The descriptor “level” refers to the number of uniform pulse groupings within a period (see the RACC-Pulse instructions in the Appendix for further details). We note that the CPU time is a function of the number of levels and periods modeled, i.e. increased complexity of the pulsing history results in an increase in the CPU time. The increase in time is the result of the extra matrices required to model the irradiation history. Hence modeling a changing flux level is quite costly. Figure 4 depicts a comparison of the radioactivity results for the operation histories investigated.

Results for the DKR-Pulsar code have also been included for comparison purposes in
Table 2: Comparison of the RACC-Pulse and RACC Code After Shutdown Total Activity Results Using the BOTS Study Nonbreeding 316 SS/H₂O Blanket Design Option

<table>
<thead>
<tr>
<th>Time After Shutdown</th>
<th>Total Activity [Ci/MW]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
</tr>
<tr>
<td>Uniform Pulsing (RACC-Pulse)</td>
<td>2.059 × 10⁶</td>
</tr>
<tr>
<td>DKR-Pulsar (Steady State)</td>
<td>9.912 × 10⁶</td>
</tr>
<tr>
<td>DKR-Pulsar (Uniform Pulsing)</td>
<td>2.201 × 10⁶</td>
</tr>
</tbody>
</table>

Parameters used in the calculations
Steady state operation - 1.5 years
Uniform pulsed operation - \( t_{\text{pulse}} = 1000 \text{ s} \); \( t_{\text{dwell}} = 7000 \text{ s} \); \# pulses = 47,304

Table 3: Comparison of CPU Time

<table>
<thead>
<tr>
<th>Code</th>
<th>Operation Mode</th>
<th>Accuracy-Truncation Tolerance^+</th>
<th>Transmutation Generations (RACC)</th>
<th>CPU Time (DEC-5000/200 RISC) (hr:mm:ss)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RACC (-Gear)</td>
<td>Steady State</td>
<td>1.0e-9</td>
<td>1</td>
<td>3:40.39</td>
</tr>
<tr>
<td>RACC-Pulse</td>
<td>Steady State</td>
<td>1.0e-5</td>
<td>1</td>
<td>22.00</td>
</tr>
<tr>
<td>RACC-Pulse</td>
<td>1 Period–1 Level</td>
<td>1.0e-5</td>
<td>1</td>
<td>28.19</td>
</tr>
<tr>
<td>RACC-Pulse</td>
<td>1 Period–3 Levels</td>
<td>1.0e-5</td>
<td>1</td>
<td>40.31</td>
</tr>
<tr>
<td>RACC-Pulse</td>
<td>3 Periods–3 Levels</td>
<td>1.0e-5</td>
<td>2</td>
<td>1:48.20</td>
</tr>
<tr>
<td>RACC-Pulse</td>
<td>1 Period–3 Levels</td>
<td>1.0e-5</td>
<td></td>
<td>Problem was too large to run on workstation</td>
</tr>
<tr>
<td>DKR-Pulsar</td>
<td>Steady State</td>
<td>(1.5e-3)</td>
<td>–</td>
<td>11.39</td>
</tr>
<tr>
<td>DKR-Pulsar</td>
<td>1 Period–1 Level</td>
<td>(1.5e-3)</td>
<td>–</td>
<td>17.33</td>
</tr>
<tr>
<td>DKR-Pulsar</td>
<td>1 Period–3 Levels</td>
<td>(1.5e-3)</td>
<td>–</td>
<td>19.13</td>
</tr>
</tbody>
</table>

^A comparison between the accuracy-truncation tolerance levels of the different codes is not meaningful. This “tolerance limit” has a different definition and is applied differently within each code. Its purpose is to illustrate that the solution methods use some sort of tolerance check.
ITER Pulsed/Intermittent Operation Parameters:
(1). Total Life Time: 12 Years
(2). Total Number of Cycles: 47304 (equivalent to 1.5 year steady-state operation time)
(3). Maximum Duty Factor of Cycle: 50%
(4). Pulse Width: 1000 seconds
(5). Fusion Power: 3 GW (2MW/m² average wall loading)

Two Types of Pulsed Operation Schemes:
(1). Homogeneous Scheme (1 period and 1 level):
   \[(1000+T_{dwell}*47304-T_{dwell}) = 12*365*24*3600\]
   \[T_{dwell} = 7000 \text{ seconds}\]

Figure 3. Uniform pulse scenario irradiation history.
Figure 4. Total after shutdown activity for different pulse history scenarios.
Table 3. Until the recent modifications were made to the RACC code for pulse operation histories, DKR-Pulsar was the only code which had the capability to perform pulsed activation calculations. The calculational scheme employed in the DKR-Pulsar code is based on the linear chain methodology [6]. The difference in CPU times thus reflects the difference in code philosophies. A word of caution regarding the RACC-Pulse calculations — as mentioned previously only one transmutation generation could be modeled due to memory limitations of the workstation. In order to perform a complete radioactivity analysis the transmutation generation parameter in the code should be set to at least 2 but preferably 3. Increasing this parameter increases the size of the nuclide matrices in the RACC-Pulse code which in turn increases the CPU time. Hence the RACC-Pulse times represent a lower bound on the CPU time. The benchmark problem modeling with the DKR-Pulsar code is more complete and hence the times listed are more representative of the actual times one can expect for a realistic calculation.

4.1 Implications for ITER

The implications for the ITER facility are rather straightforward. The RACC-Pulse code gives the blanket and shield designer the capability to perform pulsed/intermittent activation calculations. The code is quite versatile in its modeling abilities, being able to model varying flux levels, pulse widths and dwell times and maintenance periods. One must, however, be aware of the computational time, as an increase in operation history complexity increases the run time. For a detailed fine mesh blanket and shield design calculation, the run time can exceed 5 hours.

5 Conclusion and Discussion

The RACC radioactivity code now termed RACC-Pulse, has been modified by the implementation of routines which extends the code’s capabilities to pulsed/intermittent irradiation histories. The code now has the ability to model varying flux levels, pulse widths and dwell periods, varying pulsing schemes and maintenance periods. This capability gives the blanket and shield designer and safety analyst the required flexibility to model virtually any irradiation history that may be prescribed by the experimentalist of the ITER facility.

Though the RACC-Pulse code is quite flexible in its modeling capabilities, one noticeable drawback is the CPU time required by the program. If the benchmark CPU results are extrapolated to a full blown, realistic model calculation of the ITER facility (where the transmutation generation parameter is set to 3), all indications are that the calculations would require several hours of CPU time on a HP735/99 MHz workstation and the Cray-2
computer at Livermore (C-machine), particularly if the problem consists of many zones of differing composition or if a detailed fine mesh calculation is required.

The reason for this is inherent to the basic calculation philosophy (code decay scheme and problem setup) of the code and the computer architecture the code was optimized for at the time of its original development. Hence, a further reduction in CPU time can only be obtained by optimization and changes to various portions of the code unrelated to the pulsing algorithms which is beyond the scope of this work statement. The problem of CPU time should have been addressed and perhaps have been one of the criteria used for code selection by the decision making committee. The large memory requirements of the code may preclude realistic detailed calculations to be performed on small computer systems lacking sufficient memory. This is in contrast to the DKR-Pulsar code which is both faster and does not suffer from the large memory requirements.

Acknowledgement

This work was supported by the Office of Fusion Energy, U. S. Department of Energy, under Contract No. DE-FGQ2-94ER54244.A001.
References


15. B.N. Parlett, “Computations of Functions of Triangular Matrices,” Electronic Research Laboratory, University of California-Berkeley Memorandum No. ERL-M481.


18. Private communications with Dr. Fred Mann of Hanford Engineering Design Laboratory.

Appendix

A. Pulsed History Operation

The unique characteristics of RACC-Pulse is that it can model a wide variety of pulsed/intermittent operation histories including the steady state case. The steady state operation scheme and homogeneous pulsed operation scheme are typical single period operation schemes. Multi-period operation schemes are a bit more difficult to set up. A set of examples are provided in Figs. A1-A4 to illustrate the flexibility in pulsing scenario and their input parameters.

RACC-Pulse subdivides the operation history into “periods”. Within each period the power level is constant as well as the pulse width. Hence different periods can have different pulse widths and power levels. Each period can have a different number of pulse levels, e.g. the operation scheme can be steady state in the first period and in homogeneous pulsed scheme in the second period, multi-period with multilevel scheme in the third period, etc.

Fig. A1. Example 1 — Steady State Scheme.

Fig. A2. Example 2 — Homogeneous pulsed scheme.
Fig. A3. Example 3 — Single period with 2 level scheme.

Fig. A4. Example 4 — Multi-period with multilevel scheme with inhomogeneous power level.
B. Input to the RACC-Pulse Code

The following is the input for the RACC-Pulse code. Most of the input instructions are the same as for the original RACC code. Additional lines of input occur at the end of the standard input file and are the parameters for the pulsing routines. For a more detailed explanation of the standard input section, the user is referred to the original RACC manual, “Theory and Use of the Radioactivity Code RACC” by Jungchung Jung.

All of the data arrays in RACC-Pulse are read by using the standard/format free FIDO input system. Each FIDO array in RACC-Pulse must be followed by the terminator symbol, t. Certain arrays are conditional in RACC-Pulse. Those conditions are indicated in brackets []. Quantities in parentheses () stand for array dimensions and numbers following the symbol † show reference numbers for the detailed data notes in Chapter IV of the original RACC manual.

**Input Data**

(1) Title FORMAT (18A4) Problem Title

(2) Arrays

1$$ Control Integer Parameters (50)

1. ID Problem ID number
2. IDIM problem dimension (†1)
   1 - one dimension
   2 - two dimensions
   3 - three dimensions
3. IGE Geometry of system (†1)
   0 - any
   1 - slab
   2 - sphere
   3 - cylinder
   4 - torus
<table>
<thead>
<tr>
<th>No.</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.</td>
<td>IGM No. of total energy groups of input flux</td>
</tr>
<tr>
<td>5.</td>
<td>IGN No. of neutron energy groups of input flux</td>
</tr>
<tr>
<td>6.</td>
<td>IGG No. of gamma energy groups of input flux</td>
</tr>
<tr>
<td>7.</td>
<td>IM No. of fine intervals in x (r) direction (†1)</td>
</tr>
<tr>
<td>8.</td>
<td>JM No. of fine intervals in y (θ/z) direction (†1)</td>
</tr>
<tr>
<td>9.</td>
<td>KM No. of fine intervals in z (φ) direction (†1)</td>
</tr>
<tr>
<td>10.</td>
<td>IZM No. of zones in x (r) direction (†1)</td>
</tr>
<tr>
<td>11.</td>
<td>JZM No. of zones in y (θ/z) direction (†1)</td>
</tr>
<tr>
<td>12.</td>
<td>KZM No. of zones in z (φ) direction (†1)</td>
</tr>
<tr>
<td>13.</td>
<td>NPP No. of radioactivity calculation problem zones</td>
</tr>
<tr>
<td>14.</td>
<td>MS1 Mixing table length for basic material makeup (†2,3)</td>
</tr>
<tr>
<td>15.</td>
<td>MS3 Mixing table length for composite material makeup (†4)</td>
</tr>
<tr>
<td>16.</td>
<td>MS2 Mixing table length for problem zone makeup</td>
</tr>
<tr>
<td>17.</td>
<td>IVOL Problem zone volumes (†1)</td>
</tr>
<tr>
<td></td>
<td>0 - input</td>
</tr>
<tr>
<td></td>
<td>1 - calculate</td>
</tr>
<tr>
<td>18.</td>
<td>ISD System shutdown calculation</td>
</tr>
<tr>
<td></td>
<td>0 - no - only pre-shutdown calculation</td>
</tr>
<tr>
<td></td>
<td>1 - yes - both pre- and post-shutdown calculation</td>
</tr>
<tr>
<td>19.</td>
<td>NT1 No. of time steps before shutdown - 2 (always)</td>
</tr>
<tr>
<td>20.</td>
<td>NT2 No. of time steps after shutdown</td>
</tr>
<tr>
<td>21.</td>
<td>IFXA Input of group flux (†7)</td>
</tr>
<tr>
<td></td>
<td>0 - card</td>
</tr>
<tr>
<td></td>
<td>1 - ANISN file</td>
</tr>
<tr>
<td></td>
<td>2 - DOT file</td>
</tr>
<tr>
<td></td>
<td>3 - TWODANT file</td>
</tr>
<tr>
<td></td>
<td>4 - MORSE file</td>
</tr>
<tr>
<td></td>
<td>5 - VIM file</td>
</tr>
<tr>
<td></td>
<td>6 - ONEDANT file</td>
</tr>
<tr>
<td></td>
<td>7 - DKR formatted file</td>
</tr>
<tr>
<td></td>
<td>8 - any FIDO formatted file</td>
</tr>
<tr>
<td></td>
<td>if IFXA is negative, the flux is double precision</td>
</tr>
<tr>
<td>22.</td>
<td>IXSA Input of group cross section (†7)</td>
</tr>
<tr>
<td></td>
<td>0 - card</td>
</tr>
<tr>
<td></td>
<td>1 - disk/tape</td>
</tr>
</tbody>
</table>

0 - input
1 - calculate

System shutdown calculation
0 - no - only pre-shutdown calculation
1 - yes - both pre- and post-shutdown calculation

No. of time steps before shutdown - 2 (always)

No. of time steps after shutdown

Input of group flux (†7)
0 - card
1 - ANISN file
2 - DOT file
3 - TWODANT file
4 - MORSE file
5 - VIM file
6 - ONEDANT file
7 - DKR formatted file
8 - any FIDO formatted file
if IFXA is negative, the flux is double precision

Input of group cross section (†7)
0 - card
1 - disk/tape
<table>
<thead>
<tr>
<th></th>
<th>Description</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>23.</td>
<td>IDLA Input of decay data ([†7])</td>
<td>0 - card, 1 - disk/tape</td>
</tr>
<tr>
<td>24.</td>
<td>IFXB Storage of group flux ([†8])</td>
<td>0 - card, 1 - disk</td>
</tr>
<tr>
<td>25.</td>
<td>IXSB Storage of cross section ([†8])</td>
<td>0 - card, 1 - disk</td>
</tr>
<tr>
<td>26.</td>
<td>IDLB Storage of decay data ([†8])</td>
<td>0 - card, 1 - disk</td>
</tr>
<tr>
<td>27.</td>
<td>IPRFX Print group flux ([†9])</td>
<td>0 - no, 1 - only interval group flux, 2 - only zone group flux, 3 - both</td>
</tr>
<tr>
<td>28.</td>
<td>IPRXS Print group cross section ([†9])</td>
<td>0 - no, 1 - yes</td>
</tr>
<tr>
<td>29.</td>
<td>IPRDA1 Print decay data for chain construction ([†9])</td>
<td>0 - no, 1 - yes</td>
</tr>
<tr>
<td>30.</td>
<td>IPRDA2 Print decay chain table ([†9])</td>
<td>0 - no, 1 - yes</td>
</tr>
<tr>
<td>31.</td>
<td>IPRDA3 Print isotopes involved in the problem (MDX table) ([†9])</td>
<td>0 - no, 1 - yes</td>
</tr>
<tr>
<td>32.</td>
<td>IPRDB1 Print decay constants/branching ratios ([†9])</td>
<td>0 - no, 1 - yes</td>
</tr>
<tr>
<td>33.</td>
<td>IPRDC1 Print radioactivity-related data for edit ([†9])</td>
<td>0 - no, 1 - yes</td>
</tr>
<tr>
<td>No.</td>
<td>Code</td>
<td>Description</td>
</tr>
<tr>
<td>-----</td>
<td>-------</td>
<td>-----------------------------------------------</td>
</tr>
<tr>
<td>34</td>
<td>ISTART</td>
<td>Problem restart (†10)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>IDUMP</td>
<td>Core dump (†10)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>36</td>
<td>IEDT1</td>
<td>BHP (air) edit (†11)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>37</td>
<td>IEDT2</td>
<td>BHP (water) edit (†11)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>38</td>
<td>IEDT3</td>
<td>Decay heat edit (†11)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>39</td>
<td>IEDT4</td>
<td>Radioactivity edit (†11)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>IEDT5</td>
<td>Decay gamma spectrum edit (†11)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>41</td>
<td>IEDT6</td>
<td>Print system matrix/solution of equations (†12)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
2** Control Floating Parameters (10)

1. EPS Precision required for solution (†14)
2. FACFLX Input flux normalization constant (cm²-s) (†15)
   no effect if FACFLX is 0.0
3. FACVLM System volume normalization constant (cm³) (†15)
   no effect if FACVLM is 0.0
4. FACPWR System power normalization constant (MWTh) (†15)
5. RMAJOR Major radius of torus (cm) [IGE = 4] (†1)
6. RNULL5 For future use
7. RNULL4 For future use
8. RNULL3 For future use
9. RNULL2 For future use
10. RNULL1 For future use

3$$ Basic Material Numbers for Basic Material Makeup (MS1) (†3)

4$$ Constituent Isotope JZA ID Numbers for Basic Material Makeup (MS1) (†2,3)

5** Constituent Isotope Number Densities (atom/barn-cm) for Basic Material Makeup (MS1) (*3)

6** Constituent Isotope Source Densities (atom/barn-cm-s) for Basic Material Makeup (MS1).
   For RACC_Pulse all data of this array are 0.0

7$$ Composite Material Numbers for Composite Material Makeup (MS3) (†4)

8$$ Constituent Basic Material Numbers for Composite Material Makeup (MS3) (†4)
9** Constituent Basic Material Fractions for Composite Material Makeup (MS3) (†4)
10** Constituent Basic Material Source Fractions for Composite Material Makeup (MS3) (†4)
   For RACC_Pulse all data of this array are 0.0
11$$ No. of I-Fine Intervals in Each I-Zone (IZM) (†1)
12$$ No. of J-Fine Intervals in Each J-Zone (JZM) [IDIM≥2] (†1)
13$$ No. of K-Fine Intervals in Each K-Zone (KZM) [IDIM≥3] (†1)
14$$ Problem Zone Numbers for Problem Zone Makeup (MS2) (†1,5)
15$$ I-Zone Numbers for Problem Zone Makeup (MS2) (†1,5)
16$$ J-Zone Numbers for Problem Zone Makeup (MS2) [IDIM≥2] (†1,5)
17$$ K-Zone Numbers for Problem Zone Makeup (MS2) [IDIM≥3] (†1,5)
18** I-Dimensional Volume Elements (IMM) [IVOL = 0] (†1)
   IMM = IM if IDIM = 1 or IGE ≠ 4
   IMM = 2*JM otherwise
19** J-Dimensional Volume Elements (JMM) [IVOL = 0 and IDIM≥2] (†1)
   JMM = JM if IGE ≠ 4
   JMM = 2*JM if IGE = 4
20** K-Dimensional Volume Elements (KM) [IVOL = 0 and IDIM = 3] (†1)
21** I-Fine Interval Boundaries (IM + 1) [IVOL = 1] (†1)
22** J-Fine Interval Boundaries (JM + 1) [IVOL = 1 and IDIM≥2] (†1)
23** K-Fine Interval Boundaries (KM + 1) [IVOL = 1 and IDIM = 3] (†1)
24$$ Composite Material Numbers for Problem Zones (NPP)
25$$ No. of Neutron Reaction Generations to be Followed for Problem Zones (NPP) (†6)
26** Time Step Boundaries for Pre-Shutdown Calculation (2)
   0.0 and total operation time
27** Time Step Boundaries for Post-Shutdown Calculation (NT2) [ISD = 1]
28** Output Decay Gamma Source Energy Group Boundaries (IGGEDT +1)
29** Group Flux (IM*JM*KM*IGN) [IFXA = 0] (†7)
Pulsed History Parameters (not FIDO Formatted Input Data)

LINE 1  Free Format Integers (3)
  1. lscheme - scheme option
     0 - scaling and squaring technique
     1 - Schür decomposition
  2. nlevel - number of levels in any periods
  3. nperiod - number of periods in whole operating time

LINE 2  Free Format Integers (nlevel * nperiod)
  (npulses(j, i), j = 1, nlevel)
  [repeat this input card for each period]
  npulses(j, i) - number of pulses of level j in period i

LINE 3  Free Format Real Numbers (nlevel * nperiod)
  ton(i) (toff(j, i), j = 1, nlevel)
  [repeat this input card for each period]
  ton(i) - pulse width in period i. [s]
  toff(j, i) - dwell time of level j in period i [s]

LINE 4  Free Format Real Numbers (nperiod-1)
  (tdwell(i), i = 1, nperiod-1)
  tdwell(i) - dwell time between period i and i+1 [s]

LINE 5  Free Format Real Numbers (nperiod)
  (fpower(i), i = 1, nperiod)
  fpower(i) - normalization factor of power level in period i