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INPUT INSTRUCTIONS FOR RACC-P

by

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ABSTRACT

*This report describes the input instructions of a new version of the radioactivity computer code **RACC**. This version of the codes includes new methods of solutions and the treatment of the pulsed operation. The new methods are the eigenvector decomposition, the Schür decomposition, and the Páde approximation. In addition, this version employs a new comprehensive cross-section and decay data library which include new radioactivity responses.*

1. Introduction

The GEAR method [1] has been used in the radioactivity code RACC [3] to solve the transmutation system of equations which is a set of first order simultaneous differential equations. With the considerable improvement in the quality and the quantity (number of isotopes) of the decay and the cross-section data libraries [4]; it was imperative to seek different methods of solution that reduce the computation time and can be easily adopted to the treatment of the pulsed operation.

Different methods have been considered. The criteria of this consideration were based on the accuracy, the reliability, the generality, the efficiency of the method and its applicability to treat pulsed irradiation. The methods that were considered and employed are: the LSODES, the Schür decomposition, the eigenvector decomposition, and the Páde approximation of the matrix exponential function. Details of these methods are given elsewhere [5].

The solver and the editor parts of the RACC code have been rewritten to include the above methods and to interface it with the new decay and cross-section data libraries. The input part of the code has been kept as close as

possible to the original code. This reports describes the slightly modified input and illustrate the use of the different methods.

2. Methods of Solutions

2.1 GEAR

This is the original GEAR [1] solver and is triggered by setting the variable MGEAR in the integer control array (\$1) to non-zero value. In this case, RACC-P uses the same method employed in RACC for the post shutdown solutions.

2.2 LSODES

This solver [2] is based on the GEAR method. It has the advantage over the original GEAR solver [1] of making use of the sparsity structure of the transmutation matrix. As a result, sizable reduction in the required computer memory is achieved. In the steady state operation, this is the default method of solution.

2.3 Schür Decomposition

This method is used by setting the input variable MEIGEN in the integer control array (\$1) to '1'. This method is always invoked in the case of pulsed operation. Different routines from the mathematical library LAPACK [6] are used to perform the decomposition. The Parlett [7] algorithm for calculating the function of the Schür matrix is used.

2.4 Eigenvector Decomposition

Although this method is considered naive by mathematicians, it has been included to show its limitations. The Schür decomposition is performed first and if the matrix is proved well-conditioned, the LAPACK eigenvector routines are called. If the matrix is ill-conditioned or posses complex eigenvalues, the Parlett algorithm is used as above. This method is triggered by setting the variable MEIGEN to '2'.

2.5 Ward's Padé Algorithm

This algorithm [8] has been proven to be very reliable and efficient. A modified version by Van Loan [9] is used to calculate the exponential of the transmutation matrix. This method is used by setting the input variable MPADE to non-zero value.

3. Pulsed Operation

The pulsed operation is triggered by setting the input variable NPULSE in the integer control array (\$1) to the number of pulses. In this case, the first non-zero value of the time step boundaries for pre-shutdown (26*) is used as the burn time, and the second value is used as the dwell time. The value of the number of the time steps before shutdown (NT1 in \$1) must be ≥ 3 .

4. Input Instructions

This version of RACC, as the original version, uses the standard/free FIDO input format which is used by many neutronics codes. Each FIDO array in RACC must be followed by the terminator symbol, T. Certain arrays are conditional. Those conditions are indicated in brackets [] under which the arrays must be supplied. Quantities in parentheses () stand for array dimensions. To make the input clearer, comments can be inserted anywhere in the input by enclosing them between two square brackets [] or two braces {}. Comments in the input can be added to the end of a line after "/". The reader is referred to Ref. 1 for more detailed information.

4.1 Input Data

- (1) Title Problem Title 1-70 characters
- (2) Arrays
 - 1\$ Control Integer Parameters
 - 1. ID Problem ID number
 - 2. IDIM Problem dimension
 - 1 - one dimension
 - 2 - two dimensions
 - 3 - three dimensions

3.	IGE	Geometry of system 0 - any 1 - slab 2 - sphere 3 - cylinder 4 - torus
4.	IGM	No. of total energy groups of input flux
5.	IGN	No. of neutron energy groups of input flux
6.	ICG	No. of gamma energy groups of input flux
7.	IGGEDT	No. of output gamma-source energy groups [IEDT5#0]
8.	IM	No. of fine intervals in x (θ) direction
9.	JM	No. of fine intervals in y (θ/z) direction
10.	KM	No. of fine intervals in z (ϕ) direction
11.	IZM	No. of zones in x (r) direction
12.	JZM	No. of zones in y (θ/z) direction
13.	KZM	No. of zones in z (ϕ) direction
14.	NPP	No. of radioactivity calculation problem zones
15.	IVOL	Problem zone volumes 0 - input 1 - calculate
16.	MS1	Mixing table length for basic material makeup
17.	MS2	Mixing table length for problem zone makeup
18.	MS3	Mixing table length for composite material makeup
19.	IOP	Pre-shutdown output control 1 - yes - pre-shutdown outputs 0 - no - No pre-shutdown outputs
20.	ISD	System shutdown calculation 0 - no - No shutdown calculation 1 - yes - Post-shutdown calculations
21.	NT1	No. of time steps before shutdown
22.	NT2	No. of time steps after shutdown
23.	IFXA	Input of group flux 0 - card 1 - ANISN file 2 - DOT file 3 - TWOTRAN file 4 - MORSE file 5 - VIM file 6 - any FIDO formatted file 7 - ONEDANT rflux file If IFXA is negative, the flux is double precision

24. IXSA	Input of group cross section
0 - card
1 - disk/tape
25. IDLA	Input of decay data
0 - card
1 - disk/tape
26. IFXB	Storage of group flux
0 - card
1 - disk
27. IXSB	Storage of cross section
0 - card
1 - disk
28. IDLB	Storage of decay data
0 - card
1 - disk
29. IPRFX	Print group flux
0 - no
1 - only interval group flux
2 - only zone group flux
3 - both
30. IPRXS	Print group cross section
0 - no
1 - yes
31. IPRDA1	Print decay data for chain construction
0 - no
1 - yes
32. IPRDA2	Print decay chain table
0 - no
1 - yes
33. IPRDA3	Print isotopes involved in the problem (MDX table)
0 - no
1 - yes
34. IPRDB1	Print decay constants/branching ratios
0 - no
1 - yes
35. IPRDC1	Print radioactivity-related data for edit
0 - no
1 - yes
36. MF	Method of solution
11 - Adams method
21 - Gear method

37. MATED Print system matrix/solution of equations
 0 - no
 1 - system matrix
 2 - solution of ODE (atomic transmutation rates)
 3 - both
38. IEDT1 BHP (air) edit
 0 - no
 1/-1 - specific edit/and save
 2/-2 - total edit/and save
 3/-3 - both/and save
39. IEDT2 BHP (water) edit
 0 - no
 1/-1 - specific edit/and save
 2/-2 - total edit/and save
 3/-3 - both/and save
40. IEDT3 Decay heat edit
 0 - no
 1/-1 - specific edit/and save
 2/-2 - total edit/and save
 3/-3 - both/and save
41. IEDT4 Radioactivity edit
 0 - no
 1/-1 - specific edit/and save
 2/-2 - total edit/and save
 3/-3 - both/and save
42. IEDT5 Decay gamma spectrum edit
 0 - no
 1/-1 - specific edit/and save
 2/-2 - total edit/and save
 3/-3 - both/and save
43. IEDT6 Gamma dose edit
 0 - no
 1/-1 - specific edit/and save
 2/-2 - total edit/and save
 3/-3 - both/and save
44. IEDTB Beta heat edit
 0 - no
 1/-1 - specific edit/and save
 2/-2 - total edit/and save
 3/-3 - both/and save
45. IEDTG Gamma heat edit
 0 - no
 1/-1 - specific edit/and save
 2/-2 - total edit/and save
 3/-3 - both/and save

46. IEDTY	Gamma yield edit 0 - no 1/-1 - specific edit/and save 2/-2 - total edit/and save 3/-3 - both/and save
47. Debug	# 0 : stop after reading input
48. Debug	# 0 : stop after matrix construction
49. Debug	# 0 : stop after flux & cross-section processing
50. Debug	For future use
51. Debug	For future use
52. Contrl	# 0 : No zonal edit
53. Contrl	# 0 : No system edit
54. Contrl	For future use
55. Contrl	For future use
56. Contrl	=0 edit output in %; # 0 absolute edit
57. Contrl	For future use
58. Contrl	For future use
59. Contrl	For future use
60. Contrl	For future use
61. Contrl	For future use
62. Contrl	For future use
63. Contrl	For future use
64. MGEAR	# 0 : Use Gear
65. MEIGEN	# 0 : Use eigenvalue/Schür decomposition 1 - Schür decomposition 2 - Eigenvalue decomposition
66. MPADE	# 0 : Use Páde approximation
64. NPULSE	No. of pulses
65. NULL3	For future use
66. NULL2	For future use
67. NULL1	For future use

2* Control Floating Parameters

1. EPS-R	Relative precision required for solution (LSODES & GEAR)
2. EPS-A	Absolute precision required for solution (LSODES)
3. FACFLX	Input flux normalization constant (cm 2-s) no effect if FACFLX is 0.0
4. FACVLM	System volume normalization constant (cm3) no effect if FACVLM is 0.00
5. FACPWR	System power normalization constant (MW'h)
6. RMAJOR	Major radius of torus (cm) [IGE=4]

- 7. RNULL2 For future use
- 8. RNULL1 For future use
- 9. EDLIM Ignore isotopes' responses .lt. EDLIM
- 10. PRCLM Ignore isotope which contributes .LE. PRCLM % of the total edit

- 3\$ Basic Material Numbers for Basic Material Makeup (MS1)
- 7\$ Composite Material Numbers for Composite Material Makeup (MS3)
- 8\$ Constituent Basic Material Numbers for Composite Material Makeup (MS3)
- 9* Constituent Basic Material Fraction for Composite Material Makeup (MS3)
- 10* Constituent Basic Material Source Fractions for Composite Material Makeup (MS3)
- 11\$ No. of I-Fine Intervals in Each I-Zone (IZM)
- 12\$ No. of J-Fine Intervals in Each J-Zone (JZM) [IDIM $\geq$ 2]
- 13\$ No. of K-Fine Intervals in Each K-Zone (KZM) [IDIM = 3]
- 14\$ Problem Zone Numbers for Problem Zone Makeup (MS2)
- 15\$ I-Zone Numbers for Problem Zone Makeup (MS2)
- 16\$ J-Zone Numbers for Problem Zone Makeup (MS2) [IDIM = 2]
- 17\$ K-Zone Numbers for Problem Zone Makeup (MS2) [IDIM = 3]
- 18* I-Dimensional Volume Elements (IMM) [IVOL = 0]
 - IMM = IM if IDIM = 1 or IGE $\neq$ 4
 - IMM = 2IM otherwise
- 19* J-Directional Volume Elements (JMM) [IVOL = 0 and IDIM $\geq$ 2]
 - JMM = JM if IGE $\neq$ 4
 - JMM = 2JM if IGE = 4
- 20* K-Directional Volume Elements (KM) [IVOL = 0 and IDIM = 3]
- 21* I-Fine Interval Boundaries (IM + 1) [IVOL = 1]
- 22* J-Fine Interval Boundaries (JM + 1) [IVOL = 1 and IDIM $\geq$ 2]
- 23* K-Fine Interval Boundaries (KM + 1) [IVOL = 1 and IDIM = 3]
- 24\$ Composite Material Numbers for Problem Zones (NPP)
- 25\$ No. of Neutron Reaction Generations to be Followed for Problem Zones (NPP)
- 26* Time Step Boundaries for Pre-shutdown Calculation (NT1)
- 27* Time Step Boundaries for Post-shutdown Calculation (NT2) [ISD = 1]
- 4\$ Constituent Isotope JZA ID Numbers for Basic Material Makeup (MS1)
- 5* Constituent Isotope Number Densities (atom/barn-cm) for Basic Material Makeup (MS1)
- 6* Constituent Isotope Source Densities (atom/barn-cm-s) for Basic Material Makeup (MS1)
- 28* Output Decay Gamma Source Energy Group Boundaries (IGGEDT > 1) [IEDT5 $\neq$ 0]
- 29* Group Flux (IM*JM*KM*IGN) [IFXA = 0]

4.2 Example

```

1      YAEA Benchmark.....
2 1$$ +1 1 1 100 100 0 0 /id, idim, ige, ign, ign, igg, gedt
3      1 1 1 1 / IM JM KM (fine)
4      1 1 1 / IZM JZM KZM
5
6      1[NPP] 1[IVOL] 6[MS1] 1[MS2] 2[MS3]
7
8      1 1 / IOP ISD
9      2 2 / NT1 NT2 ?????
10
11 [_21] 1 1 1 /ifxa, ixsa, idla / INPUT 0(card) 1(disk)
12      0 0 0 / ifxb, ixsb, idlb / store 1=disk 0=core
13
14 [_27] 2 0 / iprfx, iprxs
15      1 1 1 / iprda1(D chain con), iprda2(D T), iprda3(mdx T)
16      1 1 / iprdbl(decay cons/branch ratio, iprdcl
17
18      21 / MF method of solution
19      3 / system_matrix/solution
20
21 { edit [1 spec], [ 2 total], [3 both], [-save] [0 no]}
22
23 0[Bhp-a] 0[Bhp-w] 0[Dheat] 0[Ci]
24 0[G-spc] 0[Rem ] 0[Bheat] 0[Gheat] 0[G-y]
25
26 [stop:a] 0 [input ] 0 [matrix cons]
27      0 [flux proc ] 0 [ ]
28      0 [ ]
29
30 [EDIT:NO?] 0 [zones ] 1 [ SYS ] 1 [ pre shut]
31      1 [Beta ] 0 [ % ] 0 [No flux writ]
32      0 [No edit but gama_s]
33      0 [write sol to 51]
34      0 [=1 M new format]
35      1 [itask in lside ]
36      0 [call mdwrt ]
37      0 [same flux & xs ]
38      0 [use gear ]
39      1 [use eigen ]
40      0 [0=Schur, +invers, -eigen ]
41      0 [use Pade(V.loan) ]
41      0 [number of pulses ]
42      F0
43      T
44
45
46 2**
47 1.0-9 / eps-relative
48 0.0 / eps-abs
49 1.00000-24 / fact_flux
50 0.00000 / fact_volume
51 1.00000 / fact_power
52 0.00000 / Rmaj
53 2R0.
54 0.00000 / Limit for Edit
55 1.00000-6 / Limit for %
56 T
57
58
59 7$$ / MSS = S( 10)
60 [ 1:Cr50 ] 1{CR50 }
61 [ 2:nat_Fe ] 2{Fe_nat }

```

```

62 T
63
64 8$$
65 [ 1:Cr50 ] 1{CR50 }
66 [ 2:nat_Fe ] 2{Fe_nat }
67 T
68
69 9**
70 [ 1:Cr50 ] 1.{CR50 }
71 [ 2:nat_Fe ] 1.{Fe_nat }
72 T
73
74 10** F0.0 T
75
76
77 11$$ / IZM- 50
78 1
79 T
80 14$$ / MS2= 11
81 1
82 T
83 15$$ /MS2
84 1
85 T
86 21** /IM= 332
87 0. 1.
88 T
89 24$$ / NPP= 11
90 1 {?}
91 T
92 25$$ F5 T / gen#
93 /*****
94
95 26** / operation time
96 0. /0.0 s
97 3.1580+07 / 1.0 y
98 T
99
100 27** / Dwell time
101 0. /0.0 s
102 3.1560+07 / 1.0 y
103 T
104
105
106
107 3$$ 1[cr] 4R2 [fe]
108 T
109
110 4$$ 4$$
111 240500 c410
112 260540 260560 260570 260580 fe12
113 T
114
115 5** 5**
116 1.00000+1 cr10
117 6.25423-1 9.89031 2.37229-1 3.01928-2 fe 1
118 T
119
120
121
122
123 6** F0.0 T
124
125 29*
126 0 +41750+10 0 +13720+ 9 0 +32380+ 8 0 +34020+ 8 0 +49830+ 8 0 +60730+ 8 1
127 0 +34680+ 8 0 +67370+ 8 0 +53870+ 8 0 +53290+ 8 0 +54780+ 8 0 +43050+ 8 2

```

128	0	+75680+	8	0	+11260+	9	0	+11440+	9	0	+15150+	9	0	+18070+	9	0	+24980+	9	3
129	0	+27120+	9	0	+32740+	9	0	+43300+	9	0	+45700+	9	0	+61180+	9	0	+62070+	9	4
130	0	+69720+	9	0	+80040+	9	0	+89860+	9	0	+88050+	9	0	+95120+	9	0	+10610+	10	5
131	0	+10550+	10	0	+10710+	10	0	+10990+	10	0	+12800+	10	0	+10190+	10	0	+10090+	10	6
132	0	+94040+	9	0	+73090+	9	0	+60510+	9	0	+65500+	9	0	+45110+	9	0	+39260+	9	7
133	0	+32130+	9	0	+44450+	9	0	+49100+	9	0	+54490+	9	0	+64450+	9	0	+63450+	9	8
134	0	+53870+	9	0	+18470+	10	0	+13080+	10	0	+14340+	10	0	+11070+	10	0	+88600+	9	9
135	0	+50110+	9	0	+36010+	9	0	+16900+	9	0	+10010+	9	0	+11410+	9	0	+24460+	9	10
136	0	+53340+	8	0	+57280+	8	0	+78120+	8	0	+22350+	9	0	+15010+	9	0	+77950+	8	11
137	0	+45450+	8	0	+23290+	8	0	+13720+	8	0	+52350+	7	0	+11150+	7	0	+85280+	6	12
138	0	+	0	0	0	+26570+	626R+	0	+	0								13	
139	T																		

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