

COMMISSION OF THE EUROPEAN COMMUNITIES

SABINE - 3

AN IMPROVED VERSION OF THE SHIELDING CODE SABINE

by

S ANT S

C. PONTI and R. VAN HEUSDEN

ESIS

1974



Joint Nuclear Research Centre Ispra Establishment - Italy Nuclear Studies Division

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Commission of the European Communities D.G. XIII - C.I.D. 29, rue Aldringen Luxembourg September 1974

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Commission of the European Communities Joint Nuclear Research Centre — Ispra Establishment (Italy) Nuclear Studies Division Luxembourg, September 1974 — 14 Pages — B.Fr. 25.—

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ABSTRACT

This report describes the new version of the programme SABINE, for one-dimensional bulk shielding calculations. The main improvements implemented into SABINE-3 are: the complete test of input data before starting the execution of a problem; a more accurate and flexible calculation of gamma-ray fluxes, that allows to save computer time; and an up-dated library that includes also data for gamma-rays arising from neutron inelastic scattering.

KEYWORDS

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1. Introduction

The code SABINE¹⁾ is used since 1967 to calculate neutron and gamma-ray attenuation in bulk shielding problems. It is widely used in European countries both in research centres and in private industries. It is applied for heating, damage, dose, and activation calculations in several types of thermal reactors and also in fast reactors.

This report describes the modifications which have been worked out to remove some inconsistency, to improve the accuracy of the results and to speed up the calculation time. As requested by many users, the input of the code is now tested before execution, and several diagnostics are provided to point out possible input errors.

Finally the cross section library has been improved by updating the gamma-ray data and including for some elements the gamma radiation produced by inelastic scattering.

This report should be considered as a supplement of ¹: it describes the new features and the differences between the new and the previous version. For all subjects not mentioned in this report, reference is made to what written in ¹. Examples of application of SABINE, as well as useful information on the check of the results for different types of shields, on comparisons between calculation and experience, on comparisons with other programs, may be found in ⁶ to ¹².

2. Neutronic Calculation

In the part of the code where the calculation of the neutron fluxes is performed, no important modifications have been introduced. The formula that determines the dependence of the thermal absorption cross section from the temperature, in the subroutine NEUTRO, has been improved.

3. Calculation of the Gamma-Ray Fluxes

Changements into this part of the program have been made in order to eliminate some sources of errors, to get a better accuracy of the results, and to simplify input data preparation.

- The temperature dependence of the thermal radiative capture c.s, which was not taken into account in the previous versions, has been introduced, with the same formula as for thermal absorption c.s.
- After having completed the neutron flux calculation, SABINE-3 may be used to compute the gamma-ray source distribution (to be introduced for instance in other computer codes), or to compute also the gamma-ray fluxes.
- Gamma-ray fluxes are now calculated at the points which are requested by specifying their abscissa z (distance from the core boundary). These points need not be equidistant or regularly distributed; they can be within the core (negative z) or within the shield (positive z).
- For each point where the gamma-ray flux is requested, the user may specify which regions should be taken into account as source regions for that point. In this way the computer effort may be minimized and important savings may be realised.
- The numerical integration over the source volume which is executed to compute the gamma-ray flux, has been improved; the errors that sometimes occurred when calculating fluxes at the interfaces (errors of 50% were pointed out) have now been removed.
- Division by zero were also frequent with the previous versions; they had no effect on the results, but produced sometimes a number of diagnostics or even stopped the running of the code. These have also been removed.
- The input data for this part of calculation has been simplified; in particular the number of coefficients of the polynomial that should fit the source distribution needs no more to be provided in input, being now computed by the code.

The program SABLIB that writes the unformatted library tape for SABINE has been modified to provide a new structure for the gamma-ray data. Furthermore it writes the library tape in a new way (with a smaller number of longer records). Previous library tapes read from SABINE are no more suitable for SABINE-3; new library tapes should be generated with the new SABLIB and the new data library.

The data needed to calculate the neutron induced gamma-ray sources may be provided for each element in to ways:

a) σ_i , i = 1,26 microscopic (n, γ) c.s. in <u>barns</u>

 c_{a} , g = 1,7 capture gamma spectrum, <u>MeV/cap</u>

In this way the gamma-ray spectrum is assumed to be independent from the neutron energy.

b)
$$\sigma_{i,\alpha}$$
 i = 1,26; g = 1,7 (n, γ) matrix, MeV·barn

This complete 26x7 matrix can account for gamma radiation produced by capture, inelastic scattering, or any other reaction that neutrons may produce with the element.

The neutron induced gamma-ray sources are calculated by SABINE-3 in the following way:

$$S_g(X) = \sum_{i=-L}^{26} \phi_i(X) P_{i,g}$$

 $S_{rr}(X)$ is the gamma-ray source density at x, for the group g, in MeV/cm³.sec.

 ϕ_i (X) is the neutron flux of the ith group at X.

L = IFGAM (see card 4 of input data), and

$$\mathsf{P}_{i,g} = \sum_{e(a)} \mathsf{N}^{e} \sigma_{i}^{e} c_{g}^{e} + \sum_{e(b)} \mathsf{N}^{e} \sigma_{i,g}^{e} \quad (\mathsf{MeV/cm})$$

e = index of the element

N^e = nuclear density in the region considered in atoms/barn.cm

The first sum is extended to those elements of the region considered, that are described as shown in (a); the second sum is extended to the elements described as shown in (b). This distinction is automatically operated by the code through the parameters contained in the data library.

5. SABINE-3 Data Libraries

The code is delivered together with two new data libraries; they differ only in the gamma-ray data. The neutron data library is essentially the same as that previously in use, except for a few corrections interesting the elements Calcium and Barium. The content of the gamma-ray data libraries is described below. The two libraries contain the same elements; they are listed in Table 1.

5.1 First Library (A)

In this library the gamma-ray data are described for all the elements in the way (a) of section 4. The changements contained as compared to the old library are listed below.

1) Gamma-ray spectra from thermal neutron cepture

For S, Ti, Ni, Cu, Zn, Ba, these data are taken from ²; for Na, Ai, Si, K, Ca, Fe, they are taken from ³. The data for Pb have not been modified because the differences versus the data published in ³ are irrelevant.

2) Neutron capture cross sections

For Na, Ni, Cu, the data were taken from ENDF/B materials 1059, 1123, 1087 and averaged with a spectrum calculated in a sodium tank. For Fe, data for material No: 1122 were averaged with a spectrum calculated in graphite. For U²³⁸ the data have been averaged with a spectrum of a PWR, taking into account the effect of the resonances.

3) Other changements

For the natural Boron, the library data account for the photon of 0.478 MeV emitted in 94% of (n, α) reactions.

5.2 Second Library (B)

This library contains complete (n, γ) matrices for ten elements: Li, C, Na, Al, Si, Fe, Ni, Cr, Cu, Pb. These matrices (see point (b) of section 4) have been generated by POPOP4⁴) taking into account all the reactions for which data were available in the POPOP4 library ⁵). The gamma-rays arising from inelastic scattering with Oxigen, may be produced only by neutrons of the first energy group; this gamma-source may be described in the way (a) of section 4.

A part from these elements, the content of this library is the same as that in library A. Note that within the gamma data library, the data of the "type (b)" elements precede the data of the other elements.

Material	ld. no.	Material	ld. no.
Material Hydrogen Deuterium Lithium Beryllium Boron Carbon Carbon Oxigen Sodium Magnesium Aluminium	ld. no. 1 2 3 4 5 6 8 11 12 13	Material Vanadium * Chromium Manganese * Iron Cobalt * Nickel * Copper * Zinc Zirconium Molybdenum	Id. no. 23 24 25 26 27 28 29 30 40 42
 Silicon Phosphorus Sulfur Water Potassium Calcium Titanium 	14 15 16 18 19 20 22	Cadmium * Barium Tungsten * Lead Uranium 235 * Uranium 238	48 56 74 82 235 238

TABLE 1

Identification numbers of the materials included in the library.

The elements indicated by * have been corrected or updated in the gamma-ray data library.

6. Input Specifications

An important new feature of SABINE-3 is the fact that before starting the calculations, the code checks the input data for consistency; if an error is found in a problem, the code prints a message, completes the check of the input data of that problem, and then goes to look for the following problem, if there is any.

Each problem is terminated by an "end card". If errors are pointed out in the input of a problem, the code looks for the "end card" of that problem, and starts reading the data for the following one.

A description of the formats and variable definitions is given below.

The cards that contain some changements compared to the original version of SABINE¹⁾ are underlined.

Further details on the meaning and effects of the input data, have to be found in $^{1)}$. The layout of input data is shown in Table 2.

Card 1 (110)

N Number of problems to be solved

Card 2 (18 A4) Title card.

Card 3 (4 110)

IGRC Index of the core geometry; 0, 1, 2, 3 for plane, cylindrical, spherical and disk geometry respectively.

- IGRS The geometry of the <u>shield</u> assumed for the calculation of <u>removal</u> neutrons and <u>primary</u> gamma radiation is
 - 0 plane slabs
 - 1 cylindrical shells
 - 2 spherical shells
- IGDS Geometrical index for the solution of the <u>diffusion equation</u> (0, 1, 2 as above)
- IGSS <u>Shield geometry for the calculation of secondary gamma-ray flux (0, 1, 2, 3, as for IGRC).</u>

Card 4 (5/10)

NREG Number of regions $(3 \le NREG \le 22)$

- IFGAM Neutron induced gamma-ray are taken into account only if generated by neutron groups with index $I \ge IFGAM$. When IFGAM, ≥ 26 no gamma-ray calculation is performed.
- NBUC The build-up factor applied to gamma radiation from core is computed assuming
 - 1 homogeneous shield
 - 2 Broder's formula
 - 3 Kitazume's formula

NBUS Similarly for gamma radiation from the shield.

- 0 Uranium-235 fission spectrum is assumed for the neutron source inside the core.
- 1 Source spectrum is input (card 5).

When MOP = 1, the code reads three cards defining the spectrum of the neutron source. When MOP = 0 cards 5 are omitted.

Card 5 (7E10.0)

MOP

FS_i; i = 1, 19 fraction of source neutrons released into the ith removal group.

A monoenergetic source e.g. in group 10, with strength 1 neutron/cm³ sec, may be defined by $FS_{10} = 1$, $FS_i = 0$ for $i \neq 10$, and $S = 1/\nu$ in card 12; $\nu \neq 2.46$ neutrons/fission.

One card 6 is required for each region (NREG cards). They need not be ordered.

Card 6 (110, 4F10.0, 315)

J	index of the region
ZR	thickness of the region (cm)
Н	transversal size
т	temperature (centigrades)
DEN	density (g/cm ³)
IGAP	1 normal region
	2 air gap in P1 approximation
	3 air gap with α and β values in input.
MBU	Build-up factor to be applied to the region. See Table 6 of 1 , 1 < MBU < 7
NEMR	Number of elements in the region NFMR ≤ 10

One card 7 is needed for each region; they need not be ordered. NDIF and the following parameters are requested only for regions 3 to NREG.

Card 7 (110, 315, 5X, E10.0, 415)

J	index of the region
$M_{\Theta}, M_{R}, M_{\Psi}$	Parameters that determine the mesh path of the numerical integration. If blank, the code will use 1, 1, 1.
ETHA	Relation accuracy for numerical integration. If blank, 0.001 will be used.
NDIF	d = ZR/NDIF is the mesh path for the solution of the diffusion equation. Recommended values are given in Table 9 of ¹).
4 ≤ NDIF ≤ 250	^D No more than 250 meshes per region, and 1000 in the whole shield are allowed.
NREM	Removal flux is calculated at each NREM th point, and in no more than 100 points of the shields.
NREM ≤ 50	
NPRT	Neutron fluxes are printed at any NPRT th mesh point, and in no more than 200 points of the shield.
NGS	Gamma sources are alculated at each NGS th point; no more than 50 source points per region and 500 for the whole shield are allowed. Not needed when no gamma calculation is required.

In the case of an air gap H and T need not be specified, set MBU = 1 and NREM = NPRT = NGS = 1.

All the parameters entered into card 7 are checked by the programme; if any of the conditions mentioned above is not verified, a message is printed.

Card 8 describes the composition; it must be entered also for the gaps. A list of ID numbers for the new library is given in Table 1.

Card 8 (15, 5 (13, E10.0))

- J Index of the region (in increasing order)
- ID, FREM a couple of values, identification and weight fraction, must be given for each element of the region; if NEMR > 5 two cards 8 should be entered for that region.

SABINE-3 offers the possibility of using removal cross sections other than the standard ones included in the SABINE-library. In this case they are entered in the following cards.

Card 9 (15)

NRC number of removal c.s. sets to be read. If NRC = 0 omit cards 10 and 11.

Card 10 (1415)

identification of the elements whose removal c.s have to be read in. ID_ NRC entries.

NRC sets of c.s. are expected, corresponding in order to the ID numbers entered in card 10.

Card 11 (7E10.0)

RCS_i 19 entries per element. Each element starts on a new card; NRC sets of 3 cards are read in.

Cards 12-14 are needed for each core region, i.e. twice; they describe the fission source distribution.

Note that the number of neutrons emitted per unit volume at the core boundary, into the jth removal group is assumed to be the product S ν FS_i, where ν = 2.46. When the source is not a fission source, FS; should sum to one and S should be such that 2.46 S be the number of source neutrons per unit volume.

Card 12 (E10.0, 6/10)

- S Fissions/cm³ sec at the outer boundary of the region. If $S \le 0$ no other information is needed for this region (omit cards 13, 14). How the radial distribution is specified?
- ISR
- 1 the coefficients of a polynomial are given
- 2 pointwise
- 3 exponential distribution.

NCFRNumber of coefficients of the polynomial (if ISR = 1); not used if ISR = 2 orNCFR <5</td>3.NWFRIf the radial distribution is given pointwise (ISR = 2), NWFR < 51 values at</td>

equidistant points must be entered. Not used if ISR = 1 or 3.

The above three quantities refer to the radial distribution and are not used in plane geometry (IGRC = 0). The three following ones refer to the source distribution vs. Z, and are not used in spherical geometry (IGRC = 2).

- ISZ How the Z distribution is specified?
 - 1 the coefficients of a polyn. are given.

2 pointwise.

- NCFZ Number of coefficients (\leq 5) to be given (ISZ = 1); not used if ISZ = 2. For Infinite cyl. geom. NCFZ should be 1.
- **NWFZ** If ISZ = 2, $NWFZ \le 51$ values at equidistant points must be entered. Not used if ISZ = 1 or for infinite cylinder.

Card 13 has to be omitted in case of plane geometry (IGRC = 0), and inserted in the other cases.

Card 13 (7E10.0)

- AR₁ First coefficient or tabulated value or value of k in the case of exponenetial radial distribution (exp. (-- k r'), see section 2.2 of ¹)
- AR2,etc Other coefficients or tabulated values.

If core geometry is not spherical (IGRC \neq 2) card 14 is necessary.

Card 14 (7E10.0)

AZ₁, AZ₂, ... Coefficients or tabulated values for the Z distribution.

Card 15 (7E10.3)

BSQ; Transverse buckling of the jth region; j = 3, NREG.

Specification of the response functions is entered into the following cards.

Card 16 (215)

NTH Number of reaction rates of threshold detectors to be calculated.

NFRD Number of region dependent responses to be calculated.

Cards 17, 18 are entered for each threshold detector (NTH times); omlt if NTH = 0.

Card 17 (15A4)

Name Name of the detector; the content of this card is printed as headline of the calculated reaction rate.

Card 18 (7E10.3)

TCS; Macroscopic c.s. of the detector for the energy range corresponding to the ith removal group; 19 values.

For each region dependent response function enter cards 19, 20; omit if NFRD = 0.

Card 19 (215, 15A4)

11, 12Response function values are entered for the energy groups 11 to 12
included.

Label To be printed as identification of the response.

One card or set of cards 20 is needed for each shielding region.

Card 20 (7E10.3)

F(11) These are the f_i values of eq. 13 in section 2.9 of ¹⁾ F(11+1) F(12) One set of cards 21,22, 23 (if requested), has to be entered for each neutron group. If there is any air gap for which the method discribed in 2.8.2 of 1 is used (IGAP = 3 in card 6), than card 21 is needed,

Card 21 (6E10.3)

 α_1, β_1 One couple of values for each of the air gaps for which IGAP = 3 in card 6. α_2, β_2 No more than 3 gaps of this type may be present.

α3,β3

Card 22 specifies, for the neutron group to which it refers, the boundary conditions at the two boundaries of the shield. Diffusion coefficients other than those computed by the code, may be applyed; if so, the DOP (D option) switch and card 23 are used.

Card 22 (6E10.3)

b1, b2	Coefficients that determine the outer and inner boundary conditions
an, a1, a2	respectively. Some examples may be found in Table 3.
DOP'	≤ 0 no effect
	> 0 read diffusion coefficients for this neutron group in card 23

> 0 read diffusion coefficients for this neutron group, in card 23.

<u>*Card 23 (7E10.3)*</u> Omit if DOT ≤ 0.

D₃, D₄, ... (NREG-2) values of the diffusion coefficient are read in for the shielding regions; use as many cards as necessary.

If D_i is positive, it will be used as diffusion coefficient of the ith region; if $D_i \leq 0$ the value calculated by the code will be used. In any case, if DOT is positive the code will print all the diffusion coefficients actually used for that group.

Cards 24 to 26 define the region independent response functions.

Card 24 (215)

NRIR	Number of region independent responses to be calculated. If NRIR = 0, omit
	cards 25, 26.
IFDOSE	Shall neutron dose rate be computed?
	0 No
	1 Yes

NRIR sets of cards 25, 26 are entered.

Card 25 (215, 15A4)

11, 12 Response function values are entered for the neutron groups 11 to 12 included.

Label Headline for the results.

Card 26 (7E10.3)

F(I1), F(I1 + 1) ... F(I2) Response function values.

If gamma source rates are not needed (IFGAM > 26), cards 27 to 32 are omitted.

Cards 27-29 describe the space distribution of the gamma sources inside the core; one set of cards must be given for each core region. Their description is the same as that of cards 12-14, and will not be repeated here; but the colums 1-10 in card 27 (fission density at the outer boundary of the region) are not read in. If the shape of the gamma-ray source is the same as that of the neutron source, cards 27-29 are the copy of cards 12-14.

Note that if S_1 – fission density at the outer edge of the first region – is zero, the cards for the first region must not be entered, and no gamma ray source is taken into account there. The source description for the second region must always be provided: if $S_2 = 0$, only the neutron induced secondaries gamma sources are calculated.

For cylindrical or disk geometries (IGSS = 1 or 3), the shape of the transversal distribution of gamma sources must be specified in the form of polynomials; enter one card 30 for each shield region, except gaps.

Card 30 (215, 6E10.0)

JIndex of the regionNCFNumber of coefficients of the polynomial (< 5)</td>A1, A2, ...Coefficients of the polynomial

For infinite cylindrical regions, only one coefficient $(A_1 = 1)$ should be given.

Card 31 (110)

NPG Number of points where the gamma-ray fluxes have to be computed.

If NPG = 0 the code will end the problem after printing the gamma-source distributions; in that case cards 32 are omitted. If NPG > 0, there are NPG cards 32, one for each point to be computed.

Card 32 (E10.0, 215, (1713))

- Z distance of the point from <u>core-reflector boundary</u>; shield-points will have positive Z, core-points will have negative Z.
- NRS number of source regions to be taken into account (all the regions, if NRS = 0).
- NR_j The gamma-ray flux at Z will be computed taking into account only the radiation originated into the regions NR_j , j = 1, NRS.

The region to which the point Z belongs is determined and printed by the programme.

The last card of each problem must always be card 33. Before reading the input of the following problem, the code looks for card 33, that is the end-card of the problem.

Card 33 (A4) End card

Enter ******** in colums 1-4 New input, if any, begins with card 2.

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Card	Columns						
no.	1 10	20	30	40	50	60	70
1	N						
2	tit	le card					
3	IGRC	IGRS	IGDS	IGSS			
4	NREG	IFGAM	NBUC	NBUS	МОР		
5	FS ₁	FS2					
6	L	ZR	н	Т	DEN	IGAP MBU	NEMR
7	L	M _O M _R	M_{Ψ}	ETHA	NDIF NREM	NPRT NGS	
8	JID	FREM I	D FREM				
9	NRC						
10	ID ₁ ID ₂	ID ₃					
11	RCS ₁	RCS ₂					
12	S	ISR	NCFR	NWFR	ISZ	NCFZ	NWFZ
13	AR ₁	AR2					
14	AZ ₁	AZ2					
15	BSQ3	BSQ4					
16	NTH NFRD						
17	name of thresh	old detector					
18	TCS ₁	TCS2					
19	11 12	name of regi	on dependent respor	ise			
20	F(I1)	F(I1+1)					
21	α1	βι					
22	bı	b ₂	ao	ai	a ₂	DOP	
23	D ₃	D ₄					
24	NRIR IFDOSE						
25	11 12	name of regi	ion independent resp	onse			
26	F(I1)	F(I1+1)					
27		ISR	NCFR	NWFR	ISZ	NCFZ	NWFZ
28	AR ₁	AR ₂					
29	AZ ₁	AZ ₂				, , 1	1
30	J NCF	Ā ₁	A ₂	A ₃			
31	NPG			Ĭ			
32	z	NRS NR1	NR ₂				
33	****						

TABLE 2 – Layout of input data

TA	BL	E.	3
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Coefficients for the inner and outer boundary conditions

Inner boundary	a 0	a 1	₽2
Neutron flux = F	0	- 1	F
Vacuum ; $J^* = 0$	2	- 1	0
Incoming current = C ; $J^+ = C$	2	- 1	40
Reflection ; $J^+ = J^-$	1	0	0
Albedo; J⁺ = h J⁻	$2\frac{h+1}{h-1}$	1	0
Outer boundary	b 1	b ₂	
Vacuum ; J ⁻ = 0	0.5	0	
Reflection ; J ⁻ = J ⁺	0	0	
Albedo; $J^- = \frac{1}{J} J^+$	$\frac{h-1}{2(b+1)}$	0	

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Alfred Nobel

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