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PROGRAM SYSTEM FOR COMPUTATION OF THE TERRESTRIAL GAMMA-RADIATION FIELD

Peter Kirkegaard and Leif Løvborg

Abstract. A system of computer programs intended for solution of the plane one-dimensional photon transport equation in the case of two adjacent media is described, and user's guides for the programs are given. One medium represents a natural ground with uniformly distributed potassium, uranium, and thorium gamma-ray emitters. The other medium is usually air with no radioactive contaminants. The solution method is the double-P_1 approximation with logarithmic energy spacing. The complete data-processing system GB contains the transport-theory code GAMP1, the code GFX for computation of scalar flux and dose rate, and a number of auxiliary programs and data files.

INIS Descriptors. EARTH CRUST, G CODES, GAMMA RADIATION, GAMMA TRANSPORT THEORY, GEOLOGIC DEPOSITS, NATURAL RADIOACTIVITY, ONE-DIMENSIONAL CALCULATIONS, PHOTON TRANSPORT, POTASSIUM, P1-APPROXIMATION, THORIUM, URANIUM, SHIELDING, ANGULAR DISTRIBUTION, DOSE RATES, ENERGY SPECTRA, NUMERICAL SOLUTION

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CONTENTS

1. INTRODUCTION

This report describes a computer program system for evaluation of terrestrial gamma-radiation fields, i.e. environmental radiation fields produced by the natural gamma-ray emitters (^{40}K and members of the thorium and the uranium decay series) in the ground. The programs are intended as an aid to the interpretation of ground and airborne gamma-ray surveys. The same subject was discussed by the authors in two earlier reports (Kirkegaard and Løvborg 1974; Løvborg and Kirkegaard 1975), but since then substantial improvements have been made both in the formulation of the model and in the data processing system. After a short review of the double-P_1 transport theory method as applied to the terrestrial flux problem there follows a description of the program system with user's guides for the individual programs. Some details in the mathematical formulation are given in Appendix A, and Appendix B contains a list of all the FORTRAN subroutines in the program system. All the computational results from the programs are normalized to unit concentration of the radioelement, i.e. to 1 ppm Th, 1 ppm U, or 1% K.

2. SOLUTION OF THE TRANSPORT EQUATION

A central part of our data processing system GB consists of the solution of the plane two-media transport equation for gamma-radiation in the double-P_1 approximation (DP1). Our present model includes the implementation of an equidistant-lethargy mesh, i.e. a logarithmic spacing of the energy (or wavelength) points. As this procedure is described elsewhere (Kirkegaard and Løvborg 1979), we shall give only a brief summary here. Many elements from our previous model (Kirkegaard and Løvborg 1974) are still pertinent; other details can be found in Appendix A of this report.

2.1. The Double-P_1 Approximation

The geometric idealizations which are made in this work are that the ground mediur (called medium I) and the air (called medium II) are both semi-infinite and have a common boundary at a plane, each medium is homogeneous, and medium I contains uniformly distributed gamma-ray emitters with a composite line spectrum in the general case. A spatial coordinate z is introduced, denoting the distance to the interface; we have $z < 0$ in medium I and $z > 0$ in medium II. The direction cosine is $\omega = \underline{i}\cdot\underline{\Omega}$, where $\underline{i}$ and $\underline{\Omega}$ are unit vectors along the z-axis and the direction of photon movement. Finally, let λ be the wavelength in Compton units. We set out to calculate the differential and angular energy flux $I(z, \omega, \lambda)$ for all z, ω, and λ. Once I is known we are able to predict scalar fluxes, dose rates, etc. I is composed of an unscattered part U and a scattered part Ψ, $I = U + \Psi$. It is easy to evaluate U in analytical form (Kogan et al. 1969; Kirkegaard and Løvborg 1974), whereas Ψ must be found as a numerical solution of the transport equation

$$(\omega\, \partial/\partial z + \mu(z, \lambda))\, \Psi(z, \omega, \lambda)$$

$$= \int_{\lambda-2}^{\lambda} \int_{4\pi} [\Psi(z,\omega',\lambda') + U(z,\omega',\lambda')]\, k(z,\lambda',\lambda)$$

$$\cdot\, \delta(1 + \lambda' - \lambda - \underline{\Omega}\cdot\underline{\Omega}')/2\pi\, d\Omega'\, d\lambda', \quad -\infty < z < \infty \qquad (1)$$

where μ is the total interaction cross section and k the scattering kernel as given by the Klein-Nishina formula (Appendix A); both μ and k are here piecewise constant functions of z. If we define $\Psi^{\pm}(z,\omega,\lambda) = \Psi(z,\omega,\lambda)H(\pm\omega)$, where H(x) is the Heaviside step function, then $\Psi = \Psi^{+} + \Psi^{-}$ for all ω, and we have the double-P_ℓ flux expansion

$$\Psi^{\pm}(z,\omega,\lambda) = \sum_{\ell=0}^{\infty} (2\ell + 1)\, \Psi_\ell^{\pm}(z,\lambda)\, P_\ell^{\pm}(\omega). \qquad (2)$$

Here $\Psi_\ell^{\pm}$ are the half-range moments, and $P_\ell^{\pm}(\omega) \equiv P_\ell(2\omega\mp1)H(\pm\omega)$, with P_ℓ standing for the usual Legendre polynomial of degree ℓ.

Insertion of (2) in (1) and truncation to a first-order expansion lead, after reduction, to the following DP1 vector equation:

$$\partial \underline{\psi}(z,\lambda)/\partial z = \mu(z,\lambda)\ \underline{\underline{M}}\ \underline{\psi}(z,\lambda) + \int_{\lambda-2}^{\lambda} k(z,\lambda',\lambda)\ \underline{\underline{P}}(\gamma) \cdot (\underline{\psi}(z,\lambda') + \underline{u}(z,\lambda'))\ d\lambda' \ . \tag{3}$$

The four DP1 moments for the scattered flux are collected in the vector $\underline{\psi} = (\psi_o^+, \psi_1^+, \psi_o^-, \psi_1^-)$; $\underline{u}$ similarly contains the DP1 moments for the unscattered flux which are computed analytically. $\underline{\underline{M}}$ is the matrix

$$\underline{\underline{M}} = \begin{bmatrix} -3 & 3 & 0 & 0 \\ 1 & -3 & 0 & 0 \\ 0 & 0 & 3 & 3 \\ 0 & 0 & 1 & 3 \end{bmatrix} \tag{4}$$

$\underline{\underline{P}}(\gamma)$ is a matrix whose elements are analytic functions of the scattering cosine γ as quoted in Appendix A.

The procedure for solving Eq. (3) numerically is a nested one with λ in the outer loop and z in the inner. We use a logarithmically constant wavelength (or energy) mesh, which gives a good computational economy. It is important to use an accurate and stable technique for evaluating the scattering integral in (3), viz.

$$\underline{j}(z,\lambda) = \int_{\lambda-2}^{\lambda} k(z,\lambda',\lambda)\ \underline{\underline{P}}(\gamma)\ \underline{\psi}(z,\lambda')\ d\lambda' \ . \tag{5}$$

We compute (5) using the analytical form of k and $\underline{\underline{P}}(\gamma)$, combined with an essentially linear variation of $\underline{\psi}(z,\lambda')$ between the logarithmically distributed mesh points $\lambda'=\lambda_j$. This suggests that the calculation be made by a semi-analytical integration technique (details are given in Appendix A). When this is done $\underline{j}(z,\lambda)$ is written as a linear combination of the flux values $\underline{\psi}(z,\lambda_j)$ in the mesh points λ_j. Of these values only $\underline{\psi}(z,\lambda_i)$, the flux at the actual wavelength $\lambda = \lambda_i$, is unknown, because $\underline{\psi}(z,\lambda_j)$ for $\lambda_j < \lambda_i$ have already been computed. Hence Eq. (3) reduces to an equation in z for the DP1 moment vector at $\lambda = \lambda_i$. Suppressing

λ, this equation reads

$$d\underline{\psi}(z)/dz = \underline{\underline{B}}\ \underline{\psi}(z) + \underline{\phi}(z) \ . \tag{6}$$

The matrix $\underline{\underline{B}}$ of this first-order differential equation system comprises elements which are constant within each medium. Eq. (6) can therefore be solved, in each medium, by the standard diagonalization procedure using the substitution

$$\underline{\psi} = \underline{\underline{Y}}\ \underline{\chi} \ . \tag{7}$$

The transformation matrix $\underline{\underline{Y}}$, which depends on the medium, contains the eigenvectors of $\underline{\underline{B}}$ as columns; $\underline{\underline{\Sigma}} \equiv \underline{\underline{Y}}^{-1}\underline{\underline{B}}\ \underline{\underline{Y}}$ is a diagonal matrix with the eigenvalues of $\underline{\underline{B}}$ in the diagonal. The transformed equation is

$$d\ \underline{\chi}(z)/dz = \underline{\underline{\Sigma}}\ \underline{\chi}(z) + \underline{h}(z) \ , \tag{8}$$

where $\underline{h}(z) \equiv \underline{\underline{Y}}^{-1}\ \underline{\phi}(z)$ is the transformed source term. For each medium (p=1,2) there is an equation of the form (8) each of which representing four (m=1,2,3,4) independent scalar equations:

$$dX_{mp}(z)/dz = \sigma_{mp}\ X_{mp}(z) + h_{mp}(z). \tag{9}$$

The complete solution of (9) is

$$X_{mp}(z) = \exp(\sigma_{mp}z)\ \left\{ \int \exp(-\sigma_{mp}z)\ h_{mp}(z)\ dz + C_{mp} \right\}, \tag{10}$$

where C_{mp} is a constant of integration. The analytical form of $X_{mp}(z)$ is not a simple one, because $h_{mp}(z)$ is a complicated function, and its complexity increases rapidly as the wavelength integration proceeds. To circumvent this difficulty we approximate $h_{mp}(z)$ with a stationary term plus a decaying exponential multiplied by a polynomial of a specified degree k:

$$h_{mp}(z) \approx h^{\infty}_{mp} + \exp(\alpha_{mp}z) \sum_{j=o}^{k} h_{jmp}\ z^{j} \ , \tag{11}$$

where α_{mp} is >0 if p=1 and <0 if p=2. The term h^{∞}_{mp} can be found analytically, whereas the other parameters are determined using

the semi-linear least-squares approximation method described by Kirkegaard and Eldrup (1972). This procedure iterates on the nonlinear parameter α_{mp} only and convergence is rapid. We use a set $\{z_i\}$ of base points (normally nine in each medium) whose distances from the interface increase logarithmically. When $h_{mp}(z)$ is parametrized in the form (11), then (10) furnishes the approximate solution

$$X_{mp}(z) = X^{\infty}_{mp} + C_{mp} \exp(\sigma_{mp} z) + \exp(\alpha_{mp} z) \sum_{j=0}^{k} \kappa_{jmp} z^j \quad . \quad (12)$$

$(m=1,2,3,4; \quad p=1,2; \quad z \leq 0 \text{ if } p=1 \text{ and } z \geq 0 \text{ if } p=2)$

The integration constants C_{mp} are determined by the requirement that $\underline{\psi}$ is finite for $z \to \pm \infty$ and continuous at $z=0$ (in the special case when medium II is vacuum, we require instead that the "downstreaming" moments Ψ_0^- and Ψ_1^- be zero at $z=0$).

2.2. Calculation of Flux and Dose

The transport-theory program GAMP1 computes the parameters in the expression (12) for the transformed DP1 moments. These parameters are X^{∞}_{mp}, C_{mp}, σ_{mp}, α_{mp}, and κ_{jmp} for $j = 0,\ldots, k$. m indicates the component of $\underline{\chi}$ (m=1,2,3,4), and p the medium (p = 1,2). Such a parameter set is given for each wavelength mesh point. We shall now demonstrate how these data can be used to reconstruct the complete radiation field and to compute integral field quantities such as flux and dose. This is the task of the code GFX.

First we carry out the inverse transformation (7) to obtain $\underline{\psi}$ from $\underline{\chi}$. This is done separately for each medium because the transformation matrix $\underline{\underline{Y}} = \underline{\underline{Y}}_p$ depends on the medium. This results in analytical expressions of the same structure as (12) for the four DP1 moments in each medium and for each wavelength point. Use of the truncated form of the expansion (2),

$$\Psi(z,\omega,\lambda) \approx \begin{cases} \Psi_0^+(z,\lambda) + 3\Psi_1^+(z,\lambda)\,(2\omega-1), & 0 < \omega < 1 \\ \Psi_0^-(z,\lambda) + 3\Psi_1^-(z,\lambda)\,(2\omega+1), & -1 < \omega < 0 \end{cases} \quad (13)$$

then makes it possible to evaluate the scattered energy flux $\Psi(z,\omega,\lambda)$ for any values of the arguments (interpolation in λ proceeds linearly between mesh points).

Next we can derive various integral quantities from the scattered flux $\Psi(z,\omega,\lambda)$ as well as from the unscattered flux $U(z,\omega,\lambda)$ by integration over ω and λ. The integration involving U results in simple analytical expressions (Kirkegaard and Løvborg 1974). In the following we shall consider the scattered flux only. The reference point may be in either medium ($-\infty < z < \infty$). When (13) is integrated over ω we obtain the differential energy flux

$$\Phi(z,E) = 2\pi \int_{-1}^{1} \Psi(z\ \omega,\lambda)d\omega = 2\pi\ (\Psi_o^+(z,\lambda) + \Psi_o^-(z,\lambda)) \qquad (14)$$

($E = f_o/\lambda$ = energy in Mev, $f_o = 0.5110058$ Mev), and from Φ we derive the number flux N (photons $cm^{-2}\ s^{-1}$), the energy flux N_e (Mev $cm^{-2}\ s^{-1}$), and the absorbed dose rate D (Mev $g^{-1}\ s^{-1}$):

$$N(z) = \int \Phi(z,E)/E\ dE = 2\pi \int (\Psi_o^+(z,\lambda) + \Psi_o^-(z,\lambda))/\lambda\ d\lambda, \qquad (15)$$

$$N_e(z) = \int \Phi(z,E)\ dE = 2\pi\ f_o \int (\Psi_o^+(z,\lambda)+\Psi_o^-(z,\lambda))/\lambda^2\, d\lambda\ , \qquad (16)$$

$$D(z) = \int \Phi(z,E)\ \mu_{ea}(z,E)\ dE$$

$$= 2\pi\ f_o \int (\Psi_o^+(z,\lambda) + \Psi_o^-(z,\lambda))\ \mu_{ea}(z,\lambda)/\lambda^2\, d\lambda\ ; \qquad (17)$$

μ_{ea} is the energy-absorption coefficient ($cm^2\ g^{-1}$). In (15), (16) and (17) the integration range is supposed to be between two specified energies. The corresponding λ-integration is carried out semi-analytically by linearizing $\Psi_o^{\pm}(z,\lambda)$ between the mesh points of λ. This procedure is analogous to the evaluation of the scattering integral (5).

Clearly the quantities (14) - (17) are composed of an upstreaming portion due to Ψ_o^+ and a downstreaming one due to Ψ_o^-. The latter represents, for $z \geq 0$, the "skyshine" flux.

3. DATA PROCESSING SYSTEM GB

A system of data files and computer programs related to the topics discussed in section 2 is in operation at the B6700 Computer Installation at Risø. This system, which is called GB, replaces the old GAMMABANK system based on magnetic tape storage (Kirkegaard and Løvborg 1974). The programs in the new system are considerably more efficient and much easier to use than the old ones, and the handling of data files is now accomplished through random-access disk-pack storage.

3.1. Data Files

Two files of basic data form an integral part of GB. Both are organized as card images with 72 EBCDIC characters per record.

The file with the title 'GB/EMITTERS' contains the emission data for the line spectra from the radionuclides Th, U, and K. All records contain the five data

ENERGY, YIELD, ILINE, NLINE, IEMIT

in the format F7.4, F7.2, 2I4, I6. The emitter code IEMIT is a four-digit number (pos. 25-28). The code for the first digit is 1 for thorium, 2 for uranium, and 3 for potassium. The last three digits form an isotope code, such that IEMIT altogether may assume the following four values: 1232 for ^{232}Th, 2238 for ^{238}U, 2235 for ^{235}U, and 3040 for ^{40}K. All records for one emitter code are placed consecutively on the file. NLINE is the number of emission lines for the actual IEMIT. ILINE denotes the sequence number of the actual line for the actual IEMIT, and ENERGY its energy. Increasing line numbers correspond to decreasing energies. YIELD denotes the intensity of the actual line in photons per 100 disintegrations. The emission data have not been changed since our previous compilation (Kirkegaard and Løvborg 1974); most of the data are taken from the compilation of Beck (1972).

The file with the title 'GB/MATERIALS' contains composition data and gamma-ray interaction cross-sections for each member of the current set of materials. The file is self-documented with the documental part in records 1-36. The organization is index-sequential. Data for each material consists of the following items:

(1) A numerical composition code for the material in the interval [1,99].
(2) A composition table with the number of elements, the density of the material (g cm^{-3}), and the weight percentages of the constituent elements.
(3) Interaction cross-sections (cm^{-1}) for the four scattering and absorption processes and their total: coherent scattering, incoherent scattering, pair production, and photoelectric effect. There are 101 cross-section data for each process, through the energy range from 10 kev to 3 Mev spaced logarithmically equidistant.

New materials can be inserted in 'GB/MATERIALS', and present materials can be deleted, using the program UPDATE.

3.2. Program GAMP1

The FORTRAN program GAMP1 executes the double-P_1 calculation outlined in section 2.1. Data for the emission spectra are taken from the file 'GB/EMITTERS', and material data from the file 'GB/MATERIALS'. An additional reader file must be supplied containing the following data:

RECORD 1: Composition codes for media I and II (0 for medium II when this is vacuum), and radioelement code (1=Th, 2=U, 3=K). The format is 2I2,I1 corresponding to a five-digit compound index.
RECORD 2: Cutoff energy in Mev. Format F10.0.
Recommended Risø standard value: 0.020.

RECORD 3: Lethargy step (i.e. relative increment in the logarithmic energy mesh), expressed in percent. Format F10.0.
Recommended Risø standard value: 3.0.

RECORD 4: Degree k of the fitting polynomial in (11). Format I5.
Recommended Risø standard value: 2.

In case the data set is multiple, retur.. to RECORD 1. Total termination via END-OF-FILE.

GAMP1 produces both printed output and disk output. The printed output serves a check purpose and contains the DP1 moments at the interface. The main output is directed to the disk file with the title 'GB/FLUX'. Output is generated consecutively for each data set. The records are written in binary (unformatted) mode. A safe upper bound for the number of data per record is 120 (corresponding to a polynomial degree k=6). Output for one input data set consists of a header record followed by a number of "flux records". The header record contains the following seven items:

1) Composition code for medium I
2) Composition code for medium II
3) Radioelement code
4) Number of flux records (NU)
5) Polynomial degree k
6) Cutoff energy in Mev (ECUT)
7) Lethargy step in absolute units (DU).

Of the NU flux records, no. I refers to the energy

$$E(I) = ECUT \times EXP\ ((NU-I) \times DU).$$

The contents of the flux records are the parameters in the expression (12) for $X_{mp}(z)$, i.e. component m of the transformed moment vector $\underline{X}$ in medium p, and the transformation matrix in (7), $\underline{\underline{Y}} = \underline{\underline{Y}}_p = \{y_{ijp}\}$. These are the data necessary to compute the DP1 moments $\{\psi_o^+, \psi_1^+, \psi_o^-, \psi_1^-\} = \underline{\psi}$. The flux record contains the data in the following order:

$\{X^{\infty}_{mp}\}$ m=1,2,3,4; p=1,2;
$\{C_{mp}\}$ " "
$\{\sigma_{mp}\}$ " "
$\{\alpha_{mp}\}$ " "
$\{\kappa_{jmp}\}$ j=0,...,k; m=1,2,3,4; p=1,2;
$\{y_{ijp}\}$ i=1,2,3,4; j=1,2,3,4; p=1,2;

The sequence of the subscripted data follows the rule that the first subscript varies most rapidly, the second subscript next rapidly, etc. The length of one flux record is 72 + 8 k. The collection of all flux records determines the complete radiation field.

The file 'GB/FLUX' serves as a data source for the program GFX which computes integral flux quantities.

3.3. Program GFX

The FORTRAN program GFX calculates number flux, energy flux, or dose rate on the basis of the output file 'GB/FLUX' produced by GAMP1. An additional reader file must be supplied containing the following data:

RECORD 1: Composition codes for media I and II (0 for medium II when this is vacuum, 99 for medium II in the DEEPFLUX case), and radioelement code (1=Th, 2=U, 3=K). The format is 2I2,I1 corresponding to a five-digit compound index.

RECORD 2: Index for calculation type, format I5:
1 = number flux
2 = energy flux
3 = dose rate

RECORD 3: Lower limit (Mev) of energy interval, format F10.0.

RECORD 4: Upper limit (Mev) of energy interval, format F10.0.

RECORD 5: Altitude z (cm) of reference point, format F10.0. Must be negative in medium I and positive in medium II.
Any value, e.g. z=0, may be used in the DEEPFLUX case.

In case of a multiple data set, return to RECORD 1. Total termination via END-OF-FILE.

The printed output from GFX is self-explanatory and includes the total flux or dose, the unscattered contribution, the scattered contribution, and a subdivision of the latter in an upstreaming and a downstreaming component.

4. AUXILIARY GB PROGRAMS

The program complex GAMP1-GFX forms the core of the GB program system. There is, however, a number of satellite programs in the system, which will be described in the following.

4.1. Program UPDATE

The FORTRAN program UPDATE inserts data for new materials in the data file 'GB/MATERIALS' described in section 3.1. The program can also delete already existing materials from the file. Elemental interaction cross-section data are read from the file 'GB/MCMASTER'. This file conforms to the ENDF/B-format and is an edited version of the Livermore photon cross-section library by McMaster et al. (1969-70) (the edition was done by the program DAMMET, version 69-1, Brookhaven National Laboratory, U.S.). UPDATE computes macroscopic cross-sections for given materials by double-logarithmic interpolation of the Livermore elemental data. The energy range 10 kev - 3 Mev is covered by a set of 101 grid values with logarithmically equidistant spacing. To run UPDATE one must supply a reader file containing one or more consecutive data blocks. A data block for a new material must have the following structure:

RECORD 1 contains the keyword NEW in col. 1-3 and the material composition code in col. 4-5, whereas col.

7-72 is a comment field containing, for example, the name of the material.

RECORD 2 contains the number of elements in col. 4-5.

RECORD 3 contains the density in g cm^{-3} in col. 1-10.

SUPSEQUENT RECORDS contain the atomic (col. 1-5) and weight percentage (col. 6-15) for each of the constituent elements. The atomic must be in ascending order.

In the case where a material is to be deleted, the d :a block must be a single record with the keyword DEL in col. 1-3 and the composition code in col. 4-5.

4.2. Program UPDATESTART

This is an interactive ALGOL program which is used to generate the input data for the program UPDATE when the composition of the material is specified in terms of oxides. The program is run from a remote terminal and each record is to be typed in free-field format upon request from the terminal. In addition to the composition code for the material, the material name, and its density, the weight percentages of the 13 following oxides are requested:

SiO_2
TiO_2
Al_2O_3
Fe_2O_3
FeO
MnO
MgO
CaO
Na_2O
K_2O
H_2O
P_2O_5
CO_2

The weight percentage of each cation and that of oxygen are calculated and stored on a disk file with the title 'GB/UPDATEINPUT'. The average atomic number and the effective number for the material are each calculated and displayed; the effective atomic number is defined as

$$Z_{eff} = \left(\frac{\sum_i Z_i^m \, w_i \, Z_i/A_i}{\sum_i w_i \, Z_i/A_i} \right)^{1/m} ,$$

where

w_i = weight percentage of element no. i
Z_i = atomic number of element no. i
A_i = atomic weight of element no. i
m = 3.2

(see, for example, Kogan et al. (1969)).

When there are no more materials to specify, an END-OF-FILE is typed, and it is now possible to run the program UPDATE with the reader file replaced by 'GB/UPDATEINPUT'. A printer copy of the input to UPDATESTART is produced.

4.3. Program PRINT

The FORTRAN program PRINT prints information either about one specific material or all the materials currently present in the data file 'GB/MATERIALS' described in section 3.1. For each material, the following information is listed:

Composition code with comment field
Density of the material in g cm^{-3}
Composition table.

A reader file must be supplied containing a single record. Either of the two following options may be taken:

1) Information for one material: if, e.g., output is wanted for material 47, then type MAT47 in col. 1-5.
2) Total catalog for all the materials: type ALL in col. 1-3.

4.4. Program CROS

The FORTRAN program CROS calculates gamma-ray interaction cross-sections (cm^{-1}) for any material in the data file 'GB/MATERIALS' described in section 3.1. An array of energies can be handled in a single problem. The desired reaction type is specified through the ENDF/B code MT for the process:

MT = 501 Total
MT = 502 Coherent scattering
MT = 504 Incoherent scattering
MT = 516 Pair production
MT = 602 Photoelectric effect.

In addition to these five we have added the option MT = 0 giving the total minus the coherent scattering cross-section, which can be regarded as an effective transport cross-section.

A reader file must be supplied with the following data:

RECORD 1: contains composition code, MT-code, and number of energies, format 3I5.
SUBSEQUENT RECORD(S) contains the array of energies (in Mev and arbitrary order), format 7F10.0.

CROS computes the set of cross-sections by double-logarithmic interpolation of the data in 'GB/MATERIALS'.

4.5. Program DEEPFLUX

The FORTRAN program DEEPFLUX may be considered as a limiting form of the program GAMP1 for $z \to -\infty$, i.e. it calculates the scattered flux deep inside medium I. The problem to be solved involves only one homogeneous medium. The source is uniform with a line spectrum. Neither the spatial variable z nor the angular variable ω enters the transport equation (1), which reduces to an equation in λ:

$$\mu(\lambda)\ \Psi(\lambda) \;=\; \int_{\lambda-2}^{\lambda} k(\lambda',\lambda)\ (\Psi(\lambda') + U(\lambda'))\ d\lambda'$$

DEEPFLUX solves this Volterra integral equation by the same numerical technique as was applied in GAMP1 to execute the wavelength integration, although here it reduces to scalar operations only. As was the case for GAMP1, the data for the emission spectra are taken from the file 'GB/EMITTERS', and the material data from the file 'GB/MATERIALS'. An additional reader file must be supplied containing the following data:

RECORD 1: Composition codes for media I and II (medium I is the medium in question and the dummy medium II is given the code 99), and the radioelement code (1=Th, 2=U, 3=K). The format is 2I2,I1 corresponding to a five-digit compound index.
RECORD 2: Cutoff energy in Mev, format F10.0.
RECORD 3: Lethargy step length in percent, format F10.0.

In case of a multiple data set, return to RECORD 1. Total termination via END-OF-FILE.

DEEPFLUX produces both printed output and a disk file 'GB/FLUX', which conforms completely with the specifications for the corresponding output file produced by GAMP1. DEEPFLUX can therefore be used in conjunction with the code GFX, in which case a dummy medium II with composition code 99 is postulated and an arbitrary altitude z, e.g. z=0, is used.

5. CONCLUSION

We have described a consistent data-processing system for solution of the one-dimensional, plane, two-media photon transport equation. The programs use efficient numerical techniques, and the data files are kept on random-access disk-pack storage. The

system is primarily intended for prediction of flux and dose in terrestrial gamma-radiation fields, where it has been applied for various assessments. Its validity has also been confirmed by experiment (Løvborg and Kirkegaard 1974). We believe, however, that the range of use can be extended beyond this, e.g. to more general one-dimensional gamma-ray shielding problems. This could probably be done without introducing radical changes in the system.

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APPENDIX A

Details in the Solution Methods

This Appendix collects various details concerning the computer models presented in this report. We do not, however, aim at giving any systematic presentation of these details.

The Klein-Nishina scattering kernel

The kernel k in (1) is g ven by

$$k(z,\lambda',\lambda) = 3/8\ n_e(z)\ \sigma_o\ \lambda'/\lambda(\lambda/\lambda'+\lambda'/\lambda-1+(1-\lambda+\lambda')^2) \qquad (A1)$$

for $\lambda-2 \leq \lambda' \leq \lambda$, and $k = 0$ otherwise. λ' and λ are the wavelengths before and after scattering. $n_e(z)$ is the electron density (cm^{-3}), which in our application is a piecewise constant function of z. Although σ_o in the free-electron model takes on the constant value 0.66516 barns/electron (the Thomson cross-section), we shall allow for a slight variability with elemental composition (hence position z) and initial wavelength λ': We determine $\sigma_o = \sigma_o(z,\lambda')$ from the requirement that the integration of (A1) matches the incoherent scattering cross-section taken from the Livermore tabulation (McMaster et al., 1969-70).

The scattering cosine γ, which enters (3), is for Compton scattering given by

$$\gamma = 1 - \lambda + \lambda'. \qquad (A2)$$

By (A2) one can express k in terms of γ and λ:

$$k = k_o(\gamma)\ \kappa(\gamma,\lambda)$$

with

$$k_o(\gamma) = 3/8\ n_e\ \sigma_o \qquad \text{(A3)}$$

and

$$\kappa(\gamma,\lambda) = \lambda^{-1}\ \gamma^3 + (\lambda^{-2}-\lambda^{-1}+1)\gamma^2+(-2\lambda^{-2} + \lambda^{-1})\gamma+\lambda^{-2}-\lambda^{-1}+1;$$

$k_o(\gamma)$ depends slightly on γ through σ_o.

Analytical expressions for the elements of the scattering matrix $\underline{\underline{P}}(\gamma)$

The 4×4 matrix $\underline{\underline{P}}(\gamma)$ which enters (3) can be written

$$\underline{\underline{P}}(\gamma) = \begin{bmatrix} a & b & c & d \\ e & f & g & h \\ -c & d & -a & b \\ g & -h & e & -f \end{bmatrix} \qquad \text{(A4)}$$

where

$$a = 6\ \pi^{-1}\ \arcsin\gamma + 3/2 - 3/2\ \gamma$$

$$b = -(18+12\gamma)\pi^{-1}\ \arcsin\gamma\ -12\ \pi^{-1}(1-\gamma^2)^{\frac{1}{2}} + 9/2 + 15/2\ \gamma$$

$$c = -6\ \pi^{-1}\ \arcsin\gamma + 3/2 + 3/2\ \gamma$$

$$d = -(18-12\gamma)\pi^{-1}\ \arcsin\gamma\ +12\ \pi^{-1}(1-\gamma^2)^{\frac{1}{2}} - 9/2 + 15/2\ \gamma$$

$$e = -4\ \pi^{-1}\ \arcsin\gamma - 1/2 + 3/2\ \gamma$$

$$f = (12+12\gamma)\pi^{-1}\ \arcsin\gamma\ +12\ \pi^{-1}(1-\gamma^2)^{\frac{1}{2}} - 9/2 - 9/2\ \gamma$$

$$g = 4\ \pi^{-1}\ \arcsin\gamma - 1/2 - 3/2\ \gamma$$

$$h = (12-12\gamma)\pi^{-1}\ \arcsin\gamma\ -12\ \pi^{-1}(1-\gamma^2)^{\frac{1}{2}} + 9/2 - 9/2\ \gamma$$

These expressions are due to Gerstl (1967). He has shown that the two infinite series

$$A(\gamma) \equiv \tfrac{1}{2} \sum_{n=0}^{\infty} (2n+1)\ c_{n0}^2\ P_n(\gamma) \tag{A5}$$

and

$$E(\gamma) \equiv \tfrac{1}{2} \sum_{n=0}^{\infty} (2n+1)\ c_{n1}^2\ P_n(\gamma) \tag{A6}$$

where

$$c_{n\ell} \equiv \int_0^1 P_n(\omega)\ P_\ell(2\omega-1)\ d\omega, \tag{A7}$$

are summated as follows:

$$A(\gamma) = 1/\pi \quad \arcsin\gamma \quad + \quad 1/2 \tag{A8}$$

$$E(\gamma) = (3+4\gamma)/(3\pi)\arcsin\gamma + 4/(3\pi)\,(1-\gamma^2)^{\frac{1}{2}} - 1/3\ \gamma - 1/2. \tag{A9}$$

(A8) and (A9) are special cases of Gerstl's "anisotropy functions". Knowledge of $A(\gamma)$ and $E(\gamma)$ is sufficient for calculation of all the elements in (A4) (Kirkegaard and Løvborg 1974). We can prove (A8) and (A9) by showing that the right member of (A8) expands in Legendre polynomials as does (A5), and similarly for (A6) and (A9). For brevity we write

$$q_\nu \equiv \frac{1\cdot 2\cdot \ldots \cdot 2\nu-1}{2\cdot 4\cdot \ldots \cdot 2\nu}\ , \quad \nu = 1,2,\ldots$$

From the Fourier expansion of the Legendre polynomials $P_n(\cos\theta)$ (Whittaker and Watson, 1952, p. 303) we obtain by integration:

$$\int_0^\pi P_{2\nu}(\cos\theta)\ d\theta = \pi\ q_\nu^2$$

and

$$\int_0^\pi \cos 2\theta\ P_{2\nu}(\cos\theta)\ d\theta = \pi\ q_\nu^2\ \frac{2\nu+1}{2\nu+2}\ \frac{2\nu}{2\nu-1}\ .$$

Partial integration and the recurrence relations for P_n next give the following formulas:

$$\int_{-1}^{1} \arcsin x \; P_{2\nu-1}(x)dx = \pi \, q_\nu^2 \frac{1}{(2\nu-1)^2} ,$$

$$\int_{-1}^{1} x \arcsin x \; P_{2\nu}(x)\, dx = \pi \, q_\nu^2 \frac{4\nu^2+2\nu+1}{4(\nu+1)^2(2\nu-1)^2} , \qquad \text{(A10)}$$

$$\int_{-1}^{1} (1-x^2)^{\frac{1}{2}} \; P_{2\nu}(x)\, dx = -\pi \, q_\nu^2 \frac{1}{2(\nu+1)(2\nu-1)} .$$

Also, for $\ell = 0$ and 1 we have simple expressions for the coefficients (A7) (Kirkegaard and Løvborg, 1974):

$$\begin{aligned}
c_{2\nu,0} &= \delta_{\nu 0} \\
c_{2\nu-1,0} &= (-1)^{\nu-1} \, q_\nu \frac{1}{2\nu-1}, \quad \nu = 1,2,\ldots \\
c_{01} &= 0 \qquad \text{(A11)} \\
c_{2\nu,1} &= (-1)^{\nu-1} \, q_\nu \frac{1}{(\nu+1)(2\nu-1)}, \quad \nu = 1,2,\ldots \\
c_{11} &= 1.6 \\
c_{2\nu-1,1} &= (-1)^{\nu} \, q_\nu \frac{1}{2\nu-1}, \quad \nu = 2,3,\ldots
\end{aligned}$$

With the formulas (A10) and (A11) it is easy to show that the Legendre expansions in question are identical.

Semi-analytical evaluation of the scattering integral

To evaluate (5) we divide the interval $[\lambda-2,\lambda]$ into subintervals whose endpoints are the logarithmically spaced wavelength points. At the same time we change the integration variable from λ' to γ. The contribution to (5) from a typical subinterval can then be written

$$\underline{I} = \int_{\gamma_1}^{\gamma_2} k_o(\gamma) \; \kappa(\gamma,\lambda) \; \underline{\underline{P}}(\gamma) \, \underline{\psi}(\gamma) \; d\gamma \qquad \text{(A12)}$$

with $\kappa(\gamma,\lambda)$ defined as in (A3) and the argument z suppressed. To calculate (A12) we postulate that $k_o(\gamma)\ \underline{\psi}(\gamma)$ varies linearly with γ in $[\gamma_1,\gamma_2]$. This amounts to stating that the product varies linearly with wavelength in the corresponding wavelength interval, and this is a reasonable approximation even for a rather coarse mesh. Then (A12) can be written

$$\underline{I} = \underline{\underline{W}}_1\ \underline{\psi}(\gamma_1) + \underline{\underline{W}}_2\ \underline{\psi}(\gamma_2)\ ;$$

if the indefinite matrix integrals $\underline{\underline{F}}(\gamma) = \int \kappa(\gamma,\lambda)\ \underline{\underline{P}}(\gamma)d\gamma$ and $\underline{\underline{G}}(\gamma) = \int \gamma\kappa(\gamma,\lambda)\ \underline{\underline{P}}(\gamma)d\gamma$ are introduced, the "weight matrices" can be written as

$$\begin{aligned}
\underline{\underline{W}}_1 &= k_o(\gamma_1)/(\gamma_2-\gamma_1)\ [\gamma_2(\underline{\underline{F}}(\gamma_2) - \underline{\underline{F}}(\gamma_1)) - (\underline{\underline{G}}(\gamma_2) - \underline{\underline{G}}(\gamma_1))], \\
\underline{\underline{W}}_2 &= k_o(\gamma_2)/(\gamma_2-\gamma_1)\ [-\gamma_1(\underline{\underline{F}}(\gamma_2) - \underline{\underline{F}}(\gamma_1)) + (\underline{\underline{G}}(\gamma_2) - \underline{\underline{G}}(\gamma_1))].
\end{aligned} \tag{A13}$$

(If $[\gamma_1,\gamma_2]$ encompasses $\gamma=\gamma_o$ corresponding to the lower limit in (5), $\underline{\underline{F}}(\gamma_1)$ and $\underline{\underline{G}}(\gamma_1)$ in (A13) should be replaced by $\underline{\underline{F}}(\gamma_o)$ and $\underline{\underline{G}}(\gamma_o)$.) The evaluation of $\underline{\underline{F}}(\gamma)$ and $\underline{\underline{G}}(\gamma)$ with (A3) and (A4) inserted for $\kappa(\gamma,\lambda)$ and $\underline{\underline{P}}(\gamma)$, can readily be accomplished with the aid of the following two tables of indefinite integrals:

Formulas for $\int x^n \arcsin x\ dx = S_n(x)\ \arcsin x + T_n(x)\ (1-x^2)^{\frac{1}{2}}$:

n	$S_n(x)$	$T_n(x)$
0	x	1
1	$-1/4 + 1/2\ x^2$	$1/4\ x$
2	$1/3\ x^3$	$2/9 + 1/9\ x^2$
3	$-3/32 + 1/4\ x^4$	$3/32\ x + 1/16\ x^3$
4	$1/5\ x^5$	$8/75 + 4/75\ x^2 + 1/25\ x^4$
5	$-5/96 + 1/6\ x^6$	$5/96\ x + 5/144\ x^3 + 1/36\ x^5$

Formulas for $\int x^n (1-x^2)^{\frac{1}{2}}\, dx = U_n \arcsin x + V_n(x)\ (1-x^2)^{\frac{1}{2}}$:

n	U_n	$V_n(x)$
0	1/2	$1/2\ x$
1	0	$-1/3 + 1/3\ x^2$
2	1/8	$-1/8\ x + 1/4\ x^3$
3	0	$-2/15 - 1/15\ x^2 + 1/5\ x^4$
4	1/16	$-1/16\ x - 1/24\ x^3 + 1/6\ x^5$

Diagonalization procedure for solution of differential system

In the vector equation (6), which represents four interlinked differential equations, the matrix $\underline{\underline{B}}$ to be diagonalized is equal to

$$\underline{\underline{B}} = \mu(z)\ \underline{\underline{M}} + \underline{\underline{R}}\ .$$

$\underline{\underline{M}}$ was defined in (4), and $\underline{\underline{R}}$ can be interpreted as a perturbation matrix originating from the scattering integral; contributions to $\underline{\underline{R}}$ come exclusively from the wavelength interval just below the current wavelength and are normally small. It can be shown that $\underline{\underline{B}}$ belongs to the same general class as $\underline{\underline{P}}$ in (A4). The characteristic polynomial of (A4) is

$$\begin{aligned} p(\sigma) = {} & \sigma^4 + (c^2 - a^2 + h^2 - f^2 - 2be - 2dg)\ \sigma^2 \\ & + (af+dg)^2 + (be+ch)^2 - (bg+ah)^2 - (cf+de)^2 \\ & - 2(ae-cg)\ (bf-dh). \end{aligned}$$

Because $\|\underline{\underline{R}}\|$ is small, $\underline{\underline{B}}$ has two pairs of real eigenvalues (as $\underline{\underline{M}}$ has). We see that the eigenproblem involves nothing more than solution of a quadratic equation in σ^2.

Application of boundary conditions

The expression (12) for the transformed flux component $X_{mp}(z)$ contains the integration constant C_{mp} to be determined from the boundary conditions for the problem. Let us assume that the eigenvalues σ_{mp} are ranked in increasing order:

$$\sigma_{1p} < \sigma_{2p} < 0 < \sigma_{3p} < \sigma_{4p}.$$

Then it is possible to obtain a finite flux for $z \to \pm \infty$ only if

$$C_{11} = C_{21} = C_{32} = C_{42} = 0.$$

The remaining integration constants are collected in a vector:

$$\underline{c} = (C_{12}, C_{22}, C_{31}, C_{41}) \quad .$$

$\underline{c}$ is determined from the requirement that $\underline{\psi}(z)$ (not $\underline{\chi}(z)$) is continuous at $z = 0$. This leads to the 4th-order linear system:

$$\underline{\underline{Y}}^{*} \, \underline{c} = \underline{\underline{Y}}_2 \, \underline{\chi}_2^{*} - \underline{\underline{Y}}_1 \, \underline{\chi}_1^{*} \, .$$

Here, $\underline{\underline{Y}}_p$ is the transformation matrix for medium p (cf. (7)), $\underline{\chi}_p^{*}$ is the vector with components $X_{mp}^{\infty} + \kappa_{omp}$, m=1,2,3,4; finally, the coefficient matrix $\underline{\underline{Y}}^{*}$ has its two first columns equal to the two first in $-\underline{\underline{Y}}_2$, and the two last columns equal to the two last in $\underline{\underline{Y}}_1$.

APPENDIX B

List of FORTRAN Subroutines in GB

PROGRAM GAMP1

Subroutine	Task
DATAIO	Reads and prints input data.
EIGINV	Solves the eigenproblem for matrix $\underline{\underline{B}}$ in (6).
EXPPOL	Estimates the parameters in (11) by a semi-linear lest-squares technique.
GAMP	Acts as a main program. Adjustable array bounds are passed to it through the parameter list.
WSCAT	Evaluates matrix quadrature weights for the scattering integral (5).

PROGRAM GFX

Subroutine	Task
DATAIO	Reads and prints input data.
PSIREC	Reads flux records from 'GB/FLUX' and reconstructs zero-order DP1 moments.
WQUADR	Evaluates wavelength group limits and quadrature weights for flux integrals.

PROGRAM UPDATE

Subroutine	Task
STAMP	Writes a record with the current date.

PROGRAM PRINT

Subroutine	Task
MPRINT	Prints information for one of the materials in 'GB/MATERIALS'.

PROGRAM DEEPFLUX

Subroutine	Task
DATAIO	Reads and prints input data.
DEEP	Performs main calculations.
WSCATD	Evaluates quadrature weights for the scattering integral.

SUBROUTINES SHARED BY SEVERAL PROGRAMS OR OF GENERAL PURPOSE

Subroutine	Called by	Task
AKERNL	GAMP1 DEEPFLUX	Calculates the Klein-Nishina scattering kernel.
COLSOL	GAMP1	Solves a positive-definite linear equation system using the decomposition made by MFSD.
COMPT	GAMP1 DEEPFLUX	Evaluates the variable part of the Compton cross-section.
DECOMP	GAMP1	Triangularizes a general linear equation system.
EXINT2	GAMP1 GFX	Calculates the second-order exponential integral $E_2(x)$.
MFSD	GAMP1	Makes a Choleski-decomposition of a positive-definite linear equation system.
MYG	GAMP1 GFX CROS DEEPFLUX	Calculates an array of photon interaction cross-sections for one of the materials in the file 'GB/MATERIALS'.
MYGEA	GFX	Calculates an array of photon energy-absorption coefficients for one of the materials in 'GB/MATERIALS'.
SOLVE	GAMP1	Solves a general linear equation system using the decomposition made by DECOMP.
SOURCE	GAMP1 GFX DEEPFLUX	Reads emission data from 'GB/EMITTERS'.

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