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CALCULATED GAMMA RAY PHOTOFRACTIONS FOR WELL-TYPE SCINTILLATION DETECTORS

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Monte Carlo calculations for the photofractions of well-type gamma ray scintillation crystals are described. Leakage of secondary gamma rays, bremsstrahlung and electrons is considered Calculated photofractions are tabulated for two commonly used well crystals. Comparisons are made between photofractions for NaI, CsI and CaI_2 scintillation crystals. Absorption and scattering within a homogeneous cylindrical source have been considered and results are given for aqueous solutions of monoenergetic sources.

1. Introduction

Scintillation counting is a widely used technique in the determination of absolute gamma ray emission rates, primarily because of the reproducibility of the detector efficiency. Sodium iodide crystals with carefully controlled dimensions and compositions are readily available to most laboratories and can be used as scintillation detectors of accurately known efficiency. The perturbing effect of scattering from surrounding media may be eliminated by counting only those interactions which deposit the full gamma ray energy in the crystal. The number of these events is proportional to the area under the photopeak, A_p, of the pulse height spectrum from the detector. By letting the factor f represent the fractional attenuation of any absorber between the source and the crystal, the absolute source strength N_0 is given by

$$N_0 = A_p/(f\varepsilon_{AP}), \tag{1}$$

where ε_{AP} = fraction of source gammas totally absorbed in the crystal (absolute peak efficiency). Conventionally, the absolute peak efficiency is written as the product

$$\varepsilon_{AP} = p \cdot \varepsilon_{AT}, \tag{2}$$

where ε_{AT} = fraction of source gammas that interact at least once in the crystal (absolute total efficiency) and p = fraction of interacting gammas that are totally absorbed (photofraction), including all secondary particles.

Here the effects of varying the source-to-crystal geometry are reflected mainly in ε_{AT} and the photofraction has been shown to be only mildly dependent on such variation. Values of the absolute total efficiency have been previously calculated for crystals with the two most common shapes: the solid right circular cylinder[1]) and the circular cylinder with coaxial cylindrical well[2]). Photofractions for solid crystals have been given by numerous authors, e.g. Heath[1]), Zerby et al.[3,4]), Miller and Snow[5]) and Jarczyk et al.[6]). Calculated photofraction values for well-type crystals, however, have not been previously available and are the subject of the present work.

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2. Calculational procedure

Monte Carlo methods were used to simulate on a digital computer the sequence of events which occur when a gamma ray is incident upon a well-type scintillation crystal. Each source gamma interacting in the crystal generates a sequence of secondary gammas and charged particles. The original interaction, together with the fate of all secondaries, constitutes a single "history". Termination of each history occurs when either the total energy of the incident gamma ray is absorbed, or any secondary gamma (with energy > 10 keV) or charged particle escapes from the crystal. The possibility of leakage of each secondary electron is taken into account, as are the bremsstrahlung photons generated along the electron track. The number of histories for which the total gamma energy is deposited within the crystal is then divided by the total number I, of interacting source gammas to give the photofraction, p. The predicted standard deviation of the photofraction obtained in this way, is given by

$$\sigma = [p(1-p)/I]^{\frac{1}{2}}. \tag{3}$$

2.1. Source geometries

Gamma rays incident on the crystal can be considered either from isotropic sources or as finite beams in which all rays are parallel to the axis of symmetry. The isotropic sources are typical of small volume radioisotope gamma emitters and include points (on or off the crystal axis), circular discs centered on the axis, or homogeneous cylinders located along the axis. Self-

absorption and scattering have been considered for the cylinder source (sect. 3.2). Beams of parallel rays incident normal to the well bottom can be used to simulate collimated sources.

2.2. Gamma interaction processes

The general flow diagram for the Monte Carlo computation is shown in fig 1. The appropriate source geometry is sampled to select a single gamma ray defined by seven variables: rectangular coordinates (x, y, z); direction cosines (u, v, w); and energy (E). If the selected source gamma is incident upon the crystal, the total distance, ρ, traveled in the crystal medium to the first interaction is calculated from

$$\rho = -\ln r/\mu, \tag{4}$$

where

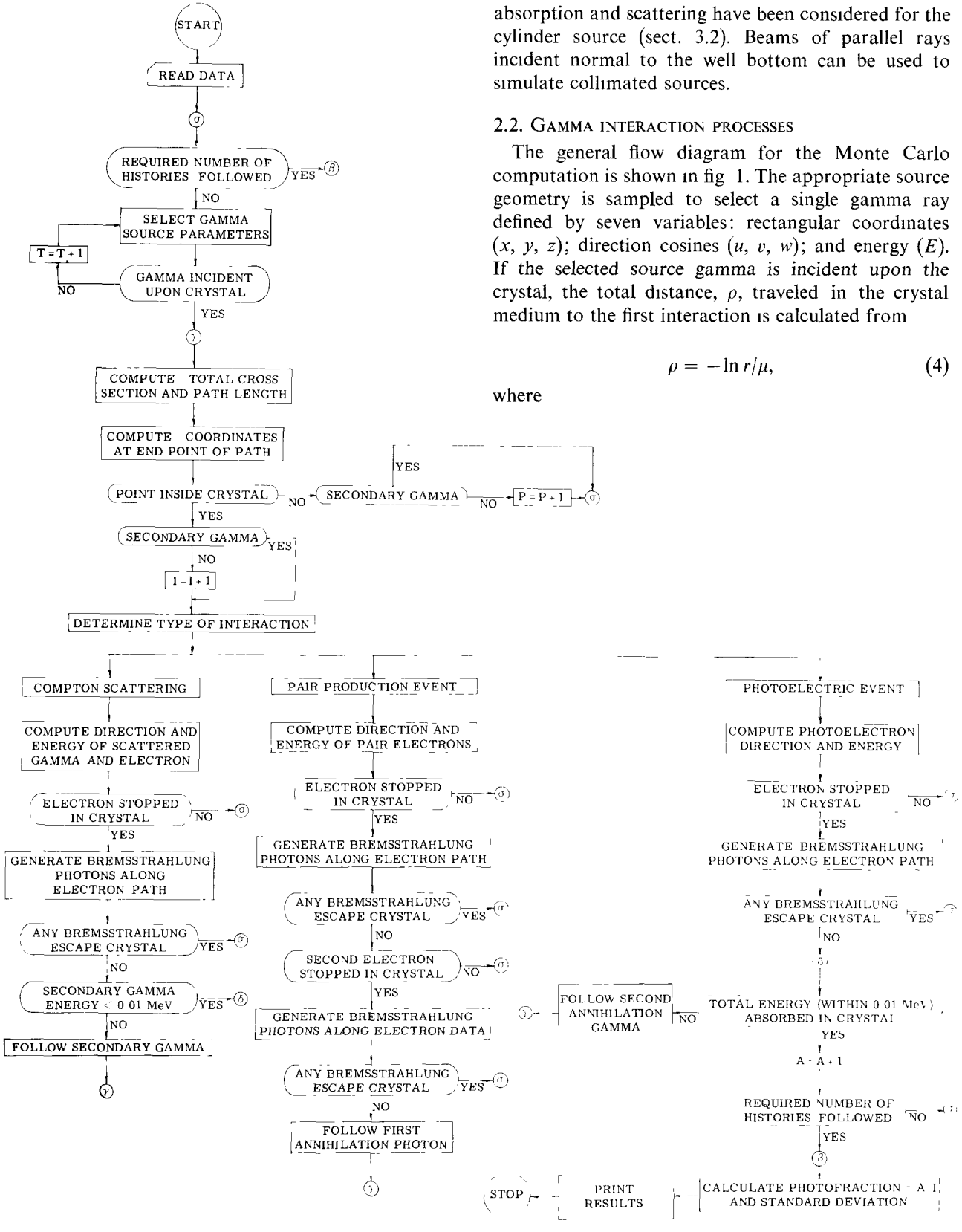


Fig 1. Diagram for Monte Carlo calculation of photofractions

r = random number obtained from a uniform distribution on the interval 0–1,
μ = total gamma ray cross section[7]) (without coherent scattering) at energy E.

If this interaction is found to occur within the crystal boundaries, the type of event is chosen by random sampling from the possible processes in proportion to their individual probabilities[7]). For gamma rays the only important interaction processes in the scintillation medium are photoelectric absorption, Compton scattering and pair production. Rayleigh (coherent) scattering has been ignored, as this process occurs only for the lowest energies where photoelectric absorption predominates and only a slight change in photon momentum results.

If a photoelectric event is sampled, the entire gamma energy is transferred to a single electron. The electron is assumed to be emitted in a direction distributed uniformly in azimuth and at an average polar angle[8]) relative to the incident gamma ray direction. Fluorescent radiation and/or Auger electrons emitted in filling the vacancy in the inner shell following a photoelectric absorption are neglected. Treatment of the photoelectron and subsequent bremsstrahlung are discussed in sections 2.3 and 2.4, respectively.

When a Compton event is chosen, the differential Klein-Nishina cross-section for free electrons is sampled by a technique of Kahn[9]) to obtain the polar angle of scattering relative to the incident gamma direction. The usual kinematic relationships are then used to obtain the energies of the scattered gamma and electron. Azimuthal symmetry is assumed. Transformations are made to relate all secondary gamma and electron directions back to the coordinate system fixed in the crystal using the method of Kleinecke[10]). The scattered gamma and electron are further followed through the crystal, as indicated in fig. 1.

If a pair production event occurs, the positron and negatron are assumed to be emitted at a mean polar angle given by Bethe and Ashkin[11]) as

$$\theta = m_0c^2/E_e, \tag{5}$$

where
m_0c^2 = electron rest mass energy,
E_e = electron kinetic energy (gamma energy minus $2m_0c^2$).

The azimuthal angles for the pair are uniformly distributed, 180° apart. The pair electrons are treated identically in slowing down and one is chosen at random to be the positron for purposes of generating annihilation radiation. Two 0.511 MeV annihilation photons are assumed to originate at the end of the positron path and are followed in the same manner as primary gamma rays.

2.3. Electron leakage

An approximate method has been used to take into account the possibility of escape through all the crystal surfaces of photo-, Compton-, and pair-electrons. For typical sizes of scintillation crystals, the fraction of all such electrons which escape is quite small and a more rigorous electron transport calculation is not warranted. The probability of escape is assumed to be a function only of the ratio ρ/R_0, where ρ is the extrapolated distance to the crystal surface and R_0 is the electron "range"[3, 12]). A random sample is obtained from the transmission curve of fig. 2 for each electron path. An electron is assumed to reach the crystal surface when

$$r \leqq P(\rho/R_0), \tag{6}$$

where
r = random number,
$P(\rho/R_0)$ = transmission probability (fig. 2),
R_0 = electron range corresponding to the initial electron energy[3, 12]).

The albedo data of Berger[14]) have been used to approximately account for that small fraction of electrons reflected from the crystal canning with only a slight loss in energy. All other electrons reaching the surface are assumed to escape from the crystal. Escape of any electron causes the history to be terminated, since the total source energy can no longer be absorbed in the crystal. If eq. (6) is not satisfied, the electron is con-

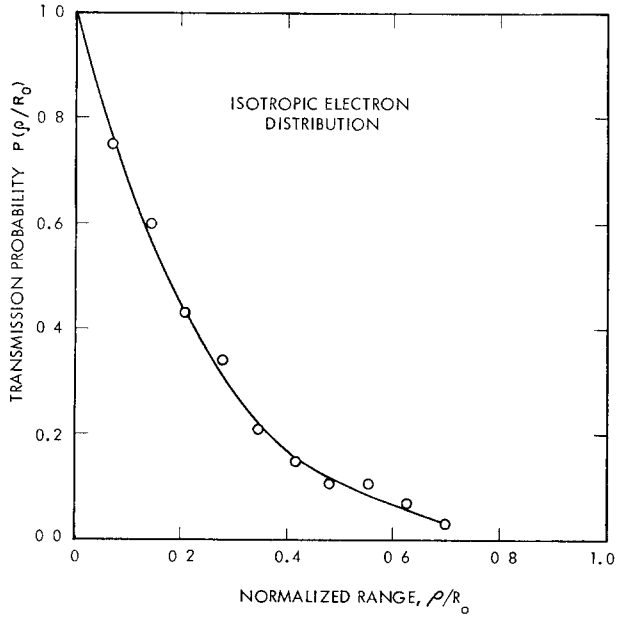


Fig 2. Electron transmission in NaI, ref.[13]).

sidered to be stopped within the boundaries and all its energy deposited in the crystal.

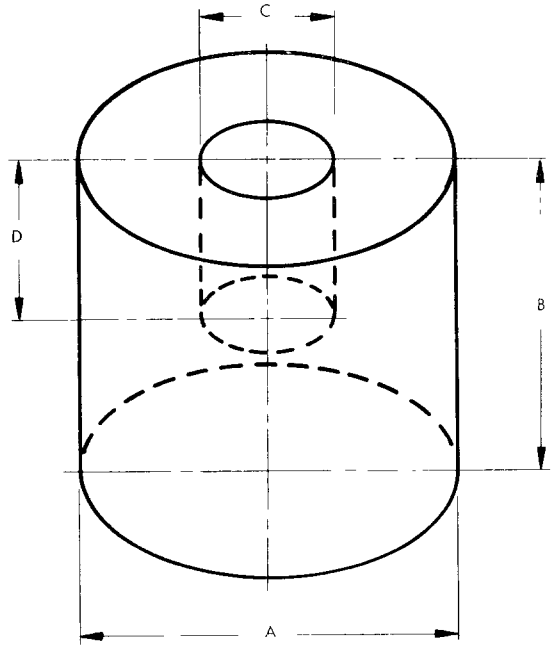
The transmission probability for electrons (fig. 2) has been calculated with the Monte Carlo program of Wainio[13]) for an isotropic, monoenergetic electron source within NaI and includes the effect of back-scattered electrons. Plotting the transmission probability vs the normalized range, ρ/R_0, yields a curve nearly independent of electron energy over the region of interest[14,15]). An isotropic, internal electron source was used in calculating these data in order to simulate the nearly random directions of incidence on the crystal boundaries.

2.4. Bremsstrahlung escape

All electrons produced in gamma ray interactions are assumed to generate bremsstrahlung photons according to the average differential spectra of Zerby and Moran[16]). Based on these differential spectra, the mean number of photons released with energy greater than $0.04\ m_0c^2$ has been calculated by Zerby[3]) and used in the present calculation to represent the average number of photons emitted while the electron is stopped. All bremsstrahlung with energy less than $0.04\ m_0c^2$ are assumed to be always absorbed in the crystal. The actual number of photons generated is obtained in a random manner by assuming that the probability for emission is given by a Poisson distribution consistent with the calculated average. For each bremsstrahlung photon released, a separate selection for energy is made from the distribution above $0.04\ m_0c^2$ according to the Monte Carlo procedure given in ref. [3]). The bremsstrahlung photons are assumed to have an isotropic angular distribution and are distributed in a random manner along the electron path. They are treated in the same manner as primary gamma rays, except that further electron or bremsstrahlung leakage are not considered. Escape from the crystal of any bremsstrahlung with energy greater than $0.04\ m_0c^2$ causes termination of the history, since total absorption of the source gamma energy is no longer possible

2.5. Secondary gamma ray escape

The secondary photons generated by primary Compton interactions and pair positron annihilation are further followed through the crystal, using the same techniques described for the primary gamma rays The coordinates of the next interaction point are calculated and tested to determine whether this point lies within the crystal boundaries. If it is outside the crystal, the secondary photon has escaped and the history is terminated. The interaction point calculation is complicated by the possibility of intersection of the photon path with the well volume. In those cases, it is assumed that the gamma ray is unattenuated through the canning and reflector on the well surface and that the well volume is vacuum. Thus, if the gamma ray cuts through the well and re-enters the crystal, the total distance traveled is increased by the length of the path through the well The case of absorption and scattering in the volume source within the well is considered in sect 3.2



	A	B	C	D
7F8	1 75	2 00	0 75	1 50
8F8	2 00	2 00	1.125	1 50

Fig 3 Well crystal dimensions (inch).

3. Calculated results

3.1. Photofractions for well crystals

Two widely used sizes of well crystals* were included in the calculation of NaI(Tl) photofraction values. As shown in fig. 3, the primary difference between the two crystals is the diameter of the well Results are given in table 1 The calculations were restricted to point isotropic sources 0 2 cm from the well bottom. The effect of various isotropic source geometries (i e. points, disks, cylinders) within the well was investigated and gave a maximum difference of $< 6\%$ from these values with most geometries showing considerably closer agreement. Similar mild dependence of photo-

* Available from Harshaw Chemical Company, Cleveland, Ohio.

TABLE 1
Well crystal photofractions isotropic point source on axis

Energy (MeV)	7F8	8F8
0 279	0.8590 ± 0 0078	0.8365 ± 0 0083
0 412	0.6460 ± 0 0107	0.6225 ± 0 0108
0 662	0.4305 ± 0 0111	0.4520 ± 0 0111
1 17	0 2775 ± 0 0100	0 2650 ± 0 0099
2.75	0.1420 ± 0 0078	0 1210 ± 0 0073
4.45	0.0785 ± 0 0060	0 0815 ± 0 0061
6 00	0.0445 ± 0 0046	0 0515 ± 0 0049
8 00	0.0235 ± 0 0034	0 0215 ± 0 0032
10 00	0.0185 ± 0 0030	0.0125 ± 0 0025

fractions on geometry is also observed for solid crystals[1])

The calculations were made for 2000 histories and the indicated standard deviations were obtained from eq. (3). When used with the ε_{AT} values of ref. [2]), these data permit calculation of peak efficiencies for the well crystals shown. Since no tabulation of calculated results can cover all possible experimental arrangements that may arise in the laboratory, the specific calculations were limited to these two commonly-used crystals. To permit extension to other cases, the computer program, designated BURP-5, has been made available through the Code Center of Argonne National Laboratory, Argonne, Illinois.

A limited investigation was made of the total absorption characteristics of CsI(Tl) and CaI_2(Eu) for a well crystal corresponding to the 8F8 dimensions. In fig 4, the results are presented in the form of the ratio of the calculated photofraction to that of NaI(Tl) at the same energy. The Monte Carlo program contains electron and bremsstrahlung data for NaI only and some error is introduced in the results for other materials at energies above 1 MeV. It is apparent that a CsI crystal will exhibit about 1.5–2.4 times the photofraction of the same size NaI crystal over the energy range of most laboratory interest. The comparison given here is based on equal crystal dimensions and the greater density of CsI (4.510 g/cm^3) over NaI (3.667 g/cm^3) accounts for a major part of this advantage. Only small CaI_2(Eu) crystals (1–2 cm^2 × 3 to 6 mm thick) have been produced to date[17]), but in order to provide a comparison, a hypothetical CaI_2 crystal with 8F8 dimensions was considered. Less than a 10% advantage for CaI_2 over NaI is indicated over the energy range considered.

3.2. Absorption and scattering in volume sources

For some gamma ray sources distributed over a finite volume, self-absorption and scattering effects may significantly reduce the effective detector efficiencies. In a review of the current literature, ref. [18]) was found to give the only calculated results in which source interactions were considered and is limited to solid crystal detectors. An investigation of this effect on total efficiencies of well crystals is described below.

The absolute peak efficiency for an ideal source defined as one with zero scattering and absorption cross sections, has been designated as ε_{AP}. Also ε'_{AP} is defined as the absolute peak efficiency for the same source geometry assuming non-zero cross sections. Analogous definitions are made for the photofractions

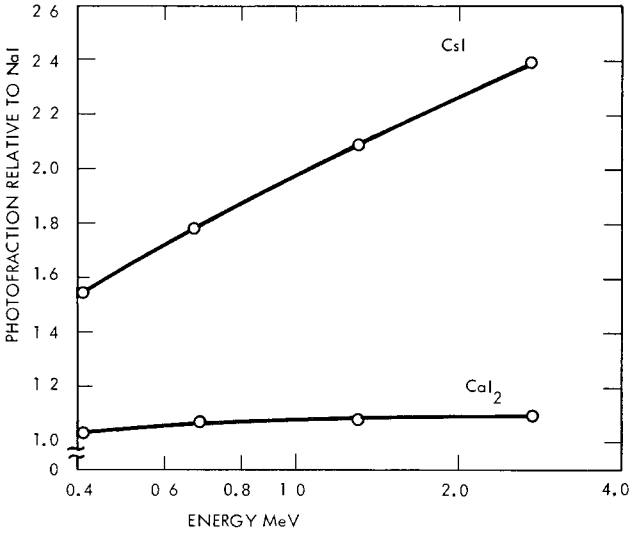


Fig 4 Ratio of CsI or CaI_2 photofraction to NaI for 8F8 well crystal

p and p' and absolute total efficiencies, ε_{AT} and ε'_{AT}. By definition

ε'_{AT} = fraction of source gamma rays that escape the source without scattering or absorption and interact at least once in the crystal.

$$\varepsilon'_{AT} = \frac{1}{V_s}\int_{\Omega}\int_{V_s}(1 - e^{-\tau x})\, e^{-\mu y}\, d\Omega\, dV_s, \qquad (7)$$

where

V_s = source volume,
y = path length in the source extrapolated in the direction of emission of a source gamma ray,
x = path length in the crystal,
$\tau(E)$ = total cross section of crystal,
$\mu(E)$ = total cross section of source,
Ω = mean solid angle subtended by the crystal at the source.

If the photofraction p' is calculated for only those

rays which escape from the source unattenuated in energy, then the absolute peak efficiency is given by

$$\varepsilon'_{AP} = p' \cdot \varepsilon'_{AT}, \quad (8)$$

where

p' = photofraction given by the ratio A'/I',

A' = number of gamma rays that deposit the total source energy in the crystal,

I' = number of gamma rays interacting at least once in the crystal.

Scattering and absorption within the source will affect both the photofraction and the total efficiency, but in many cases the change in photofraction will be negligibly small If we ignore the possibility of gamma rays scattered in the crystal re-entering the well and interacting in the distributed source, then the approximation that $p' = p$ is, at worst, equivalent to considering the photofraction for all points within the source to be equal As discussed in sect. 3.1, the latter approximation is generally good to within a few per cent for sources within the well and we have consequently limited consideration of source self-absorption to its effect on ε_{AT}. Eq. (7) was numerically evaluated by Gaussian quadrature for the case of a homogeneous aqueous solution completely filling the well of an 8F8 size NaI crystal Results, together with those for the equivalent transparent source, are given in table 2. When used with the photofraction data of table 1, approximate values of the peak efficiency ε'_{AP} can be obtained for this geometry The computer program for solution of eq. (7) for any well-crystal is designated BURP-2 and is also available from ANL Code Center.

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TABLE 2

Absolute total efficiencies for volume source in 8F8 NaI well crystal

Energy (MeV)	ε'_{AT}	ε_{AT}	Energy (MeV)	ε'_{AT}	ε_{AT}
0 01	0 0697	0 8760	0 60	0 2589	0 2890
0 015	0 2388	0 8760	0 80	0 2261	0 2491
0 02	0 4158	0 8758	1 00	0 2049	0 2234
0 03	0 5908	0 8742	1 50	0 1728	0 1855
0 04	0 6539	0 8756	2 00	0 1567	0 1667
0.05	0 6774	0 8749	3 00	0 1429	0 1505
0.06	0 6883	0 8737	4 00	0 1385	0 1444
0 08	0 7003	0 8705	5 00	0 1365	0 1429
0 10	0 7051	0 8652	6 00	0 1371	0 1429
0 15	0 6703	0 8046	8 00	0 1404	0 1455
0 20	0 5698	0 6725	10 00	0 1452	0 1499
0 30	0 4081	0 4710	15 00	0 1581	0 1624
0 40	0 3284	0 3750	20 00	0 1689	0 1731
0 50	0 2849	0 3207	30 00	0 1864	0 1907

ε'_{AT}: attenuation in aqueous source solution considered
ε_{AT} no attenuation in source.

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