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User's Manual for PHOEL-2, a Monte Carlo Computer Code for Calculating Energies of Photoelectrons and Compton Electrons in Water

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82

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FOR CALCULATING ENERGIES OF PHOTOELECTRONS AND COMPTON ELECTRONS IN WATER

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CONTENTS

	<u>Page</u>
Highlights	v
Abstract	1
1. Introduction	1
2. Photoelectric and Compton Cross Sections for Water	2
3. Treatment of Photoelectrons	6
4. Treatment of Compton Electrons	6
5. User's Input to PHOEL-2	8
6. Operation of the Code	10
7. Numerical Checks	13
References	18

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HIGHLIGHTS

A Monte Carlo computer code, PHOEL-2, is described for generating the energies of photoelectrons and Compton electrons in water irradiated by photons having an arbitrary energy spectrum. Options exist for allowing at most only a single Compton scattering, for following photons through successive Compton scattering events until a photoelectron is produced, and for suppressing the photoelectric effect. An Auger electron is assumed to be produced following the ejection of a K-shell photoelectron from oxygen. The basic physical data and their mathematical treatment in PHOEL-2 are described. Pair production is not included. This user's manual describes the operation of the code.

USER'S MANUAL FOR PHOEL-2, A MONTE CARLO COMPUTER CODE
FOR CALCULATING ENERGIES OF PHOTOELECTRONS AND COMPTON ELECTRONS IN WATER

J. E. Turner, R. N. Hamm, H. A. Wright, J. T. M6dolo and G. M. A. A. Sordi

ABSTRACT

A Monte Carlo computer code, PHOEL-2, is described for generating the energies of photoelectrons and Compton electrons in water irradiated uniformly by photons having an arbitrary energy spectrum. The code treats input photons individually on the basis of the energy-dependent cross sections for Compton scattering and for the photoelectric effect. Options exist for (1) following each photon through successive Compton scattering events until it disappears by photoelectric absorption or (2) allowing at most only a single Compton scattering event per input photon. The photoelectric effect can be turned "on" or "off" with either option. If energetically possible, the photoelectron is assumed to come from the oxygen K shell; otherwise, it originates in the L shell. An Auger electron of energy 0.508 keV is assumed to be emitted following the creation of a K vacancy. The basic numerical data used in PHOEL-2, their mathematical treatment and the operation of the code are described. Detailed comparisons made with the work of Cormack and Johns for ^{60}Co and monoenergetic x rays confirm the numerical validity of results obtained with the code. Some of the data of Cormack and Johns are extended by including successive Compton scatterings for the same photon and by including the photoelectric effect and Auger electrons. PHOEL-2, which replaces an earlier code PHOEL, can be obtained from the Radiation Shielding Information Center at Oak Ridge National Laboratory. The new version differs from the old by (1) employing a more realistic handling of the photoelectric cross section as a function of energy, (2) compiling electron spectra instead of storing the energies of every electron produced, (3) eliminating some former input restrictions and (4) using a different random number generator. PHOEL-2 does not treat pair production, which should be included for water at photon energies above about 2000 keV.

1. INTRODUCTION

The Monte Carlo computer code PHOEL-2 was written to generate the initial energies of Compton electrons and photoelectrons produced in an infinite water phantom irradiated uniformly by photons of arbitrary spectrum. Although pair production is neglected, PHOEL-2 can be used at any energy for the Compton and photoelectric effects. An earlier

version of this code, called PHOEL,¹ was used² to produce a source term for a detailed Monte Carlo code for calculating electron transport and energy degradation in liquid water.^{3,4} The latter electron code has been used extensively to study secondary electron slowing down spectra, dose distributions, G values for various products in liquid water and relative biological effectiveness (RBE) for low-LET radiations at low doses.^{5,6}

PHOEL-2 contains a number of improvements over its predecessor, PHOEL:

1. The photoelectric cross section is treated more accurately as a function of energy.
2. The secondary electron energies that are generated are compiled in energy bins (specified by the user) rather than being stored individually for printer or tape output.
3. The code has been streamlined by removing some former input restrictions (e.g., requiring an even number of input photons for ⁶⁰Co) and by using a different random number generator.

PHOEL-2 is available from the Radiation Shielding Information Center, Oak Ridge National Laboratory.

2. PHOTOELECTRIC AND COMPTON CROSS SECTIONS FOR WATER

Values of the total mass attenuation coefficient μ/ρ (cm²/g) and the Compton collision cross section σ (10⁻²⁷ cm²/electron) given by Evans⁷ are shown in columns 2 and 3 of Table 1. (Energies are specified in keV throughout PHOEL-2.) These values are taken directly from Evans' Table XII and Table III. The mass attenuation coefficient for Compton collisions, given by $\sigma N_0/\rho$, where $N_0 = 3.34 \times 10^{23}$ electrons/cm³ and $\rho = 1$ g/cm³ for water, is shown in column 4. The mass attenuation coefficient for the photoelectric effect, τ/ρ , shown in column 5, is the difference between columns 2 and 4. The ratio, τ/μ , of the photoelectric and total cross sections used in PHOEL-2 is given in column 6. The last column in Table 1 shows, for comparison, the corresponding entries computed from values of σ and τ given in Table II of Cormack and Johns' paper.⁸

A curve plotted through Evans' values is shown in Fig. 1 together with points from Cormack and Johns' table. The differences arise from the larger photoelectric cross section used by Cormack and Johns. The

Table 1. Compton and photoelectric mass attenuation coefficients for water

Photon energy E (keV)	Total attenuation μ/ρ (cm ² /g)	Compton collision cross section σ (10 ⁻²⁷ cm ² /electron)	Compton attenuation $\sigma N_0/\rho$ (cm ² /g)	Photoelectric attenuation τ/ρ (cm ² /g)	τ/μ^a	τ/μ^b
10	4.99	640.5	0.214	4.78	0.958	0.957
15	1.48	629.0	0.210	1.27	0.858	
20	0.711	618.0	0.206	0.505	0.710	0.740
30	0.337	597.6	0.200	0.137	0.407	0.457
40	0.248	578.7	0.193	0.0547	0.221	0.266
50	0.214	561.5	0.188	0.0265	0.124	0.160
60	0.197	545.7	0.182	0.0147	0.075	0.099
80	0.179	517.3	0.173	0.00622	0.035	0.049
100	0.168	492.8	0.165	0.00340	0.020	0.024
150	0.149	443.6	0.148	0.000838	0.006	
200	0.136	406.5	0.136	0.000229	0.000	

^aR. D. Evans, "Compton Effect," p. 218 in *Encyclopedia of Physics*, Vol. 34, S. Flügge (ed.) Springer, Berlin, 1958.

^bD. V. Cormack and H. E. Johns, "Electron Energies and Ion Densities in Water Irradiated with 200 keV, 1 MeV and 25 MeV Radiation," *Brit. J. Radiol.* 25, 369 (1952).

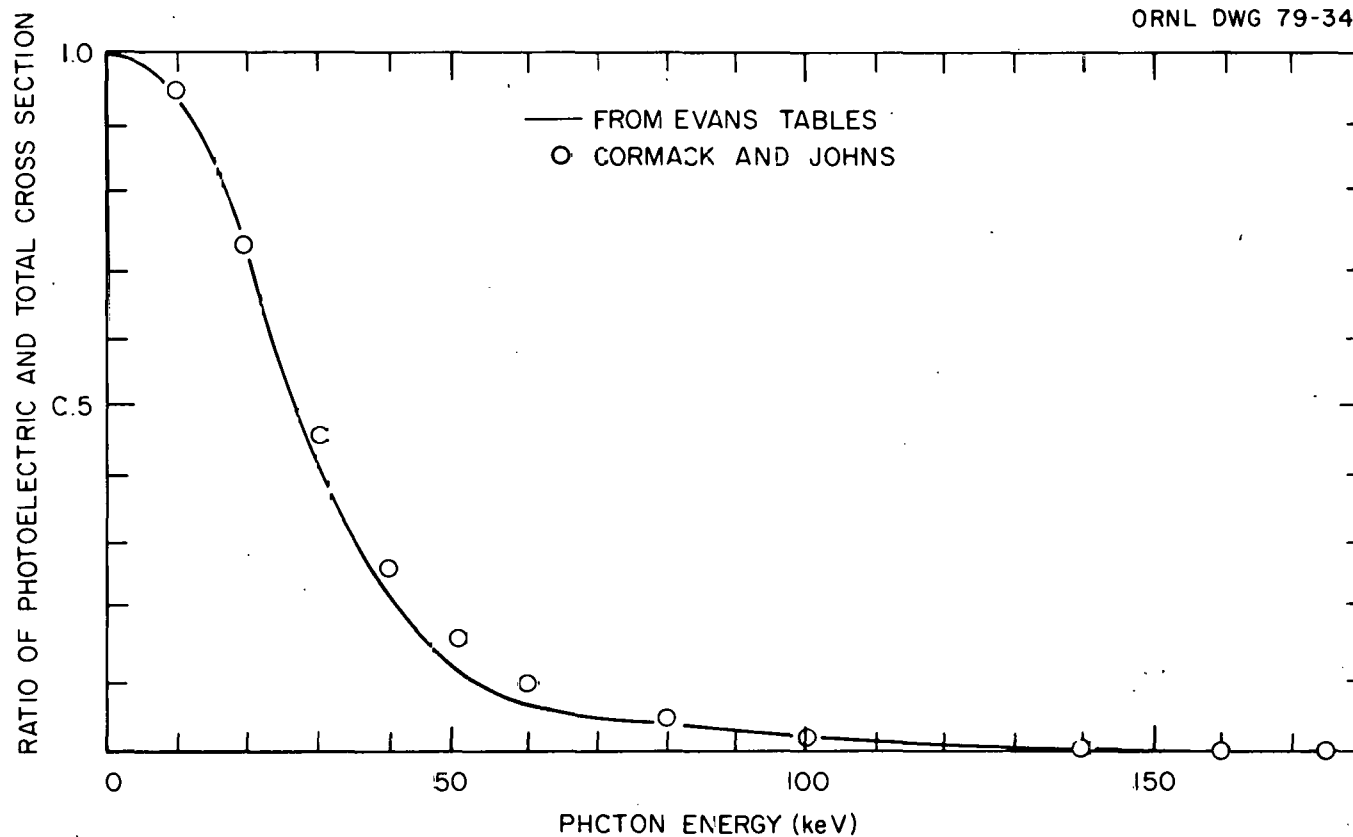


Fig. 1. Ratio of photoelectric and total cross sections as a function of energy for photons in water. The solid curve was computed from tables given by Evans,⁷ which provide the values used in PHOEL-2. For comparison, the points show some values given by Cormack and Johns.⁸

Compton cross sections in Cormack and Johns and Evans agree, both having been obtained directly from the Klein-Nishina formula. Based on Evans' values, we assume that the photoelectric cross section is negligibly small above 175 keV.

The numbers τ/μ in column 6 of Table 1 represent the probabilities that a photon of energy E will produce a photoelectron instead of being Compton scattered. It is seen from Fig. 1 that linear interpolation between entries in such a table will give a good approximation to τ/μ if a few more points are included in regions where the curvature is large. The additional points needed can be obtained by reading from the original plot of Fig. 1 on graph paper. The values used in PHOEL-2, obtained in this way, are given in Table 2; and linear interpolation is used to obtain τ/μ for values of E between the entries. Table 2 appears in the subroutine SORSIN as $E1(K)$ and $F(K)$, the number of entries (16 in Table 2) being specified by an integer NBR in the code.

Table 2. Values used in PHOEL-2 for probability that a photon of energy E produces a photoelectron instead of being Compton scattered

Photon energy E (keV) $E1(K)$	Probability τ/μ $F(K)$	Photon energy E (keV) $E1(K)$	Probability τ/μ $F(K)$
0	1.000	45	0.167
5	0.995	50	0.124
10	0.957	55	0.096
15	0.858	60	0.075
20	0.710	80	0.035
30	0.407	100	0.020
35	0.300	150	0.006
40	0.221	175	0.000

3. TREATMENT OF PHOTOELECTRONS

PHOEL-2 treats individual photons on a statistical basis. If the energy of a photon is greater than 175 keV, then it can only be Compton scattered. If the photon energy is less than 175 keV, then the code picks a random number and decides by linear interpolation in Table 2 whether it is Compton scattered or produces a photoelectron.

The threshold energy for producing a K-shell vacancy in oxygen is 0.532 keV. If $E \geq 0.532$ keV, then a photoelectron of energy $T = E - 0.532$ is assumed to be emitted. Since the fluorescent yield from oxygen is very small, it is assumed, further, that creation of the K vacancy is followed immediately by release of an Auger electron. The average L-shell binding energy in oxygen is about 0.012 keV. Therefore, the energy of the Auger electron is assumed to be 0.508 keV, the difference between the K-shell binding energy and twice the L-shell energy. If $0.532 > E > 0.012$ keV, then a photoelectron of energy $T = E - 0.012$ keV is assumed to be produced from the L shell. If $E < 0.012$ eV, nothing further happens to the photon; however, the total number and energy of these photons are tabulated.*

4. TREATMENT OF COMPTON ELECTRONS

The cross section $d\sigma/dT$ for producing Compton electrons of kinetic energy T is given by Eq. (26.7) of a review article by Evans⁹:

$$\frac{d\sigma}{dT} = \frac{\pi r_0^2}{m_0 c^2 \alpha^2} \left[2 + \frac{T}{E - T} \left(\frac{1}{\alpha^2} + \frac{E - T}{E} - \frac{2}{\alpha} \frac{E - T}{T} \right) \right] \frac{\text{cm}^2}{\text{keV electron}} \quad (1)$$

Here

$$r_0 = \frac{e^2}{m_0 c^2} = 2.18 \times 10^{-13} \text{ cm} = \text{classical electron radius}$$

$$m_0 c^2 = 511 \text{ keV} = \text{electron rest energy}$$

*The probability is very small that the calculated energy after Compton scattering will be less than 0.012 keV. No photons with $E \leq 0.012$ keV have turned up thus far in computations with PHOEL-2 involving several hundred thousand photons.

$$\begin{aligned}
 T &= \text{kinetic energy of Compton electron} \\
 E &= \text{photon energy} \\
 \alpha &= \frac{E}{m_0 c^2} .
 \end{aligned}$$

The unnormalized cumulative distribution $S(E, T)$ for producing a Compton electron of energy T or less is obtained by integrating Eq. (1). We find

$$\begin{aligned}
 S(E, T) &= \int_0^T \frac{d\sigma}{dT} dT \\
 &= \frac{\pi r_0^2 T}{m_0 c^2 \alpha^2} \left[\frac{2E - T}{2E} + \frac{2}{\alpha} + \frac{2E - T}{\alpha^2 (E - T)} - \frac{E}{T} \left(1 - \frac{2}{\alpha} - \frac{2}{\alpha^2} \right) \ln \left(1 - \frac{T}{E} \right) \right]. \quad (2)
 \end{aligned}$$

The energy of the Compton electron can vary from zero to a maximum given by

$$T_{\max} = \frac{2\alpha E}{1 + 2\alpha}. \quad (3)$$

Therefore, the normalized probability that a photon of energy E produces a Compton electron of energy T or less is given by

$$P(E, T) = \frac{S(E, T)}{S(E, T_{\max})}. \quad (4)$$

The energy T of the electron produced by Compton scattering of a photon of energy E is obtained as follows in PHOEL-2. The quantity $S(E, T_{\max})$ is first computed from Eqs. (2) and (3). A random number between 0 and 1 is selected for P , and the difference

$$D(E, T) = S(E, T) - PS(E, T_{\max}) \quad (5)$$

is formed. The transcendental equation

$$D(E, T) = 0 \quad (6)$$

is then solved for T by an iterative procedure.

The method of finding the solution of Eq. (6) in PHOEL-2 is straightforward. Since $0 < P < 1$, the function $D(E, T)$ will be positive when $T =$

T_{\max} and negative when $T = 0$. Furthermore, $S(E,T)$ is a monotonic function of T for any E ; and so $D(E,T)$ changes sign exactly once in the interval $0 \leq T \leq T_{\max}$, namely, at the point T_0 which is the root of Eq. (7). To find T_0 approximately, the code calculates $D(E,T)$ successively at equally spaced points, starting with $T = 0.9 T_{\max}$ and proceeding to $0.8 T_{\max}$, etc., until the first negative value of D is obtained. (If $D = 0$, then the root has been found.) When D is first negative, T_0 lies within the last interval of length $0.1 T_{\max}$ covered. This interval is subdivided into ten intervals of length $0.01 T_{\max}$ and the procedure repeated to determine T_0 to within $0.01 T_{\max}$. This new interval is further subdivided to find T_0 to within an interval $0.001 T_{\max}$. The midpoint of this last interval is used for the value of T_0 .

Whereas a photon disappears when it produces a photoelectron, a photon of reduced energy $E - T$ still exists following Compton scattering. In its standard form, PHOEL-2 traces the history of each photon through successive Compton scatterings until it produces a photoelectron. As an option, the history of a photon can be terminated after a single Compton scattering. The two required statements are given in the deck as "comment" cards, which can be turned around to bypass multiple Compton scattering. With either option, the average energy of the first Compton electrons produced by photons from the input spectrum is compiled in the program. It is sometimes useful to compare this average Compton energy with published values (e.g., Evans^{7,9}) as a check that the program is operating properly.

5. USER'S INPUT TO PHOEL-2

The user's input cards to PHOEL-2 are listed in Table 3. The first card in the data set gives NBR, the number of entries (16) in Table 2. The next four cards give the values of the pairs $E_1(K), F(K)$. These cards could be changed to use a different numerical representation of the ratio of the photoelectric to total cross section. This table is the first thing printed in the output of PHOEL-2. The code is dimensioned so that $NBR \leq 101$.

The next data card gives the number N of values $EN(I), PR(I)$, with $I \leq 101$, which represent the cumulative input photon spectrum. The

Table 3. Input cards
(All energies in keV)

Number of cards	Contents	Format	Remarks
1	NBR	I3	$NBR \leq 101$
4	E1(K),F(K)	8F10.4	Ratio photoelectric/total cross section
1	N	I3	$N \leq 101$
1+	EN(I),PR(I)	8F10.4	Input photon spectrum
1	NCO	I1	Set NCO = 1 for ^{60}Co and 0 for all other cases
1	NPBINS	I5	$NPBINS \leq 101$
1+	PES(K)	16F5.0	Photon energies making bin edges
1	NEBINS	I5	$NEBINS \leq 101$
1+	EES(K)	16F5.0	Electron energies marking bin edges
1	NPHOT	I6	Number of input photons

pairs start with $PR(1) = 1.0$ at the highest photon energy $EN(1)$. For a continuous photon spectrum, the pairs end with $PR(N) = 0.0$ at the lowest energy $EN(N)$. The energy E of a photon from a continuous spectrum is selected randomly from these pairs by linear interpolation. For monoenergetic photons, $N = 1$; for ^{60}Co , $N = 2$. The next 1+ cards give the pairs of numbers $EN(I), PR(I)$ describing the input photon spectrum. For monoenergetic photons, there is only a single card, with $PR(1) = 1.0$ and $EN(1) = E$, the photon energy in keV. For ^{60}Co , there is also only one card, with $PR(1) = 1.0$, $EN(1) = 1332.0$, $PR(2) = 0.5$ and $EN(2) = 1173.0$. Other spectra can be represented by specifying up to 101 pairs of values, starting with the highest energy. The spectrum, which is read in SORSIN, is printed at the end of a run.

The next card specifies NCO, an integer in I1 format. If $NCO = 1$, PHOEL-2 will give a spectrum of photons of alternating energies $EN(1)$ and $EN(2)$. This scheme is appropriate for ^{60}Co , which emits equal numbers of photons at two energies. If this option is not desired, then some other numeral (e.g., $NCO = 0$) must appear here.

The code maintains a tally of the numbers of photons it chooses from the input spectrum in various energy ranges. This is done to provide the spectrum of photons actually used in a calculation, which, of course, should agree statistically with the spectrum read into the code. A series of energy bins is set up for scoring the energy of a photon selected from the input spectrum. The next card in the data set gives NPBINS, the number of values of energy used to mark the boundaries between NPBINS - 1 successive energy bins. The energy values PES(K) appear on the following 1+ cards, up to 100 bins being allowed ($NPBINS \leq 101$). The total number of photons and the relative number in the various energy bins are tabulated and printed out at the end of the calculation. Only the energies of original photons chosen from the input spectrum are counted in this tabulation; the reduced energies of photons after Compton scattering are not.

A similar set of bins is set up for tabulating the electron spectrum generated by PHOEL-2. The next card gives NEBINS (≤ 101) and the following 1+ cards the electron energies EES(K) that mark the boundaries between adjacent bins. The number of electrons/keV per photon from the input spectrum in each of the bins is tabulated and printed. The total number of electrons is also printed.

The last card in the data set specifies NPHOT, the number of photons to be used for the input photon spectrum.

In addition, the output also lists the average initial Compton energy, mentioned above, as well as the number and total energy of any photons that occur with $E < 0.012$ keV, the assumed oxygen L-shell ionization threshold.

6. OPERATION OF THE CODE

A flow diagram for PHOEL-2 is shown in Fig. 2. The subroutine SORSIN is first called, in which the data cards are read and some of the input information is printed. Bins are set up in SORSIN for tabulating energies, and tallies IPN and IEN for the numbers of photons and electrons in each bin are initialized to 0. A monitor K2 that counts electrons is set equal to 0, as well as the number K1 and total energy ESUM of electrons with $E < 0.012$ keV. An integer ICO = 0 is specified, which generates photons of alternating energies if NCO = 1.

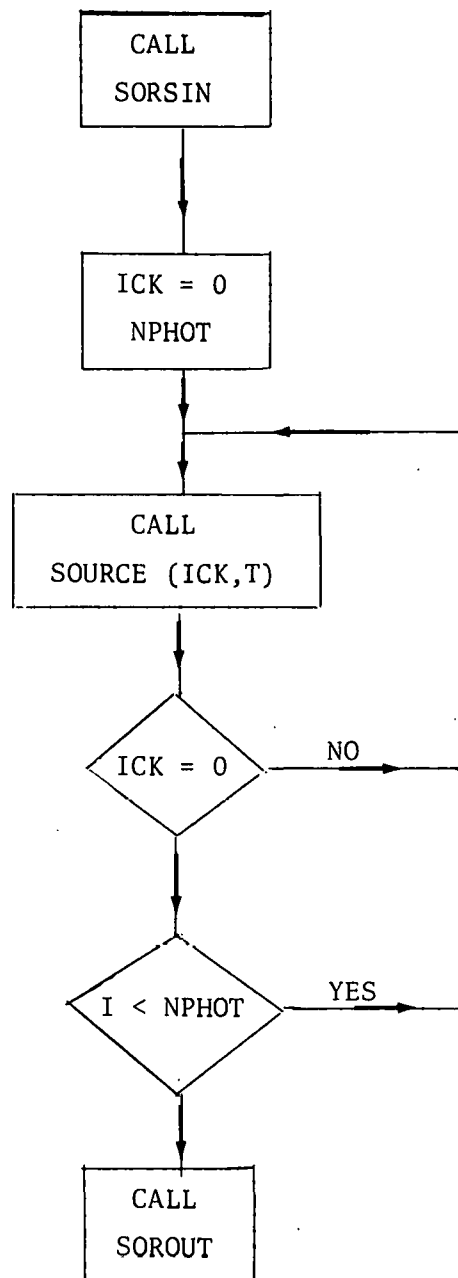


Fig. 2. Flow diagram of main program of PHQFI-2.

As indicated in Fig. 2, the main program then sets another integer $ICK = 0$ and calls the subroutine `SOURCE (ICK,T)`. This subroutine selects a photon of energy E from the input photon spectrum and returns to the main program with a value T for the energy of an electron it produces and a value for the integer ICK . The integer $ICK = 0$ indicates that a new photon will be chosen from the input spectrum when `SOURCE` is called again. The integer $ICK = 1$ indicates that a photon was Compton scattered and that the scattered photon of reduced energy will be treated next in `SOURCE` before another photon is selected from the input spectrum. (When turned around, two comment cards near the end of `SOURCE` always give $ICK = 0$, corresponding to single Compton scattering only.) As long as $ICK = 1$, the main program continues to go back to `SOURCE` for another electron energy without selecting another photon from the input spectrum. A photoelectron will eventually be produced. If it is from the L shell, then `SOURCE` returns to the main program with that photoelectron energy and $ICK = 0$, indicating that the photon is gone and that no more electrons will be produced until another photon is chosen from the input spectrum. If the photoelectron is from the K shell, then `SOURCE` returns to the main program with the electron energy and $ICK = 2$, indicating that there is a K vacancy. The main program then calls `SOURCE` again, which produces another (Auger) electron of energy 0.508 keV and sets $ICK = 0$, indicating that no more electrons will be produced by that original photon. (If a scattered photon should occur with energy < 0.012 keV, then `SOURCE` will return with $ICK = 0$.)

PHOEL-2 repeats this procedure until `NPHOT` photons from the input spectrum have been processed. `SOROUT` is then called, which tabulates and prints the statistical data generated.

PHOEL-2 running time depends on the number of photons used, `NPHOT`, as well as their energies. The CPU times on the IBM 360/91 are given in Table 4 for several cases with monoenergetic photons. The numbers of secondary electrons per photon in the input spectrum are also given.

Table 4. Sample data from three runs with monoenergetic photons

Photon energy E (keV)	CPU (IBM 360/91) time in seconds		Number of electrons per input photon
	NPHOT = 10^3	NPHOT = 10^4	
50	2.6	22.8	5.82
500	7.8	73.2	15.2
1,000	8.2	80.4	16.0

7. NUMERICAL CHECKS

PHOEL-2 has been checked numerically in a number of ways. First, as already mentioned, the average energy TAVG of electrons from the first Compton scattering of a photon from the input spectrum is tabulated. Values of TAVG computed with PHOEL-2 for monoenergetic photons with $E = 40, 100, 500, 1000$ and 5000 keV agree with the average Compton recoil energies given in Table 8 of Evans⁹ and Table III of Evans.⁷

In addition, detailed distributions of initial Compton energies were computed for monoenergetic photons in the energy range 10-220 keV. In particular, we used Table II of Cormack and Johns⁸ as a check of PHOEL-2, using only single Compton scattering and turning off the photoelectric effect.

Some additional information was generated from PHOEL-2, as shown in Fig. 3, which was calculated by using NPHOT = 25,000 photons with $E = 70$ keV. The dashed lines show the numbers from Cormack and Johns' Table II,⁸ which were also obtained exactly from PHOEL-2 with single Compton scattering and no photoelectric effect. The solid lines give the results obtained with the photoelectric effect turned on. As seen from Fig. 1, a 70-keV photon produces a photoelectron in about 4% of the collisions. Thus, we expect an average of $0.04 \times 25,000 = 1,000$ photoelectric events from among a sample of 25,000 70-keV photons. There would also be about 1,000--or possibly fewer--Auger electrons (L-shell vacancies do not produce Auger electrons) in addition to 24,000 Compton electrons in this "first-collision" calculation. Thus, a total of about 26,000 electrons is expected. In the run for Fig. 3, PHOEL-2 generated 26,022 electrons

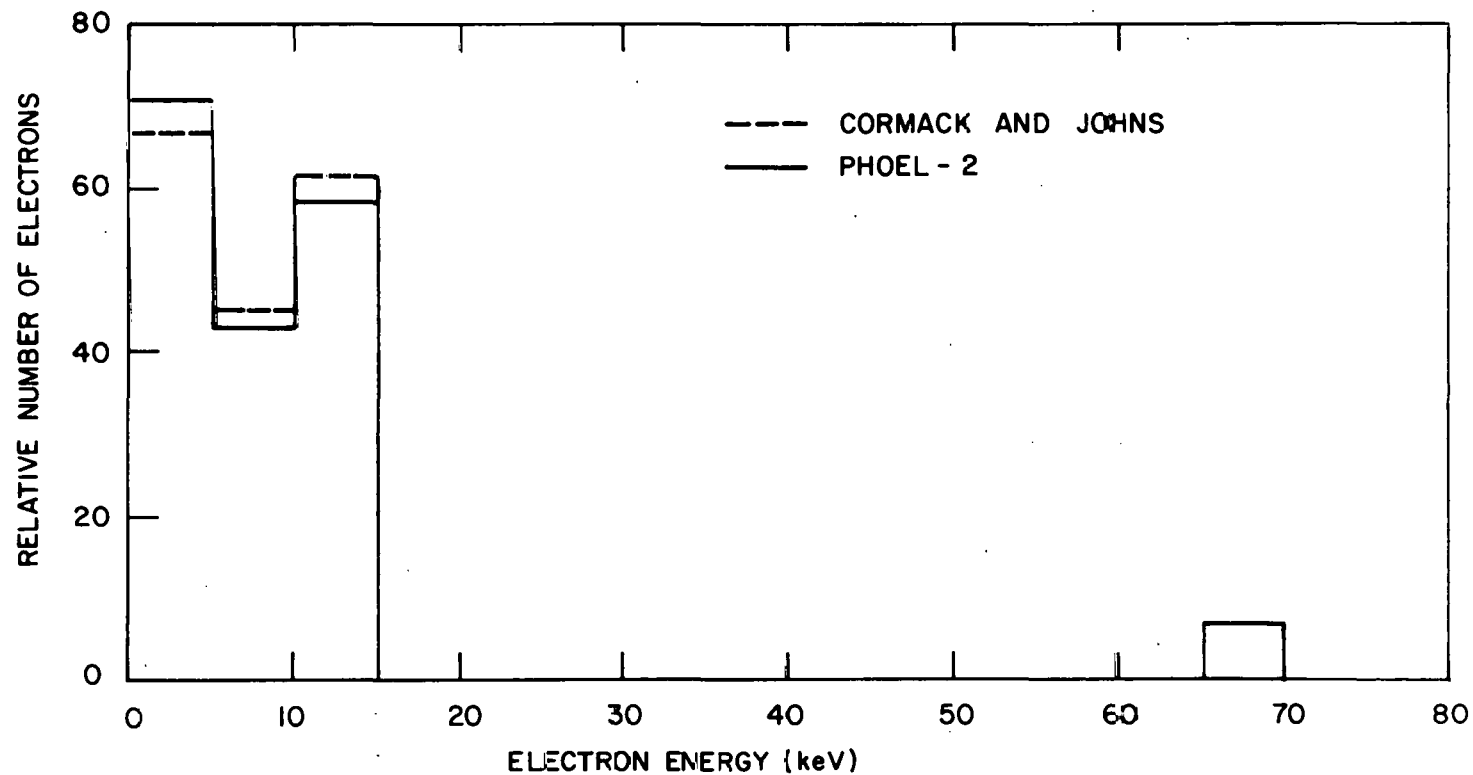


Fig. 3. Initial energies of electrons calculated with PHOEL-2 for 70-keV photons in water. Dashed lines agree with Cormack and Johns⁸ for Compton electrons. Solid lines result when photoelectrons and Auger electrons are included. The spectrum is plotted here to compare directly with Cormack and Johns' Table II (number of electrons/cm³ per unit fluence). The normalization used with PHOEL-2 is such that the first dashed entry, 71.4 in the 0-5 keV interval, represents 0.0814 electrons/keV per incident photon.

1022 more than NPHOT, indicating that there were 23,978 Compton electrons 1022 photoelectrons and 1022 Auger electrons. The solid lines in Fig. 3 show that inclusion of the photoelectric effect modifies the data in Cormack and Johns' Table II in a straightforward way. The number of electrons for each of their entries at 70 keV is reduced by 4%, this being the fraction of input photons that do not produce Compton electrons. In addition, 4% of the total number of electrons at 70 keV in their table appear in the 65-70 keV interval as photoelectrons and 4% get added back into the lowest box, 0-5 keV, as the 0.508-keV Auger electrons.

Other detailed calculations were made with PHOEL-2 for the initial Compton electron energy spectra produced by 220-keV monoenergetic photons and by ^{60}Co photons. The detailed spectrum of initial Compton energies at 220 keV agreed quite well with that given in Cormack and Johns' Table II, as shown in Fig. 4. Agreement with their Table IV for ^{60}Co was satisfactory, although not as close as expected. Percentage differences between the two sets of calculations are largest where the electron spectrum is largest. With NPHOT = 25,000, the statistical variation expected in PHOEL-2 at the highest value in Cormack and Johns' Table IV (900-1000 keV) is $\sim 2\%$. We obtained a value $\sim 5\%$ greater than theirs. Our results in the next lower bin, between 800-900 keV, is about this much lower than theirs, so that both sets of calculations agree when averaged over the interval 800-1000 keV. Increasing NPHOT to 100,000 did not improve agreement.

Another calculation for ^{60}Co was made tabulating electron energies in a much finer mesh for comparison with Cormack and Johns' Fig. 5. This comparison is shown here in Fig. 5, which was computed with NPHOT = 100,000. The curves from the two sets of calculations have the same area. PHOEL-2 appears to give a somewhat flatter spectrum than that of Cormack and Johns for $E \lesssim 700$. The reason for the discrepancy in these details is not known.

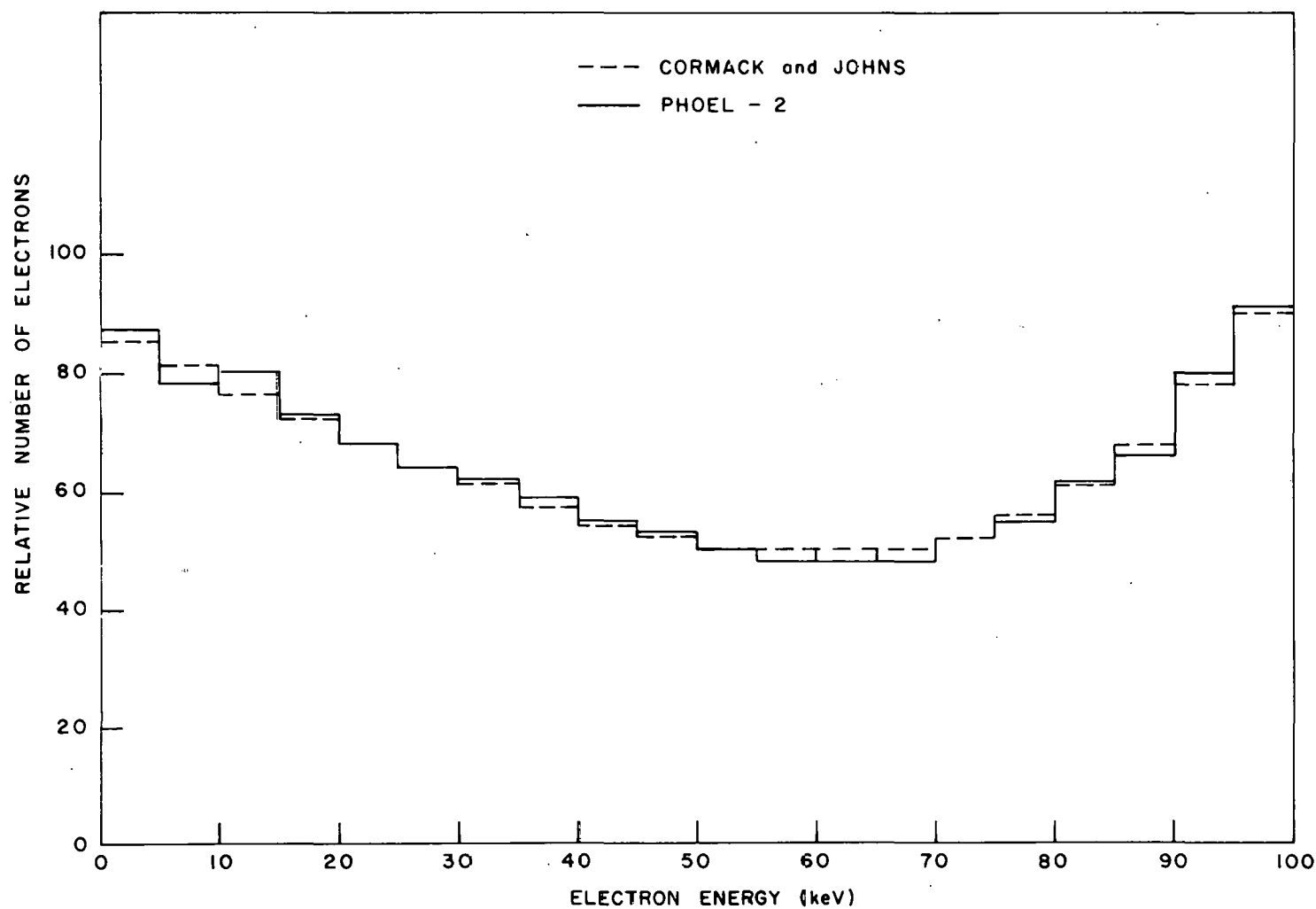


Fig. 4. Comparison of initial Compton energies calculated with PHOEL-2 (solid lines) and by Cormack and Johns (dashed lines) for 220-keV photons. Differences are consistent with expected statistical fluctuations (NFHOT = 25,000).

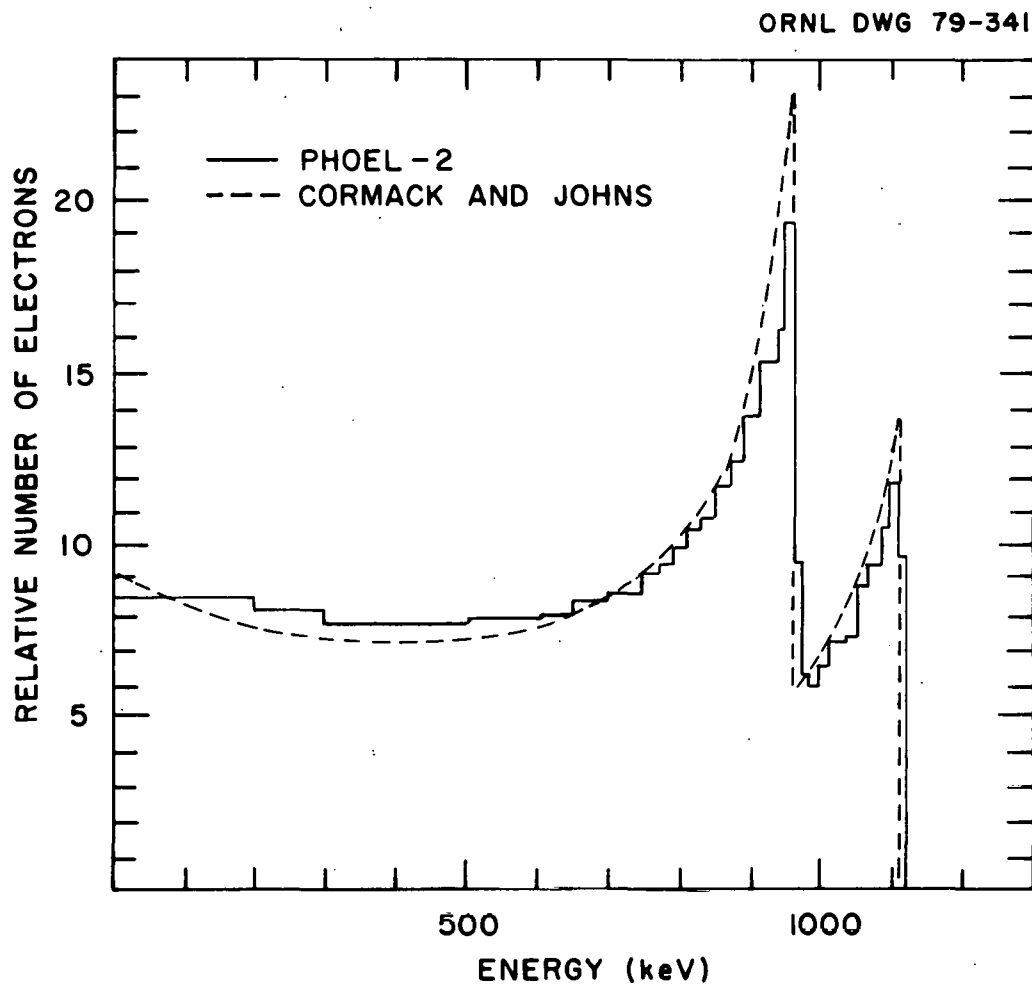


Fig. 5. Detailed comparison of initial energy distribution of Compton electrons produced by ^{60}Co radiation as calculated with PHOEL-2 (solid line histogram) and by Cormack and Johns⁸ (dashed curve).

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