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Russell K. Hobbie

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MacDose: A simulation for understanding radiological physics

Russell K. Hobbie
School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455[a]

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MacDose simulates the interaction of photons in matter in order to help students understand several concepts that are important in radiological physics. Its operation and the techniques used for the simulation are described, along with examples of the simulations.

INTRODUCTION

There are several subtle concepts that students of radiological physics must learn in order to understand how photons interact with matter. MacDose is a simulation program designed to help students learn this material through a set of exercises.[1] The program can also be used to demonstrate the concepts in the classroom. This paper describes the techniques used in MacDose and shows some of the simulations.

Development of MacDose began in 1987 when Tao-qu Chen wrote the simulation routines as a master's project. The object was not to do an accurate simulation, but rather to develop one good enough to help students understand the concepts, yet rapid enough so that it could be done in real time. After her work was completed in May 1988, it took another two summers to provide the user interface, properly manage event handling and display update, develop student exercises, and add the ability to consider subsequent photon interactions in an approximate manner.[2]

I. WHAT MacDose DOES

MacDose allows the user to specify the energy and the number of photons in a parallel beam that strikes a sample of water. Photon energies from 1 keV to 100 MeV are allowed. The photons interact with water in much the same way as they do with soft tissues in the body. MacDose has three windows which can be moved, resized, zoomed, and scrolled in the standard Macintosh fashion. One shows the Simulation, one is for numerical Results, and one provides a Graph of Energy Transferred and Energy Absorbed versus depth. The Simulation window normally displays the most recent 25 photons. The total number of photons in the simulation can be set by the user. If less than 25, it is also the number shown in the Simulation window. An option in later versions of MacDose allows the thickness of the lines to be doubled. This is useful when televising the screen for classroom use. [A Control Panel Document, VideoSync, available from APDA (Ref. 3), adjusts the refresh rate so that the screen can be televised without flicker.] Figure 1 shows a simulation with 40-keV photons using the thicker lines. Three photons underwent Compton scattering; the other two show the photoelectric effect. Ten-MeV photons are used in Fig. 2; the first (topmost) is an example of pair production, the second and fifth show Compton scattering, and the third and fourth are unattenuated.

The user can keep a Log File of the results of a simulation. The file can be read by a spreadsheet or a statistical analysis program to reduce some of the labor of analyzing the simulation. The contents of the windows can be printed. The contents of the Simulation and Graph windows can be copied to the Clipboard and from there to the Scrapbook or another application. (The contents of the Results window are transferred through the Log File.) A dialog box allows the user to select the energy of the photon beam, the thickness of the sample in the beam direction, the seed for the random number sequence used in the simulation, and whether or not subsequent photons interact. A recent verion provides an option to show only electron tracks in the Simulation window.

MacDose runs on a Macintosh Plus or later machine. If a color monitor is used, the incident photons are black, electrons are red, and scattered photons are blue. The simulations can be printed in color on a color printer such as an Imagewriter-II printer with a four-color ribbon, even if the Macintosh has a monochrome display. MacDose is compatible with Multifinder and System 7 and runs in the background. Typical execution speeds for 100-keV photons are 100 photons per minute on a Macintosh Plus or SE, and 425 photons per minute on a Macintosh II or SE/30.

Students must learn three mechanisms by which photons transfer energy to matter and their relative important at different energies. Using the notation (particle in, particle out), they are the photoelectric effect (γ,e), Compton scattering $(\gamma,\gamma' e)$, and pair production $(\gamma,e^- e^+)$. Three other interactions have been ignored: coherent scattering (γ,γ) does not transfer energy, though it is an important mechanism for contrast degradation in diagnostic radiology; triplet production $(\gamma,e^- e^- e^+)$ has not been included, even though it contributes 8% at 10 MeV and 12% for 100-MeV photons interacting with water; and photonuclear interactions have been ignored.

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[a] E-mail address: hobbie@mailbox.mail.umn.edu.

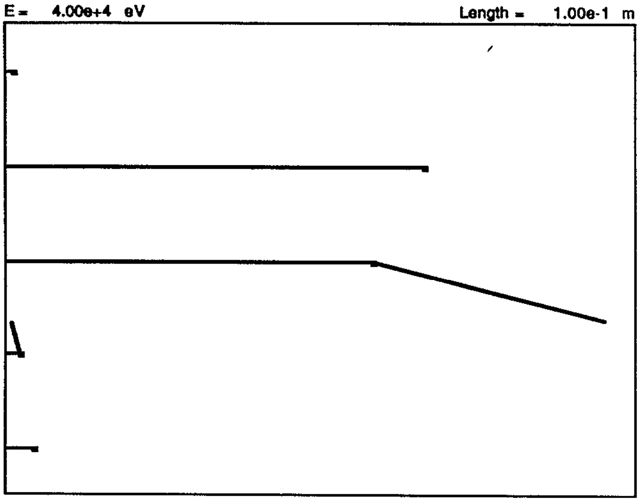

FIG. 1. The Simulation window, for the interaction of five 40-keV photons. The thick-track option has been used. Two photons underwent Compton scattering; the other three show the photoelectric effect.

After a photoelectric interaction in the K-shell, the oxygen atom has an excitation of about 500 eV; the subsequent fluorescence photons and Auger electron are not included. Two mechanisms by which charged particle energy is converted back to photon energy are also ignored: the production of photons from electrons and positrons by bremsstrahlung, and the annihilation of positrons in flight.

Students must understand the distinction between several stochastic quantities and their expectation values. These quantities are defined[4] in Table I.

TABLE I. Examples of stochastic quantities and related nonstochastic quantities.

Stochastic	Nonstochastic
Fraction of photons passing through a sample in a given experiment	attenuation $= e^{-\mu x}$
Energy transferred to charged particles in a specified volume	kerma = expectation value of energy transferred per unit mass in the limit of infinitesimal mass
Energy imparted to matter in a specified volume is the energy which remains in the volume	absorbed dose = expectation value of the energy imparted to matter per unit mass in the limit of infinitesimal mass

Another distinction is between the energy transferred to electrons in a volume of material and the energy absorbed in the volume. The former is the amount of energy transferred from photons to electron kinetic energy in the volume. The energy absorbed is the kinetic energy transferred from electrons to other atoms and molecules in the volume as the electrons move through the material and slow down. It is the energy absorbed which causes the response of a radiation detector or radiation damage such as tissue injury. Some of the energy transferred to electrons in a given volume of material will be absorbed "downstream" if the electrons have enough energy to travel a significant distance. Similarly, some of the energy absorbed in a volume will have been transferred to the electrons "upstream." Figure 3 compares the stochastic quantities, energy transferred and energy absorbed, for one particular simulation of 10-MeV photons striking a 20-cm-thick sample.

One of the most difficult concepts to appreciate quantitatively is the increase in energy transferred and energy absorbed because photons produced in the interactions (primarily in Compton scattering and annihilation radiation) also interact. It is easy to accept the idea that these subsequent photons interact, yet to have no intuitive sense for the magnitude of the effect, or of how many of the secondary photons travel upstream, or of the energies at which subsequent photon interactions are important. Since it is impossible to develop an analytic expression for subsequent interactions, students (and faculty, myself included) usually ignore them. Nevertheless, secondary photons can double the entrance dose at some energies and increase the dose deep in the tissue by factors of up to 100. MacDose provides an option to include subsequent interactions of

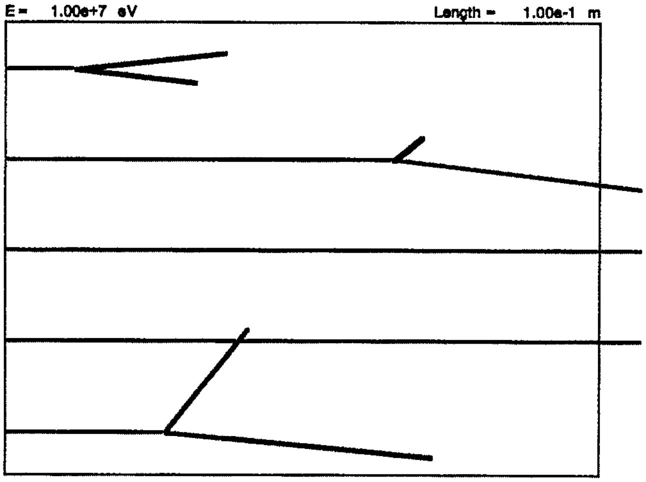

FIG. 2. The Simulation window with 10-MeV photons, showing pair production, Compton scattering, and no interaction.

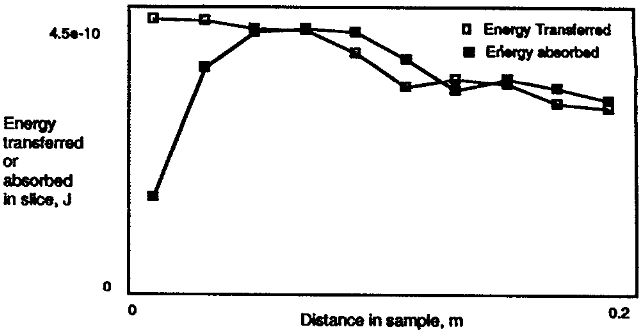

FIG. 3. Graph of Energy Transferred and Energy Absorbed versus depth for 10 MeV photons in a 20-cm-thick sample.

the Compton-scattered and annihilation radiation photons. Because all photon interactions have been rotated into the plane of the display, both for ease of viewing and to speed up the simulation, the energy transferred and absorbed by the secondary photons is only approximate. However, the importance of the effect is shown clearly. Figure 4 shows a simulation of four 100-keV photons ignoring and including subsequent interactions. Figure 5 shows electron tracks only, for 25 primary photons of 100 keV. Figure 6 plots energy transferred to electrons by all radiation and by primary radiation for 100-keV photons. The line marked "calculated" is from the standard relationship $\Psi_0 e^{-\mu x}(\mu_{\rm tr}/\rho)$.[5]

The "skin-sparing" effects of high-energy photons are striking. Figure 7 shows the electron track distribution for 250 photons of energy 100 keV, 1.25 MeV, and 8 MeV. Subsequent interactions are included.

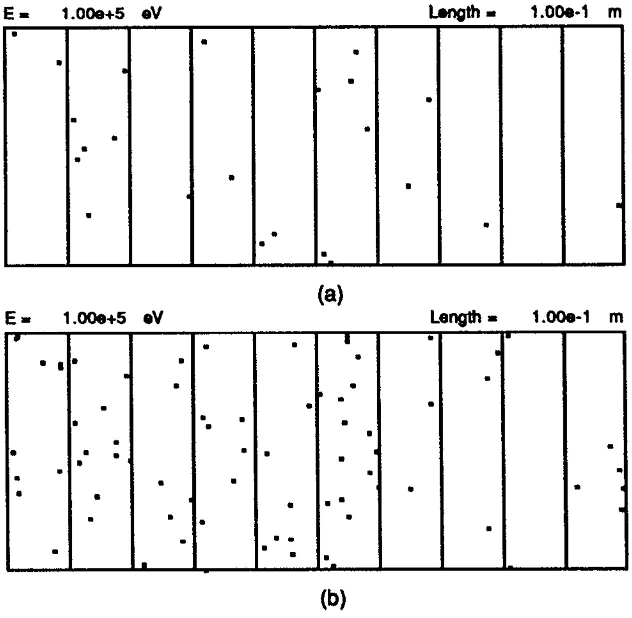

FIG. 5. Only electron tracks are shown resulting from the interaction of 25 100-keV photons. (a) Primary interactions only; (b) subsequent interactions are included.

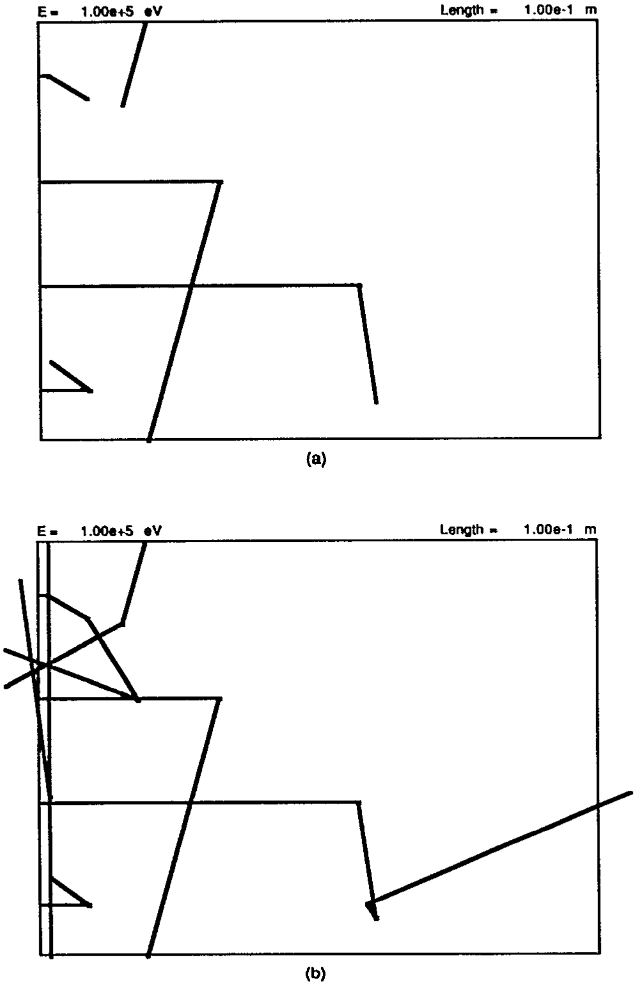

FIG. 4. Four 100-keV photons are shown (a) without and (b) with subsequent interactions.

II. THE SIMULATION

The simulation of each photon is initiated by a call to procedure `SinglePhoton`, which calls the appropriate procedures and functions shown in Table II. A procedure calls those indented below it.

Many procedures rely on a series of pseudorandom numbers r, uniformly distributed on the interval (0,1), which are obtained by transformation from the `Random` function in the Macintosh Toolbox.

To determine how far the photon travels before interacting, `RandExpDecay` uses the fact that $f = e^{-\mu x}$ is the fraction surviving at distance x, so $x = -\ln(r)/\mu$. The relative probabilities of photoelectric effect, Compton scattering, and pair production are $p_{\rm Comp} + p_{\rm pp} + p_{\rm pe} = 1$. Procedure `WhichDecay` selects another random number r. If $r < p_{\rm Comp}$, it is Compton scattering; if $p_{\rm Comp} \leqslant r < (p_{\rm Comp} + p_{\rm pp})$, it is pair production; otherwise, it is photoelectric effect. The probabilities as a function of energy are calculated using the Klein–Nishina expression

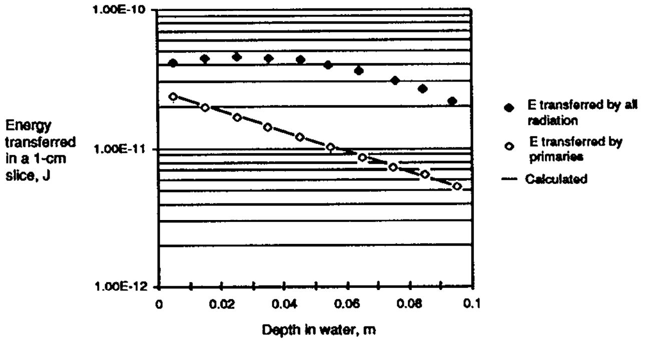

FIG. 6. Energy transferred to electrons by all radiation and by primary radiation for 100-keV photons. The line marked "calculated" is from $\Psi_0 e^{-\mu x}(\mu_{\rm tr}/\rho)$.

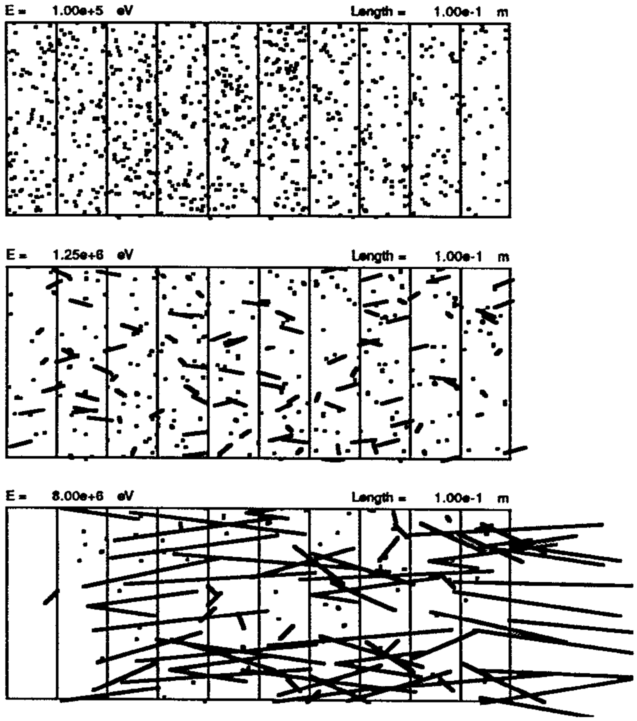

FIG. 7. The electron track distribution for 250 photons of energy 100 keV, 1.25 MeV, and 8 MeV. Subsequent interactions are included. The skin-sparing effect of high-energy photons is clearly observable.

TABLE II. Procedures and functions called in the simulation of each photon. Procedures call other procedures indented below them. Calls in parentheses are used only when subsequent photon interactions are being considered.

```
SinglePhoton
  RandExpDecay
  WhichDecay
  RandDirection
  Photoelectric
    Range
    DrawElectron
  ComptonScat
    WhatAngleBin
    ComptonEnergy
    RandExpDecay
    Range
    DrawElectron
    TraceRay
    (SecondaryPhoton)
  PairProduction
    TraceRay
    DrawElectron
    RandExpDecay
    Range
    (SecondaryPhoton)
SecondaryPhoton
  WhichDecay
  RandDirection
  PhotoElectric
  ComptonSec
    AngleDensity
    WhatAngleBin
    RandExpDecay
    ComptonEnergy
    DrawElectron
    TraceRay
    SecondaryPhoton
  SecPair
    DrawElectron
    Range
    RandExpDecay
    SecondaryPhoton
    TraceRay
```

for the total Compton cross section, a piecewise quadratic approximation for pair production, and a piecewise power law approximation for the photoelectric effect.

For Compton scattering, it is necessary to determine the scattering angle. Scattering is into one of $i = 1...24$ bins of width 7.5°. When the beam energy is first set, `AngleDensity` uses the Klein–Nishina formula to calculate and store a monotonically increasing set of probabilities p_i such that

$$p_i = \frac{\int_0^{2\pi i/24} (d\sigma_{\mathrm{KN}}/d\Omega) 2\pi \sin\theta \, d\theta}{\int_0^{2\pi} (d\sigma_{\mathrm{KN}}/d\Omega) 2\pi \sin\theta \, d\theta}.$$

For each Compton interaction `WhatAngleBin` selects another random number r and assigns the bin number so that $p_{i-1} < r \leqslant p_i$. Compton scattering kinematics determine the energy of the photon and the angle and energy of the recoil electron. `RandDirection` determines whether the photon scatters to the left or to the right. The photon travels a random distance calculated by `RandExpDecay` using the correct attenuation coefficient for its energy.

Photoelectrons are emitted in the forward direction. This gives an inaccurate simulation when the photoelectron track is long enough to be seen.

For pair production, the positron is assumed to have kinetic energy T_+ distributed randomly and uniformly[6] between $0.2E$ and $0.8E$, where E is the sum of the kinetic energies of the electron and positron, $E = h\nu - 2m_e c^2$. Then, $T_- = E - T_+$.

All electrons and positrons travel in straight lines of length R_{CSDA}, where R_{CSDA} is the range calculated in the continuous–slowing–down–approximation. Although the electron paths are tortuous because of multiple scattering, R_{CSDA} is nearly the same as the projected range (maximum penetration in an absorber) for light elements.[7]

All scattering events are drawn in the plane of the display. This does not affect the energy transferred or energy absorbed by primary interactions, but it does mean that the contributions of subsequent interactions to the energy transferred and energy absorbed are only approximate.

`MacDose` is written in Macintosh Programmer's Workshop Pascal. Drawing photon and electron tracks on the screen is relatively easy because of the system routines available on the Macintosh. The sample has a size on the screen defined by a rectangle in `QuickDraw` coordinates. The end points of a photon "track" are calculated in physical coordinates, then transformed to `QuickDraw` coordinates. The length of a scattered (or annihilation radiation) photon track is determined by another call to `RandExpDecay`. Procedure `TraceRay` draws the track. If the track leaves through the top or bottom edge of the rectangle, it is made to re-enter at the other edge and continue its path. Instances of this are seen in Fig. 4. Thus the sample and beam are effectively infinite in extent perpendicular to the incident beam.

Procedure `DrawElectron` calls `TraceRay` to draw electron or positron tracks. It also calls `CalcSlices`, which considers the sample to be divided into ten slices and keeps track of the energy transferred to electrons and the energy absorbed in each slice. Separate functions based on empirical approximations are used to determine R_{CSDA} from the electron or positron kinetic energy and to calculate the remaining kinetic energy from the residual range.

When subsequent photon interactions are to be considered, it is necessary to call `SecondaryPhoton` for each Compton-scattered photon or annihilation–radiation photon. Angles of emergence of additional photons or electrons are determined with respect to the direction of the original photon. Rotating all scatterings into the plane of view introduces errors in the calculated values of energy transferred and energy absorbed due to subsequent photons. Before a secondary chain is followed, the current random number seed is saved. At the end of the secondary chain, it is restored to its original value. Thus, if simulations with and without subsequent photons are compared and each simulation started with the same seed, the pattern of primary interactions is identical (Fig. 4). This feature is crucial to showing students the effect of subsequent interactions.

All floating point calculations are done using the standard Apple numeric environment (SANE). Using the special 32-bit fixed-point types Fixed and Fract (Ref. 8) designed for rapid graphics calculations might give faster simulations, but I have not tried them.

III. CONCLUSION

Personal computers are now fast enough so that relatively complex simulations can be done in real time. This makes it possible to consider using such simulations for teaching purposes. `MacDose` has been presented as an example. Future extensions of `MacDose` should include a plane interface between two different media, since secondary photon interactions perturb the dose near the boundary. Electron trajectories should be made more realistic, and more accurate three-dimensional calculations should be done when subsequent interactions are included.

REFERENCES

1. `MacDose` with the exercises and an Instructor's Guide is distributed at a nominal cost by Medical Physics Publishing Corp., Room B27, 1300 University Ave., Madison, WI 53706.
2. I would like to acknowledge the assistance of the Microcomputer Group at the University of Minnesota.
3. Apple Programmers Development Association, 20525 Mariani Ave., Mail Stop 33G, Cupertino, CA 95014-6299.
4. More rigorous definitions are found in many places, such as F. H. Attix, *Introduction to Radiological Physics and Radiation Dosimetry* (Wiley, New York, 1986).
5. Attix, *op. cit.*, p. 22.
6. This is a rectangular approximation to the actual energy distribution, which can be found in Attix, *op. cit.*, p. 149.
7. Attix, *op. cit.*, pp. 184–185.
8. *Inside Macintosh* (Addison-Wesley, Reading, MA), IV-63.