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CEPXS/ONELD Version 2.0: A Discrete Ordinates Code Package for General One-Dimensional Coupled Electron-Photon Transport

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ABSTRACT

CEPXS/ONELD is the only discrete ordinates code capable of modelling the fully-coupled electron-photon cascade at high energies. Quantities that are related to the particle flux such as dose and charge deposition can readily be obtained. This deterministic code is much faster than comparable Monte Carlo codes. The unique adjoint transport capability of CEPXS/ONELD also enables response functions to be readily calculated. Version 2.0 of the CEPXS/ONELD code package has been designed to allow users who are not expert in discrete ordinates methods to fully exploit the code's capabilities.

I. INTRODUCTION

CEPXS/ONELD is a code package that solves the one-dimensional transport equation for the coupled electron-photon cascade at high energies (greater than one keV.) Accurate description of this cascade is important in areas as diverse as the "hardening" of electronics that are exposed to nuclear and space radiation environments and in radiation therapy for cancer. In the ONELD code, the transport equation is solved by a finite-differencing method called discrete ordinates[1]. While this method has a long history in neutral particle transport[2], the discrete ordinates approach has only recently been applied to electron transport.[3-6] The most extensively used method for electron transport remains Monte Carlo. The Monte Carlo method can readily model the most complex three-dimensional configurations. However, it can require large amounts of computer CPU time. The main advantage of discrete ordinates codes is that they are usually less expensive to run on a computer.

The CEPXS/ONELD code package consists of four codes: the multigroup cross section generating code, CEPXS; the preprocessor code, PRE1D; the discrete ordinates transport code, ONELD; and the postprocessor code, POST1D. PRE1D creates the input for the discrete ordinates code and POST1D assembles the output that is desired by the user.

A number of significant new capabilities are included in Version 2.0 of CEPXS/ONELD that were absent in Version 1.0.[7-9] The most significant enhancement is that the finite differencing schemes that are associated with the discrete ordinates method are automatically selected by the code. Thus users who are not familiar with discrete ordinates techniques can correctly use the code. In this latest version of CEPXS/ONELD, adjoint or

inverse transport calculations, kerma predictions, and transport in one-dimensional spherical and cylindrical geometries are allowed. Version 2.0 will be released to the user community early in calendar year 1992.

II. DISCRETE ORDINATES vs. MONTE CARLO

The main advantage that the discrete ordinates method has over Monte Carlo is that precise solutions are possible for much less computational cost. Precision or relative accuracy is important when the difference between quantities that are close in magnitude must be determined. For instance, a charge deposition profile for a photon source is difficult to calculate because of such cancellation effects. Monte Carlo precision can be improved by either increasing the number of particle histories or by implementing problem-dependent biasing schemes. However, computational cost scales with the number of histories; and biasing, while more efficient, usually requires considerable expertise and extensive code modifications.

The main disadvantage of discrete ordinates codes is that, while the relative accuracy of the predictions can be high, absolute accuracy is dependent on the finite-differencing approximations used. A discrete ordinates solution will converge to the proper solution of the transport equation as the spatial, energy, and angular approximations are refined. In discrete ordinates codes, the flux is obtained on a spatial domain that is divided into meshes, an energy domain that is divided into groups, and an angular domain that is represented by a few discrete directions or characteristics. Convergence can always be obtained by using more groups, discrete directions, and spatial meshes. However, like increasing the number of particle histories in Monte Carlo, such refinements also increase computational cost. Ideally, the finite-differencing approximations should be tailored to the specific problem in order to optimize efficiency. For instance, in some calculations, the spatial mesh need only be refined at material discontinuities. But, like biasing in Monte Carlo, the knowledge required to tailor these approximations is usually available only to the expert.

In order to make the discrete ordinates method truly accessible to the non-expert for coupled electron-photon transport, CEPXS/ONELD Version 2.0 was designed to automatically select the group structure, spatial mesh, and angular characteristics that are needed to produce converged solutions. This is done on the basis of the type of source and the geometry. In this paper, the method that CEPXS/ONELD uses to select problem-specific finite-differencing schemes is not described.

The continuous-energy Monte Carlo codes[10-12] that are available for electron transport are not capable of adjoint or inverse transport. While a single forward transport prediction permits a variety of quantities and distributions to be found for a single source, a single adjoint prediction allows a single quantity to be calculated for a variety of sources. A quantity is defined as some moment of a distribution. For instance, the dose in a layer is a quantity that is obtained from a dose profile distribution. An adjoint calculation yields response functions from which

a specific quantity can be calculated for sources with arbitrary energy and angular distributions.

Discrete ordinates and Monte Carlo codes also differ in their requirements for computer resources. While discrete ordinates codes usually require much less CPU time than Monte Carlo codes, they can demand much more computer memory to store the finite-differenced form of the transport equation. At Sandia, CEPXS/ONELD is run on either a virtual memory machine such as a VAX 8600 or on machines with large disk memory such as the CRAY YMP or the IBM RISC/6000 Workstation, Model 550.

III. CALCULATIONS

In this section, we present examples of calculations performed with CEPXS/ONELD Version 2.0 that demonstrate the capabilities of this latest version. In the first example, the dose profile is predicted for ^{60}Co gamma-rays incident on a slab of lithium fluoride followed by a slab of lead. For this demonstration, the gamma-ray source is modelled as a mono-energetic photon beam (1.33 MeV) that is normally incident on the first slab of LiF.

In Figure 1, the dose profile obtained with CEPXS/ONELD is compared to the dose profile produced by the Monte Carlo code, TIGERP.[10,13] The predictions assume a unit number fluence of photons. A million particle histories were used in the Monte Carlo calculation in order to evaluate the dose profile to within 2% statistical error. In this calculation, only the biasing schemes that are available without code modification (such as electron trapping[13]) were used.

In this example, the spatial, energy, and angular grids were automatically selected by CEPXS/ONELD. It chose a variable spatial mesh with 63 meshes, variable energy group structures for both electrons and photons (68 groups for each particle species), and sixteen angular characteristics. In Figure 1, the dose at the center of each spatial mesh is plotted. Note that the spatial mesh is refined in the vicinity of material discontinuities. While the profiles that are obtained with the two codes are similar, the computational efforts involved are not. The combined cost of running both CEPXS and ONELD on the CRAY YMP/416 at Sandia is about 85 seconds of CPU time. The Monte Carlo prediction required about 2880 seconds of CPU time on the same machine.

The CEPXS/ONELD code can also predict both the collisional kerma profile and the dose profile in the same calculation. Collisional kerma[14] represents the dose if secondary electrons deposit locally the energy that they would lose in collisional interactions. The energy that these electrons would lose in radiative interactions is assumed to entirely escape. The collisional kerma and dose profiles for the Lif/Pb slab problem are shown in Figure 2. Note that these profiles are in close agreement away from the material discontinuities.

In the second example, CEPXS/ONELD is used in adjoint mode to predict the dose response function per unit number fluence that is deposited in a calcium fluoride thermoluminescent dosimeter (TLD) for normally-incident

photons (Figure 3.) In the one-dimensional calculation, the TLD is modelled as a slab of CaF, surrounded by slabs of aluminum. In this example, CEPXS/ONELD automatically selected 86 variable energy groups for both electrons and photons, a variable spatial mesh composed of 60 meshes, and sixteen angular characteristics. Hence the adjoint response function contains dose information for mono-energetic photons with 86 different energies. Monte Carlo predictions with the TIGER[10] code are also shown for comparison at three different energies.

In this adjoint calculation, pair production was allowed, but positrons were treated as electrons. Under this approximation, dose predictions are approximately correct but charge deposition predictions are distorted. However, the user can request that CEPXS/ONELD treat positrons as particles that are distinct from electrons. This doubles the cost of running the ONELD code.

The adjoint calculation actually yields more dose information than is shown in Figure 3. The entire set of response functions that are calculated by CEPXS/ONELD in adjoint mode are shown in Figure 4. These response functions represent the dose that would be deposited by gamma-rays that are incident at more oblique angles, per unit number fluence. With this set of response functions, the TLD dose can be calculated for any gamma-ray source.

In the final example, CEPXS/ONELD is used for electron-photon transport in one-dimensional spherical geometry. In Figure 5, the dose profiles that are predicted by both CEPXS/ONELD and the three-dimensional Monte Carlo code, ACCEPT[10,13], are shown for the case in which a plane-wave of mono-energetic electrons is incident on an aluminum sphere. A unit number fluence of electrons is assumed. The dose profiles represent the dose per unit electron fluence that is deposited in a spherical shell of aluminum at the specified radius.

CONCLUSIONS

The CEPXS/ONELD Version 2.0 code package offers a versatile and easy-to-use tool for calculating the high-energy electron-photon cascade in one-dimensional geometries. Since defaults exist for the finite-differencing approximations, the user is not required to be an expert in discrete ordinates techniques. Version 2.0 of CEPXS/ONELD allows users to easily perform adjoint or inverse transport calculations. These predictions are useful for parameter studies in which a quantity such as the dose in a layer must be determined for a variety of sources. Kerma predictions and calculations in curvilinear geometries can also be obtained.

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FIGURES

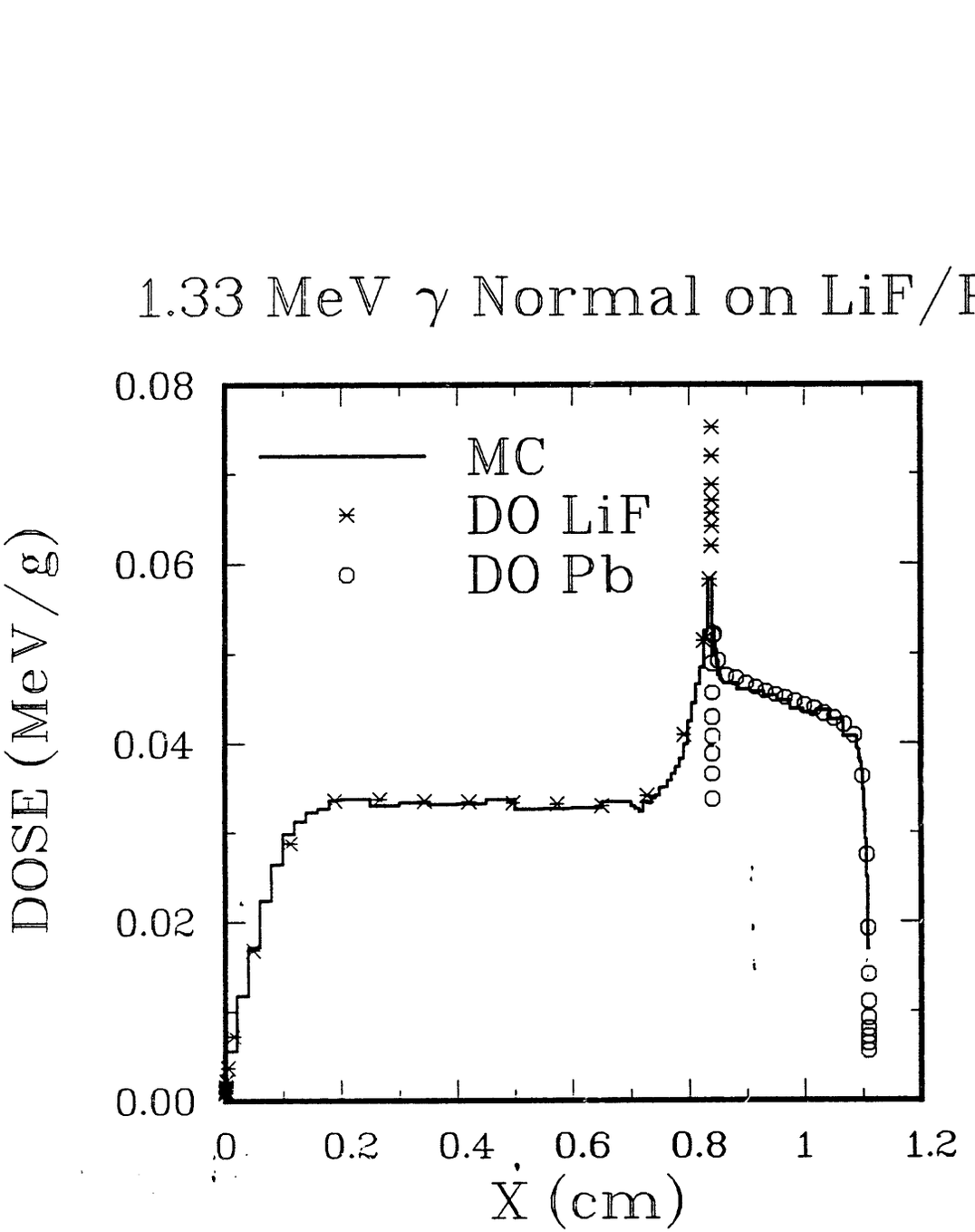
1. Dose profile in .84-cm thick slab of LiF followed by a .27-cm thick slab of lead for 1.33 MeV normally-incident gamma-rays. Predictions are obtained with TIGERP (MC) and CEPXS/ONELD (DO). Fluence is one photon/cm^2.

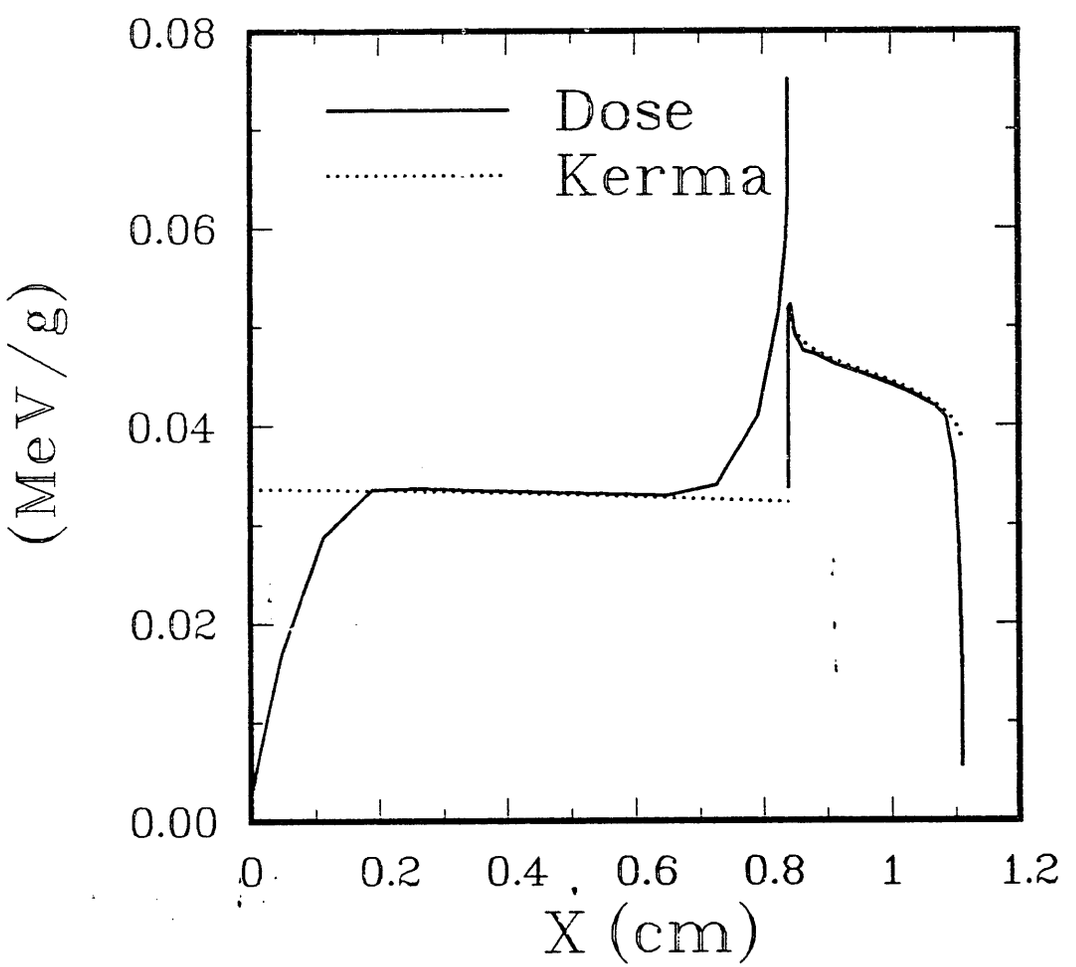
2. Dose and kerma profile calculated by CEPXS/ONELD in a .84-cm thick slab of LiF followed by a .27-cm thick slab of lead. Fluence is one photon/cm^2.

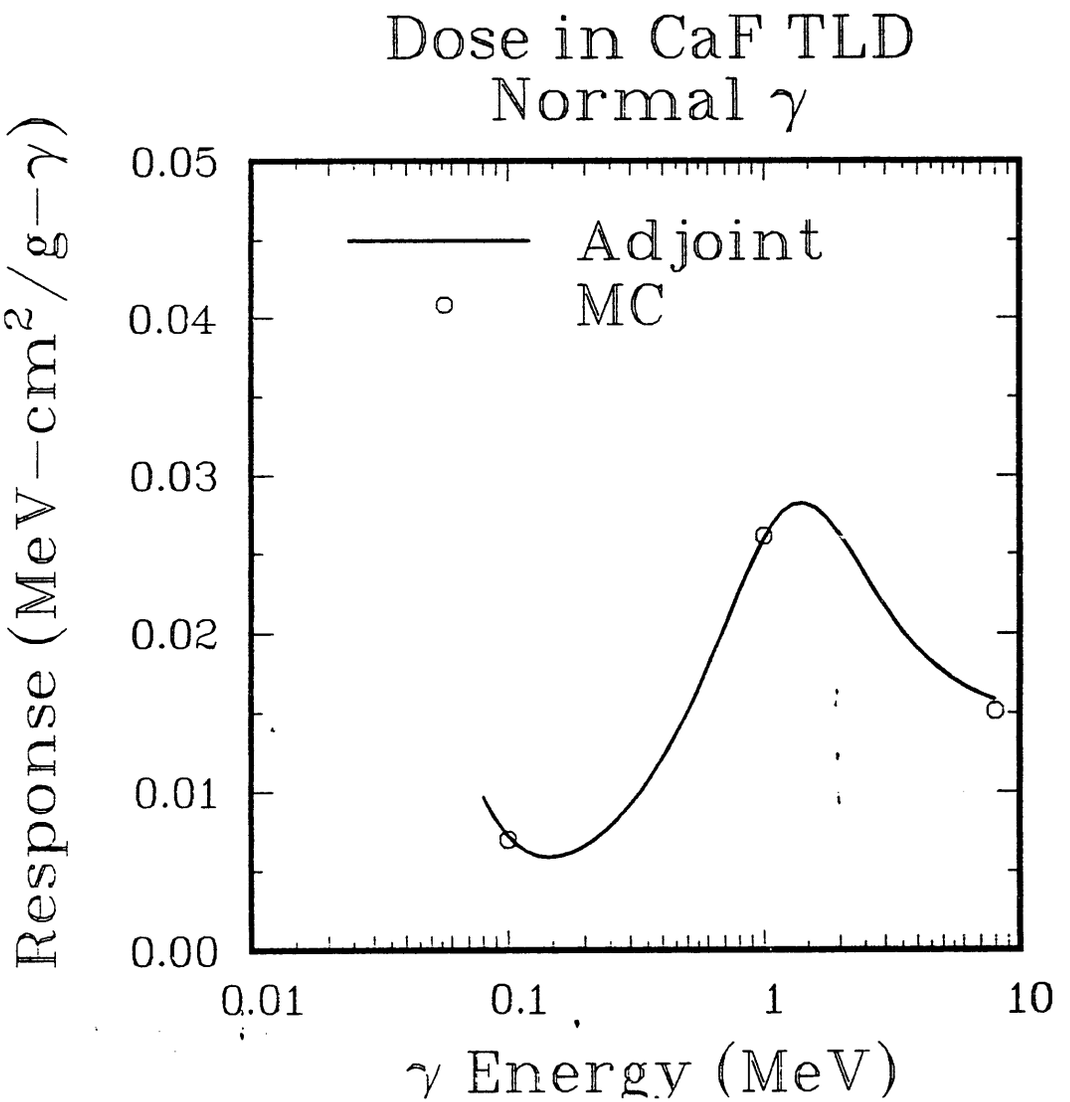
3. The dose response function that is calculated by CEPXS/ONELD in adjoint mode for normally-incident gamma-rays of mono-energetic energy from 8.0 MeV to .08 MeV that are normally incident on a CaF TLD. The TLD is represented as a .0899-cm thick layer of CaF surrounded by .0363-cm thick layers of aluminum. Monte Carlo calculations (MC) with TIGERP are shown at three energies (8.0, 1.0, and .1 MeV.)

4. The entire set of dose response function that are calculated by CEPXS/ONELD in adjoint mode for mono-energetic gamma-rays that are incident on a slab representation of a CaF TLD. The response functions correspond (in order of increasing magnitude) to gamma-rays that are incident at 8^{o} (near normal), 19°, 30°, 41°, 52°, 63°, 74°, 85°, and 96°.

5. The dose profile calculated by CEPXS/ONELD (DO) and ACCEPT (MC) for a plane-wave of 1.0 MeV electrons incident on an aluminum sphere of radius .2107 cm. Fluence is one electron/cm^2.


1.33 MeV γ Normal on LiF/Pb
MC
DO LiF
DO Pb
DOSE (MeV/g)
0.08
0.06
0.04
0.02
0.00
0
0.2
0.4
0.6
0.8
1
1.2
X (cm)


1.33 MeV γ Normal on LiF/Pb
Dose
Kerma
0.08
0.06
0.04
0.02
0.00
(MeV/g)
0
0.2
0.4
0.6
0.8
1
1.2
X (cm)


Dose in CaF TLD
Normal γ
Adjoint
MC
Response (MeV−cm²/g−γ)
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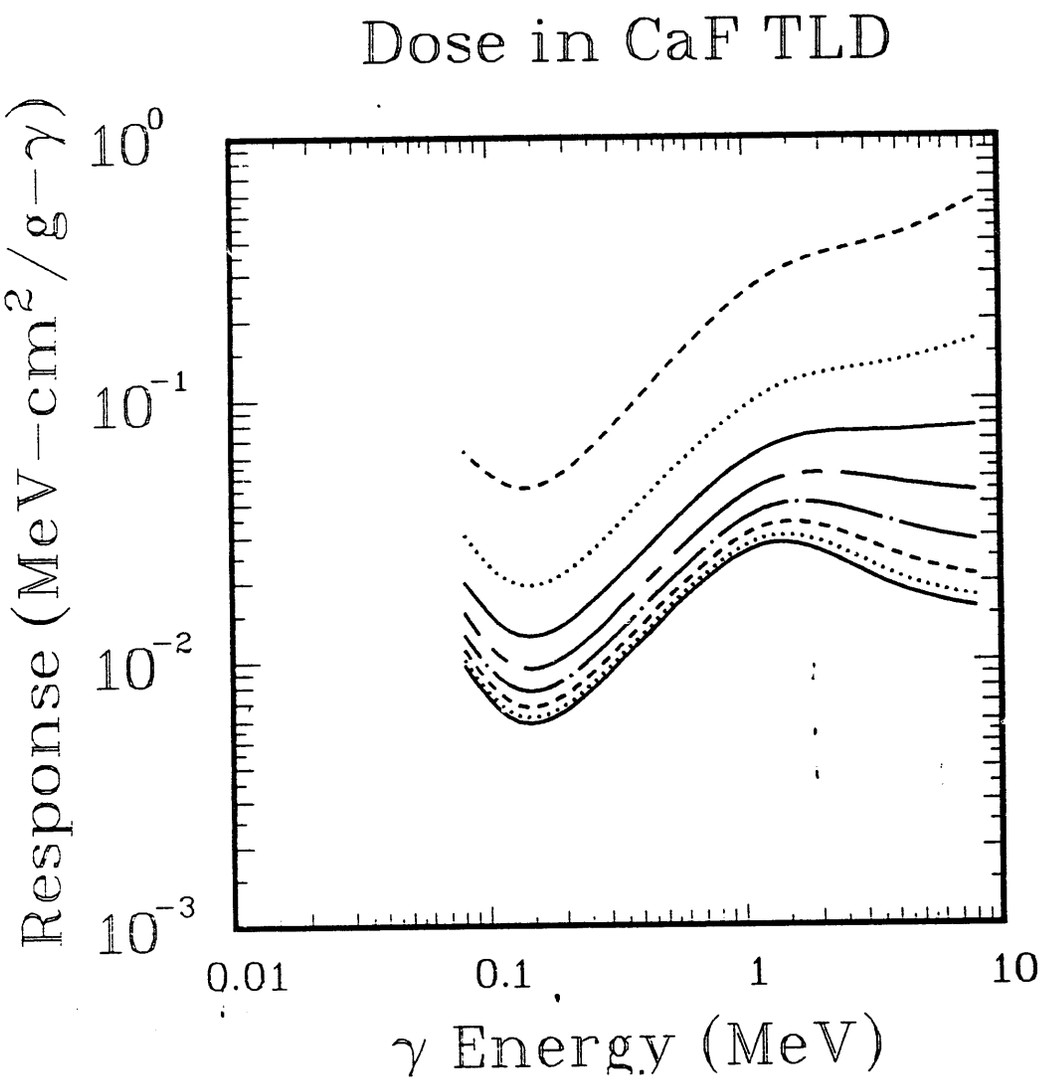
0.04
0.03
0.02
0.01
0.00
0.01
0.1
1
10
γ Energy (MeV)


Dose in CaF TLD
Response (MeV−cm²/g−γ)
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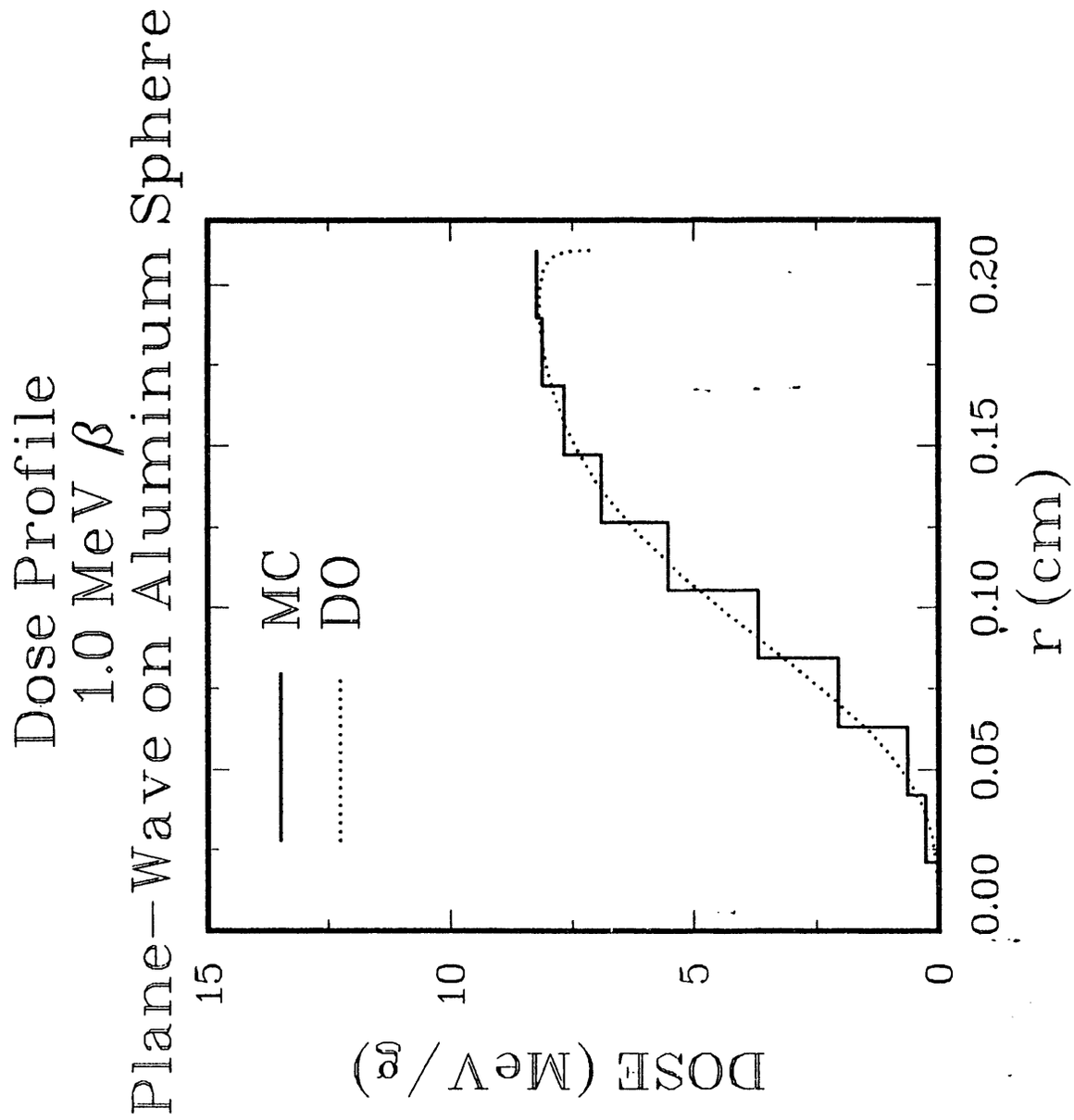
10⁻¹
10⁻²
10⁻³
0.01
0.1
1
10
γ Energy (MeV)

DISCLAIMER



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