LA-UR · 95-2068

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TITLE: MULTIGROUP BOLTZMANN FOKKER PLANCK ELECTRON-PHOTON TRANSPORT CAPABILITY IN MCNP[TM1]

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SUBMITTED TO: ANS Winter Meeting, San Francisco, CA, 10/30 - 11/2/95

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FORM NO. 836 R4
ST. NO. 2629 5/81

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CONF-951006--19

Multigroup Boltzmann Fokker Planck Electron-Photon Transport Capability in MCNP[TM1].

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Introduction

The MCNP code system has a robust multigroup transport capability which includes a multigroup Boltzmann-Fokker-Planck (MGBFP) transport algorithm to perform coupled electron-photon or other coupled charged and neutral particle transport in either a forward or adjoint mode. This paper will discuss this capability and compare code results with other transport codes.

Description of the MGBFP capability in MCNP

The multi-group formalism for performing charged particle transport was pioneered by Morel and Lorence[2] for use in deterministic transport codes such as ONEDANT. With a first order treatment for the continuous slowing down approximation (CSDA) operator, this formalism is equally applicable to a standard Monte Carlo multigroup transport code as discussed by Sloan[3]. Unfortunately, a first order treatment is not adequate for many applications. Morel, et. al.[4], have addressed this difficulty by developing a hybrid multigroup/continuous energy algorithm for charged particle which retains the standard multigroup treatment for large angle scattering, but

1.MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory

exactly treats the CSDA operator. As is the case with standard multigroup algorithms, adjoint calculations are readily performed with the hybrid scheme. This algorithm has been implemented in the MCNP code system.

The process for performing a MCNP/MGBFP calculation involves executing three codes. First the multigroup cross section generating code is exercised. For coupled electron-photon multigroup cross sections the CEPXS[2] code was used. Next these need to be cast into a suitable form for use in the MCNP code which is done with the CRSRD[5] code (a general purpose multigroup cross section translation code available to XTM sponsors). Here CRSRD adjusts the discrete ordinate moments into a Radau quadrature form that can be used by a Monte Carlo code. CRSRD also generates a set of multigroup response functions for dose or charge deposition which can be used for response estimates for a forward calculation or sources in an adjoint calculation. Finally, the MCNP code is executed using these adjusted multigroup cross sections.

Results

Forward Calculations

We present two cases using the MGBFP option of the MCNP code. The first is a bremsstrahlung converter or radiation machine head configuration. This calculation has a mono-energetic 10 MeV pencil beam of electrons normally incident on slabs of either aluminum (Al) or tungsten (W) a fifth of an electron range thick. Figure 1 shows the electron and photon transmitted and

reflected spectra. The MGBFP results are compared with the continuous energy Monte Carlo code ITS-TIGER[6] since they utilize the same electron/photon interaction database. Figure 2 shows the fractional difference in energy deposition in the slabs. In both figures the agreement between the two calculational methodologies is usually within 10% which is quite good. The slight deviation in photon spectrum below 1 MeV is due to a statistical artifact since an independent calculation for 1 MeV electron source gave similarly good agreement.

Another stressing problem for the MGBFP methodology is the calculation of the dose enhancement or unequilibrium dose at dissimilar material interfaces where the absorbed energy will differ from the equilibrium value, by as much as a factor of ten or twenty. The ability of the code to accurately calculate that is a litmus test for the methodology. Moreover, this problem was chosen to have a photon source to demonstrate that the methodology could equally well be used for either electron or photon sources. The problem has a 100 keV pencil photon beam normally incident on a 2.54×10^{-3} cm (1 mil) slab of gold abutting a 1 mil slab of silicon where the dose is tallied in zones 0.5 microns thick. Figure 3 shows the comparison of the MCPN/ MGBFP calculation and TIGERP and CEPXS/ONELD. Once again the agreement between the methodologies is usually within 10% which is good.

Adjoint Calculations

One of the main reasons to use the MGBFP is the capability to perform an adjoint calculation. One of the advantages of the MCNP code system for performing an adjoint calculation is that the normalization can be naturally incorporated in the code run as standard tallies of the code[5].

This can be seen by recalculating the dose for the problem in Figure 1 by using the adjoint method. The dose estimated from the adjoint calculation is 3.268(7%) and the forward calculation is 3.063(1%). The forward and adjoint calculations are within 10% of each other and within the statistical error bounds.

Conclusions

The MGBFP methodology for performing charged particle transport with MCNP has been presented and been validated with independent calculation for simple 1D geometries. The results of forward and adjoint Monte Carlo calculations show the broad range of applicability of this methodology. Furthermore the MCNP/MGBFP calculation shows no signs of degrading computational performance and may actually greatly improve it for certain applications.

Future work includes addition of other charged particle species such as protons or other heavy ions. Application of the methodology to more complex geometries and utilization of the adjoint capability for estimating dose or importances in CT voxel descriptions of radiation treatment patients.

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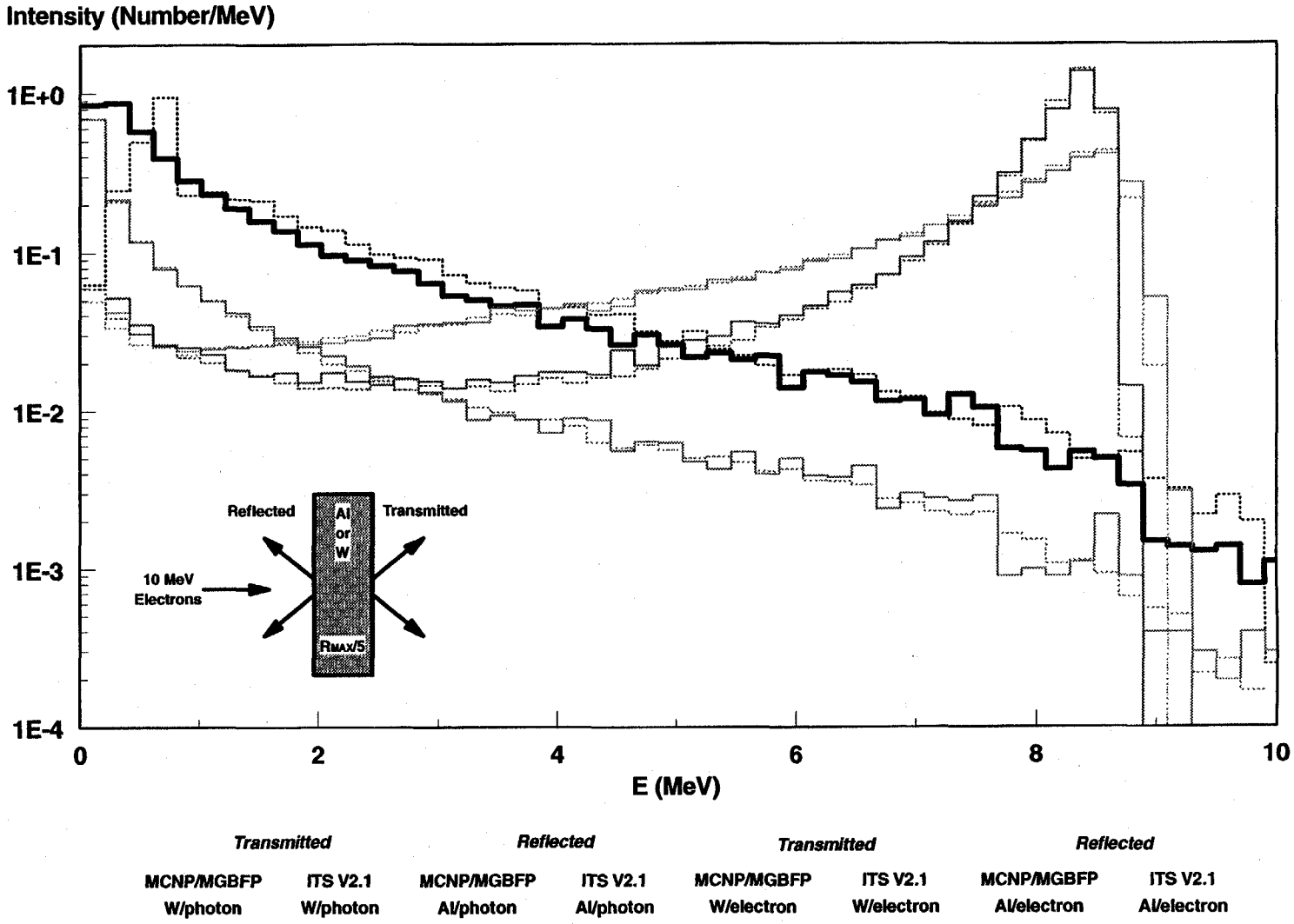

Figure 1: Reflected and transmitted electron and photon spectra generated by 10 MeV electrons incident on slabs of tungsten and aluminum

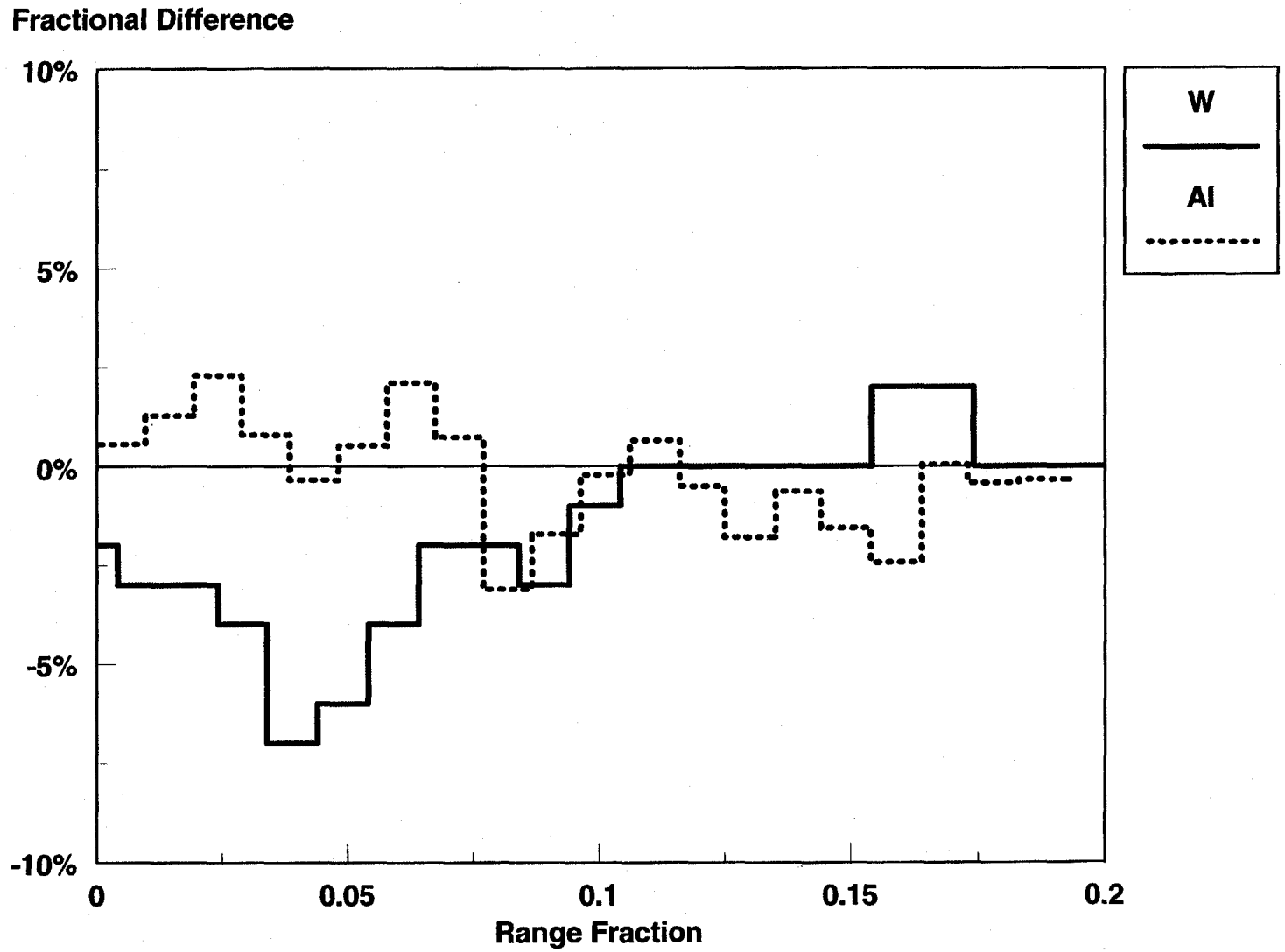

Figure 2: Fractional difference in dose calculation for MCNP/MGBFP and ITS normali[illegible]o ITS results for 10 MeV electrons incident on slabs of tungsten and aluminum

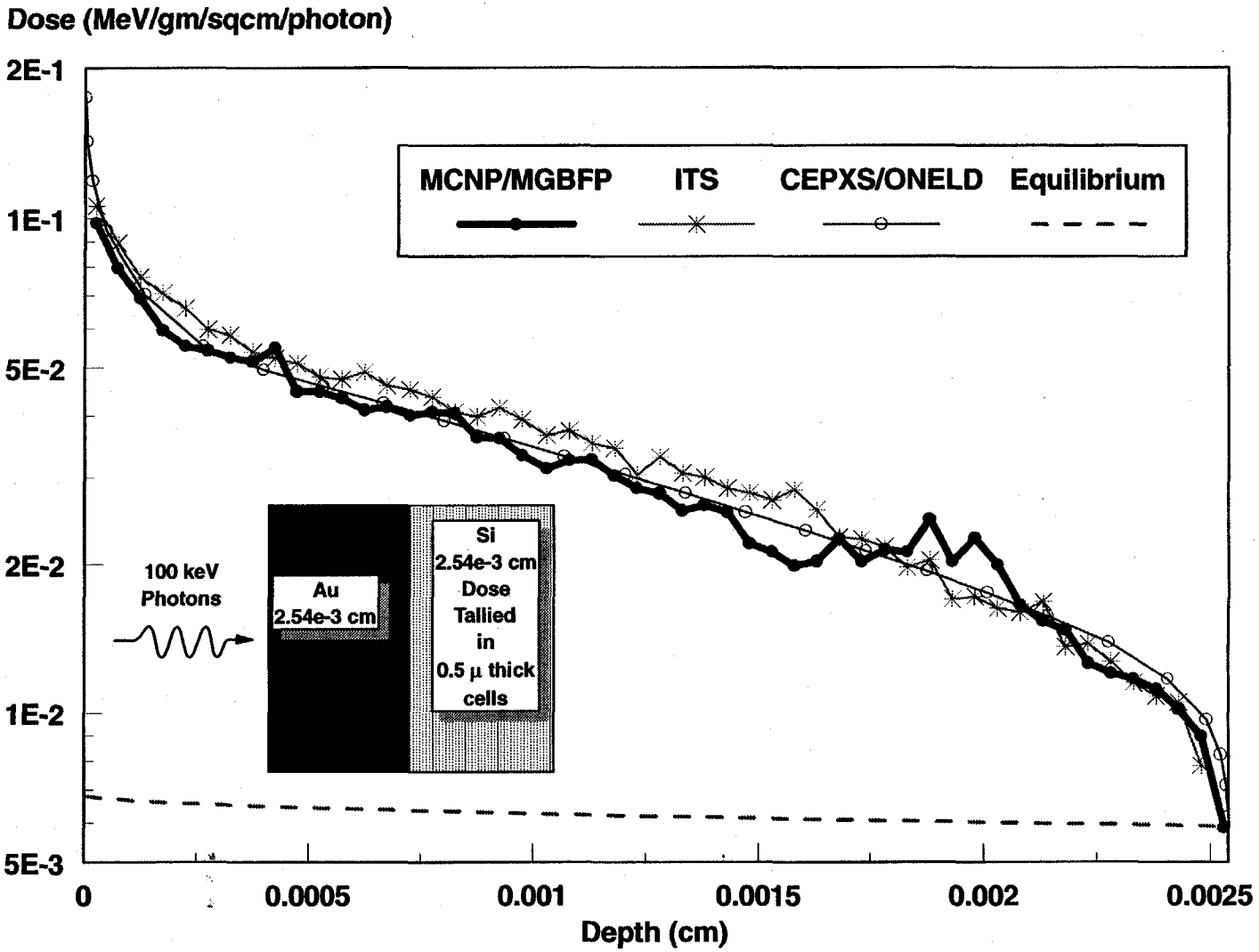

Figure 3: Dose deposited in 1 mil of Si generated from 100 keV photons incident on 1 mil Au abutting the Si. The Si was zoned into 0.5 micron cells to tally the energy deposited.