ITS: The Integrated TIGER Series of Electron/Photon Transport Codes - Version 3.0

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Abstract

The ITS system is a powerful and user-friendly software package permitting state-of-the-art Monte Carlo solution of linear time-independent coupled electron/photon radiation transport problems, with or without the presence of macroscopic electric and magnetic fields of arbitrary spatial dependence. Version 3.0 is a major upgrade of the system with important improvements in the physical model, variance reduction, I/O, and user friendliness. Improvements to the cross-section generator include the replacement of Born-approximation bremsstrahlung cross sections with the results of numerical phase-shift calculations, the addition of coherent scattering and binding effects in incoherent scattering, an upgrade of collisional and radiative stopping powers, and a complete rewrite to Fortran 77 standards emphasizing Block-IF structure. Improvements in the Monte Carlo codes include significant variance reduction from reorganized logic for electron trapping and Russian Roulette, angular dependent output of particle fluxes, explicit line radiation in flux and escape outputs, an option for photon transport only, more accurate sampling of collision loss straggling, extended implementation of full automatic subzoning, increased error checking, and extensive improvements in code clarity and maintainability.

I. INTRODUCTION

The ITS system is a system of general-purpose time-independent, multimaterial, multidimensional coupled electron/photon Monte Carlo transport codes that combine collisional transport with transport in externally applied macroscopic electric and magnetic fields over the energy range from 1 GeV down to 1 keV. In the six years since the release of Version 1.0 [1-4], our experience, as well as feedback from a worldwide user community, has suggested a number of improvements to the system. Version 3.0 is the first major upgrade of ITS and represents a systematic effort at a more comprehensive implementation of these improvements [5].

Figure 1 is a brief description of the physical model employed in Version 3.0. The only completely new physical process that has been added is the coherent scattering of photons. It is clear that a model that includes these phenomena constitutes a very sophisticated description of the generation and transport of the electron/photon cascade.

PHYSICAL MODEL

- Production and Transport of $e^+/e^-/\gamma$ Cascade
  - (a) Electron/Positron Interactions
    - Energy loss straggling
    - Elastic scattering
    - Production of knock-on electrons
    - Impact ionization followed by production of fluorescence photons and/or Auger electrons
    - Bremsstrahlung production
    - Production of annihilation radiation
  - (b) Photon Interactions
    - Photoelectric absorption with the production of photoelectrons, Auger electrons, and fluorescence photons
    - Incoherent scattering with the production of scattered electrons
    - Coherent scattering
    - Pair production
- Transport in Macroscopic Electric (voids) and Magnetic Fields of Arbitrary Spatial Dependence

Fig. 1 Physical model of ITS, Version 3.0

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Figure 2 shows the member codes of the system. The TIGER, CYLTRAN, and ACCEPT codes are the standard codes of the system in one, two/three, and three dimensions, respectively. The P codes (TIGERP, CYLTRANP, and ACCEPTP) are the versions of the codes that include the more detailed ionization/relaxation model that was originally taken from the SANDYL code [6]. Finally, the M codes (CYLTRANM and ACCEPTM) are the versions of the codes that combine collisional transport with transport in macroscopic electric and magnetic fields [7].

Features / Geometry	Standard Codes	P Codes Enhanced Ionization/Relaxation	M Codes Macroscopic Fields
1-D	TIGER	TIGERP	
2-D/3-D	CYLTRAN	CYLTRANP	CYLTRANM
3-D	ACCEPT	ACCEPTP	ACCEPTM

Fig. 2 Member codes of ITS

The objectives of the 3.0 project were to improve upon similar objectives of the original system: (1) to improve the accuracy of the physical model, (2) to improve the efficiency of the Monte Carlo simulations, (3) to expand and improve upon the I/O capability, and (4) to generally make the software more user friendly. In the following sections we discuss some of the modifications vis-a-vis the original system (Version 1.0) directed toward achieving these objectives.

II. IMPROVEMENTS IN THE PHYSICAL MODEL

We begin with a discussion of some of the more important improvements in the physical model.

There have been two major and primarily empirical improvements to the electron collision energy loss straggling. First, it was observed that the mean of the Landau straggling distribution was not sufficiently consistent with the collisional stopping power. This was corrected [8] by extending Landau's universal function to higher values of the independent variable, improving the accuracy of the tabulation and sampling of this function, and choosing a cutoff value of the independent variable that results in a mean energy loss that is consistent with the stopping power. In Fig. 3, a comparison of predictions of the energy deposition profile in water by normally incident 20.0 MeV electrons (which we believe to be near the worst case) shows that the older version of ITS underpredicted deposition ahead of the backscatter peak by just over 5%. The superiority of Version 3.0 has been indirectly verified against on-axis measurements of the energy deposition. Secondly, an improvement in the Blunck-Leisegang correction [9] to the Landau distribution leads to more accurate simulation of electron transport at lower energies and in higher-atomic-number media. The resulting improvement in the simulation of the backscatter of low-energy electrons from tantalum is demonstrated in Fig. 4.

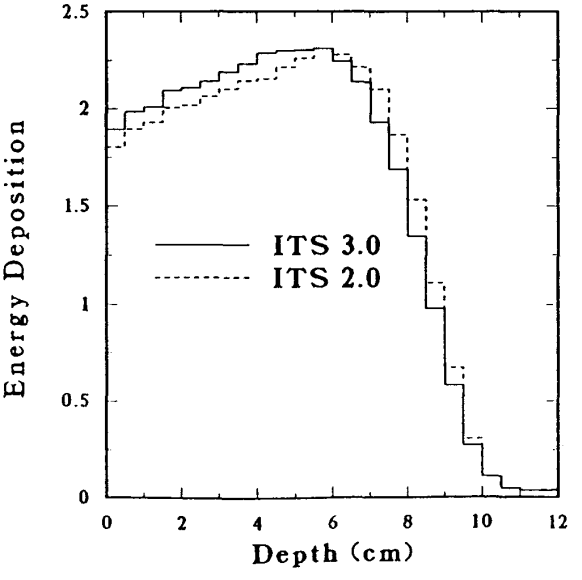

Fig. 3 Energy deposition in water by normally incident 20 MeV electrons

Below an electron energy of 2.0 MeV, the Bethe-Heitler Born-approximation-based bremsstrahlung cross sections, differential in photon energy [10], that were used in Version 1.0 were replaced by the more accurate results based on numerical phase-shift calculations for the screened

Coulomb potential [11-13]. Figure 5 demonstrates that Version 3.0 predicts harder thick-target bremsstrahlung spectra in this energy region. When these spectra are used as sources in simulations of a pulse-height-distribution measurement obtained from a Van de Graaf facility [14], it is seen in Fig. 6 that Version 3.0 provides a substantially better prediction of the continuum. The bremsstrahlung cross sections at higher energies have also been improved.

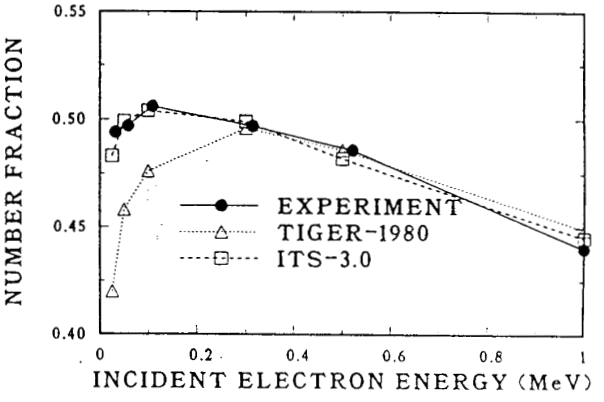

Fig 4. Backscatter of normally incident electrons from tantalum

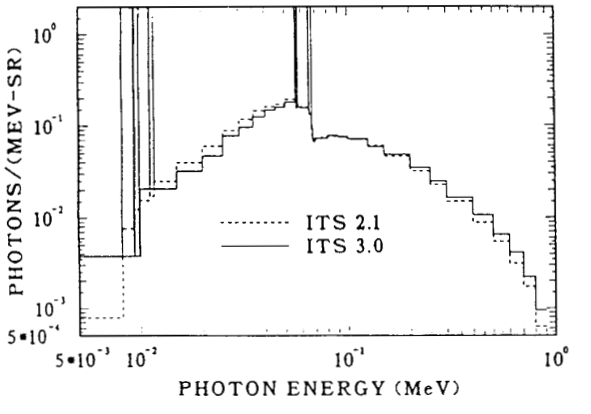

Fig 5. Forward radiation produced by 0.9-MeV electrons normally incident on 0.09 mm of tantalum

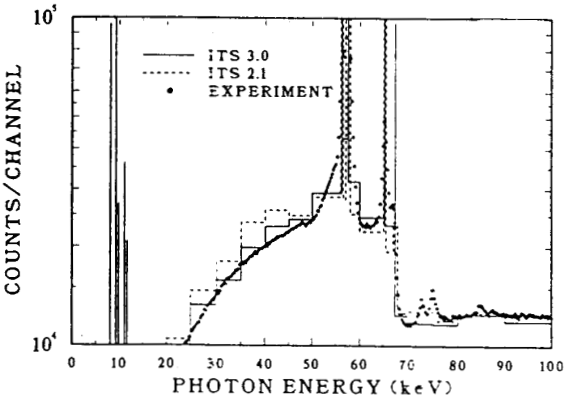

Fig 6. Comparison of the pulse-height spectrum measured with a germanium detector with those predicted using the source photon spectra from Fig 5

The latest electron collisional stopping powers from ICRU report 37 [15] were implemented in Version 3.0. These data were derived from an improved data base of mean ionization energies and an improved algorithm for calculating the density-effect correction that accounts for conductor/non-conductor differences. The stopping powers can differ by as much as a few percent from those of the original version of ITS. Also, the radiative stopping powers were made consistent with the improved bremsstrahlung cross sections.

There are two major changes to the physical model employed for photon transport [16-20]. First, coherent scattering is included for the first time in ITS. Moreover, the coherent scattering also includes binding effects. Secondly, in an incoherent scattering event, the sampled energy-angle distribution for the scattered photon now includes binding effects in contrast to previous versions which used the simpler Klein-Nishina theory. Coherent scattering is expected to be significant at low photon energies, especially for low-atomic-number media. Figure 7 shows the dependence of photon backscattering from 5 mean free paths of water on the energy of the normally incident photons, with and without the effects of these improvements to photon transport. At 10 keV, these effects increase the backscatter by about 60%. Even more striking, they increase the

transmission of scattered photons by a factor of four at the same source energy. But transmission is dominated by unscattered photons, whose number is sufficiently reduced due to the increase in the total cross section that net transmission actually increases.

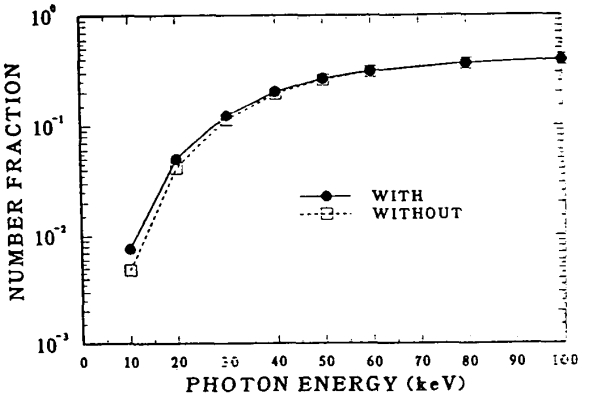

Fig 7. Photon backscatter from five mean free paths of water with and without coherent scattering and binding corrections to both coherent and incoherent scattering

III. IMPROVED VARIANCE REDUCTION

We turn now to some of the modifications that affect the Monte Carlo efficiency.

As the primary motivation for initiating the 3.0 project, we decided to permanently incorporate into the system a broadbased modification we had evolved from past experience that terminated electron histories much more efficiently. This was important because, after all, electron transport is much more expensive than photon transport. Briefly, this modification amounted to an extensive reorganization of the logic to more effectively utilize existing options for trapping electrons and for killing photon generated secondary electrons via Russian Roulette. It also eliminated a previously existing possibility for obtaining misleading results through overbiasing. With this new logic, we have achieved run-time reductions of up to 40% in our standard set of test problems.

The logical extension of the more efficient termination of electron histories is to simply ignore electron transport altogether. Consequently, in Version 3.0 we provide the user with an option for photon transport only. With these very sophisticated and fast photon Monte Carlo codes, we have achieved run time reductions up to an order of magnitude in test problems. This is a powerful option for applications involving low-energy photon sources where (1) the finite ranges of the electrons are negligible and (2) radiation by those electrons is negligible. It is especially useful where accurate simulation of line radiation transport is important.

The capability for automatic subzoning has been greatly extended in Version 3.0. Let us first briefly explain what is meant by automatic subzoning. The software must track particles through all regions bounded by material discontinuities. However, if the boundaries are not material discontinuities, but only logical boundaries of subzones of the same material that are present only to obtain spatially dependent profiles of some sort within that material, e. g., energy and charge deposition, then tracking across such boundaries is usually not necessary. In the latter case one is usually only interested in locating some point among the subzones. This is a process that requires much less memory and computation than particle tracking. Moreover, major reductions in user input can also be achieved from the implementation of this fully automatic subzoning because the user is relieved of what can be the onerous task of describing each individual subzone.

The combinatorial-geometry logic of the ACCEPT codes was taken from a local version of the MORSE code [21-22]. Over the years since the original implementation, certain inaccuracies, inconsistencies, and inefficiencies have been identified. Diagnoses of these problems were hampered by the fact that the coding was essentially uncommented. In version 3.0 these routines have been carefully revised and heavily commented. Indeed, the core analytic geometry routine was completely rewritten with the result that we now routinely achieve 10-15% reductions in run time.

Similar problems were encountered with the logic for enhanced ionization/relaxation in the P codes. This was contained within a single, very complex subroutine written in an obtuse and archaic style of Fortran with negligible commenting. In version 3.0 this routine was decomposed into a cascade of routines corresponding to each of the atomic shells

and much commenting was added. The advantages in clarity and maintainability more than compensate for the slight increase in run time.

IV. IMPROVED OUTPUT

We continue to expand upon a user-friendly system of internal error checking and diagnoses. Emphasis is first and foremost upon detection of errors at the earliest possible moment. This allows rapid termination before propagation of an error that may necessitate a lengthy debug. Secondly, once an error condition is detected, an attempt is made to provide an error message that is as informative as possible. Finally, if the error occurs while the Monte Carlo is in progress, the current history and batch numbers and the initial random number of the current history are provided. The latter permits debugging to procede by rerunning only the offending history, thus avoiding what may be a costly repetition of the entire run.

In the original version, only the spectra of the spatially dependent particle fluxes were given. In Version 3.0 this has been expanded to include the full angular distribution as well.

Perhaps the most interesting improvement, however, is the more comprehensive treatment of line radiation. Whereas line radiation in the original version was combined with the continuum photon spectra, in Version 3.0, a comprehensive and separate accounting is made of the contribution of line radiation to both photon flux and photon escape. For example, the coupled energy and angular distribution of the continuum is immediately followed by separate angular distributions for each of the lines. Annihilation radiation is given first, followed by each contributing fluorescence line identified by shell transition and transition energy.

A number of users have indicated that it would also be nice to have particle currents at internal boundaries. Although it would be difficult, and probably not cost effective to do this in general for multidimensional geometries, this default output has been added to the TIGER codes.

V. CONCLUSIONS

In this discussion we have only given the briefest descriptions of some of the more important improvements to the ITS system. There have been numerous other modifications of a lesser nature that substantially improve the overall user friendliness of the software. In particular, the Fortran has been extensively rewritten and restructured in such a way as to enhance the clarity, maintainability, and portability of the system.

VI. ACKNOWLEDGMENTS

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