

SAND2004-4782
Printed September 2004

ITS5 Theory Manual

Document Rev. 1.2

September 17, 2004
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1 Scope

This document describes the modeling of the physics (and eventually features) in the Integrated TIGER Series (ITS) codes [Franke 04] which is largely pulled from various sources in the open literature (especially [Seltzer 88], [Seltzer 91], [Lorence 89], [Halbleib 92]), although those sources often describe the ETRAN Code from which the physics engine of ITS is derived, not necessarily identical.

This is meant to be an evolving document, with more coverage and detail as time goes on. As such, entire sections are still incomplete. Presently, this document covers the continuous-energy ITS codes with more completeness on photon transport (though electron transport will not be completely ignored). In particular, this document does not cover the Multigroup code, MCODES (externally applied electromagnetic fields), or high-energy phenomena (photon pair-production). In this version, equations are largely left to the references though they may be pulled in over time.

2 General Limitations

A simulation is only as good as the underlying model. The continuous-energy ITS codes (without externally applied electromagnetic fields) is modeled after the linear, time-independent Boltzmann Equation for photons and electrons (additional assumptions on how the electrons are handled will be discussed shortly), which essentially says particles stream between collision points. The frequency and type of collisions are given in terms of cross sections which are probabilities per path length. The physics is embodied in the details of what happens at collision points, which may include how the energy and direction of the incoming particle change, whether the incoming particle is absorbed, and how many new particles emerge including details of their energies and directions.

Here, “time independence” means that neither the source nor material properties depend on time. The Boltzmann Equation is “linear” which means the particle interactions do not modify the material properties and the particles do not interact with each other.

The cross sections are based upon those of elements of neutral atoms. In particular, molecular and solid-state effects are not modeled. These effects tend to be of greater importance at lower energies. The Atomic Form Factor associated with photon coherent scattering is particularly sensitive to this (e.g. see [Poletti 02]). The sole case where ITS addresses molecular or solid-state effects (at least approximately) is the parameters for the Bethe stopping power of electrons, where alternate values are used for low-Z elements depending on whether it is used in a compound or whether it is a gas or solid [Berger 88].

The modeled cross sections tend to be rather smooth functions of energy, except for discontinuities in photon cross sections at edge energies. Real cross sections [Hubbell 99] exhibit oscillations near these edge energies, so the codes may be less accurate for mono-energetic photons near edge energies of the material they are transporting through. For the case of a spectrum of photons, such effects are believed to quickly wash out. Similarly, real electron cross sections may exhibit large oscillations for small angular deflections due to solid-state effects. This suggests transport codes such as ITS “are not intended or suitable for applications in the thin-film, plural scattering regime, where interference effects depending on the structure of the material play an important role” [Berger 88].

For 3D calculations, distances of 1nm for the non-CAD codes, or 10 nm for the CAD codes (including a CG-only simulation using an executable from the CAD codes) must be “small” compared to zone thicknesses in the modeled geometry. In tracking, when a particle is moved to a boundary, the 3D codes determine which zone is entered next by making a query at a point slightly beyond the boundary (based on these distances) in the direction of the particle.

Generally, electron transport is more approximate than photon transport. Electron transport is treated in a “Class I” [Berger 63] condensed-history approach, where the accumulated effects of scattering over a path length are treated instead of individual interactions (details are given in the sections on electron transport). Since individual scatters are not modeled along the path length, the path length should be fairly small compared to regions of interest (sometimes a third is sufficient [Jensen 88], though this will depend on the

application). From an angular-deflection perspective, this path length is the ITS “substep” (see section 4), which in principle (but not with the present implementation) can be reduced to an arbitrary size. Presently, ITS uses unstable recursion relations which translate to a fixed, small number of terms to be summed [Seltzer 88], which would be insufficient for convergence for very small path lengths. From an energy-straggling perspective, the path length is the “step” size. Also, the present implementation in ITS uses several nearest-neighbor algorithms, the effects of which should be better characterized.

3 Photon Transport

Photons move in straight lines between collision sites and are modeled as such. The frequency of collisions is determined by the total cross section of all (modeled) photon interactions. A distance to collision is sampled based on an exponential distribution. In the continuous-energy members of the ITS codes, this sampling is done mechanically assuming photon collision forcing is in effect. First, the distance to boundary of the current zone is calculated and the natural probability of an interaction along that distance to boundary is calculated. If the user had requested photon collision forcing in that zone, this natural probability would be used to modify the weight of the photon which would interact with the user’s specified probability. By default, the natural probability is used as the “forcing” probability which is mathematically equivalent to no forcing at all.

The details of what happens at a collision site are specified by the modeling of the type of collision which occurred. The relative probability of any one interaction is given by the relative size of the corresponding cross sections.

When no interaction occurs in a given zone, the photon is moved to the boundary. The next zone is determined in slightly different ways depending on the dimensionality of the member code:

- In the 3D codes (ACCEPT), a point is chosen a certain distance beyond the boundary in the direction of the photon. This distance is 1 nm for non-CAD and 10 nm for CAD (including the CG-only option in CAD). The zone containing that point is identified as the next zone for the photon.
- In the 2.5D codes (CYLTRAN), the next zone is determined by comparing to either the axial or radial boundaries of a set of candidate zones based on the surface exited from the previous zone.
- In the 1D codes (TIGER), the new zone index is simply one greater or smaller than the previous zone, depending on the direction of the photon.

After being moved (to either a boundary or collision site – if the photon has not been absorbed), the process of sampling distance to collision repeats (until the photon has escaped the boundaries of the model geometry). No sampling of distance to collision occurs in void regions.

The pre-processed data of the cross sections from NIST for each interaction are given as values on an 80-point energy grid (spanning the range of 1 keV to 1 GeV) for each element. Higher-Z (atomic number) elements will have more energy points, as the energy range is broken up into “tables” between the edge energies (at which the photoelectric cross sections have discontinuities in energy). These values are mapped onto a fine grid (of about 3000 energy points – the grid is adaptive with more points added near edge-energy discontinuities) by log-log quadratic interpolation. (The XCOM [Berger 87] program, upon which our methods are based, uses different interpolation procedures. XCOM uses log-log cubic spline interpolation above the K-edge, and log-log linear interpolation below. Spot checking values obtained from our fine grid and XCOM’s interpolation methods, the differences are generally less than 1% and often much less away from edge energies. There is evidence NIST [Seltzer 93] may be exploring use of log-log Hermite polynomial interpolation “to avoid the occasional numerical excursion found for cubic splines,” so the best interpolation scheme may be a moving target.) Values are then used in the Monte Carlo with a simple nearest-neighbor lookup, where the energy at which the cross section is evaluated is the geometric mean of the endpoints of the energy bin.

Cross sections for compounds are obtained from weighted sums over the corresponding coefficients (i.e. fractions of weights of the atomic constituents) for the elements. [Berger 87]

3.1 Interactions Modeled

3.1.1 Photoelectric Effect

The total photoelectric absorption cross sections are based on calculations from Scofield [Scofield 73]. However, these cross sections were not renormalized using the relativistic Hartree-Fock correction factors supplied by Scofield since reviews of Saloman and Hubbell [Saloman 87] indicate that agreement with experiment is better when the renormalization is not done. Although these cross sections were also used in the publicly released ITS 3.0 in 1992 [Halbleib 92], the medical physics community apparently has only recently “rediscovered” the benefit of use of these (non-renormalized) cross sections [DeMarco 02].

The accuracy of the photoelectric cross sections are given in [Hubbell 99] as:

Photon energy range	Solid	Gas
0.5-1 keV	10-20%	5%
1-5 keV	5%	5%
5-100 keV	2%	2%
100 keV – 10 MeV	1-2%	1-2%
10 MeV – 100 GeV	2-5%	2-5%

Strictly speaking, this table is comparing measurements to the EPDL data set, but again these are based on the same non-renormalized Scofield calculations (with a slightly different interpolation scheme). This assessment comes from a systematic comparison [Saloman 88] to the massive NIST database where, for example in the 5-100 keV range, almost each element is compared with measurements from several sources.

This is the dominant interaction cross section for low-energy photons.

3.1.1.1 Photoelectron Production

The probability of having a particular shell ionized is the ratio of the photoelectric cross section evaluated on either side of the discontinuity at the shell edge energy (for photon energies above that edge energy, but otherwise assumed to independent of the photon’s energy). For the standard codes, only the K-shell of the highest-Z element in each material is treated. For the PCODES, all elements are treated down to an average-M and average-N shell.

The angle of the emerging photo-electron (with respect to the parent photon) is described by the Fischer distribution at lower energies and Sauter formula at higher energies (both can be found in [Lorence 89]). For the standard codes (non-PCODES), the switching energy is 50 keV [Seltzer 88] and the distributions have been pre-calculated by NIST on thirteen energies and 21 equi-probable reduced-angle bins. The sampling proceeds by linearly interpolating on energy and an angular term, $(1-\beta\cos\theta)$, which is a typical factor in the Bethe-Heitler formulas. For the PCODES, the switching energy is a function of atomic number [MacCallum 73] and the distributions are sampled analytically by either direct sampling from Fischer or a rejection technique for the Sauter distribution.

The energy of the emerging photo-electron is the difference between the energy of the photon having the photoelectric interaction and the binding energy of the atomic shell involved. For the standard codes, the binding energies are those from [Carlson 75]. The binding energies for the PCODES are set to be consistent with the NIST photoelectric edge energies. For shell energies below 1 keV for the PCODES, we use the binding energies of [Carlson 75]. Binding energies are generally well known, and the differences in these data sets tend to be less than 1%.

3.1.1.2 Relaxation

If a shell has been ionized through the photoelectric event, the residual shell binding energy must relax through the production of fluorescence photons or Auger electrons. For each shell, the data which are needed are the fluorescence efficiency and relative probabilities of which other shell(s) may be involved which in turn affects the energies of the emitted fluorescence photons or Auger electrons.

In the standard codes, only the K-shell is treated. A 1984 fit (over atomic number Z) is used for the K-shell fluorescence efficiencies. See [Hubbell 94] for discussion and latest suggestion of tabulated values. Efficiencies for high-Z materials (which generate the most fluorescence) are rather stable to the 1% level. Low-Z elements such as Al have changed by about 20% over the years, and is now known to about 10% [Hubbell 94]. The branching ratios (which K-shell fluorescence or which Auger electrons) are taken from [Bambynek 72]. The assessment of agreement of these fluorescence branching ratios to measured values are as large as 20% for low-Z and of the order of 7% at high Z [Bambynek 72].

The data for the PCODES (which need similar data but for more shells, including Coster-Kronig transitions for the L shells) come from 10 references cited in [Halbleib 75]. At this time, it is not clear which quantity came from which source.

3.1.2 Incoherent Scattering

The total cross section for incoherent (Compton) scattering is taken from [Hubbell 75] obtained from using a product of the analytic Klein-Nishina formula and non-relativistic Hartree-Fock incoherent-scattering functions $S(Z,x)$ (where x is the momentum transfer and Z is the atomic number). The sampling of the angle of the scattered photon is performed by sampling from the Klein-Nishina cross section then rejecting on $S(Z,x)$ for large energies (energies larger than 0.003 MeV times the square root of an effective atomic number for the given material), otherwise sampling on $S(Z,x)$ and rejecting on Klein-Nishina. We are consistent in using the same $S(Z,x)$ to sample from the total or differential (in angle) cross sections. When the Klein-Nishina cross section is sampled, Kahn's method [Kahn 56] is used for energies less than 5 MeV while Koblinger's method [Koblinger 75] is used otherwise. Both methods use analytic expression and are mathematically equivalent (but not necessarily as efficient) in their range of validity. Koblinger's method cannot be used below about 1.4 MeV since one of the terms, treated as a probability, becomes negative. The switching energies were determined by NIST as good choices for efficient sampling times.

When evaluating the incoherent scattering functions, cubic spline interpolation is used (which is additionally log-log for momentum transfers larger than 2 inverse Angstroms). $S(Z,x)$ is assumed to be unity above momentum transfers of 100 inverse Angstroms. When x is sampled from $S(Z,x)$, cubic spline interpolation is used on the cumulative probability function.

For compounds, an effective (normalized to unity for large x) incoherent scattering function is used as [Seltzer 89]

$$S_{\text{eff}}(x) = \sum_i w_i (Z_i / A_i) [S(x, Z_i) / Z_i] / \langle Z / A \rangle$$

where

$$\langle Z / A \rangle = \sum_i w_i (Z_i / A_i).$$

Once the angle of the scattered photon is determined, its energy and that of the emerging electron are determined by Compton kinematics.

Hubbell [Hubbell 97] assessed the incoherent-scattering function approach to be 5% or better in forward scattering angles and for low and medium Z materials. For large angles and high Z values this approach may be too high by as much as 20%. He also refers to S-Matrix theory which may provide more accurate cross sections than the use of the incoherent scattering function, but admits more comparisons with experimental data are needed. Meanwhile, there is interest in a simpler theory but one which can incorporate Compton Doppler broadening – which is thought to have a very minor effect on energy deposition (due to energy deposition being the integral of the broadened quantity) but a dramatic effect on for example, a pulse height distribution. Evaluations by NIST [Rao 04] on this alternate approach to modeling Compton scattering resulted in differences in the total cross sections by less than 1% above 50 keV, but could be as large as 10% at 5 keV for particular elements. They conclude “We note, unfortunately, that there is a scarcity of absolute experimental data for total scattering cross sections.” [Rao 04] (We have a student intern implementing a form of the Compton Doppler broadening so we can eventually make our own assessments of its impact on our applications.)

3.1.3 Coherent Scattering

The total cross sections for coherent (Rayleigh) scattering is taken from [Hubbell 79] obtained from using a product of the analytic Thompson formula combined with relativistic Hartree-Fock atomic form factors $F(Z,x)$ (where x is the momentum transfer and Z is the atomic number). The sampling of the angle of the scattered photon is performed by sampling from the Thompson cross section then rejecting on $F(Z,x)$ for small energies (energies smaller than 0.002 MeV times a power of an effective atomic number for the given material), otherwise sampling on $F(Z,x)$ and rejecting on the Thompson formula. Unlike those used for the total cross sections (used to determine the relative probability of having a Coherent interaction), the $F(Z,x)$ used for the angle sampling are the non-relativistic Hartree-Fock atomic form factors of [Hubbell 75].

When evaluating the atomic form factors, cubic spline interpolation is used (which is additionally log-log for momentum transfers larger than 0.1 inverse Angstroms). $F(Z,x)$ is assumed to be zero above a material-dependent momentum transfer (calculated as x for which $F(Z,x)=1.E-6$). When x is sampled from $F(Z,x)$, cubic spline interpolation is used on the cumulative probability function which is additionally logarithmic in momentum transfer for sampled probabilities greater than 0.1 inverse Angstroms.

For compounds, an effective (normalized to unity at $x=0$) atomic form factor is used as [Seltzer 89]

$$F_{\text{eff}}(x) = \sum_i w_i (Z_i^2 / A_i) [F(x, Z_i) / Z_i^2] / \langle Z / A \rangle$$

where

$$\langle Z / A \rangle = \sum_i w_i (Z_i / A_i).$$

It is assumed no energy loss is associated with a coherent scattering interaction.

3.1.4 Pair Production

Pair production is not yet discussed.

4 Electron Transport

Electron transport is treated in a “Class I” [Berger 63] condensed-history approach, where the accumulated effects of scattering over a path length are treated instead of individual interactions. Path lengths are treated on two levels [Seltzer 88] in ITS. For energy-loss sampling, a “step” size is defined as the distance over which a specified average energy loss occurs (the ITS default is about 8% so that, after 8 steps the electron’s energy is, on the average, halved.). These step sizes are naturally mapped to a logarithmic energy grid on which most of the electron cross sections are evaluated. This step is further divided into multiple (from 2-15 with larger numbers for higher atomic number of the material) substeps to help capture the spatial variation (“wiggleness” [Seltzer 91]) of real electron tracks. The spatial displacement over a substep is described in the following section on “transport mechanics”.

4.1 Transport Mechanics

ITS uses the simplest transport mechanics scheme [Berger 63]: straight-line motion in the direction of the unscattered electron, with the accumulated angular deflection imposed at the end of the substep. Other approaches (attempting to better describe the “wiggleness” of the scattered electrons over a substep) include straight-line motion with explicit path length corrections [Seltzer 91], single or multiple hinges [Kawrakow 98], or sampling from distributions generated from single-scattered codes (which describe

where the electron ends up, but not how it got there). [Of those, the single randomly-placed hinge has some attractive properties (approximately preserving moments) while maintaining simplicity for boundary crossing. This may be explored in future versions of ITS.]

4.1.1 Boundary Crossing Details

With the simple straight-ahead transport, the spatial location of a boundary crossing is straight forward. However, the machinery of the condensed-history algorithms, which is based on precalculating sampling distributions over a pre-determined pathlength, need to be modified, since both the step and substep pathlengths have been truncated.

The energy of an electron which has crossed a boundary is resampled based on truncated step-size. This energy loss is applied to the electron at the boundary. The energy loss of the truncated subset is simply the scaled energy loss (based on the full step) for that fraction of the substep. This introduces a lack of correlation of the energy loss along the substeps already traversed, but attempts to maximize the pathlength used in the sampling (i.e. a truncated step instead of a truncated substep). On the average, the mean energy deposited will be preserved, but the energy straggling (spread) for the energy deposited will be different from the energy straggling of the energy lost by the electron on the other side of the boundary.

The angular deflections are now sampled with a procedure [Jensen 88] which represents the multiple angular scattering distribution as a combination of a modified Gaussian [Berger 88] with a single-scattering large-angle tail. If the pathlength is sufficiently short, only the single scattering angular deflections will be sampled. The number of large-angle single scatters (or total single scattering when the path length is too small to have multiple scattering) is based on a Poisson distribution of the average number of those scatters. The single-scattering distributions (for these truncated substeps) are represented analytically as screened Rutherford distributions, even below 256 keV, using Seltzer's modified screening parameter [Seltzer 88] to preserve the first transport moment of the more accurate phase-shift calculations. This accumulated scattering is then imposed at the boundary (i.e. the end of the truncated substep). Finally, accumulated scatterings which bring the particle back into the present zone (i.e., have not crossed the boundary) are rejected.

The number of any secondaries produced is simply scaled back by the ratio of the truncated to full substep.

4.2 Interactions Modeled

4.2.1 Collisional Energy Loss

The energy loss over a step is sampled from a modified [Seltzer 91] Landau/Blunck-Leisegang distribution. Two modifications were made by Seltzer: (1) a finite maximum energy loss was determined to preserve the mean stopping power (calculated from the Bethe formula for the total stopping power), and (2) a semi-empirical correction to the width which dramatically improves comparisons with experiment for smaller step sizes. Within a step, the sampled energy loss is partitioned equally among the substeps.

4.2.2 Elastic Scattering

The Goudsmit-Saunderson (GS) distribution is an infinite series whose coefficients involve the transport moments (angular moments) of the single-scattering cross section. The method of evaluation used in ITS was largely developed in the late 50's early 60's when computational power was very limited so a premium was placed on analytic manipulations. A more robust method has been described in [Berger 88].

At energies above 256 keV, the cross section is represented as the product of a screened Rutherford with the ratio of the Mott to Rutherford. In [Berger 88], Berger gives a table of the estimated error as about 5% in U at 274 keV (falling off at higher energies or lower-Z). The screening parameter η is essentially that of Moliere, but modified by Seltzer [Seltzer 88] which we use to smooth the transition to the use of phase-shift calculations below 256 keV. Seltzer's modification is designed to approximately preserve the first transport moment of the phase-shift cross section. The Mott to Rutherford ratio is treated as numerical data from NIST: evaluated for every element ($Z=1$ to 100) at 18 energies and 5 angles (every 45 degrees). (The data includes a similar tabulation of Mott-positrons to Rutherford ratios.) The function is interpolated by

piecewise quadratic (Lagrange) interpolation in energy. Finally, this cross section is expanded in powers of $(1-\cos\theta+\eta)$ where five coefficients are determined by matching exactly at 5 angles (every 45 degrees).

At energies below 256 keV, phase-shift calculations [Riley 75] have been performed and expanded in a 12-parameter fit of a sum of different powers of $(1-\cos\theta+B)$ combined with a sum of a few Legendre Polynomials, where B is one of the fitting parameters. The fitting coefficients have been determined to preserve the first twenty transport moments of the phase-shift calculations. (We do have numerical tables of Berger's extension of Riley's cross sections to 1 MeV.[Berger 93])

By representing the single scattering cross section in this way, the transport-moment integrals (to determine the GS coefficients) can be done analytically using recursion relations, which unfortunately are unstable. To maintain accuracy the series is summed to 240 terms (with the next term representing the unscattered probability) in the forward direction when $\eta < 1.E-4$. When $\eta > 1.E-4$, the series is summed to $\exp(1.794-.397\ln \eta)$, but never less than 10, in the backward direction [Seltzer 88].

Each coefficient is evaluated at two energies: at the beginning and end of the substep (which is centered within the corresponding step). The same angular distribution will then be used throughout the step. Though this may introduce some bias in situations where a boundary is crossed before the step cycle can be completed. This permits the coefficients of a 2-parameter fit [Spencer 55] to describe the energy dependence of the GS coefficients, so they may be integrated analytically over energy (i.e. over the substep) to account for the energy loss of the electron over the substep.

The final distribution is represented as the delta-function plus a histogram in angle (with a default size of 33 bins, more closely spaced at small angles). All of these computations take place within the cross section generating code XGEN, so that the Monte Carlo need only sample from the cumulative probability of that histogram. The cumulative distribution is normalized to the complement of the delta-function scattering.

4.2.3 Inelastic Scattering

The angular deflections due to inelastic scattering are approximated by increasing the elastic-scattering cross section by $(Z+1)/Z$ while the GS coefficients are determined. With this treatment, the large-angle collisions will be uncorrelated with the associated larger energy loss. This increases the cross section at all angles, so the resulting distribution is reduced by $Z/(Z+1)$ at all angles greater than the kinematical cutoff angle [Seltzer 88]. An alternative procedure, incorporating the correction perhaps a little more consistently, has been suggested in [Berger 88].

4.2.4 Bremsstrahlung

Bremsstrahlung production is sampled from a Poisson distribution over each substep. The energy of each photon is subtracted from the parent electron (hence the two are correlated unlike knock-on production). The starting position of the photon is sampled uniformly along the substep path. The angular distribution of the bremsstrahlung photon is sampled from Bethe-Heitler cross sections (Born approximations) [Koch 59] differential in both energy and angle of the emitted photon. Phase-shift calculations for these angular distributions are also available at or below 500 keV [Kissel 83] and the differences discussed in [Seltzer 91]. The direction of the parent electron is taken to be that at the beginning or end of the substep, whichever is closer. This can lead to measurable artifacts [Faddegon 93] and a simple solution has been proposed [Hughes 97] though not yet implemented in ITS.

The bremsstrahlung cross sections, differential in energy, are discussed more fully in [Seltzer 88b]. For energies below 2 MeV, they include phase-shift calculations of Pratt [Pratt 77] (with linear extrapolation to include $Z=1$ and Z above 92 to 100). Seltzer evaluates "agreement is generally within the combined limits of experimental uncertainty and a theoretical uncertainty estimated to be 5 to 10%." [Seltzer 88b]

4.2.5 Knock-ons

The production of knock-on electrons is sampled according to the Moller cross section (which ignores binding effects). The angular distribution of the knock-ons is based on Moller kinematics with the

reference direction of the parent electron taken to be that at the beginning or end of the substep, whichever is closer. The starting positions of these knock-ons are sampled uniformly over the substep.

No change of the parent electron's energy (or direction) is made since this is already taken into account through using the total stopping power and Landua/Blunck-Leisegang distribution (and our treatment of inelastic scattering). Hence, the energy loss due to knock-ons are uncorrelated from the parent electron.

4.2.6 Impact Ionization

4.2.6.1 Vacancy Relaxation

5 Geometry Tracking

6 Tallies

7 Biasing Options

8 Source Descriptions

9 Statistics

10 Random Number Generators

11 References

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