Acuros® XB advanced dose calculation for the Eclipse™ treatment planning system

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Introduction

The Acuros XB advanced dose calculation (Acuros XB) algorithm was developed to address two strategic needs of external photon beam treatment planning: accuracy and speed. In external photon beam radiotherapy, heterogeneities introduced by materials such as lung, bone, air, and non-biologic implants may significantly affect patient dose fields, especially in the presence of small or irregular fields. Acuros XB uses a sophisticated technique to solve the Linear Boltzmann transport equation (LBTE) and directly accounts for the effects of these heterogeneities in patient dose calculations. Acuros XB provides comparable accuracy to Monte Carlo methods in treatment planning for the full range of X-ray beams produced by clinical linear accelerators, 4 MV – 25 MV with exceptional calculation speed and without statistical noise.

Additionally, Acuros XB calculations are minimally sensitive to the number of fields in a plan such that calculation of the dose in a RapidArc® radiotherapy technology plan is almost as fast as for a single field. The effect of which is that while single field dose calculations are somewhat slower than with Eclipse Analytical Anisotropic Algorithm (AAA), Acuros XB is significantly faster for RapidArc.

Acuros XB is fully integrated into the Eclipse distributed calculation framework (DCF) as a new dose calculation algorithm and uses the multiple-source model originally derived for AAA. Therefore, the user will also appreciate that AAA beam data can be imported in the Acuros XB beam model and only requires reconfiguration before it is ready to be used for dose calculations.
Background

The Boltzmann transport equation (BTE) is the governing equation which describes the macroscopic behavior of radiation particles (neutrons, photons, electrons, etc.) as they travel through and interact with matter. The LBTE is the linearized form of the BTE, which assumes that radiation particles only interact with the matter they are passing through, and not with each other, and is valid for conditions without external magnetic fields. For a given volumetric domain of matter, subject to a radiation source, under the above conditions the solution to the LBTE would give an “exact” description of the dose within the domain. However, since closed form solutions (analytic solutions) to the LBTE can only be obtained for a few simplified problems, the LBTE must be solved in an open form, or non-analytic, manner.

There are two general approaches to obtaining open form solutions to the LBTE. The first approach is the widely known Monte Carlo method. Monte Carlo methods do not explicitly solve the LBTE; they indirectly obtain the solution to this equation. The second approach is to explicitly solve the LBTE using numerical methods [ref. 1]. Methods used to explicitly solve the LBTE equation, such as those of Acuros XB, are relatively new to the medical physics community.

Both Monte Carlo and explicit LBTE solution methods such as Acuros XB are “convergent.” That is, with sufficient refinement both approaches will converge on the same solution of the LBTE. The achievable accuracy of both approaches is equivalent and is limited only by uncertainties in the particle interaction data and uncertainties in the problem being analyzed. In practice, neither Monte Carlo nor explicit LBTE solution methods are exact, and both methods produce errors. In Monte Carlo, errors are random and result from simulating a finite number of particles and following each particle as it interacts with a medium. When Monte Carlo methods employ techniques to accelerate solution times or reduce noise (de-noising), systematic errors may be introduced. In the explicit LBTE solution methods, errors are primarily systematic and result from discretization of the variables in space, angle, and energy. Larger steps in the discretization process result in a faster solution, but less accuracy. In both methods, a trade-off exists between speed and accuracy. Differences between the two methods may also result from the treatment of charged particle Coulomb interactions. Model- or correction-based algorithms such as pencil beam or collapsed cone convolution are only convergent under the exact conditions in which their dose kernels are generated.

The impetus behind the development of explicit LBTE solution methods was to provide a rapid alternative to Monte Carlo simulations, which are known to be time intensive. A second benefit of LBTE is the absence of statistical noise. Many of the methods contained within Acuros XB were originally developed in a prototype solver called Attila®, which was co-authored by the founders of Transpire, Inc. while at Los Alamos National Laboratory [ref. 2, 3]. The development of the Acuros XB external photon beam prototype was funded in part through an SBIR Phase II Grant from the National Cancer Institute.
Acuros XB in Eclipse – Source Model

Acuros XB in Eclipse leverages the existing AAA machine source model. This model consists of four components:

- **Primary source** – user-defined circular or elliptical source located at the target plane which models the bremsstrahlung photons created in the target that do not interact in the treatment head.

- **Extra focal source** – Gaussian plane source located at the bottom of the flattening filter, which models the photons that result from interactions in the accelerator head outside the target (primary in the flattening filter, primary collimators, and secondary jaws).

- **Electron contamination** – represents the dose deposited in the build-up region not accounted for by the primary and extra-focal source components.

- **Photons scattered from wedge** – represents the scatter from hard wedges, where present. Implemented with a dual Gaussian model, where the width of the Gaussian kernel increases with distance from the wedge.

A detailed description regarding these sources can be found in the paper on AAA photon dose calculation by Sievinen et al. [ref. 8].
Acuros XB in Eclipse – Patient Transport and Dose Calculation

(The Acuros XB solution methods are briefly described here, with a detailed overview provided in the Appendix.)

The Acuros XB patient transport consists of four discrete steps, which are performed in the following order:

1. Transport of source model fluence into the patient
2. Calculation of scattered photon fluence in the patient
3. Calculation of scattered electron fluence in the patient
4. Dose calculation

Steps 1 through 3 are performed to calculate the electron fluence in every voxel of the patient. Once the energy dependent electron fluence is solved, the desired dose quantity (dose-to-medium or dose-to-water) is computed in Step 4. Step 1 is the only step repeated for each beam, and Steps 2 through 4 are performed once, regardless of the number of beams. In the case of RapidArc, each beam will have a large number of orientations, and Step 1 is repeated at each orientation and Steps 2 through 4 are performed just once.

In Step 1, the machine sources are modeled as external sources and ray tracing is performed to calculate the uncollided photon and electron fluence distributions in the patient.

In Steps 2 and 3, Acuros XB discretizes in space, angle, and energy, and iteratively solves the LBTE.

In Step 4, the dose in any voxel of the problem is obtained through applying an energy dependent fluence-to-dose response function to the local energy dependent electron fluence in that voxel. Acuros XB supports two dose reporting options: dose-to-water ($D_w$) and dose-to-medium ($D_m$). When $D_m$ is calculated, the energy dependent response function is based on the material properties of that voxel. When $D_w$ is calculated, the energy dependent fluence-to-dose response function is based on water.

Therefore, to calculate dose, Acuros XB must have a material map of the imaged patient. Unlike convolution/superposition algorithms, where heterogeneities are generally handled as density based corrections applied to dose kernels calculated in water, Acuros XB explicitly models the physical interaction of radiation with matter. To do this accurately, Acuros XB requires the chemical composition of each material in which particles are transported through, not only the density. To enable this, Eclipse provides Acuros XB with a mass density and material type in each voxel of the image grid. The Acuros XB material library includes five biologic materials (lung, adipose tissue, muscle, cartilage, and bone) and 16 non-biologic materials, with a maximum supported density of 8.0 g/cc (steel).
In Figure 1, an illustration of the differences between $D_W$ and $D_M$ are presented for a $5 \times 5 \text{ cm}^2$ 6 MV field on a water-bone-lung slab phantom. Also shown are results for “scaled water density”, in which the entire phantom was assigned water material, with varying density according to the region. As shown, $D_W$ and $D_M$ are identical in water voxels upstream of the bone, and are nearly identical in the lung downstream of the bone. This is expected since in both cases, the electron transport field is identical, and only the electron energy deposition interaction is different. However, for “scaled water density” there are significant differences in the build-up region before the bone, in the bone, and in the lung downstream of the bone. These differences highlight the significance of using the actual material composition as opposed to scaling the density of water material.

Figure 1. Acuros XB depth dose comparison between different dose reporting modes for a $5 \times 5 \text{ cm}^2$ 6 MV field on a water-bone-lung slab phantom. For “scaled water density”, the entire phantom consisted of water material, but with the density scaled in each region (1.85 g/cc in bone region, and 0.26 g/cc in lung).
In Figure 2, differences between \( D_W \) and \( D_M \) are presented for a 5 x 5 cm\(^2\) 18 MV field for the biologic materials in Acuros XB.

**Figure 2.** Acuros XB depth dose curves for dose-to-water (\( D_W \)) and dose-to-medium (\( D_M \)) for a 5x5 cm\(^2\) 18 MV beam on a slab phantom containing: water (1.0 g/cc), cartilage (1.1 g/cc), bone (1.85 g/cc), lung (0.26 g/cc), adipose tissue (0.92 g/cc), and muscle (1.05 g/cc)
Comparison with Monte Carlo

Since Monte Carlo methods are well known in the radiotherapy community, a useful way to understand the methods in Acuros XB is to highlight where and why differences between Acuros XB and Monte Carlo can occur, which are discussed below.

Dose-to-water and dose-to-medium

Both Acuros XB and Monte Carlo methods calculate $D_M$ based on energy deposition, and as shown in the included figures, produce very similar results. However, when calculating $D_W$ in non-water materials, Acuros XB and Monte Carlo methods employ different approaches.

Acuros XB calculates the energy dependent electron fluence using the material compositions of the patient, regardless of whether $D_W$ or $D_M$ is selected. When $D_W$ is selected, in non-water materials this is analogous to calculating the dose received by a volume of water which is small enough to not significantly perturb the energy dependent electron fluence. Due to the very short range of low energy electrons, this volume may be much smaller than either the dose grid voxel size or detectors used to experimentally measure $D_W$. This effect is most significant for bone and non-biologic, high density materials such as aluminum, titanium, and steel. In such cases, when comparing Acuros XB to experimental measurements of $D_W$, it is recommended to explicitly model a small water volume representing the detector in Acuros XB.

Monte Carlo methods will generally calculate $D_M$, and employ stopping power ratios to convert $D_M$ to $D_W$ [ref. 5]. To illustrate the expected differences between the approaches of Acuros XB and Monte Carlo in calculating $D_W$, Figure 3 shows a comparison between energy deposition ratios (water/medium) [ref. 4] and collisional stopping power ratios (water/medium) [ref. 6] in different biologic materials as a function of electron energy. The energy deposition ratios (Figure 3 - left) show the ratio of $D_W/D_M$ which would be calculated by Acuros XB, and the collisional stopping power ratios (Figure 3 - right) show the ratio of $D_W/D_M$ which would be calculated by Monte Carlo methods.

![Figure 3](left) Energy deposition ratios (water/medium) and (right) collisional stopping power ratios (water/medium), as a function of electron energy (MeV). The ratio between dose-to-water and dose-to-medium in Acuros XB is reflected in the energy deposition ratios; and for Monte Carlo in the collisional stopping power ratios.
Although Acuros XB and Monte Carlo use different methods, calculating $D_w$ in a non-water medium is a theoretical quantity, and therefore neither approach is correct or incorrect.

**Electron cutoff energy**

Acuros XB employs an electron cutoff of 500 keV (kinetic energy, not including electron rest mass energy). Electrons passing below this energy are assumed to dump all of their energy in the voxel in which they are located. When comparing Acuros XB and Monte Carlo in voxels containing very low density lung or air, the choice of electron cutoff energy may result in differences between the two solvers. However, such differences will generally be isolated to the low density voxels, and will not significantly influence the dose in adjacent tissue.

**Implementation differences**

As discussed earlier, Acuros XB and Monte Carlo methods are unique in radiotherapy in that both methods explicitly solve for the electron fluence, without the use of pre-calculated dose kernels. As mentioned earlier, neither method is exact and in practice differences will occur.

A simple way to understand the different approaches between Acuros XB and Monte Carlo is as follows: Analog Monte Carlo methods simulate a finite number of particles, and stochastic errors result from a finite number of particles being tracked. Acuros XB simulates an infinite number of particles, and systematic errors are introduced by discretization in space, angle, and energy. In Acuros XB, the discretization settings are specified internally to provide an optimal balance of speed and accuracy for patient treatment planning conditions. This is analogous to a Monte Carlo code which internally sets a limit on the statistical uncertainty.
Acuros XB Calculation Options

The Acuros XB implementation in Eclipse is very similar to that of AAA. A few key points related to the Acuros XB implementation are summarized below, and several differences with AAA are highlighted.

**Calculation grid voxel size:** The Acuros XB calculation grid voxel size can range from 1 to 3 mm. AAA currently supports a voxel size range between 1 and 5 mm.

**Dose reporting mode:** In Acuros XB, $D_M$ or $D_W$ can be selected as dose reporting options. This concept does not exist in AAA.

**Plan dose calculation:** This is a unique option for Acuros XB. In Acuros XB, the calculation time has a very weak dependence on the number of fields, since the majority of the calculation time is spent calculating the scattered photon and electron fluence, which is performed once for all fields in the plan. When a separate Acuros XB calculation is performed for each field, the scatter calculation phase has to run for every field, which significantly increases the calculation time. Since field weights cannot be edited when plan dose calculation is selected, this option is well suited for rapidly calculating intensity-modulated radiation therapy (IMRT) and RapidArc plans. However, in 3D conformal planning where field weights may be individually changed during optimization, plan dose calculation would generally be turned off.

**Material specification:** Material determination is done in two ways for Acuros XB. The default method used to determine the material composition of a given voxel in a 3D image is based on the HU value. The HU value in the voxel is converted to mass density using the CT calibration curve. This curve can be configured by the users for their specific CT scanner. Once mass density is known in a voxel, the material is determined based on a hard coded look up table stored in the Varian system database. This automatic conversion is used for all voxels with mass density below 3.0g/cc. Any voxel with density higher than 3.0g/cc requires user assignment. Furthermore, the automatic material assignment only assigns biological materials to voxels. Based on their mass density, voxels will be assigned lung, adipose tissue, muscle, cartilage, or bone. Even very low density regions are automatically assigned a material, either lung or air. Users have the option to manually override the automatic material assignment.

**Configuration:** Since Acuros XB uses the same source model as AAA, no additional beam data is needed and the AAA configured data can be imported into the Acuros XB model directly. AAA beam data imported in Acuros XB will need to be reconfigured and all configuration steps will need to be run again to optimize the source model for Acuros XB. The preconfigured beam data available for AAA is also available for Acuros XB. For every DCF version, preconfigured beam data for AAA and Acuros XB is available.
Acuros XB Validation Examples

A brief sampling of Acuros XB validation cases with heterogeneities are provided below. Note that in order to fully validate Acuros XB against Monte Carlo N-Particle eXtended (MCNPX), the MCNPX computations were run with a very large number of particles to create results that were very smooth and without statistical uncertainties that may have influenced the validations of Acuros XB. In practice typical Monte Carlo results are much less smooth and statistical uncertainties are clearly visible. Additional validation results can be found in the literature [ref. 7].

The Acuros XB material library includes 13 non-biologic materials. Figure 4 and Figure 5 compare $D_M$ results from Acuros XB and MCNPX on a slab phantom containing 12 of the 13 non-biologic materials for 6 MV and 20 MV.

![Figure 4. Depth dose comparison (dose-to-medium) between Acuros XB and MCNPX for a 6X 10 x 10 cm$^2$ field on a multi-material slab phantom. Slab materials are as follows: (1) Polystyrene – 1.05 g/cc, (2) Epoxy – 1.04 g/cc, (3) Aluminum – 2.7 g/cc, (4) PMMA – 1.19 g/cc, (5) Titanium alloy – 4.42 g/cc, (6) Radel – 1.30 g/cc, (7) Wood – 0.70 g/cc, (8) PEEK – 1.31 g/cc, (9) PVC – 1.38 g/cc, (10) Acetal – 1.42 g/cc, (11) PVDF – 1.77 g/cc, (12) PTFE – 2.20 g/cc.](image-url)
The highest density material supported in Acuros XB is stainless steel, with a maximum density of 8.0 g/cc. Figures 6 through 8 present an extreme case where a 2 x 2 x 2 cm³ steel implant (8.0 g/cc) is placed in a water phantom inside an 18 MV 10 x 10 cm² field. As shown, both codes are in close agreement, even in the high gradient electron disequilibrium regions surrounding the implant.

**Figure 5.** Depth dose comparison (dose-to-medium) between Acuros XB and MCNPX for a 20X 10x10 cm² field on a multi-material slab phantom. Slab materials the same as in Figure 4.

**Figure 6.** Phantom containing a 2 x 2 x 2 cm³ 8.0 g/cc steel implant used in Figures 7 and 8. Acuros XB dose contours shown (dose-to-medium) for an 18 MV 10 x 10 cm² field.
Figure 7. Depth dose comparison between Acuros XB and MCNPX for an 18 MV 10 x 10 cm² field impinging on the steel insert phantom shown in Figure 1. Dose-to-medium shown in both codes with dose normalized to 100% at depth of 4.875 cm.

Figure 8. Lateral depth dose comparison (depth of 4.875 cm) between Acuros XB and MCNPX for an 18 MV 10 x 10 cm² field impinging on the steel insert phantom shown in Figure 1. Dose-to-medium shown in both codes with dose fields normalized to 100% at centerline depth of 4.875 cm.
Figures 9 through 11 present comparisons between Acuros XB and Monte Carlo for a half cork (0.19 g/cc) phantom for 5 x 5 cm² fields and 6 MV and 15 MV beam energies.

**Figure 9.** Phantom containing a half cork slab (0.193 g/cc) used in Figures 10 through 13. Acuros XB dose contours shown (dose-to-medium) for a 6 MV 5 x 5 cm² field.

**Figure 10.** Depth dose comparison between Acuros XB and MCNPX for a 5 x 5 cm² 15 MV field on the half cork slab phantom shown in Figure 9. Depth dose line located 1.125 cm OAX on the cork side. Dose-to-medium shown in both codes with dose normalized to 100% at depth of 4 cm.
Figure 11. Lateral dose comparison between Acuros XB and MCNPX for case shown in Figure 10, at depths of 4.625, 17.875, and 21.125 cm.

Figure 12 presents comparisons between Acuros XB and Monte Carlo for 2 x 2 cm² 6 MV fields on a water phantom containing a 2 x 2 x 10 cm³ block of air, which simulates an esophagus.

Figure 12. Depth dose comparison between Acuros XB and MCNPX for a 2 x 2 cm² 6 MV field on a phantom containing a 2 x 2 x 10 cm³ air block representing an esophagus. Electron energy cutoff for both Monte Carlo and Acuros XB is 500 keV.
Figure 13 shows the result of an Acuros XB RapidArc dose comparison with the Radiological Physics Center (RPC) head and neck phantom. TLD measurements are within 2% of calculated dose for the 3 mm x 3 mm calculation grid size.

![Figure 13. Acuros XB RapidArc plan for Radiological Physics Center (RPC) Head and Neck Phantom (figure courtesy of Firas Mourtada, Ph.D., UT MD Anderson Cancer Center).](image)

<table>
<thead>
<tr>
<th>TLD position</th>
<th>Measured dose (cGy)</th>
<th>Acuros XB, Heterogeneity “on”; Dose to medium</th>
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<tr>
<td></td>
<td>Treatment 1</td>
<td>Treatment 2</td>
</tr>
<tr>
<td>TLD_54_I</td>
<td>621.4</td>
<td>621.9</td>
</tr>
<tr>
<td>TLD_54_S</td>
<td>591.2</td>
<td>603.5</td>
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<tr>
<td>TLD_66_Iant</td>
<td>745.3</td>
<td>742.4</td>
</tr>
<tr>
<td>TLD_66_Ipost</td>
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</tr>
<tr>
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<td>360.9</td>
</tr>
<tr>
<td>TLD_CORD_S</td>
<td>357.3</td>
<td>357.2</td>
</tr>
</tbody>
</table>

Averaged percentage error (%) 1.89%

Table 1. Measured (TLD) vs calculated doses for RapidArc plan shown in Figure 13 above. Measurement is within 2% of calculation averaged over all TLD locations (courtesy of Firas Mourtada, Ph.D., UT MD Anderson Cancer Center).
Acuros XB Calculation Times

Calculations of a single or few fields are longer with Acuros XB than AAA. For a 10 x 10 cm² 6 MV field on a 30 x 30 x 30 cm³ water phantom, Acuros XB will calculate the dose on a 2.5 mm voxel grid in about 85 seconds (Dell T5500 with dual quad-core Xeon 2.27 GHz processors and 24 GB DDR3 RAM). AAA will require approximately 10 seconds for a similar case. For a 5 x 5 cm² field on the same phantom, Acuros XB will require about 40 seconds. Larger fields and higher energies take longer to calculate, as do phantoms containing large amounts of bone. Most of the Acuros XB calculation time is in solving for the scattered photon and electron fluencies, which are performed only once for all beams in the plan. As a result, Acuros XB calculation times scale very weakly with the number of fields. However, AAA calculation times scale linearly with the number of fields. As a result, the relative calculation speed of Acuros XB increases with increasing numbers of fields in the plan. For cases with larger numbers of fields, i.e., RapidArc, Acuros XB exploits spatial adaption to speed-up calculations in low dose, low gradient regions.

Acuros XB becomes significantly faster than AAA for cases with a large number of fields, i.e., RapidArc. As an example, the calculation times for several RapidArc cases are provided in Table 2 below, with screenshots of the Acuros XB dose calculation for the lung and head/neck case shown in Figures 14 and 15.

<table>
<thead>
<tr>
<th>Case</th>
<th>Acuros XB</th>
<th>AAA</th>
<th>Improvement over AAA</th>
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</thead>
<tbody>
<tr>
<td>Lung (57 control points, Fig. 14)</td>
<td>1 min 26 s</td>
<td>3 min 35 s</td>
<td>2.5x</td>
</tr>
<tr>
<td>Lung (114 control points, Fig. 14)</td>
<td>2 min 7 s</td>
<td>6 min 15 s</td>
<td>3.0x</td>
</tr>
<tr>
<td>Head &amp; Neck (89 control points, Fig. 15)</td>
<td>2 min 43 s</td>
<td>8 min 23 s</td>
<td>3.1x</td>
</tr>
<tr>
<td>Head &amp; Neck (178 control points, Fig. 15)</td>
<td>4 min 13 s</td>
<td>16 min 12 s</td>
<td>3.8x</td>
</tr>
<tr>
<td>Prostate (89 control points, not shown)</td>
<td>2 min 7 s</td>
<td>5 min 46 s</td>
<td>2.7x</td>
</tr>
<tr>
<td>Prostate (178 control points, not shown)</td>
<td>3 min 8 s</td>
<td>11 min 21 s</td>
<td>3.6x</td>
</tr>
</tbody>
</table>

Table 2. Acuros XB and AAA calculation times shown for representative RapidArc cases. All times shown on a Dell T5500 (Hyper-threading off for Acuros XB) with 2.5 mm voxel grids. Calculation times include both source model and patient transport components.
It should be noted that Acuros XB is considerably faster on the Varian Eclipse Dell T5500 machines than on the Dell T5400 machines, even with similar clock speeds. The limited memory bandwidth of the DDR2 memory on T5400 machines prevents Acuros XB from effectively scaling on all available cores (AAA does not exhibit this behavior). However, this bottleneck is removed with the DDR3 memory on T5500 machines, allowing Acuros XB to scale much more efficiently on available cores. This results in almost a factor of two speed-up on the T5500 (compared with the T5400) for some cases. Additionally, it is recommended to run Acuros XB with hyperthreading turned off, as hyperthreading may also degrade performance.
Conclusion

The Acuros XB advanced dose calculation algorithm was developed and implemented in Eclipse to address the accuracy and speed requirement for modern techniques in radiation therapy including IMRT and RapidArc. Acuros XB provides comparable accuracy in treatment planning conditions to benchmarked Monte Carlo methods for the full range of X-ray beams produced by clinical linear accelerators, 4 MV – 25 MV. Validation has been performed to assure dose calculation accuracy in typical and challenging phantom and patient geometries with excellent results.

References

Appendix

Acuros XB solution methods – patient transport

The Acuros XB patient transport consists of four discrete steps, which are performed in the following order:

1. Transport of source model fluence into the patient.
2. Calculation of scattered photon fluence in the patient.
3. Calculation of scattered electron fluence in the patient.
4. Dose calculation

Steps 1 through 3 are performed to calculate the electron fluence in every voxel of the patient. Once the energy dependent electron fluence is solved for, the desired dose quantity (dose-to-medium or dose-to-water) is computed in Step 4. Step 1 is the only step repeated for each field orientation, and Steps 2 through 4 are performed once, regardless of the number of orientations.

Material specification

Prior to initiating Step 1, Acuros XB must have a material map of the imaged patient. Unlike AAA, where heterogeneities are generally handled as density-based corrections applied to dose kernels calculated in water, Acuros XB explicitly models the physical interaction of radiation with matter. To do this accurately, Acuros XB requires the chemical composition of each material in which particles are transported through, not only the density. To enable this, Eclipse provides Acuros XB with a mass density and material type in each voxel of the image grid. The Acuros XB material library includes five biologic materials (lung, adipose tissue, muscle, cartilage, and bone) and 16 non-biologic materials, with a maximum supported density of 8.0 g/cc (steel).

The fundamental material data used by Acuros XB are known as macroscopic atomic cross sections. A macroscopic cross section is the probability that a particular reaction will occur per unit path length of particle travel, so it has units of cm⁻¹. The cross sections also describe the angular and energy behavior probabilities associated with any given interaction. Macroscopic cross sections are composed from two values: the microscopic cross section for a given reaction (generally given in barns/atom = 10⁻²⁴ cm²/atom and symbolized by \( \sigma \)) and the mass density of the material (\( \rho \), given in g/cm³). The expression for the macroscopic cross section, \( \sigma \), is:

\[
\sigma = \frac{N_a \rho}{M} \bar{\sigma}
\]

where

\( M = \) Mass of the atom in atomic mass units (AMU)

\( N_a = \) Avogadro’s number
Acuros XB uses coupled photon-electron cross sections produced by CEPXS [ref. 4]. For photon interactions, CEPXS includes Compton scatter (also known as incoherent scatter), the photo-electric effect, and pair production. CEPXS does not account for Rayleigh scatter (also known as coherent scatter), the effect of which is insignificant for dose distributions at energies typical in photon beam radiotherapies.

**The LBTE**

In Steps 1 through 3, Acuros XB solves the time-independent three-dimensional system of coupled Boltzmann transport equations (LBTE) shown below (for brevity the dependent variables have been suppressed in the equations):

**Eq. 1**

\[
\hat{\Omega} \cdot \nabla \Psi^\gamma + \sigma^\gamma_t \Psi^\gamma = q^\gamma + q^\gamma_e,
\]

**Eq. 2**

\[
\hat{\Omega} \cdot \nabla \Psi^e + \sigma^e_t \Psi^e - \frac{\partial}{\partial E} \left( S_R \Psi^e \right) = q^e + q^e_e + q^e_e + q^e_x,
\]

where

- \( \Psi^\gamma \) = Angular photon fluence (or fluence if not time integrated), \( \Psi^\gamma (\vec{r}, E, \hat{\Omega}) \), as a function of position, \( \vec{r} = (x, y, z) \), energy, \( E \), and direction, \( \hat{\Omega} = (\mu, \eta, \zeta) \).
- \( \Psi^e \) = Angular electron fluence, \( \Psi^e (\vec{r}, E, \hat{\Omega}) \).
- \( q^\gamma \) = Photon-to-photon scattering source, \( q^\gamma (\vec{r}, E, \hat{\Omega}) \), which is the photon source resulting from photon interactions.
- \( q^e \) = Electron-to-electron scattering source, \( q^e (\vec{r}, E, \hat{\Omega}) \), which is the electron source resulting from electron interactions.
- \( q^\gamma_e \) = Photon-to-electron scattering source, \( q^\gamma_e (\vec{r}, E, \hat{\Omega}) \), which is the electron source resulting from photon interactions.
- \( q^e_e \) = Electron-to-photon scattering source, \( q^e_e (\vec{r}, E, \hat{\Omega}) \), which is the photon source resulting from electron interactions.
- \( q^\gamma_x \) = Extraneous photon source, \( q^\gamma (E, \hat{\Omega}) \), for point source \( P \), at position \( \vec{r}_p \).
  This source represents all photons coming from the machine source model.
- \( q^e \) = Extraneous electron source, \( q^e (E, \hat{\Omega}) \), for point source \( P \), at position \( \vec{r}_p \).
  This source represents all electrons coming from the machine source model.
- \( \sigma^\gamma_t \) = Macroscopic photon total cross section, \( \sigma^\gamma_t (\vec{r}, E) \), units of cm\(^{-1}\).
- \( \sigma^e_t \) = Macroscopic electron total cross section, \( \sigma^e_t (\vec{r}, E) \), units of cm\(^{-1}\).
- \( \sigma_t \) = Macroscopic total cross section, \( \sigma_t (\vec{r}, E) \), units of cm\(^{-1}\).
- \( S_R \) = Restricted collisional plus radiative stopping power, \( S_R (\vec{r}, E) \).
The first term on the left hand side of Equations 1 and 2 is the streaming operator. The second term on the left hand side of Equations 1 and 2 is the collision or removal operator. Equation 2 is the Boltzmann Fokker-Planck transport equation, which is solved for the electron transport. In Equation 2, the third term on the left represents the continuous slowing down (CSD) operator, which accounts for Coulomb ‘soft’ electron collisions. The right hand side of Equations 1 and 2 include the scattering, production, and the external source terms from the AAA source module (\( q^\gamma \) and \( q^e \)).

The scattering and production sources are defined by:

Eq. 3

\[
q^{\gamma\gamma}(\vec{r}, E, \hat{\Omega}) = \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma^{\gamma\gamma}_s(\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}')\Psi^{\gamma}(\vec{r}, E', \hat{\Omega}') ,
\]

Eq. 4

\[
q^{\gamma e}(\vec{r}, E, \hat{\Omega}) = \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma^{\gamma e}_s(\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}')\Psi^{e}(\vec{r}, E', \hat{\Omega}') ,
\]

Eq. 5

\[
q^{e e}(\vec{r}, E, \hat{\Omega}) = \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma^{e e}_s(\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}')\Psi^{e}(\vec{r}, E', \hat{\Omega}') ,
\]

where

\( \sigma^{\gamma\gamma}_s = \) Macroscopic photon-to-photon differential scattering cross section
\( \sigma^{\gamma e}_s = \) Macroscopic photon-to-electron differential production cross section
\( \sigma^{e e}_s = \) Macroscopic electron-to-electron differential scattering cross section

The basic assumptions used in Equations 1 and 2 are briefly summarized as follows: Both charged pair production secondary particles are assumed to be electrons instead of one electron and one positron. Also, the partial coupling technique is assumed, whereby photons can produce electrons, but electrons do not produce photons. Regarding the latter, the energy from Bremsstrahlung photons is assumed to be negligible and is discarded.

These assumptions have only a minor effect on the energy deposition field, and are similar to those employed in clinical Monte Carlo codes. A primary assumption of Equation 2 is that the Fokker-Planck operator (of which the CSD operator is the first order term), is used for Coulomb, or “soft”, interactions that result in small energy losses. Catastrophic interactions that result in large energy losses are represented with the standard Boltzmann scattering. This can be seen as the deterministic equivalent to electron condensed history models in Monte Carlo.
To represent the anisotropic behavior of the differential scattering and production sources, in a mathematically practical manner, the macroscopic differential scattering cross sections are expanded into Legendre polynomials, $P_l(\mu_0)$, where $\mu_0 = \hat{\Omega} \cdot \hat{\Omega}'$. This expansion allows the differential scattering or production cross section(s) to be expressed as:

**Eq. 6**

$$
\sigma_{s}^{\gamma \gamma'/ee}(\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}') = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} \sigma_{s,l}^{\gamma \gamma'/ee}(\vec{r}, E' \rightarrow E)P_l(\mu_0),
$$

Similarly, the angular fluence appearing in the scattering source is expanded into spherical harmonics moments:

**Eq. 7**

$$
\Psi(\vec{r}, E', \hat{\Omega}') = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \phi_{l,m}(\vec{r}, E')Y_{l,m}(\hat{\Omega}'),
$$

where

- $Y_{l,m}(\hat{\Omega})$ = Spherical harmonic functions
- $l, m$ = Angular indices
- $\phi_{l,m}(\vec{r}, E')$ = Spherical harmonics moments of the angular fluence, calculated as:

$$
\int_{4\pi} d\Omega' Y_{l,m}^{*}(\hat{\Omega}')\Psi(\vec{r}, \hat{\Omega}', E),
$$

where * denotes the complex conjugate

$\sigma_{s}^{ee}$ = Macroscopic electron-to-electron differential scattering cross section

Equations 6 and 7 are exact. Additionally, for purely isotropic scattering, $l = 0$ is also exact. However, Acuros XB sets a limit on the scattering order, $l \leq 7$, and hence the number of spherical harmonic moments kept in the scattering/production source. Using the Legendre addition theorem, the scattering and production sources become:

**Eq. 8**

$$
q_{\gamma\gamma'/ee}(\vec{r}, E, \hat{\Omega}) = \sum_{l=0}^{7} \sum_{m=-l}^{l} \int dE' \sigma_{s,l}^{\gamma\gamma'/ee}(\vec{r}, E' \rightarrow E)\phi_{l,m}(\vec{r}, E')Y_{l,m}(\hat{\Omega}).
$$
**Step 1: Transport of source model fluence into the patient**

The external photon and electron sources, \( q^\gamma \) and \( q^e \), are modeled as anisotropic point sources in Acuros XB. At each static beam phase space (i.e. control point), a separate point source exists for each of the AAA sources. For the primary source, the anisotropy of \( q^\gamma \) is described through a 2D fluence grid, in which both the particle fluence and energy spectra are spatially variable. For the extra-focal and wedge scatter sources, the anisotropy of \( q^\gamma \) is described through a 3D fluence grid, and the energy spectra is spatially constant. For the electron contamination source, the anisotropy of \( q^e \) is described through a 3D fluence grid, and the energy spectra is spatially constant. All point sources are located at the target for the respective control point.

For a photon point source, \( q^\gamma (E, \hat{\Omega}) \) located at position, \( \vec{r}_p \), Equation 1 becomes:

**Eq. 9**

\[
\hat{\Omega} \cdot \nabla \Psi^\gamma + \alpha^\gamma \Psi^\gamma = q_i^\gamma + q^\gamma (E, \hat{\Omega}) \delta (\vec{r} - \vec{r}_p),
\]

where

\[
\delta = \text{Dirac-delta function}
\]

The principle of linear superposition may be used to define the photon angular fluence as the summation of uncollided and collided fluence components,

**Eq. 10**

\[
\Psi^\gamma = \Psi^\gamma_{unc} + \Psi^\gamma_{coll},
\]

where

\( \Psi^\gamma_{unc} \) = Uncollided, or unscattered, photon angular fluence. Refers to photons which have not yet interacted with the patient/phantom.

\( \Psi^\gamma_{coll} \) = Collided, or scattered, photon angular fluence. Refers to photons which were produced or scattered by a photon interaction in the patient/phantom.

Substituting Equation 10 into Equation 9, leads to the following equation for the uncollided photon fluence:

**Eq. 11**

\[
\hat{\Omega} \cdot \nabla \Psi^\gamma_{unc} + \alpha^\gamma \Psi^\gamma_{unc} = q^\gamma (E, \hat{\Omega}) \delta (\vec{r} - \vec{r}_p),
\]
A property of Equation 11 is that \( \Psi_{unc}^{\gamma} \) can be solved for analytically. Doing so provides the following expression for the uncollided photon angular fluence from a point source:

**Eq. 12**

\[
\Psi_{unc}^{\gamma}(\vec{r}, E, \vec{\Omega}) = \delta(\vec{\Omega} - \vec{\Omega}_{\vec{r}, \vec{r}_p}) q^{\gamma}(E, \vec{\Omega}) \frac{e^{-\tau(\vec{r}, \vec{r}_p)}}{4\pi |\vec{r} - \vec{r}_p|^2},
\]

where

\[
\vec{\Omega}_{\vec{r}, \vec{r}_p} = |\vec{r} - \vec{r}_p|, \quad \text{where } \vec{r}_p \text{ and } \vec{r} \text{ are the source and destination points of the ray trace, respectively.}
\]

\[
\tau(\vec{r}, \vec{r}_p) = \text{The optical distance (measured in mean-free-paths) between } \vec{r} \text{ and } \vec{r}_p.
\]

Equation 12 is solved for each primary, extra focal, and wedge source in the calculation, to compute \( \Psi_{unc}^{\gamma} \) throughout the patient. The electron contaminant source is modeled in a similar manner, but with the inclusion of the CSD operator to account for charged particle interactions.

**Step 2: Transport of scattered photon fluence in the patient**

Once Equation 12 is solved, \( q_{unc}^{\gamma} \) is calculated according to Equation 8, and is considered a fixed source in Equation 13, which is solved to compute \( \Psi_{coll}^{\gamma} \) throughout the patient:

**Eq. 13**

\[
\hat{\Omega} \cdot \nabla \Psi_{coll}^{\gamma} + \sigma_{e}^{\gamma} \Psi_{coll}^{\gamma} = q_{coll}^{\gamma} + q_{unc}^{\gamma},
\]

where

\( q_{unc}^{\gamma} = \) First scattered photon source. Refers to photons which are created or scattered from the first photon interaction inside the patient/phantom.

\( q_{coll}^{\gamma} = \) Secondary scattered photon source. Refers to photons which are created or scattered from secondary photon interactions inside the patient/phantom.
Step 3: Transport of scattered electron fluence in the patient

Once Equation 13 is solved, \( q_{\text{coll}} \) is calculated according to Equation 8, and is considered a fixed source in Equation 14. Similarly, from the solution to Equation 12, \( q_{\text{unc}} \) is calculated according to Equation 8, and is also considered a fixed source in Equation 14. Equation 14 is solved to compute \( \Psi^e \) throughout the patient:

\[
\hat{\Omega} \cdot \nabla \Psi^e - \frac{1}{E} \frac{\partial}{\partial E} \sum_{\nu} \Psi^e = q_{\text{coll}} + q_{\text{unc}} + q^e,
\]

where

\( q_{\text{unc}} \) = First scattered electron source. Refers to electrons which are created or scattered from the first photon interaction inside the patient/phantom.

\( q_{\text{coll}} \) = Secondary scattered electrons source. Refers to electrons which are created or scattered from secondary photon interactions inside the patient/phantom.

Discretization methods

Acuros XB discretizes in space, angle, and energy to iteratively solve Equations 12 through 14, the methods of which are discussed below.

Spatial discretization

The computational grid in Acuros XB consists of spatially variable Cartesian elements, where the local element size is adapted to achieve a higher spatial resolution inside the beam fields, with reduced resolution in lower dose, lower gradient regions outside the beam penumbra. Commonly referred to as adaptive mesh refinement (AMR), the mesh is limited to refinement in factors of 2 (from one level to the next) in any direction, allowing for localized refinement to resolve areas of sharp gradients. Spatial discretization is performed through using a linear discontinuous Galerkin finite-element method [ref. 1], providing a linear solution variation throughout each element, with discontinuities permitted across element faces. The first scattered photon and first produced electron sources, obtained from solving Equation 12, are also represented as linear varying functions in each element, since these sources are used for the linear discontinuous discretization of Equations 13 and 14. To accurately integrate these first scattered sources, the analytic solution is computed at a density inside the primary beam and penumbra of at least 8 ray traces per output grid voxel.
Energy discretization

Energy discretization is performed through the standard multigroup method [ref. 1], which is used in both the energy dependence of Equations 12 and 13 and the Boltzmann scattering in Equation 14. In energy, the energy derivative of the continuous slowing down (CSD) operator in Equation 14 is discretized using the linear discontinuous finite-element method [ref. 3]. The Acuros XB cross section library includes 25 photon energy groups and 49 electron energy groups, although not all groups are used for energies lower than 20 MV.

Angular discretization

For the spatial transport of the scattered particle field, the discrete ordinates method is used to discretize in angle [ref. 1]. The discrete ordinates method consists of requiring Equations 13 and 14 to hold for a fixed number of directions, $\hat{\Omega}_n$. These discrete directions are chosen from an angular quadrature set that also serves to compute the angular integrals in Equation 5 for the generation of the scattering source. Square-Tchebyshev legendre quadrature sets are used and the quadrature order ranges from $N=4$ (32 discrete angles) to $N=16$ (512 discrete angles). The angular quadrature order varies both by particle type and energy. Higher energy particles have longer mean free paths, or ranges for electrons, and thus for each particle type, the angular quadrature order is increased with the particle energy.

Spatial transport cutoff

Acuros XB employs a spatial cutoff for photon energies below 1 keV and electron energies below 500 keV. When a particle passes below the cutoff energy, any subsequent interactions are assumed to happen locally in that voxel.

Additional errors may also be present from the internally set convergence tolerances in Acuros XB. These tolerances control how tightly the inner iterations in Acuros XB are converged in energy group. These errors will generally be on the order of 0.1% of the local dose in any voxel.
Step 4: Dose calculation

Once Acuros XB solves for the electron angular fluence for all energy groups, the dose in any output grid voxel, \( i \), of the problem is obtained through the following:

\[
D_i = \int_0^\infty dE \int_4\pi d\hat{\Omega} \frac{\sigma_{ED}^e(r', E)}{\rho(r')} \Psi^e(r', E, \hat{\Omega}),
\]

where

\[
\sigma_{ED}^e = \text{Macroscopic electron energy deposition cross sections in units of MeV/cm} \\
\rho = \text{Material density in g/cm}^3
\]

Acuros XB supports two dose reporting options: dose-to-water (\( D_W \)) and dose-to-medium (\( D_M \)). When \( D_M \) is calculated, \( \sigma_{ED}^e \) and \( \rho \) are based on the material properties of output grid voxel, \( i \). When \( D_W \) is calculated, \( \sigma_{ED}^e \) and \( \rho \) are based on water. Since Equation 15 is calculated as an internal post processing operation after the energy dependent electron fluence is solved, both \( D_M \) and \( D_W \) can be theoretically obtained from a single transport calculation.