SAND2020-3581

SANDIA REPORT

Printed March 2020

RAPTURE User's Guide

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ABSTRACT

This User's Guide serves as a brief introduction to the RAPTURE radiation effects analysis code. It includes an overview of the input format, RAPTURE's error- and consistency-checking of the user-provided input files, the automatic-differentiation and convergce-checking schemes employed by RAPTURE, and the RAPTURE output files. A variety of example problems are included in this Guide which collectively demonstrate RAPTURE's current capabilities and provide a suite of test problems and template input files for the user. This Guide includes, for each problem, the problem description, RAPTURE input files, and comparison of the RAPTURE solution with solutiong generated with the Monte Carlo transport code ITS, the legacy deterministic code ADEPT, and, where possible, published experimental results. An appendix includes a description of all keywords and options in the RAPTURE input file.

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NOMENCLATURE

Table 0-1.

Abbreviation	Definition
AWE	Atomic Weapons Establishment
DOE	Department of Energy
GUI	Graphical User Interface
SNL	Sandia National Laboratories
S_N	Discrete ordinates method of angular discretization
P_N	Legendre Moments method of scattering
QoI	Quantity of Interest

1. THE RAPTURE CODE

1.1. Overview

RAPTURE is a coupled photon-electron radiation-effects analysis tool for one-dimensional slab geometries. RAPTURE is applicable to a variety of radiation-effects problems, uses a straightforward and verbose input format, can be run on a variety of operating systems, and is actively supported by developers in the Radiation Effects Theory Department at Sandia National Laboratories (SNL) and the Radiation Science Group at the Atomic Weapons Establishment (AWE). RAPTURE serves as a modern alternative to the legacy code ADEPT.

Many photon-electron radiation effects problems are adequately modelled with one-dimensional slab geometries due to the highly forward-peaked anisotropic scattering displayed by these particles. RAPTURE is also valuable as a scoping tool to inform the discretization of multi-dimensional problems. The space and energy discretizations necessary to converge QoIs in a representative one-dimensional problem can inform the meshing of a two- or three- dimensional problem.

RAPTURE uses the deterministic transport code SCEPTRE[9][10] and the photon-electron cross-section generation code CEPXS[5] to perform radiation transport calculations, inheriting the extensive history of verification and validation efforts associated with these codes. Modern software design practices including version control, unit and regression testing, and a portable release system distinguish RAPTURE from the legacy code ADEPTand its predecessors [7][8][4]. RAPTURE, SCEPTRE, and CEPXSare production codes that are actively supported by developers at SNL and AWE.

The RAPTURE input file uses the verbose XML format which emphasises clarity and avoids ambiguity in the problem description. The input file describes the problem to be solved but does not require the user to specify the numerical methods that are to be used to solve the problem. The user must specify the problem geometry, the materials present in the problem, the radiation source that drives the problem, and the quantities of interest (QoIs) that motivate the problem. The problem geometry is characterized in terms of thicknesses. Materials are described by density and the mass fraction of the constituent elements. Radiation sources may be mono-energetic, constant in energy, or a spectrum defined by a probability density function (PDF) or cumulative distribution function (CDF). RAPTURE supports a variety of QoIs, including energy deposition, charge deposition, or kerma in a region of interest, reflected or transmitted spectra, or response functions for energy deposition or kerma. Comprehensive error checking and verbose error messages alert the user to mistakes in the input file before calculations begin.

Discretization and solution of the problem specified in the input file is automatically performed by RAPTURE. RAPTURE generates a spatial mesh, a multigroup energy discretization and multigroup cross sections, and an angular discretization based upon the radiation source and the QoI(s). The radiation transport problem is solved using these physics-informed space, angle, and energy discretizations. The discretization of the phase space is iteratively refined until all QoIs converge to a user-specified tolerance. The physics-based rules in RAPTURE are similar to the heuristic rules found in ADEPTbut the addition of a convergence study improves the reliability and accuracy of the RAPTURE results as compared to results generated by ADEPT.

RAPTURE produces as output text files and plots of the QoI(s) requested by the user and a collection of the input files necessary to rerun the fully-converged SCEPTREproblem to reproduce the reported solution. All of the input and output files used to produce the final, converged solution are also collected and presented alongside the reported QoI.

RAPTURE is released under a commercial copyright from Sandia National Laboratories. The licence is free. RAPTURE is released via Docker, a free commercial product that enables cross-platform portability [1]. RAPTURE and all necessary libraries are compiled and installed by the development team and packaged as a Docker Container. Users install RAPTURE by downloading and installing Docker, obtaining the RAPTURE Docker Container from SNL, and then loading the RAPTURE Container in Docker. No compilation is required on the part of the user. This release method supports users that wish to run RAPTURE in Linux, Windows, and Apple environments.

1.2. Physics Codes

RAPTURE is a wrapper for the photon-electron cross section generation code CEPXSand the radiation-transport code SCEPTRE. RAPTURE inherits the extensive history of testing, verification, and validation associated with these codes and benefits from the ongoing development on these projects. RAPTURE is extensible as additional features are added to CEPXSor SCEPTREor as new sources of cross-section data become available for use by SCEPTRE.

Photon, electron, and positron cross sections are calculated using CEPXS, the Coupled Electron-Photon Cross Section generation code [5]. CEPXSgenerates multigroup-Legendre cross sections for the interaction of these particles with background materials. CEPXSalso produces cross sections for quantities of interest including charge deposition, energy deposition, kerma, heating, and damage.

A modern successor to CEPXSis being developed by SNL and AWE. In addition to replicating CEPXS' current capabilities the SKEPTXScode will include additional sources of cross-section data and will enable the development of novel representations of the cross-section data. SKEPTXSwill generate cross-sections for low-energy (sub-keV) photons and electrons, which is not available in ADEPTor its predecessors. SKEPTXSmay also eventually generate cross sections for light ions. Research is ongoing into the development of finite-element-in-energy and finite-element-in-angle cross sections for use in SCEPTRE. RAPTURE will transition from CEPXSto SKEPTXSwhen SKEPTXSis released in order to take advantage of these features.

Radiation transport calculations are performed by SCEPTRE2.0, the Sandia Computational Engine for Particle Transport for Radiation Effects [9][10]. SCEPTREis a deterministic radiation transport code, discretizing the spatial variable with a finite-element method, the energy variable with the multigroup method, and the angular variable with the discrete ordinates method. SCEPTREsolves the linear Boltzmann transport equation in one-, two-, and three-dimensional geometries and has the capability to solve either the first-order or second-order form of the Boltzmann transport equation.

RAPTURE, SCEPTRE, and SKEPTXSutilize modern software engineering practices and contain comprehensive unit, integration, and method of manufactured solutions tests.

1.3. Input and Output Files

This section contains a qualitative overview of the RAPTURE input file and a description of the output files produced by RAPTURE. A complete description of the RAPTURE input options is included in Section 2 of this manual.

The RAPTURE input file is constructed with XML formatting. This verbose format thoroughly and explicitly characterizes the problem to be solved. This decreases the potential for mistakes in the problem description but results in lengthy input files. A future release of RAPTURE may support a lighter-weight input format like JSON in addition to XML. The input file must contain sections describing the problem geometry, composition of the problem, driving sources, and quantities of interest.

Extensive error checking is performed by RAPTURE to ensure that the input file is complete and self-consistent. Each entry in the XML input deck is checked to ensure both that the XML tag is recognized and that the specified option is allowed. This avoids errors in which portions of the input deck are silently ignored by RAPTURE. The consistency of the input deck is checked thoroughly before physics calculations are performed to catch errors (and warn the user of potential errors) before setting up and solving the physics calculations. Thorough error checking and verbose error and warning messages at this stage of the calculation provide timely and clear feedback to the user.

Once error checking of the input deck is successfully completed RAPTURE generates an initial discretization of the user- specified problem, solves the radiation transport problem and calculates the QoIs, and performs a convergence study on the QoIs as a function of the discretization of the problem. Once the QoIs are converged RAPTURE collects and organizes output for the user. This output includes the user-specified QoIs in both tabular and plot form and all of the files used in the calculation of the converged QoIs. These files include the CEPXSinput file used to generate the multigroup cross sections and the SCEPTREinput files used to generate the spatial mesh, solve the transport problem, and post- process the solution to compute QoIs. Collecting and preserving these input decks documents the exact problem specification that produced the fully-converged RAPTURE results.

1.4. Driving Sources

RAPTURE supports a variety of driving radiation sources. Sources may be photons or electrons normally or isotropically incident on the left boundary of the slab geometry. Sources may be mono-energetic, constant in energy, or described by a spectrum provided to RAPTURE as a tabular data file. Spectrum sources may be described as either a probability density function (PDF) or as a cumulative distribution function (CDF) in units of particles per energy. For problems in which the QoI is transmitted or reflected radiation the driving spectrum is included in the plot of the QoI. Source strengths are characterized as either a number of particles or an energy fluence in units of joules (or joules per square centimeter).

The driving source is considered in the discretization of the energy variable. Energy group boundaries are added to accurately capture mono-energetic and constant radiation sources. Source spectra that particles below the cutoff energy of 1 keV are modified based on the quantity of interest. For reaction rate QoIs related to the number of particles (such as charge deposition) the total number of particles contained in the source spectrum is preserved. For reaction rate QoIs related to the total amount of energy in the driving source that energy is preserved. In both cases the number of particles in the lowest-energy group is modified to preserve the quantity relevant to the QoI. For problems in which the QoI is spectrum the input spectrum is truncated at 1 keV without modifying the lowest-energy group.

The initial release of RAPTURE does not explicitly model positrons created by high-energy photons. These particles are initially approximated in the generation of cross sections by CEPXS. The positron treatment used by CEPXSdepends upon the RAPTURE QoI. For problems with a QoI related to charge deposition the positrons are approximated as depositing their energy locally. This preserves charge but slightly skews energy deposition. For problems with an energy deposition QoI positrons are approximated as electrons, which slightly skews charge deposition but yields a good approximation of energy deposition. A future release of RAPTURE will directly model positrons and preserve both charge and energy.

Future releases of RAPTURE will include several improvements to source modeling in RAPTURE. These will include support for sources incident at angles besides normal incidence on the left face of the problem, source strengths specified in units of particles or units of energy fluence, explicit treatment of sources with components below 1 keV, and the ability to specify multiple mixed sources in a single problem.

1.5. Quantities of Interest

RAPTURE supports the calculation of three broad categories of QoIs: radiation spectra, reaction rates, and response functions. The first category of QoIs include transmitted and reflected photon and electron spectra. These are output as tabular data files and as plots which include the driving radiation spectrum. Spectra QoIs are converged based on the number of particles of each species exiting through the left or right face of the problem for reflection and transmission QoIs, respectively.

Reaction rate QoIs include energy deposition, kerma, and charge deposition. Future releases of RAPTURE may allow users to specify addition reaction rate QoIs. Reaction rates may be requested in per mass or per volume units and are reported in every spatial cell, as region-integrated values, and as local minima and maxima with the associated position of these extrema. Reaction rate QoIs are converged based upon the region-integrated values for regions of interest specified in the input deck.

Response functions may be specified as the QoI for any of the reaction rate QoIs. These QoIs return the adjoint spectra through the left face of the slab. The response functions are generated by performing adjoint radiation transport calculations. RAPTURE calculations for response functions do not accept an input source; rather, the cross sections that describe the response of interest form a volumetric source in the region of interest. SCEPTREincludes an adjoint capability which is utilized for these calculations. The response function QoIs are converged based upon the number of particles in the radiation spectrum on the left face of the problem.

A single RAPTURE problem may contain multiple spectra QoIs or multiple reaction rate QoIs or a single response function QoI. Problems with reaction rate QoIs may contain multiple reactions and multiple regions of interest. Problems with spectra QoI may specify both transmission and reflection spectra for both photons and electrons. Response function QoIs require a RAPTURE calculation per QoI.

1.6. Automatic Discretization in RAPTURE

RAPTURE handles the discretization of the space, angle, and energy variables for the user. Heuristic rules are used to establish an initial discretization for each of these three variables. A convergence study is performed to determine the necessary resolution in each variable. The following sections outline the discretization scheme used in each variable, the heuristic rule used to initially discretize the variable, the mesh refinement scheme used to converge the QoI, and the convergence scheme used to ensure that each variable is appropriately discretized.

1.7. Spatial Discretization

The spatial dimension is discretized into using linear discontinuous finite elements. This scheme subdivides the one-dimensional slab into spatial cells and solves a system of linear equations for the solution in every cell. Cell thicknesses vary across the problem; cells are very thin at material discontinuities and near the problem boundaries and grow logarithmically as distance from a discontinuity increases. This “feathering” of the spatial mesh is intended to resolve boundary-layer effects.

The initial discretization is chosen based upon the radiation source, the QoI, and material properties of each region. Problems with electron sources, charge deposition QoIs, or electron spectrum QoIs require resolving the range of low-energy electrons, especially near the boundaries of the region of interest. For these types of problems the smallest spatial cells are chosen to resolve the range of the lowest-energy electron groups and the largest cells are limited by the range of electrons in the highest-energy groups. Similarly, spatial cell thicknesses for problems with photon spectra QoIs or energy deposition QoIs are bounded by the mean free path of the lowest-energy and highest-energy photon groups. Maximum cell sizes are also bounded such that each cell is no more than ten percent of the region’s thickness in centimeters.

The midpoint of each spatial region is established before the spatial meshing is started. Cell thicknesses grow logarithmically as the distance from material discontinuities increases until the maximum cell thickness is reached or the midpoint between material discontinuities is reached.

The spatial mesh is iteratively refined by scaling the maximum and minimum cell sizes by a factor of one half per iteration. Note that this does not double the number of spatial cells used in each iteration due to the nonlinear method in which the minimum and maximum cell sizes are determined and the logarithmic growth of the cell sizes between these values.

1.8. Angular Discretization

The angular variable is discretized using the discrete ordinates (or S_N) method, a discretization scheme common to deterministic radiation transport. `RAPTURE` uses a Gauss-Lobatto quadrature. This quadrature set includes the directions $\cos(\theta) = \pm 1.0$ in addition to the standard Gauss quadrature directions. This quadrature set is well-suited to one-dimensional radiation-effects calculations as it allows normally-incident radiation sources to be exactly represented. This removes an approximation inherent in the use of a Gauss-Legendre quadrature set (as in `ADEPT`) which requires approximating normally-incident sources by placing them in the angular bin closest to $\cos(\theta) = 1.0$.

`RAPTURE` currently allows only isotropic and normally-incident radiation sources. A future release of `RAPTURE` will include the ability to specify sources at angles besides $cos(\theta) = 1.0$. In these cases the problem geometry will be scaled such that the source is normally-incident, the problem will be solved on this scaled geometry, and then the QoI will be scaled back to the user-specified dimensions.

Radiation scattering is modelled by expanding the radiation source as a Legendre polynomial (the P_N approximation). An initial scattering order of P_5 is applied. The angular quadrature order is chosen such that it can exactly integrate polynomials of the scattering order. An S_{12} angular quadrature set is paired with the P_5 scattering source. At each iteration in the convergence study the scattering order is increased by one and the discrete ordinates order is chosen such that it can exactly integrate the scattering source.

1.9. Energy Discretization

The energy variable is discretized with the multigroup method. This scheme divides the continuous energy variable into discrete energy groups and then represents energy-dependent quantities with piecewise-constant or step finite elements. The problem's upper energy bound is set by the upper energy of the radiation source; the lower energy bound is set at 1 keV. Energy groups are chosen so that they are of constant width in log space. `RAPTURE` uses a single set of group boundaries for both photons and electrons, although additional group boundaries may be added to the group structure used for either particle species in order to characterize the problem source.

`RAPTURE` includes mono-energetic and constant sources by modifying the log-spaced energy-group structure applied to the source particle. Constant sources are represented by the addition of group boundaries that correspond to the limits of the constant source. Mono-energetic sources are included by the addition of an energy group with width equal to one percent of the source energy centered at the source energy. For example, a mono-energetic source at 1 MeV is represented by a group 10 keV wide with group bounds at 995 keV and 1005 keV. Both constant and mono-energetic sources may span multiple groups if a group boundary exists between the upper and lower limits of the source.

Mesh refinement is performed by doubling the number of log-spaced energy groups used for both particle species. This doubling is performed before group boundaries are added to represent the source.

Research is ongoing to determine an optimal energy-discretization scheme for `RAPTURE`. Problem-specific physics-informed group structures should reduce the number of energy groups required to resolve the energy-dependent photon and electron fluxes, reducing both the time required to solve each transport problem and the number of mesh-refinement iterations necessary to resolve the QoIs. These physics-informed group structures may be generated by choosing group boundaries such that they correspond to shell edges, which create discontinuities in otherwise smoothly-varying cross sections. Placing energy group bounds at the shell edge energies should improve the multigroup approximation of the cross sections and the solution. This approach is complicated by the large number of edges that are present in problems with multiple materials.

In the future finite-element-in-angle and finite-element-in-energy cross sections may be produced by SKEPTXSand used by SCEPTRE. In theory a linear-discontinuous representation of the energy variable should show significant advantages over the piecewise-constant multigroup representation. If these discretization schemes offer significant advantage over the traditional multigroup-Legendre method these schemes will be implemented in RAPTURE.

1.10. Convergence Study

The space, angle, and energy discretizations used by RAPTURE are initially chosen based upon heuristic rules related to the physics of the problem to be solved. A convergence study is performed to verify that the QoIs reported by RAPTURE are accurate and free of discretization errors. It should be noted that this discretization study cannot guarantee that the solution is free of discretization errors, but when paired with the physics-informed initial discretization the user may be confident in the RAPTURE results.

The finite element method employed to discretize the spatial variable is guaranteed to monotonically converge towards the correct solution as the mesh is refined. Unfortunately, no such guarantees exist for the multigroup method employed to discretize the energy variable or the discrete ordinates method applied to the angular variable. It is possible that the finite-element-in-angle and the finite-element-in-energy methods under development in the SCEPTREand SKEPTXSprojects may produce discretizations for these variables that do carry these guarantees, and if so, they may be incorporated in RAPTURE.

The convergence scheme used by RAPTURE may be described in terms of “outer” iterations, in which the space, angle, and energy variables are refined simultaneously, and “inner” calculations, in which each variable is independently refined. Each outer iteration consists of four inner calculations: a base calculation using the current space, angle, and energy discretizations, a calculation using a refined spatial mesh, a calculation using a refined angular mesh, and a calculation using a refined energy mesh. The QoI(s) are calculated for each of the four inner calculations. Another outer iteration is required if any of the refined calculations produce a QoI that differs from the base QoI by more than the user-specified tolerance. The base calculation in the next outer iteration uses the refined meshes for each variable that was not yet converged in the current outer iteration. For each variable, if the inner iteration does not result in a change to the QoI, the base mesh is not refined for the next outer iteration.

The outer iterations always contains an inner calculation with a refined mesh in the space, angle, and energy variables. These calculations are performed even if refining a particular variable did not produce a change in the QoI(s) in a previous outer iteration. As RAPTURE performs the four inner calculations in parallel this does not generally result in increased runtime. This scheme ensures that the discretization error in the three variables is comparable.

The spatial mesh is coupled to the energy mesh through the electron range and the photon mean free path. As the energy group structure is refined the average energy in the lowest group decreases, decreasing the particle's characteristic length in that energy group. Similarly the average energy in the highest energy group increases as the mesh is refined, increasing the characteristic length of particles in that energy group. In scenarios in which the inner calculations suggest that the spatial mesh does not need to be refined the minimum and maximum spatial cell sizes are not halved for the next outer iteration; however, the minimum and maximum cell sizes will change if the energy mesh is refined.

The cost associated with refining the meshes is multiplicative. The cost associated with refining the angular variable is small. However, refining the space and energy meshes each result in a factor of approximately two increase in the solve time. In the case where the first outer iteration concludes that both the energy and the spatial meshes need to be refined, the second outer iteration's base problem is almost four times as expensive as the base problem in outer iteration one. Outer iteration two's calculation using the refined spatial mesh is about eight times as expensive as outer iteration one's base calculation.

Each SCEPTREcalculation is performed one a single processor. If four processors are available RAPTURE will automatically perform the convergence study in parallel. If fewer than four processors are available than the calculation is performed serially.

Upon convergence RAPTURE collects and presents the most refined QoI data. Although the iterative convergence scheme has determined that meshes used in the base calculation were fine enough to resolve the QoI, as the more-refined calculations have already been performed there is no penalty in presenting this information to the user. For spectrum QoIs RAPTURE returns the calculation with the finest energy group structure. For reaction rate QoIs the calculation with the finest spatial mesh is returned.

1.11. Release

Cross-platform compatibility is achieved using the commercial product Docker[1]. Docker provides a virtual Linux environment that may be run on Windows, Apple, or Linux computers. A RAPTURE release consists of a Docker container that includes RAPTURE, SCEPTRE, CEPXS, and the third-party libraries required by those codes. The RAPTURE installation process for users consists of downloading and installing Docker, obtaining a current RAPTURE Docker container, and loading the RAPTURE container in Docker.

This section will be updated with more detailed instructions when the Docker release is ready.

1.12. Future Releases of RAPTURE

The RAPTURE code is under active development at SNL and AWE. After the initial RAPTURE 1.0 release a series of minor releases will incorporate additional features. These will include source specification at angles other than normal incidence, the ability to specify source strengths in units of energy in addition to units of particles, the explicit treatment of positrons, the ability for the user to specify an energy group structure, and the ability for a user to specify a spatial mesh or to provide a spatial mesh file. The XML input format may also be supplemented by a lighter-weight JSON interface.

Additional features may be added to RAPTURE if there is sufficient user interest in the features. This could include libraries of laboratory or experimental radiation sources and a collection of standard materials. Additional QoIs, such as the ability to generate response functions for charge deposition, could be implemented if such features are desired by the radiation-effects community.

A major update to RAPTURE will occur when the cross-section generation code SKEPTXSis released by Sandia National Laboratories. SKEPTXSwill enable sub-keV calculations by incorporating data sets not found in CEPXS. SKEPTXSmay also generate finite-element-in-angle and finite-element-in-energy cross sections that may improve the convergence properties of the angle and energy meshes used by SCEPTRE.

Feature requests and bug reports are accepted at rapture-help@sandia.gov.

1.13. Conclusion

The RAPTURE code is a valuable tool for the analysis of one-dimensional coupled photon-electron radiation transport problems. Given a problem description and a desired quantity of interest, RAPTURE determines the space, angle, and energy discretization necessary to resolve the solution and calculate a converged QoI. Built on the SCEPTREand CEPXScodes, RAPTUREinherits the extensive testing, verification, and validation efforts associated with modern production codes. In addition to current capabilities, RAPTURE's use of SCEPTREallows the rapid incorporation of methods development in SCEPTREand the CEPXSsuccessor SCEPTXS. These features make RAPTURE a valuable and practical tool for a variety of applications.

2. RAPTURE INPUT

This section documents the RAPTURE input file. All mandatory and optional components of the input file are described in detail in this section. An alphabetical reference of all RAPTURE input keywords is included in Appendix A.

The RAPTURE input is divided into several sections: Materials Input, Geometry Input, Radiation Source Input, and QoI Input. Each of these components are explained in detail in the following subsections.

RAPTURE performs extensive error checking of the user input before beginning CEPXSor SCEPTREcalculations. The error checking associated with each section of the input deck is explained in the appropriate section. Integral-level testing includes checking that each entry in the RAPTURE input is expected; misspelled XML tags will yield an error rather than a silent failure. Missing or duplicated sections of the input will cause an error. Error messages include the exact cause of the error to assist the user in fixing the RAPTURE input.

The RAPTURE input deck is not case sensitive (with one important exception discussed in the section describing the radiation source input). Although this avoids many potential errors in setting up the XML tags it can potentially introduce subtle errors in the input deck. The user is encouraged to think carefully about material and region names to avoid these potential errors.

2.1. Materials Input

The materials input section of the RAPTURE input is contained within <material_input> XML tags and contains all of the materials present in the problem. Each material must contain a unique name defined with the <name> keyword, a mass density in units of gram per centimeter cubed specified with the <mass_density> keyword, and the list of each element present in the material, each of which is defined using the <element> keyword. Each element is defined by its atomic symbol <symbol> and mixed according to mass fraction <mass_fraction>. For each material the elemental mass fractions must sum to 1.0.

RAPTURE recognizes the special material "void." This material is entered without specifying a density of elemental composition.

```
   <Materials_Input>
    <Material>
      <Name>copper</Name>
      <Mass_Density>8.90</Mass_Density>
      <Element>
        <symbol>Cu</symbol>
      </Element>
    </Material>
    <Material>
      <Name>water</Name>
      <Mass_Density>1.00</Mass_Density>
      <Element>
        <Symbol>H</Symbol>
        <Mass_Fraction>0.1121</Mass_Fraction>
      </Element>
      <Element>
        <Symbol>O</Symbol>
        <Mass_Fraction>0.8879</Mass_Fraction>
      </Element>
    </Material>
    <Material>
      <Name>void</Name>
    </Material>
  </Materials_Input>
```

RAPTURE's error checking of this section of the user input will check that each material name is unique, each element is recognized, that each density is greater than zero, and that mass fractions for each material sum to 1.0.

2.2. Geometry Input

The geometry input section <geometry_input> defines the 1-D slab geometry. The problem geometry is defined as a series of regions with keyword <region>. The geometry must contain at least one region. Each region must contain a name <name>, a thickness <thickness> in units of centimeters, and composition <composition>. Each composition must name one of the materials defined in the <materials> section of the `RAPTURE` input deck.

```
<Geometry_Input>
  <Region>
    <Name>Conductor</Name>
    <Thickness>0.025</Thickness>
    <Composition>Copper</Composition>
  </Region>
</Geometry_Input>
```

The maximum cell size used in the spatial discretization of a region may be specified on a per-region basis using the keyword <maximum_element_size>. The maximum element size is specified in units of centimeters and must be smaller than the region for which it is specified. Although it is not recommended the user may use the <spacing> keyword to specify either “linear” or “logarithmic” mesh spacing on a per-region basis.

```
<Geometry_Input>
  <Region>
    <Name>WetLayer</Name>
    <Thickness>1.0</Thickness>
    <Composition>Water</Composition>
    <Spacing>logarithmic</Spacing>
  </Region>
  <Region>
    <Name>Conductor</Name>
    <Thickness>0.025</Thickness>
    <Composition>Copper</Composition>
    <Maximum_Cell_Size>0.0025</Maximum_Cell_Size>
    <Spacing>linear</Spacing>
  </Region>
</Geometry_Input>
```

2.3. Radiation Source Input

A variety of radiation sources may be defined to drive a RAPTURE calculation. These sources are defined in the <radiation_source_input> section of the RAPTURE input deck. This section is necessarily more complex than the preceding sections. All "forward" RAPTURE calculations must include at least one radiation source. All external sources impinge upon the left face of the slab. RAPTURE problems that take advantage of SCEPTRE's adjoint mode to calculate response functions must not include a <radiation_source_input> section.

Each source is defined with the <source> keyword and must contain:

- a <radiation_type> keyword, either "photon" or "electron",
- a <source_format> keyword, either "mono-energetic", "constant", or "tabular",
- a <source_angular_distribution> keyword, either "plane-wave" or "isotropic".

If "plane-wave" is specified as the <source_angular_distribution> keyword the angle of the source on the left face of the slab may be specified using the <angle> keyword. The angle is defined in units of degrees measured from normal; that is, an angle of 0 is normally-incident. If the "plane-wave" is specified for the angular distribution and the <angle> keyword is not specified a normally-incident source is assumed. The initial release of RAPTURE does not support plane wave sources at incident angles besides zero degrees; a future release of RAPTURE will enable this functionality.

If the <source_format> is specified as either "mono-energetic" or as "constant" the <source_energy> keyword must be provided. Energies are specified in units of MeV. Mono-energetic sources are defined with a single energy. Constant sources are defined with the endpoints of the source, starting with the upper energy bound of the source and followed by the lower energy bound of the source. Sources below 1 keV are not accepted. RAPTURE will report an error if a mono-energetic source is defined with more than one energy, if the <energy> keyword for a constant source does not contain exactly two doubles in decreasing order, or if an energy below 1 keV is specified.

Complicated spectra may be provided by setting the <source_format> keyword to "tabular" and providing the <spectrum_file_name> and <spectrum_file_format> keywords. The <spectrum_file_name> keyword must contain either the absolute or relative path (relative to the RAPTURE input file) to a text file containing the radiation source. Unlike other fields in the RAPTURE input file the spectrum file name is case-sensitive. The use of spaces in the spectrum file name is discouraged. The spectrum file format may be either "PDF" or "CDF", referring to a probability density function or cumulative density function, respectively. RAPTURE will report an error if it can not find the source file specified in this section or if the source file is not in the format expected by RAPTURE.

The text file containing the driving spectrum is a two-column comma- or space-separated list. Comments may be included at the top of the file by starting a line with a leading "#". The first column contains the energy, in units of MeV, ordered from low energy to high energy. The second column contains either the PDF or CDF values of the spectrum in **units of particles**. Please carefully note these units; the specification of a spectrum source has proven to be the most error-prone portion of the RAPTURE input deck. CDFs must start at 0.0 and end at 1.0. PDFs must integrate to 1.0. An example spectrum is included in the test problems released with `RAPTURE`. `RAPTURE` will report an error if the source file does not follow this format, if a CDF does not begin at 0.0 and end at 1.0, or if a PDF does not integrate to 1.0.

The source strength is specified with the <source_strength> keyword. This keyword must be provided for each source and is specified in units of particles. A default value of one particle is applied if this keyword is not included in the source specification. A future release of `RAPTURE` will expand this keyword to allow the user to specify the source strength in units of either particles or energy.

Multiple constant or mono-energetic sources may be specified for a single problem. Spectrum sources are limited to a single source per problem. A future release of `RAPTURE` will allow users to specify plane-wave sources at angles besides normal incidence; however, if a problem contains multiple sources, all sources will need to be specified for the same incident angle.

An example radiaton source input containing both a constant source and a mono-energetic source is included below.

```
<Radiation_Source_Input>
  <Source>
    <Radiation_Type>photon</Radiation_Type>
    <Source_Format>constant</Source_Format>
    <Source_Energy>6.00000 5.041829</Source_Energy>
    <Source_Angular_Distribution>plane-wave</Source_Angular_Distribution>
    <Angle>0</Angle>
    <Number_Of_Source_Particles>1.0</Number_Of_Source_Particles>
  </Source>
  <Source>
    <Radiation_Type>electron</Radiation_Type>
    <Source_Format>mono-energetic</Source_Format>
    <Source_Energy>1.0</Source_Energy>
    <Source_Angular_Distribution>isotropic</Source_Angular_Distribution>
    <Number_Of_Source_Particles>1.0</Number_Of_Source_Particles>
  </Source>
</Radiation_Source_Input>
```

The following section of a RAPTURE input deck demonstrates the specification of a tabular source using a text source file is co-located with the RAPTURE input file.

```
<Radiation_Source_Input>
  <Source>
    <Radiation_Type>photon</Radiation_Type>
    <Source_Format>tabular</Source_Format>
    <Spectrum_File_Name>example_pdf_spectrum.txt</Spectrum_File_Name>
    <Spectrum_File_Format>cdf</Spectrum_File_Format>
    <Source_Angular_Distribution>plane-wave</Source_Angular_Distribution>
    <Angle>0</Angle>
    <Number_Of_Source_Particles>1.0</Number_Of_Source_Particles>
  </Source>
</Radiation_Source_Input>
```

A example PDF source spectrum file (truncated for length) is included below. The full example spectrum is included in the appendices associated with the test problems.

```
# example_pdf_spectrum.txt
# 50 keV endpoint bremsstrahlung
# Mev    cdf
0.013  0.00000
0.014  0.00353
 ...
 ...
0.045  0.99257
0.046  0.99776
0.047  0.99880
0.048  1.00000
```

2.4. QoI Input

The final component of the RAPTURE input deck is the <qoi_input> section. Each RAPTURE input must include this section. Multiple QoIs may be defined within an input deck. Each QoI is defined with the <qoi> keyword and must contain the keyword <qoi_type>, which may be "transmittance", "reflectance", or "reaction_rate". Reaction rate QoIs are defined with the keywords

- <reaction>, which may be "energy_deposition", "charge_deposition", or "kerma",
- one or more <region_of_interest>, which must name one of the named regions defined in the <geometry_input>,
- <per_unit_mass_or_volume>, an optional keyword which may be set to "mass" or "volume". If unspecified this keyword defaults to "mass".

An example of a <QoI_Input> section of a RAPTURE input deck is included below showing two different reaction rate QoIs.

```
<QoI_Input>
  <QoI>
    <QoI_Type>reaction_rate</QoI_Type>
    <Reaction>energy_deposition</Reaction>
    <Region_Of_Interest>conductor</Region_Of_Interest>
  </QoI>
  <QoI>
    <QoI_Type>reaction_rate</QoI_Type>
    <Reaction>kerma</Reaction>
    <Region_Of_Interest>WetLayer</Region_Of_Interest>
    <Per_Unit_Mass_Or_Volume>volume</Per_Unit_Mass_Or_Volume>
  </QoI>
</QoI_Input>
```

The <QoI_input> block for a problem with a reflectance or transmittance QoI is simpler than the block required to define a reaction rate QoI,

```
<QoI_Input>
  <QoI>
    <QoI_Type>reflectance</QoI_Type>
  </QoI>
  <QoI>
    <QoI_Type>transmittance</QoI_Type>
  </QoI>
</QoI_Input>
```

Response functions or adjoint QoI may be specified for any of the reaction rate QoIs. Problems with response function QoIs are identified by setting the keyword <adjoint_mode> to "true" and defining the energies for which a response function is desired with the <energy_range> keyword, which expects the upper and lower energy bounds in MeV. Adjoint QoI are not supported for the spectrum QoIs transmittance or reflectance. An example adjoint QoI is displayed below.

```
<QoI_Input>
  <Tolerance>0.01</Tolerance>
  <Adjoint_Mode>true</Adjoint_Mode>
  <Energy_Range>6.0 0.001</Energy_Range>
  <QoI>
    <QoI_Type>reaction_rate</QoI_Type>
    <Reaction>energy_deposition</Reaction>
    <Region_Of_Interest>conductor</Region_Of_Interest>
    <Per_Unit_Mass_Or_Volume>mass</Per_Unit_Mass_Or_Volume>
  </QoI>
</QoI_Input>
```

A relative tolerance may be set with the <tolerance> keyword, as illustrated in the previous input deck.

`RAPTURE` will report an error if the <adjoint_mode> keyword is set to true and a <radiation_source_input> section is included in the input deck or if a spectrum QoI is specified. An error will be thrown if the energy range does not contain two doubles ordered from large to small, or if the second energy is below 1 keV.

3. TEST SUITE

This section describes the suite of tests that are distributed with `RAPTURE` to ensure the correct execution of the software. Table 3 provides a brief summary of the capabilities tested within each input deck, with each test discussed in further detail in the following sections. The input decks for each of the tests (including the `ADEPT` and ITS TIGER decks used to generate the comparisons) are listed in Appendix B.

Test ID	Source type	QoI	Transport	Section
1	Photon	Energy deposition	Forward	3.1
2	Electron	Charge deposition	Forward	3.2
3	Electron	Leakage	Forward	3.3
4	Electron	Leakage	Forward	3.4
5	Photon	Energy deposition	Adjoint	3.5
6	Photon	Charge deposition	Forward	3.6

Table 3-1. An overview of the `RAPTURE` test suite.

3.1. Test 1

Test 1 is designed to test the forward mono-energetic photon transport capability of RAPTURE. The problem is based on Case VII.1 from [6] and sees a 6 MeV photon beam incident on a 4 cm slab of tungsten. The resultant energy deposition profile from RAPTURE is compared against that computed by ITS TIGER in Figure 3-1.

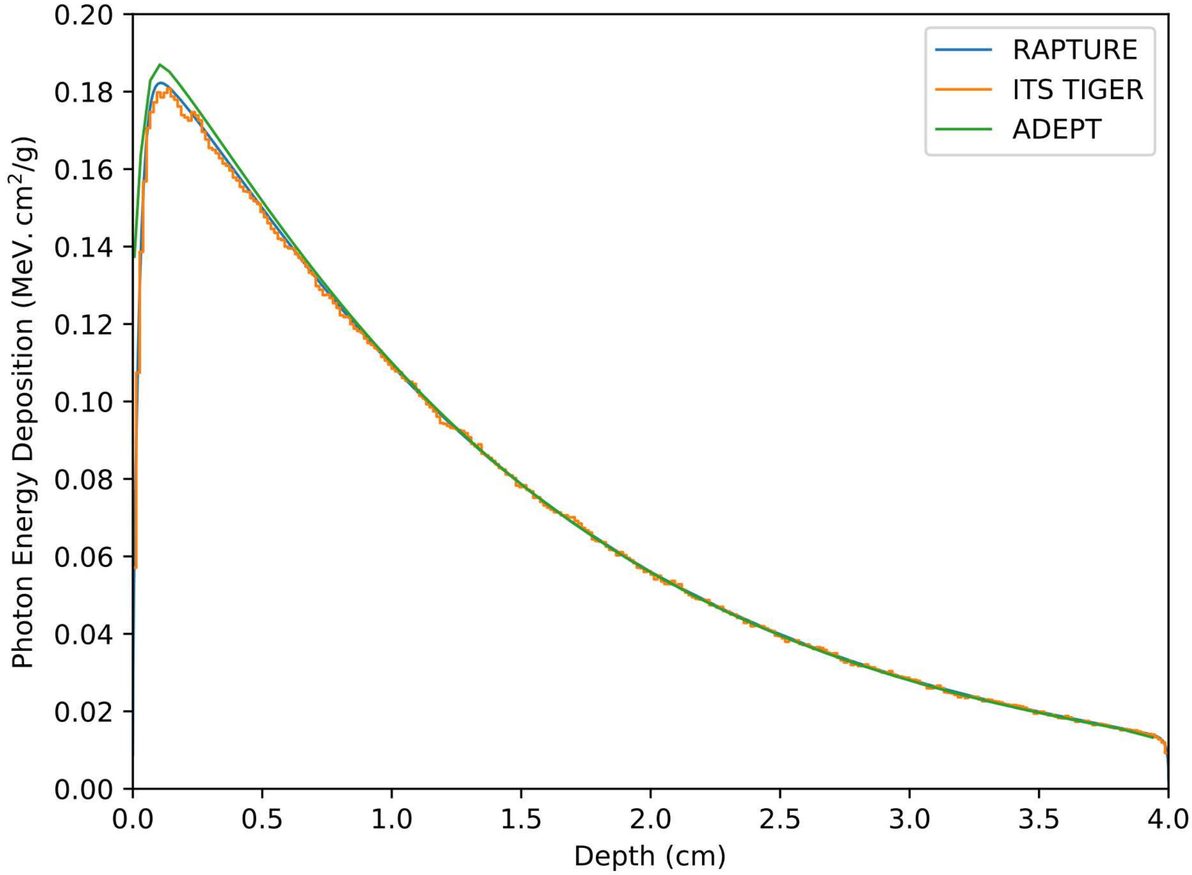

Figure 3-1. A comparison of the energy deposition profiles calculated by RAPTURE and ITS TIGER.

3.2. Test 2

Test 2 is designed to test the forward mono-energetic electron transport capability of RAPTURE. The problem is based on Case III.1 from [6] and sees a 1 MeV electron beam incident on a $0.5\,\mathrm{g\,cm^{-2}}$ slab of plastic. The resultant charge deposition profile from RAPTURE is compared against that computed by ITS TIGER and ADEPT, and against experimental data[3], in Figure 3-2.

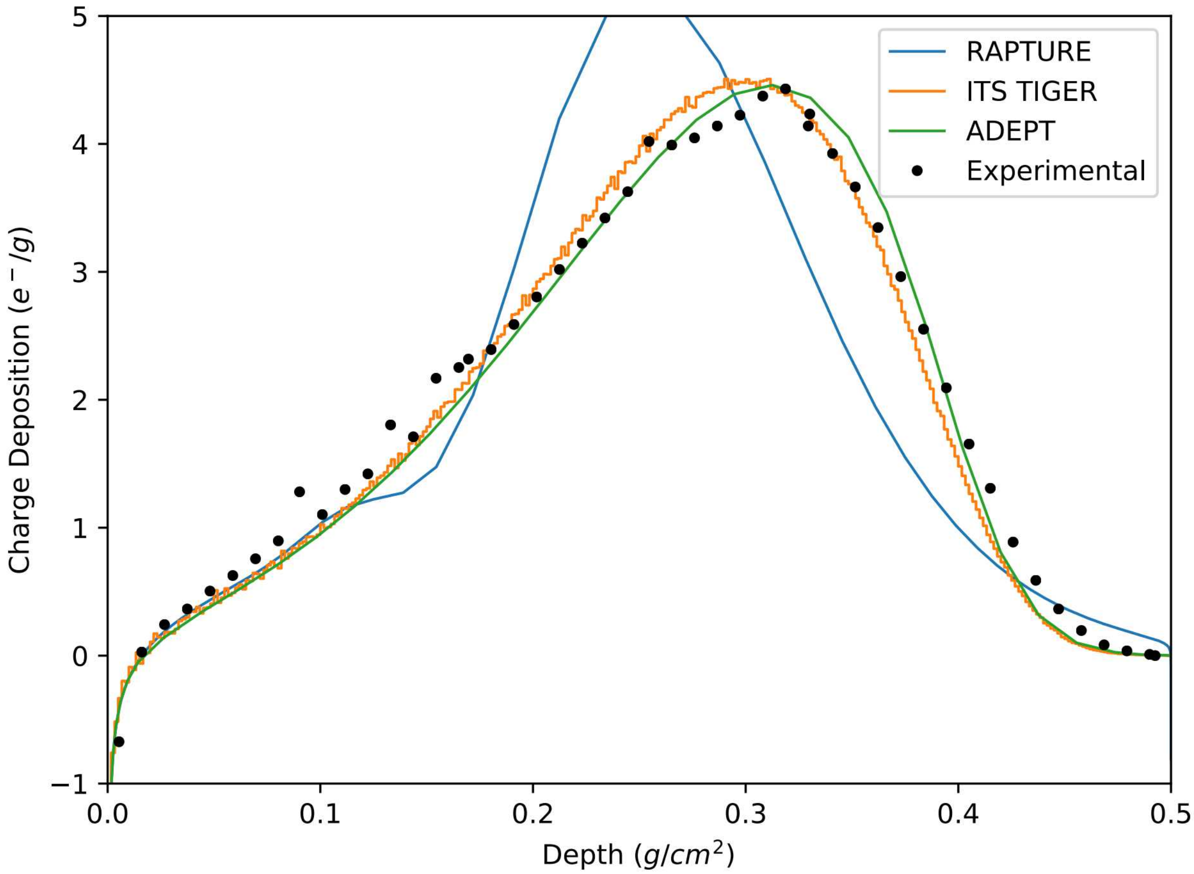

Figure 3-2. A comparison of the charge deposition profiles calculated by RAPTURE, ITS TIGER and ADEPT with experimental data.

3.3. Test 3

Test 3 is designed to test the forward mono-energetic electron transport capability of RAPTURE. The problem is based on Case VI.1 from [6] and sees a 1 MeV electron beam incident on a 0.0815 cm slab of aluminium. The resultant reflectance and transmission spectra from RAPTURE are compared against those computed by ITS TIGER and ADEPT and against (digitised) experimental data[11], in Figures 3-3 and 3-4.

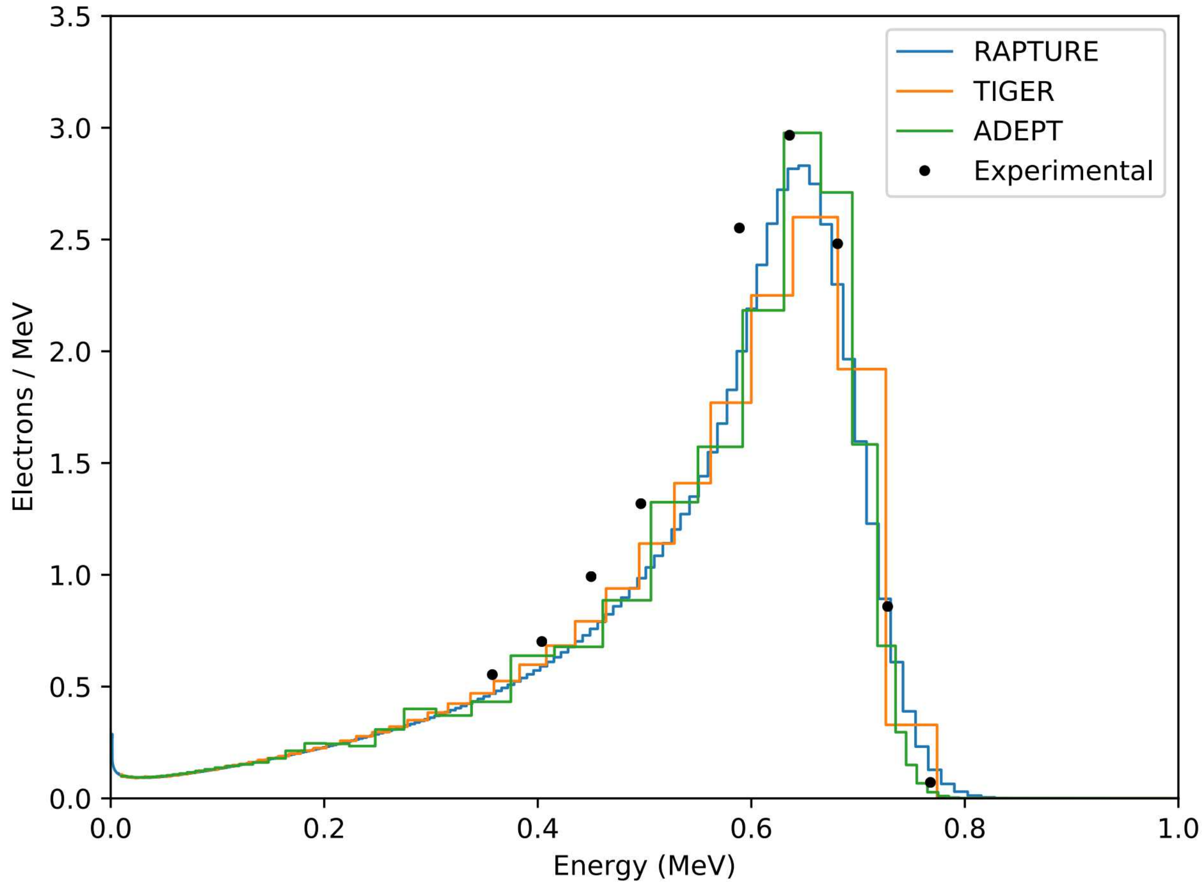

Figure 3-3. A comparison of transmission spectra calculated by RAPTURE, ITS TIGER and ADEPT with (digitised) experimental data.

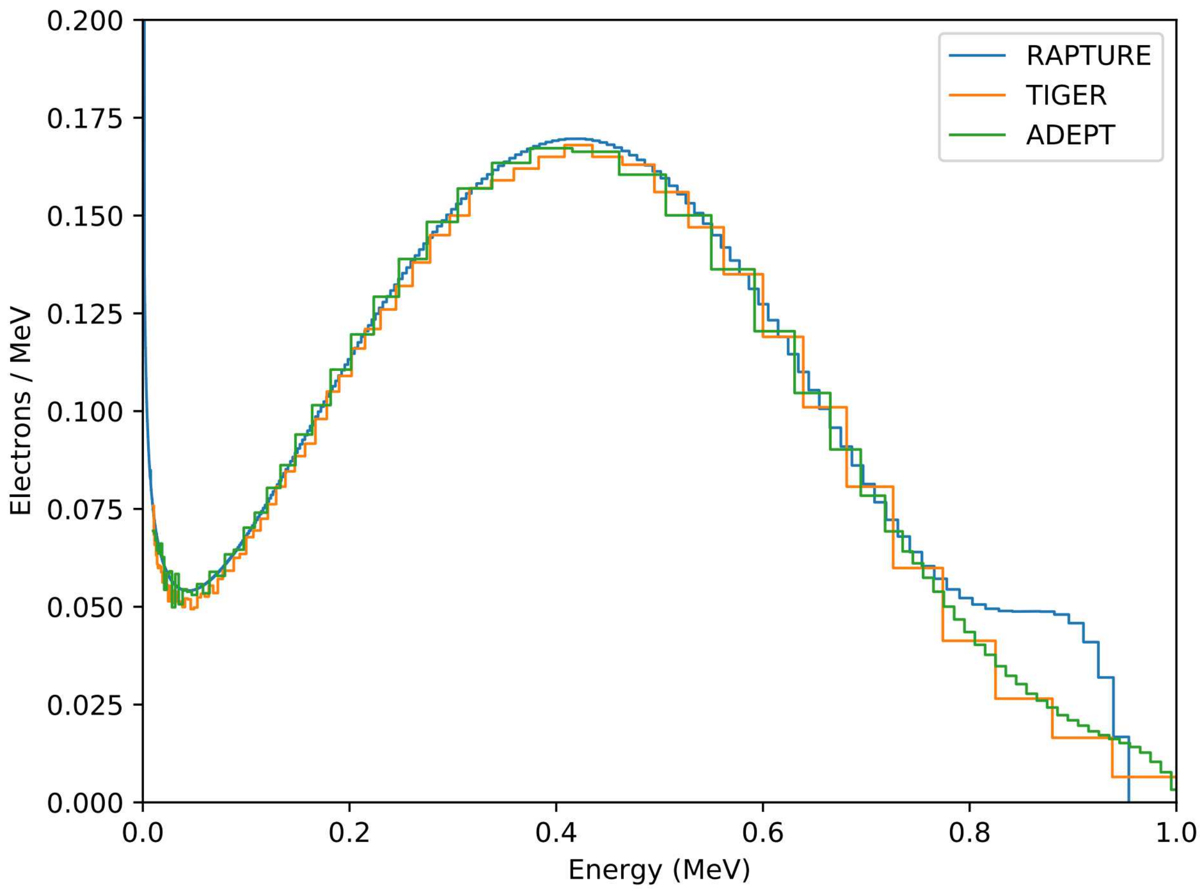

Figure 3-4. A comparison of reflectance spectra calculated by `RAPTURE`, ITS TIGER and `ADEPT`.

3.4. Test 4

Test 4 is designed to test the forward photon spectrum transport capability of RAPTURE. The problem is based on Case X.3 from [6] and sees a 50 keV end-point energy bremsstrahlung beam incident on a 0.0025 cm slab of tantalum. The resultant reflectance and transmission spectra from RAPTURE are compared against those computed by ITS TIGER and ADEPT and against experimental data[2] in Figures 3-5 and 3-6.

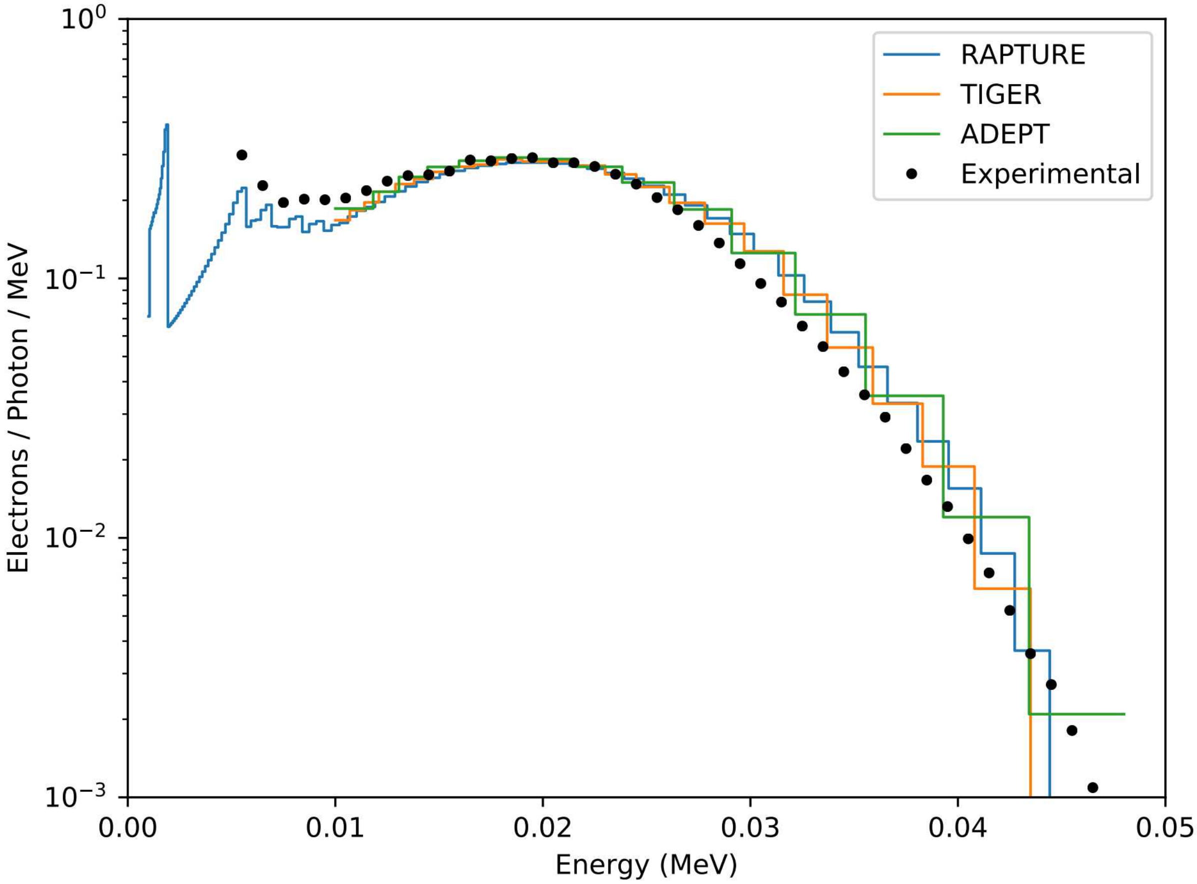

Figure 3-5. A comparison of transmission spectra calculated by RAPTURE and ITS TIGER and ADEPT with experimental data[1].

[1] Note that each spectrum is normalised to the number of photons transmitted per source photon.

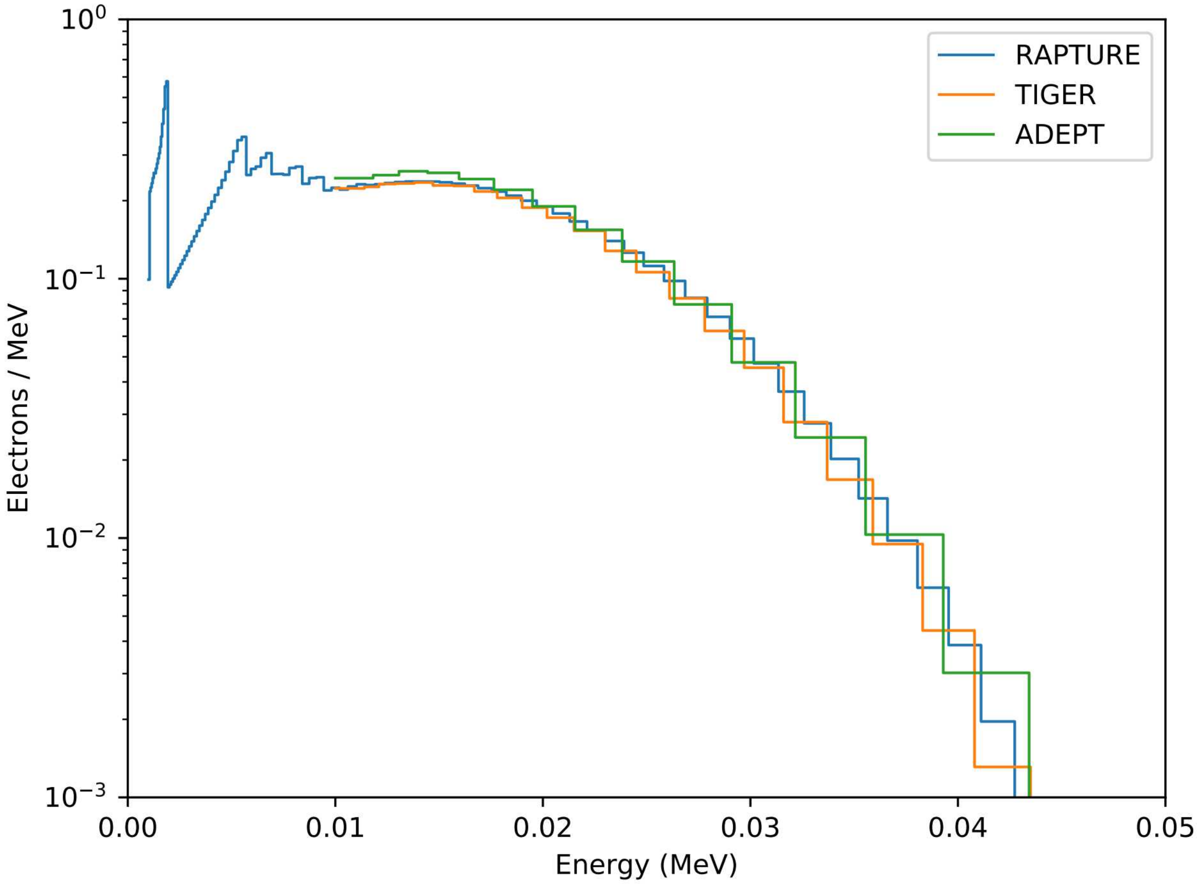

Figure 3-6. A comparison of reflectance spectra calculated by `RAPTURE` and ITS TIGER and `ADEPT`.

3.5. Test 5

Test 5 is designed to test the adjoint capability of `RAPTURE` and is constructed to be the adjoint analog of Test 1. The resultant response function from `RAPTURE` is compared against those computed by ITS TIGER and `ADEPT` in Figure 3-7.

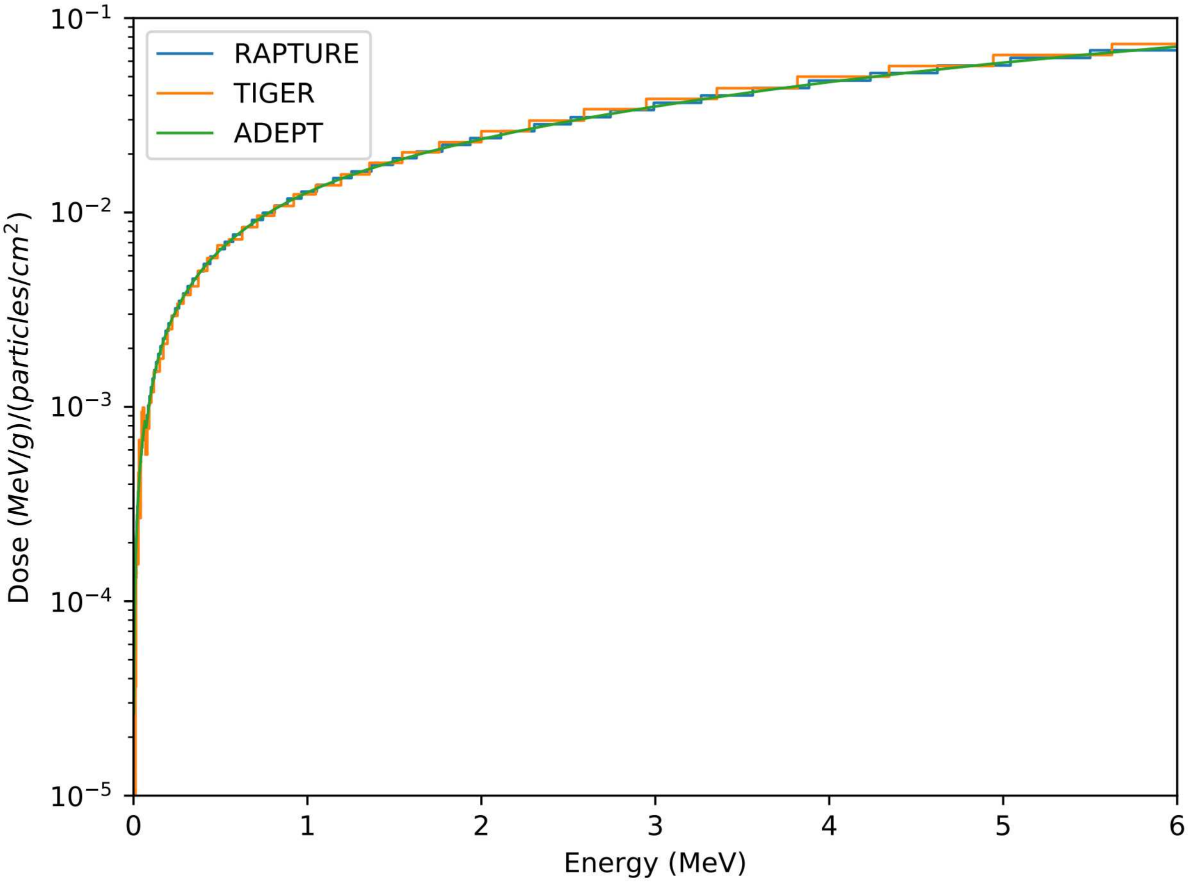

Figure 3-7. A comparison of response functions calculated by `RAPTURE` and ITS TIGER and `ADEPT`.

3.6. Test 6

Test 6 is designed to test the forward photon transport capability of `RAPTURE`. The problem sees a constant source of photons between 10.0 keV and 1.0 MeV, incident onto a simple copper cable. The resultant charge deposition profile from `RAPTURE` is compared against that computed by ITS TIGER and `ADEPT` in Figure 3-8.

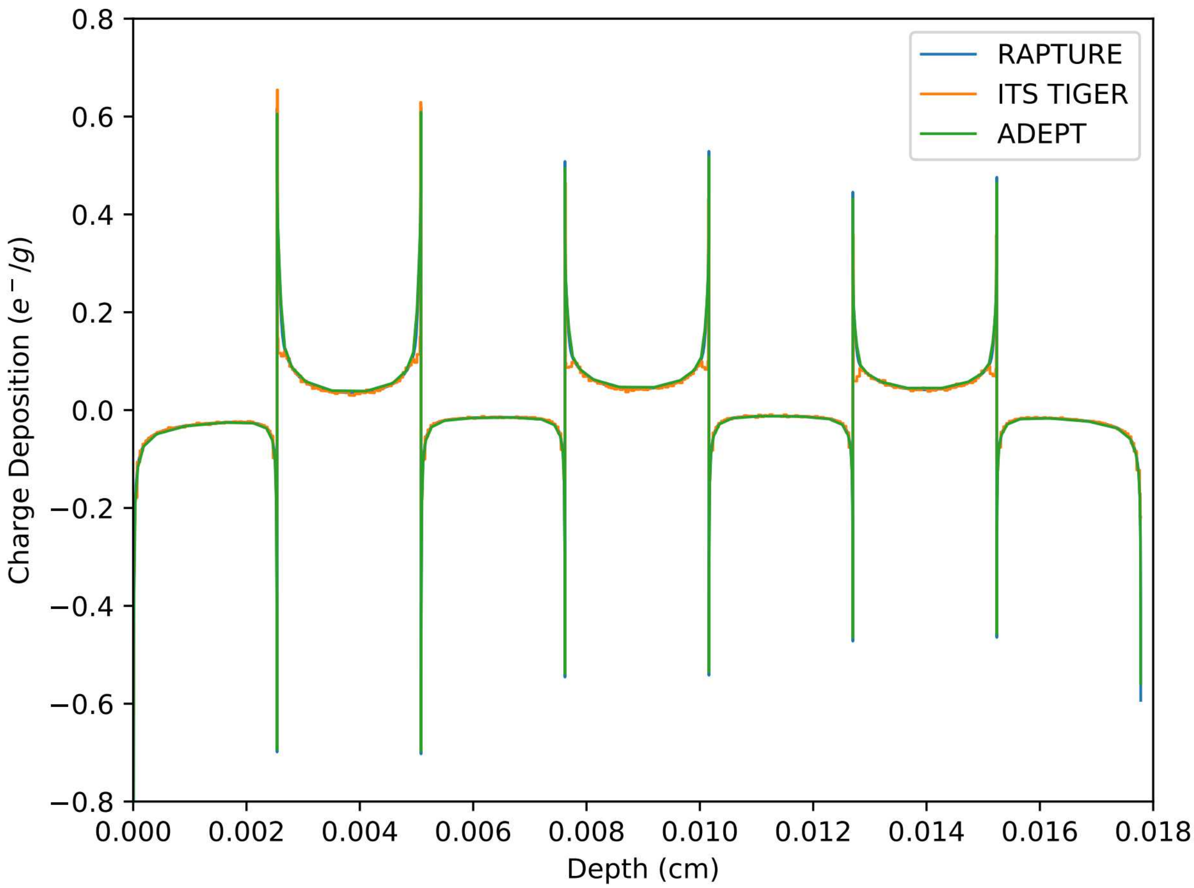

Figure 3-8. A comparison of the charge deposition profiles calculated by `RAPTURE`, ITS TIGER and `ADEPT`.

REFERENCES

[1] Inc. Docker. Docker-Build, Ship, and Run Any App, Anywhere. www.docker.com.

[2] K. W. Dolan. X-ray-induced electron emission from metals. *Journal Of Applied Physics*, 46(6), June 1975.

[3] A. R. Frederickson and S. Woolf. Electron Beam Current Penetration in Semi Infinite Slabs. *IEEE Transactions on Nuclear Science*, 28(6), December 1981.

[4] L. J. Lorence Jr. CEPXS/ONELD Version 2.0: A Discrete Ordinates Package for General One-Dimensional Coupled Electron-Photon Transport. *IEEE Transactions on Nuclear Science*, 39(4):1031, 1992.

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[7] L. J. Lorence Jr, W. E. Nelson, and J. E. Morel. Coupled Electron-Photon Transport Calculations Using the Method of Discrete Ordinates. *IEEE Transactions on Nuclear Science*, 32(6):4416, 1985.

[8] J. E. Morel and L. J. Lorence Jr. Recent Developments in Discrete Ordinates Electron Transport. *Transactions of the American Nuclear Society*, 52:384, 1986.

[9] S. Pautz, B. Bohnhoff, C. Drumm, and W. Fan. Parallel Discrete Ordinates Methods in the SCEPTRE Project. In *Proceedings of the International Conference on Mathematics*, Computational Methods and Reactor Physics, Saratoga Springs, NY, May 2009. American Nuclear Society. CD-ROM.

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[11] D. H. Rester and J. H. Derrickson. Electron Transmission Measurements for Al, Sn, and Au Targets at Electron Bombarding Energies of 1.0 and 2.5 MeV. *Journal Of Applied Physics*, 42(2), February 1971.

APPENDIX A. Quick reference

Angle

Description: Defines the angle of incidence of a plane-wave radiation source in degrees.

Default: `0.0` (normally-incident)

Parent: `Source`

Children: None

Composition

Description: The name of the material that composes this region. This must match one of the names defined in the material section.

Default: None

Parent: `Region`

Children: None

Element

Description: Encapsulates the definition of a single constituent of the material.

Default: None

Parent: `Material`

Children: `Symbol`, `Mass_Fraction`

Geometry_Input

Description: Encapsulates the region definitions.

Default: None

Parent: `RAPTURE_Input`

Children: `Region`

Material

Description: Encapsulates the definition of a single material.

Default: None

Parent: `Materials_Input`

Children: `Name`, `Mass_density`, `Element`

Materials_Input

Description: Encapsulates the material definitions.

Default: None

Parent: RAPTURE_Input

Children: Material

Mass_Density

Description: The mass density of the material in g/cm^3. section.

Default: None

Parent: Material

Children: None

Mass_Fraction

Description: The mass fraction for this element. Mass fractions for a material must sum to unity.

Default: 1.0

Parent: Element

Children: None

Name

Description: A unique name for the material or region. In the case of a mateial, note that 'void' is a special case and does not allow the mass density or elemental composition to be defined.

Default: None

Parent: Region/Material

Children: None

Number_Of_Source_Particles

Description: A float defining the scaling of the radiation source.

Default: 1.0

Parent: Source

Children: None

Per_Unit_Mass_Or_Volume

Description: Report the QoI normalised by mass (g) or volume (cm^3).

Default: mass

Parent: QoI

Children: None

`QoI`

Description: Encapsulates the definition of a single QoI.

Default: None

Parent: `QoI_Input`

Children: `QoI_Type`, `Reaction`, `Region_Of_Interest`, `Per_Unit_Mass_Or_Volume`

`QoI_Input`

Description: Encapsulates the QoI definitions.

Default: None

Parent: `RAPTURE_Input`

Children: `Tolerance`, `QoI`

`QoI_Type`

Description: Either `Transmittance`, `Reflectance` or `Reaction_Rate`.

Default: None

Parent: `QoI`

Children: None

`Radiation_Source_Input`

Description: Encapsulates the radiation source definitions.

Default: None

Parent: `RAPTURE_Input`

Children: `Source`

`Radiation_Type`

Description: The type of radiation source. This can be either `Photon` or `Electron`.

Default: None

Parent: `Source`

Children: None

`RAPTURE_Input`

Description: Encapsulates all of the information required for a RAPTURE run.

Default: None

Parent: None

Children: `Materials_Input`, `Geometry_Input`, `Radiation_Source_Input`, `QoI_Input`

Reaction

Description: Either Charge_Deposition, Energy_Deposition, Kerma or Damage.

Default: None

Parent: **QoI**

Children: None

Region

Description: Encapsulates the definition of a single region.

Default: None

Parent: **Geometry_Input**

Children: **Name**, **Thickness**, **Composition**

Region_Of_Interest

Description: Define the region for which the QoI is required. This must match the unique name of a **Region**.

Default: None

Parent: **QoI**

Children: None

Source

Description: Encapsulates the definition of a single radiation source.

Default: None

Parent: **Radiation_Source_Input**

Children: **Radiation_Type**, **Source_Format**, **Spectrum_File_Name**, **Spectrum_File_Format**, **Source_Energy**, **Source_Angular_Distribution**, **Angle**, **Number_Of_Source_Particles**

Source_Angular_Distribution

Description: This can be either Plane-Wave or Isotropic.

Default: None

Parent: **Source**

Children: None

Source_Energy

Description: Defines a mono-energetic radiation source, in MeV.

Default: None

Parent: **Source**

Children: None

Source_Format

Description: This can be either `Mono-Energetic`, `Constant` or `Tabular`.

Default: None

Parent: `Source`

Children: None

Spectrum_File_Format

Description: The description of the radiation source energy spectrum. This can be `PDF` or `CDF`.

Default: None

Parent: `Source`

Children: None

Spectrum_File_Name

Description: The file path of the data file containing the radiation source energy spectrum.

Default: None

Parent: `Source`

Children: None

Symbol

Description: The symbol of the element.

Default: None

Parent: `Element`

Children: None

Thickness

Description: The thickness of the region in cm.

Default: None

Parent: `Region`

Children: None

Tolerance

Description: Defines a fractional tolerance criteron for convergence.

Default: `0.005`

Parent: `QoI_Input`

Children: None

APPENDIX B. Test Suite Code Listings

B.1. Test 1

```
<RAPTURE_Input>
  <Materials_Input>
    <Material>
      <Name>Tungsten</Name>
      <Mass_Density>19.3</Mass_Density>
      <Element>
        <Symbol>W</Symbol>
      </Element>
    </Material>
  </Materials_Input>
  <Geometry_Input>
    <Region>
      <Name>Tungsten_slab</Name>
      <Thickness>4.0</Thickness>
      <Composition>Tungsten</Composition>
    </Region>
  </Geometry_Input>
  <Radiation_Source_Input>
    <Source>
      <Radiation_Type>photon</Radiation_Type>
      <Source_Format>mono-energetic</Source_Format>
      <Source_Energy>6.0</Source_Energy>
      <Source_Angular_Distribution>plane-wave</Source_Angular_Distribution>
      <Angle>0</Angle>
      <Number_Of_Source_Particles>1.0</Number_Of_Source_Particles>
    </Source>
  </Radiation_Source_Input>
  <QoI_Input>
   <Tolerance>0.01</Tolerance>
    <QoI>
      <QoI_Type>reaction_rate</QoI_Type>
      <Reaction>energy_deposition</Reaction>
      <Region_Of_Interest>Tungsten_slab</Region_Of_Interest>
      <Per_Unit_Mass_Or_Volume>mass</Per_Unit_Mass_Or_Volume>
    </QoI>
  </QoI_Input>
</RAPTURE_Input>
```

Listing B.1 RAPTURE test 1 deck

```
title 1
Test 1
geometry 1
 1 300 4.0
photons 1
energy 6.0
position
 surface zmin
cutoffs 0.01 0.01
histories-per-batch 3200
batches 320
```

Listing B.2 ITS TIGER test 1 deck

```
title 1
Test 1 material deck
* Material 1 - Tungsten
material w 1.0
density 19.3
energy 6.0
```

Listing B.3 ITS TIGER test 1 material deck

```
title 1
Tungsten deposition
material w
layers 1
 1 4.0
photon-source
 full-coupling
energy 6.0
plane-wave 0.0
output
 edep
```

Listing B.4 ADEPT test 1 deck

B.2. Test 2

```
<RAPTURE_Input>
  <Materials_Input>
    <Material>
      <Name>Plastic</Name>
      <Mass_Density>1.0</Mass_Density>
      <Element>
        <Symbol>C</Symbol>
        <Mass_Fraction>0.742</Mass_Fraction>
      </Element>
      <Element>
        <Symbol>H</Symbol>
        <Mass_Fraction>0.093</Mass_Fraction>
      </Element>
      <Element>
        <Symbol>O</Symbol>
        <Mass_Fraction>0.165</Mass_Fraction>
      </Element>
    </Material>
  </Materials_Input>
  <Geometry_Input>
    <Region>
      <Name>Plastic_slab</Name>
      <Thickness>0.5</Thickness>
      <Composition>Plastic</Composition>
    </Region>
  </Geometry_Input>
  <Radiation_Source_Input>
    <Source>
      <Radiation_Type>electron</Radiation_Type>
      <Source_Format>mono-energetic</Source_Format>
      <Source_Energy>1.0</Source_Energy>
      <Source_Angular_Distribution>plane-wave</Source_Angular_Distribution>
      <Angle>0</Angle>
      <Number_Of_Source_Particles>1.0</Number_Of_Source_Particles>
    </Source>
  </Radiation_Source_Input>
  <QoI_Input>
   <Tolerance>0.01</Tolerance>
    <QoI>
      <QoI_Type>reaction_rate</QoI_Type>
      <Reaction>charge_deposition</Reaction>
      <Region_Of_Interest>Plastic_slab</Region_Of_Interest>
      <Per_Unit_Mass_Or_Volume>mass</Per_Unit_Mass_Or_Volume>
    </QoI>
  </QoI_Input>
</RAPTURE_Input>
```

Listing B.5 RAPTURE test 2 deck

```
title 1
Test 2
geometry 1
 1 300 0.5
electrons
energy 1.0
position
 surface zmin
cutoffs 0.01 0.01
histories-per-batch 320000
batches 32
```

Listing B.6 ITS TIGER test 2 deck

```
title 1
Test 2 material deck
* Material 1 - Plastic
material c 0.742 h 0.093 o 0.165
density 1.0
energy 1.0
```

Listing B.7 ITS TIGER test 2 material deck

```
title 1
Test 2
material c 0.742 h 0.093 o 0.165
density 1.0
layers 1
 1 0.5
electron-source
 full-coupling
energy 1.0
plane-wave 0.0
output
 cdep
```

Listing B.8 ADEPT test 2 deck

B.3. Test 3

```
<RAPTURE_Input>
  <Materials_Input>
    <Material>
      <Name>Al</Name>
      <Mass_Density>2.6989</Mass_Density>
      <Element>
        <Symbol>Al</Symbol>
      </Element>
    </Material>
  </Materials_Input>
  <Geometry_Input>
    <Region>
      <Name>Al_slab</Name>
      <Thickness>0.0815</Thickness>
      <Composition>Al</Composition>
    </Region>
  </Geometry_Input>
  <Radiation_Source_Input>
    <Source>
      <Radiation_Type>electron</Radiation_Type>
      <Source_Format>mono-energetic</Source_Format>
      <Source_Energy>1.0</Source_Energy>
      <Source_Angular_Distribution>plane-wave</Source_Angular_Distribution>
      <Angle>0</Angle>
      <Number_Of_Source_Particles>1.0</Number_Of_Source_Particles>
    </Source>
  </Radiation_Source_Input>
  <QoI_Input>
   <Tolerance>0.01</Tolerance>
    <QoI>
      <QoI_Type>reflectance</QoI_Type>
    </QoI>
    <QoI>
      <QoI_Type>transmittance</QoI_Type>
    </QoI>
  </QoI_Input>
</RAPTURE_Input>
```

Listing B.9 RAPTURE test 3 deck

```
title 1
Test 3
geometry 1
 1 350 0.0815
electrons 1
energy 1.0
position
 surface zmin
electron-escape
 nbine 108 user
  9.380419e-01 8.799225e-01
  8.254042e-01 7.742637e-01 7.262918e-01 6.812921e-01
  6.390805e-01 5.994843e-01 5.623413e-01 5.274997e-01
  4.948168e-01 4.641589e-01 4.354005e-01 4.084239e-01
  3.831187e-01 3.593814e-01 3.371148e-01 3.162278e-01
  2.966349e-01 2.782559e-01 2.610157e-01 2.448437e-01
  2.296736e-01 2.154435e-01 2.020950e-01 1.895736e-01
  1.778279e-01 1.668101e-01 1.564748e-01 1.467799e-01
  1.376857e-01 1.291550e-01 1.211528e-01 1.136464e-01
  1.066050e-01 1.000000e-01 9.380419e-02 8.799225e-02
  8.254042e-02 7.742637e-02 7.262918e-02 6.812921e-02
  6.390805e-02 5.994843e-02 5.623413e-02 5.274997e-02
  4.948168e-02 4.641589e-02 4.354005e-02 4.084239e-02
  3.831187e-02 3.593814e-02 3.371148e-02 3.162278e-02
  2.966349e-02 2.782559e-02 2.610157e-02 2.448437e-02
  2.296736e-02 2.154435e-02 2.020950e-02 1.895736e-02
  1.778279e-02 1.668101e-02 1.564748e-02 1.467799e-02
  1.376857e-02 1.291550e-02 1.211528e-02 1.136464e-02
  1.066050e-02 1.000000e-02 9.380419e-03 8.799225e-03
  8.254042e-03 7.742637e-03 7.262918e-03 6.812921e-03
  6.390805e-03 5.994843e-03 5.623413e-03 5.274997e-03
  4.948168e-03 4.641589e-03 4.354005e-03 4.084239e-03
  3.831187e-03 3.593814e-03 3.371148e-03 3.162278e-03
  2.966349e-03 2.782559e-03 2.610157e-03 2.448437e-03
  2.296736e-03 2.154435e-03 2.020950e-03 1.895736e-03
  1.778279e-03 1.668101e-03 1.564748e-03 1.467799e-03
  1.376857e-03 1.291550e-03 1.211528e-03 1.136464e-03
  1.066050e-03 1.000000e-03
cutoffs 0.01 0.01
histories-per-batch 32000
batches 320
```

Listing B.10 ITS TIGER test 3 deck

```
title 1
Test 3 material deck
* Material 1 - Aluminium
material al 1.0
density 2.6989
energy 1.0
```

Listing B.11 ITS TIGER test 3 material deck

```
title 1
Test 3
material al 1.0
density 2.6989
layers 1
 1 0.0815
electron-source
 full-coupling
energy 1.0
plane-wave 0.0
cutoff 0.01
output
 curre
```

Listing B.12 ADEPT test 3 deck

B.4. Test 4

```
<RAPTURE_Input>
  <Materials_Input>
    <Material>
      <Name>Tantalum</Name>
      <Mass_Density>16.654</Mass_Density>
      <Element>
        <Symbol>Ta</Symbol>
      </Element>
    </Material>
  </Materials_Input>
  <Geometry_Input>
    <Region>
      <Name>Ta_slab</Name>
      <Thickness>0.0025</Thickness>
      <Composition>Tantalum</Composition>
    </Region>
  </Geometry_Input>
  <Radiation_Source_Input>
    <Source>
      <Radiation_Type>photon</Radiation_Type>
      <Source_Format>tabular</Source_Format>
      <Spectrum_File_Name>rapture_test_4_spectrum.txt</Spectrum_File_Name>
      <Spectrum_File_Format>cdf</Spectrum_File_Format>
      <Source_Angular_Distribution>plane-wave</Source_Angular_Distribution>
      <Angle>0</Angle>
      <Number_Of_Source_Particles>1.0</Number_Of_Source_Particles>
    </Source>
  </Radiation_Source_Input>
  <QoI_Input>
   <Tolerance>0.01</Tolerance>
    <QoI>
      <QoI_Type>reflectance</QoI_Type>
    </QoI>
    <QoI>
      <QoI_Type>transmittance</QoI_Type>
    </QoI>
  </QoI_Input>
</RAPTURE_Input>
```

Listing B.13 RAPTURE test 4 deck

```
# 50 keV endpoint bremsstrahlung
# Mev cdf
0.013 0.00000
0.014 0.00353
0.015 0.00833
0.016 0.01545
0.017 0.02595
0.018 0.04075
0.019 0.06115
0.020 0.08695
0.021 0.11795
0.022 0.15385
0.023 0.19405
0.024 0.23775
0.025 0.28395
0.026 0.33235
0.027 0.38185
0.028 0.43175
0.029 0.48125
0.030 0.53025
0.031 0.57825
0.032 0.62435
0.033 0.66875
0.034 0.71105
0.035 0.75095
0.036 0.78825
0.037 0.82305
0.038 0.85495
0.039 0.88425
0.040 0.91055
0.041 0.93365
0.042 0.95355
0.043 0.97005
0.044 0.98315
0.045 0.99257
0.046 0.99776
0.047 0.99880
0.048 1.00000
```

Listing B.14 RAPTURE test 4 spectrum

+

```
title 1
Test 4
geometry 1
 1 200 0.0025
photons 1
spectrum 36
1.0000 0.9988 0.9978 0.9926 0.9832
0.9701 0.9536 0.9337 0.9106 0.8843
0.8550 0.8231 0.7883 0.7510 0.7111
0.6688 0.6244 0.5783 0.5303 0.4813
0.4318 0.3819 0.3324 0.2840 0.2378
0.1941 0.1539 0.1180 0.0870 0.0612
0.0408 0.0260 0.0155 0.0083 0.0035
0.0000
0.0480 0.0470 0.0460 0.0450 0.0440
0.0430 0.0420 0.0410 0.0400 0.0390
0.0380 0.0370 0.0360 0.0350 0.0340
0.0330 0.0320 0.0310 0.0300 0.0290
0.0280 0.0270 0.0260 0.0250 0.0240
0.0230 0.0220 0.0210 0.0200 0.0190
0.0180 0.0170 0.0160 0.0150 0.0140
0.0130
position
 surface zmin
electron-escape
 nbine 61 user
  4.641589e-02 4.354005e-02 4.084239e-02
  3.831187e-02 3.593814e-02 3.371148e-02 3.162278e-02
  2.966349e-02 2.782559e-02 2.610157e-02 2.448437e-02
  2.296736e-02 2.154435e-02 2.020950e-02 1.895736e-02
  1.778279e-02 1.668101e-02 1.564748e-02 1.467799e-02
  1.376857e-02 1.291550e-02 1.211528e-02 1.136464e-02
  1.066050e-02 1.000000e-02 9.380419e-03 8.799225e-03
  8.254042e-03 7.742637e-03 7.262918e-03 6.812921e-03
  6.390805e-03 5.994843e-03 5.623413e-03 5.274997e-03
  4.948168e-03 4.641589e-03 4.354005e-03 4.084239e-03
  3.831187e-03 3.593814e-03 3.371148e-03 3.162278e-03
  2.966349e-03 2.782559e-03 2.610157e-03 2.448437e-03
  2.296736e-03 2.154435e-03 2.020950e-03 1.895736e-03
  1.778279e-03 1.668101e-03 1.564748e-03 1.467799e-03
  1.376857e-03 1.291550e-03 1.211528e-03 1.136464e-03
  1.066050e-03 1.000000e-03
cutoffs 0.01 0.01
histories-per-batch 320000
batches 320
```

Listing B.15 ITS TIGER test 4 deck

```
title 1
Test 4 material deck
* Material 1 - Tantalum
material ta 1.0
density 16.654
energy 0.05
```

Listing B.16 ITS TIGER test 4 material deck

```
title 1
Test 4
material ta 1.0
density 16.654
layers 1
 1 0.0025
photon-source
 full-coupling
spectrum 36
1.0000 0.9988 0.9978 0.9926 0.9832
0.9701 0.9536 0.9337 0.9106 0.8843
0.8550 0.8231 0.7883 0.7510 0.7111
0.6688 0.6244 0.5783 0.5303 0.4813
0.4318 0.3819 0.3324 0.2840 0.2378
0.1941 0.1539 0.1180 0.0870 0.0612
0.0408 0.0260 0.0155 0.0083 0.0035
0.0000
energies
0.0480 0.0470 0.0460 0.0450 0.0440
0.0430 0.0420 0.0410 0.0400 0.0390
0.0380 0.0370 0.0360 0.0350 0.0340
0.0330 0.0320 0.0310 0.0300 0.0290
0.0280 0.0270 0.0260 0.0250 0.0240
0.0230 0.0220 0.0210 0.0200 0.0190
0.0180 0.0170 0.0160 0.0150 0.0140
0.0130
plane-wave 0.0
cutoff 0.01
output
 curre
```

Listing B.17 ADEPT test 4 deck

B.5. Test 5

```
<RAPTURE_Input>
  <Materials_Input>
    <Material>
      <Name>Tungsten</Name>
      <Mass_Density>19.3</Mass_Density>
      <Element>
        <Symbol>W</Symbol>
      </Element>
    </Material>
  </Materials_Input>
  <Geometry_Input>
    <Region>
      <Name>Tungsten_slab</Name>
      <Thickness>4.0</Thickness>
      <Composition>Tungsten</Composition>
    </Region>
  </Geometry_Input>
  <QoI_Input>
    <Tolerance>0.01</Tolerance>
    <Adjoint_Mode>true</Adjoint_Mode>
    <Energy_Range>6.0 0.001</Energy_Range>
    <QoI>
      <QoI_Type>reaction_rate</QoI_Type>
      <Reaction>energy_deposition</Reaction>
      <Region_Of_Interest>Tungsten_slab</Region_Of_Interest>
      <Per_Unit_Mass_Or_Volume>mass</Per_Unit_Mass_Or_Volume>
    </QoI>
  </QoI_Input>
</RAPTURE_Input>
```

Listing B.18 RAPTURE test 5 deck

```
title 1
Test 5
adjoint
geometry 1
 1 1 4.0
source-surfaces 1
 surface zmin
photon-surface-source
 nbint 1 plane-wave
detector-response
 dose
  material 1
  location
   volume 1
no-intermediate-output
histories-per-batch 320000
batches 320
```

Listing B.19 MITS TIGER test 5 deck

```
mits
photon-source
 full-coupling
cutoff 0.01 0.01
electrons
 log 50
photons
 log 50
no-lines
energy 6.0
material w 1.0
density 19.3
```

Listing B.20 CEPXS test 5 material deck

```
title 1
 Test 5
maxlcm 15000000
material w
layers 1
 1 4.0
photon-source
 full-coupling
mono 6.0
plane-wave 0.0
adjoint
 max-energy 6.0
 dose 1
output
 edep
```

Listing B.21 ADEPT test 5 deck

B.6. Test 6


```
<RAPTURE_Input>
  <Materials_Input>
    <Material>
      <Name>Copper</Name>
      <Mass_Density>8.90</Mass_Density>
      <Element>
        <symbol>Cu</symbol>
      </Element>
    </Material>
    <Material>
      <Name>Kapton</Name>
      <Mass_Density>1.42</Mass_Density>
      <Element>
        <Symbol>H</Symbol>
        <Mass_Fraction>0.026362</Mass_Fraction>
      </Element>
      <Element>
        <Symbol>C</Symbol>
        <Mass_Fraction>0.691133</Mass_Fraction>
      </Element>
      <Element>
        <Symbol>N</Symbol>
        <Mass_Fraction>0.07327</Mass_Fraction>
      </Element>
      <Element>
        <Symbol>O</Symbol>
        <Mass_Fraction>0.209235</Mass_Fraction>
      </Element>
    </Material>
  </Materials_Input>
  <Geometry_Input>
    <Region>
      <Name>TopElectricalShield</Name>
      <Thickness>0.00254</Thickness>
      <Composition>Copper</Composition>
    </Region>
    <Region>
      <Name>TopInsulator</Name>
      <Thickness>0.00254</Thickness>
      <Composition>Kapton</Composition>
    </Region>
    <Region>
      <Name>FirstConductor</Name>
      <Thickness>0.00254</Thickness>
      <Composition>Copper</Composition>
    </Region>
    <Region>
      <Name>MiddleInsulator</Name>
      <Thickness>0.00254</Thickness>
      <Composition>Kapton</Composition>
    </Region>
```

```
    <Region>
      <Name>BottomConductor</Name>
      <Thickness>0.00254</Thickness>
      <Composition>Copper</Composition>
    </Region>
    <Region>
      <Name>BottomInsulator</Name>
      <Thickness>0.00254</Thickness>
      <Composition>Kapton</Composition>
    </Region>
    <Region>
      <Name>BottomElectricalShield</Name>
      <Thickness>0.00254</Thickness>
      <Composition>Copper</Composition>
    </Region>
  </Geometry_Input>
  <Radiation_Source_Input>
    <Source>
      <Radiation_Type>photon</Radiation_Type>
      <Source_Format>constant</Source_Format>
      <Source_Energy>1.000 0.010</Source_Energy>
      <Source_Angular_Distribution>plane-wave</Source_Angular_Distribution>
      <Angle>0</Angle>
    </Source>
  </Radiation_Source_Input>
  <QoI_Input>
    <Tolerance>0.01</Tolerance>
    <QoI>
      <QoI_type>reaction_rate</QoI_type>
      <reaction>charge_deposition</reaction>
      <region_of_interest>TopInsulator</region_of_interest>
      <region_of_interest>MiddleInsulator</region_of_interest>
      <region_of_interest>BottomInsulator</region_of_interest>
      <per_unit_mass_or_volume>mass</per_unit_mass_or_volume>
    </QoI>
  </QoI_Input>
</RAPTURE_Input>
```

Listing B.22 RAPTURE test 6 deck

```
title 1
 Test 6
geometry 21
 1 2 0.000020
 1 50 0.002500
 1 2 0.000020
 2 2 0.000020
 2 50 0.002500
 2 2 0.000020
 1 2 0.000020
 1 50 0.002500
 1 2 0.000020
 2 2 0.000020
 2 50 0.002500
 2 2 0.000020
 1 2 0.000020
 1 50 0.002500
 1 2 0.000020
 2 2 0.000020
 2 50 0.002500
 2 2 0.000020
 1 2 0.000020
 1 50 0.002500
 1 2 0.000020
photons 1
spectrum 35
1.00000 0.86966 0.75614 0.65727
0.57115 0.49615 0.43082 0.37393
0.32437 0.28122 0.24362 0.21089
0.18237 0.15753 0.13590 0.11706
0.10065 0.08636 0.07392 0.06307
0.05363 0.04541 0.03825 0.03201
0.02657 0.02184 0.01772 0.01413
0.01100 0.00828 0.00591 0.00384
0.00204 0.00048 0.00000
1.00000 0.87096 0.75858 0.66069
0.57544 0.50119 0.43652 0.38019
0.33113 0.28840 0.25119 0.21878
0.19055 0.16596 0.14454 0.12589
0.10965 0.09550 0.08318 0.07244
0.06310 0.05495 0.04786 0.04169
0.03631 0.03162 0.02754 0.02399
0.02089 0.01820 0.01585 0.01380
0.01202 0.01047 0.01000
position
 surface zmin
cutoffs 0.01 0.01
histories-per-batch 3200000
batches 320
```

Listing B.23 ITS TIGER test 6 deck

```
title 1
 Test 6 material deck
* Material 1 - Copper
material cu 1.0
density 8.9
* Material 1 - Kapton
material h 0.026362 c 0.691133 n 0.07327 o 0.209235
density 1.42
energy 1.0
```

Listing B.24 ITS TIGER test 6 material deck

```
title 1
 Test 6
maxlcm 15000000
material cu 1.0
density 8.9
material h 0.026362 c 0.691133 n 0.07327 o 0.209235
density 1.42
layers 7
 1 0.00254
 2 0.00254
 1 0.00254
 2 0.00254
 1 0.00254
 2 0.00254
 1 0.00254
photon-source
 full-coupling
spectrum 35
1.00000 0.86966 0.75614 0.65727
0.57115 0.49615 0.43082 0.37393
0.32437 0.28122 0.24362 0.21089
0.18237 0.15753 0.13590 0.11706
0.10065 0.08636 0.07392 0.06307
0.05363 0.04541 0.03825 0.03201
0.02657 0.02184 0.01772 0.01413
0.01100 0.00828 0.00591 0.00384
0.00204 0.00048 0.00000
energies
1.00000 0.87096 0.75858 0.66069
0.57544 0.50119 0.43652 0.38019
0.33113 0.28840 0.25119 0.21878
0.19055 0.16596 0.14454 0.12589
0.10965 0.09550 0.08318 0.07244
0.06310 0.05495 0.04786 0.04169
0.03631 0.03162 0.02754 0.02399
0.02089 0.01820 0.01585 0.01380
0.01202 0.01047 0.01000
plane-wave 0.0
output
 cdep
```

Listing B.25 ADEPT test 6 deck

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