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MCNP6 Subroutine for Simulating a D-T Neutron Source in Ti-T Targets

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Introduction

- A deuterium-tritium (D-T) neutron source defined with the SOURCE subroutine for MCNP5 was released in the Shielding Integral Benchmark Archive and Database (SINBAD) [1].
  - The subroutine simulated deuteron transport in a titanium-tritium (Ti-T) target and calculated the properties of neutrons from D-T fusion.
  - The code implementation was based on the Stopping and Range of Ions in Matter (SRIM) code.
  - The MCNP5 source subroutine is not compatible with MCNP6.

- The goal of this work was to refactor the MCNP5 (D-T) fusion neutron SOURCE subroutine for MCNP6.3.

MCNP Source Definition

- Each MCNP problem requires a source, defined in one of four ways:
  - SDEF, KSRC, SSR, or a user defined source [2].
- **SDEF**
  - Allows the user to create a source by defining each source parameter as a specific value, a user defined distribution, or as a function of another source variable.
- **KSRC**
  - Allows the user to define initial source points, used for criticality calculations.
- **SSR**
  - The surface source read card, reads in a surface source created by a previous MCNP calculation with the SSW card.
- **User defined source**
  - Implement the **SOURCE** Fortran subroutine to supply starting particle parameters. Requires access to the MCNP source code.

SOURCE and SRCDX Subroutines

- The SOURCE subroutine is required by MCNP when the SDEF, KCODE, or SSR cards are not in an MCNP input file.
- The SOURCE subroutine must supply parameters for each source particle, including the x-y-z position, u-v-w cosine direction, energy, time, weight, particle type, starting cell, and starting surface if applicable.
  - See Table 5.16 in MCNP6.3 Manual for the variable names.
- If the problem includes F5 tallies or DXTRAN spheres and the source has an anisotropic angular distribution, the SRCDX subroutine is required [2].
- The SRCDX subroutine is for calculating the probability of a source particle being emitted in the direction of a detector or DXTRAN sphere (PSC).
  - PSC is a variable used in the MCNP code.

D-T Neutron Source Physics

- The SINBAD D-T neutron source included physics for deuterium ion transport in Ti-T and neutron production.
- Deuterium Ion Transport:
  - Sample a free flight path and update the deuteron position with the new location.
  - Process a collision and update the deuteron angle and energy.
  - Check the deuteron position and energy and either start a next free flight path or initialize a new particle.
- Neutron Production:
  - At deuterium ion collision, determine if a D-T reaction occurs by rejection sampling.
  - If there is a reaction, calculate the resulting neutron energy and direction.
  - Use rejection to sample the position of the starting neutron.

Deuterium Ion Transport

- Deuterons are initialized with a user input beam energy and position.
- Stochastic Iteration Method:
  - Transport deuterons until a neutron is produced.
- The deuteron flight path is sampled from a maximum free flight path.
  - The maximum flight path is calculated with the maximum reduced impact parameter and the reduced center of mass energy of the deuteron, shown in Eq. 1 and 2.
  - The reduced parameters correct for the charge shielding effects of inner electrons by the Bohr radius, a.

$$\frac{p_{max}}{a} = (\xi + \xi^{0.5} + 0.125\xi^{0.1})^{-1}$$

Eq. 1: Equation for impact parameter p. ξ depends on the deuteron energy and minimum energy transfer. The Bohr radius, a, is used for the reduced values.

$$FFP = (\pi p_{max}^2 N)^{-1}$$

Eq. 2: Equation for the free flight path, where N is the atom density of the material.

Deuterium Ion Transport (cont.)

- The deuteron energy is reduced by the material stopping power.
  - The stopping power is dependent on the deuteron energy and is interpolated for the energy before the flight.
  - The energy loss is the stopping power multiplied by the flight distance and corrected by the Bohr straggling effect.
- The deuteron position is updated, and a collision is processed.
  - For a deuteron reduced center of mass energy greater than 10 MeV, Rutherford scattering is used to determine the scattering angle.
  - Otherwise, the method described by Biersack and Haggmark is used to calculate the scattering angle [3].
  - The scattering angle is then used to update the deuteron direction and calculate the energy reduction by kinematics.

Deuterium Ion Transport (cont.)

- After the collision, if the energy of the deuteron is below 10 KeV, a new deuteron will be initialized.
- If the y position is greater than the thickness of the target or negative, a new deuteron will be initialized.
- The D-T reaction is then sampled:
  - If a neutron is produced, the deuteron transport loop will exit. Otherwise, a next free flight will be sampled for the current deuteron.

Neutron Production

- The incident deuteron cross section and Legendre moments for Tritium are used to construct a probability density function (PDF) for a D-T reaction.
- After each collision, a random direction cosine is sampled for the neutron and used with the deuteron energy to interpolate a value of the PDF.
- A probability value is uniformly sampled below the maximum of the PDF and the rejection technique is used to determine if a reaction occurred.
- If a reaction is sampled, the neutron direction and deuteron energy are used with relativistic kinematics to calculate the neutron energy.
- The neutron position is sampled in a circle about the user input position using the beam width. The circle is in the y plane at the face of the target.

User Inputs

- Several parameters for the SOURCE subroutine must be input by the user.
- This is accomplished using the RDUM card in an MCNP input file.
- Eight entries of the RDUM card must be populated and correspond to, in order:
  - The deuteron beam energy, tritium to titanium atomic ratio, x, y, and z positions, deuteron beam width, reaction flag, and starting cell.
- The y position must be positive.
- The reaction flag allows selection between D-T and D-D reactions by choosing 1 or 2, respectively.
  - D-D reactions had not been tested for MCNP5 subroutine.

SINBAD SRCDX Subroutine

- A SRCDX subroutine was included due to the anisotropy of the D-T neutron source.
- The SRCDX subroutine is supplied the direction to a detector or DXTRAN sphere by MCNP.
- The SOURCE subroutine passes in a distribution of neutron emission angles, the direction of the progenitor deuteron, and the D-T reaction PDF.
- The angle between the detector and deuteron direction is calculated, μ_0.
- The PSC is calculated using the D-T reaction PDF and μ_0:
  - The PDF is evaluated at the angle μ_0 and integrated over energy.
  - The PSC is calculated as the ratio of the previous integral to the integral of the PDF over energy and angle.

SINBAD D-T Source Modernization

- Both subroutines were originally written in Fortran 77 to work with MCNP5.
- In this work, the subroutines were converted to modern Fortran for use with MCNP6.3 and many outdated Fortran practices were removed and replaced.
- Improved code robustness through explicit variable type assignment and better error checking.
- General improvements were made to the readability and efficiency including the change to column-major array access.
- The new subroutines were then used with MCNP6.3, and the results were analyzed.

Verification – Code-to-Code Comparison

- To verify the new SOURCE/SRCDX subroutines, the results calculated by the old Fortran 77 and new modern Fortran subroutines were compared.
  - Goal of updating the code with the same functionality
- The new and old SOURCE/SRCDX subroutines were assembled as two Fortran programs.
- A test problem was created to call the SOURCE/SRCDX subroutines 1E6 times, and the starting particle parameters were placed in histograms for comparison.
- The results were expected to be identical since the same random number generator and seed were used for each version.

Results – Subroutine Comparison

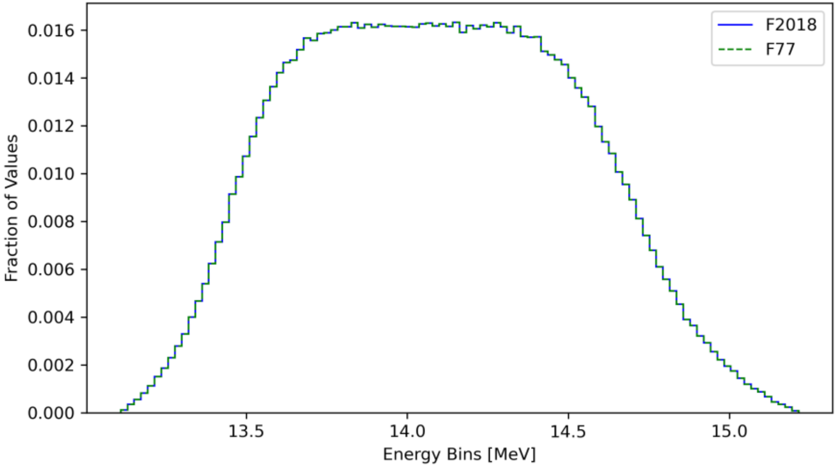

Figure 1. Comparison of the neutron energies for the F2018 and F77 SOURCE subroutines.

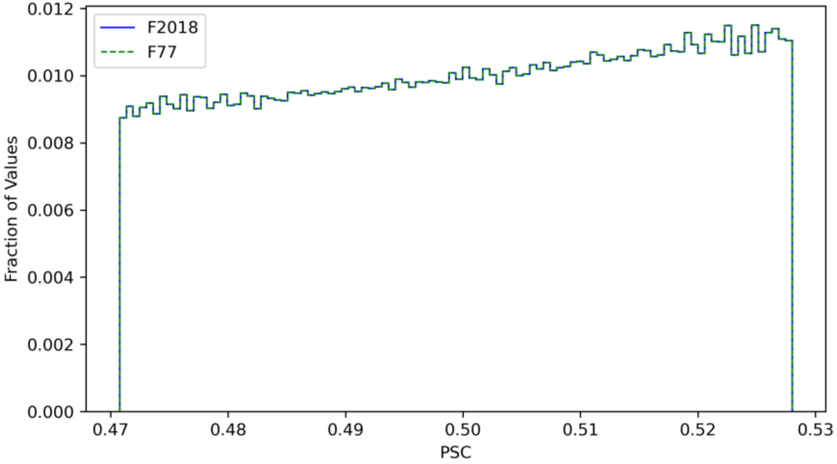

Figure 2. Comparison of the PSC for the F2018 and F77 SOURCE and SRCDX subroutines.

Results – Subroutine Comparison

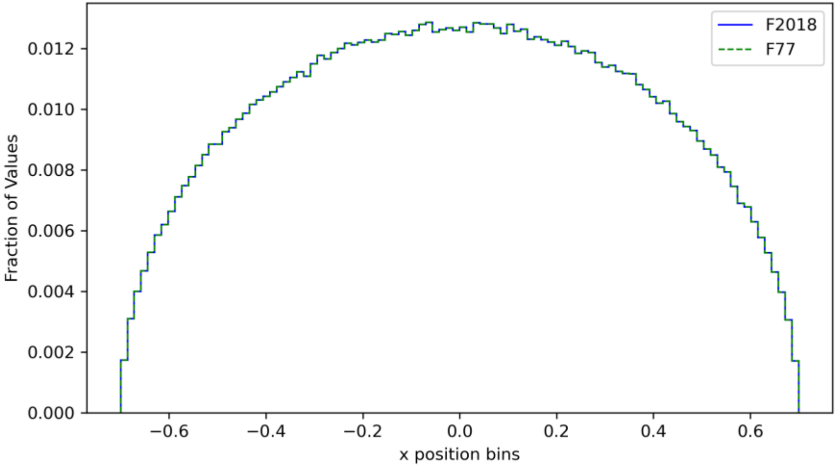

Figure 3. Comparison of the neutron starting x position for the F2018 and F77 SOURCE subroutines.

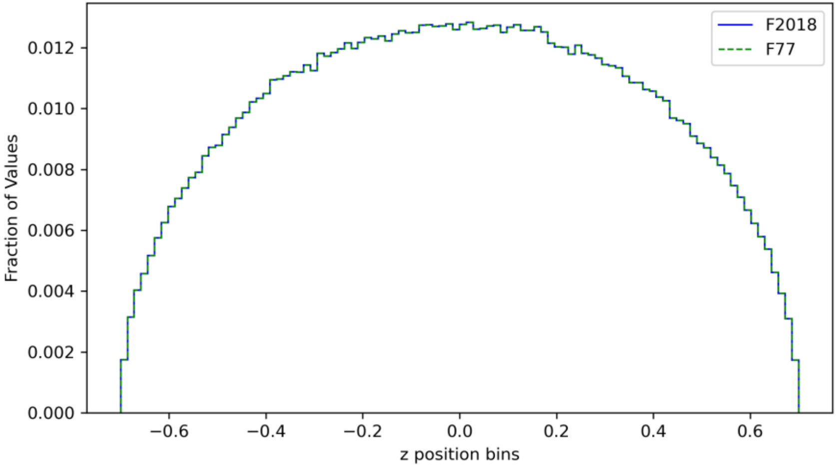

Figure 4. Comparison of the neutron starting z position for the F2018 and F77 SOURCE subroutines.

Results – Subroutine Comparison

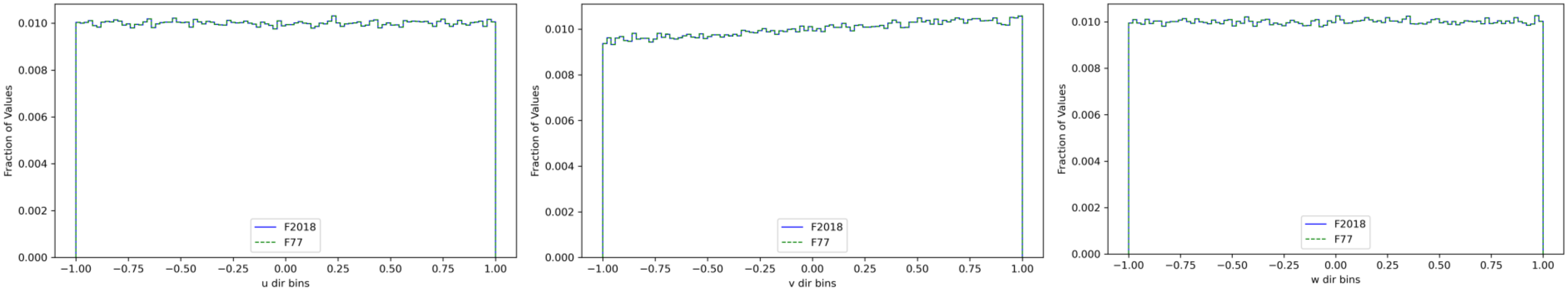

Figure 5. Comparison of the neutron angular distribution for the F2018 and F77 SOURCE subroutines. Shown is the u direction (left), v direction (middle), and w direction (right).

OKTAVIAN Experiments in SINBAD

- The D-T neutron source subroutines were used in an MCNP model of the OKTAVIAN benchmark experiment, also included in SINBAD [4].
- The experiment featured a spherical shield sample with a Ti-T target at the center.
- Deuterons were accelerated into the target to produce fusion neutrons and investigate the properties of several shields of differing materials.
- Tally cell 10.9 m from the source, necessitating variance reduction.

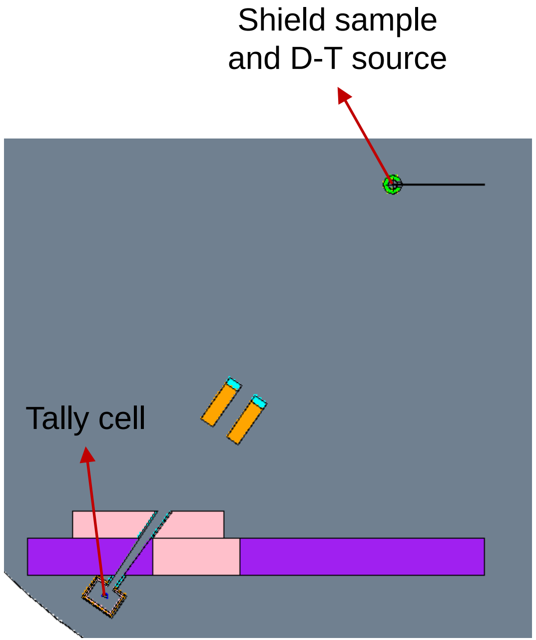

Figure 6. MCNP model of the OKTAVIAN experimental layout.

Results – MCNP Calculations

- The modernized subroutines were used in MCNP calculations for the OKTAVIAN benchmark.
  - The aluminum, 40 cm silicon, and 60 cm silicon models were analyzed.
- Two calculations were performed for each model, one with SDEF and one using the SOURCE and SRCDX subroutines.
- For each source method, a calculation was also performed to analyze the source spectrum alone.
  - These calculations consisted of only the Ti-T target and a sphere F2 tally.

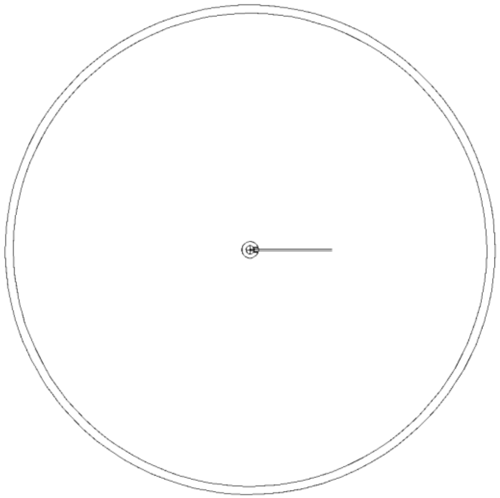

Figure 6: MCNP geometry for the source spectrum calculations.

Results – MCNP Calculations

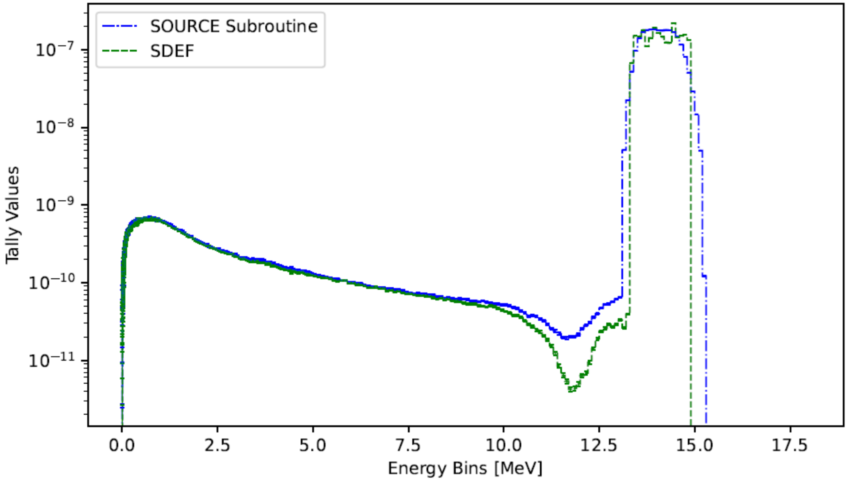

Figure 8. Source neutron energy spectrum comparison for the SOURCE subroutine and SDEF methods. Normalized by bin width.

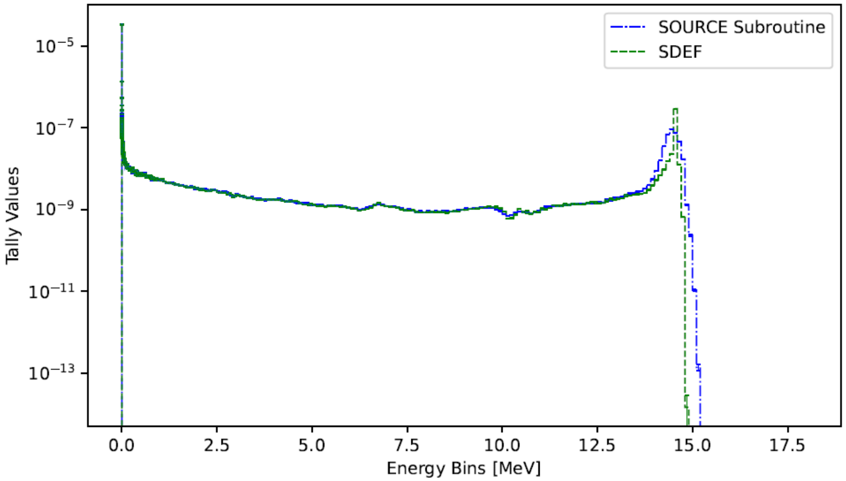

Figure 9. Neutron energy spectrum comparison for the SOURCE subroutine and SDEF methods with the aluminum model. Normalized by bin width.

Results – MCNP Calculations

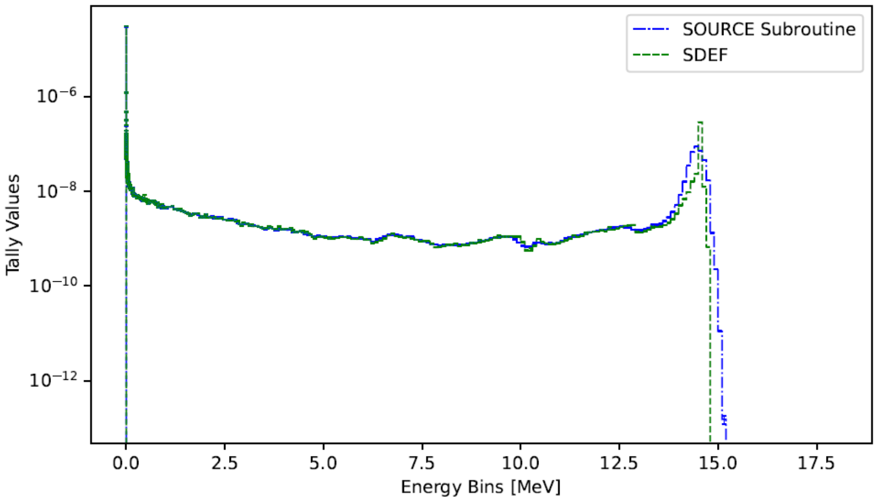

Figure 10. Neutron energy spectrum comparison for the SOURCE subroutine and SDEF methods with the 40cm silicon model. Normalized by bin width.

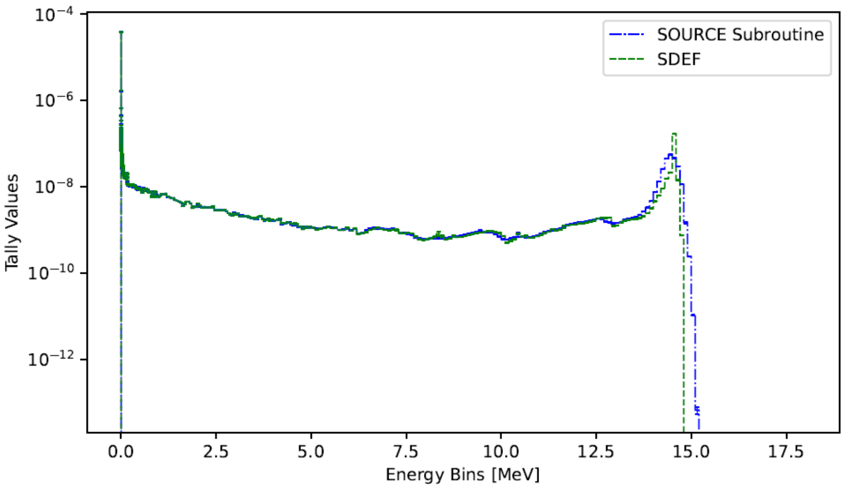

Figure 11. Neutron energy spectrum comparison for the SOURCE subroutine and SDEF methods with the 60cm silicon model. Normalized by bin width.

Conclusions

- The SINBAD D-T neutron SOURCE and SRCDX subroutines were modernized for use with MCNP6.3.

- The verification results indicate that the modernized subroutines are functionally the same as the old subroutines.

- The MCNP calculations show that the SOURCE subroutine results are close to an approximately equivalent D-T neuron source implemented with SDEF.

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[3] J.P. BIERSACK, L.G. HAGGMARK, A Monte Carlo computer program for the transport of energetic ions in amorphous targets, Nuclear Instruments and Methods, Volume 174, Issues 1–2, 1980, Pages 257-269, ISSN 0029-554X, https://doi.org/10.1016/0029-554X(80)90440-1.

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