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Comparison Of The 3-D Deterministic Neutron Transport Code Attila® To Measure Data, MCNP And MCNPX For The Advanced Test Reactor

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To Measured Data, MCNP and MCNPX
For the Advanced Test Reactor

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Abstract An LDRD (Laboratory Directed Research and Development) project is underway at the Idaho National Laboratory (INL) to apply the three-dimensional multi-group deterministic neutron transport code (Attila®) to criticality, flux and depletion calculations of the Advanced Test Reactor (ATR). This paper discusses the development of Attila models for ATR, capabilities of Attila, the generation and use of different cross-section libraries, and comparisons to ATR data, MCNP, MCNPX and future applications.

1.0 Introduction

This report discusses the Advanced Test Reactor (ATR), a brief overview of the Attila [1] three-dimensional deterministic neutron transport code, the model development for ATR with Attila and the SolidWorks® CAD tool, the results of the comparisons to fresh core data and depletion benchmarks. Additional discussion is given on future plans for the Attila code at INL.

The Advanced Test Reactor is operated and maintained by the Idaho National Laboratory (INL) for the Department of Energy (DOE). ATR tests and experiments are responsible for much of the world's data on material response to reactor environments. The ATR has nine flux traps in its core and achieves a close integration of flux traps and fuel by means of the serpentine fuel arrangement shown in Figure 1.0.

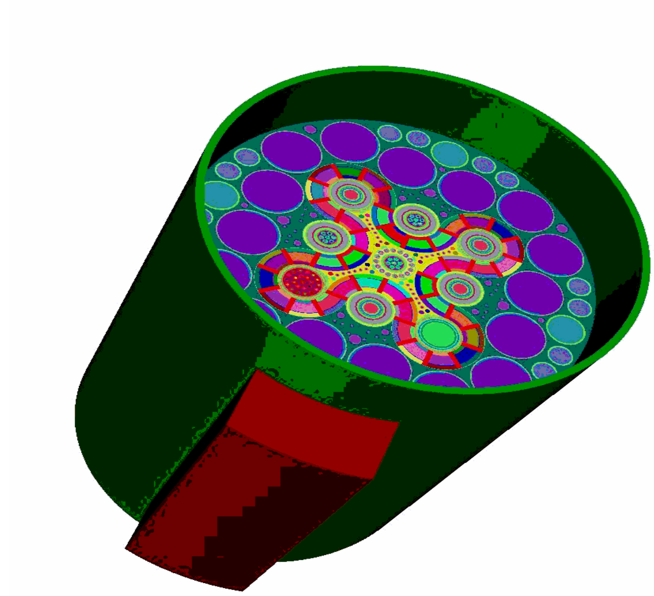


Figure 1.0 ATR Reactor and Core

The nine flux traps within the four corner lobes of the reactor core are almost entirely surrounded by fuel, as is the center flux trap position. The remaining four flux trap positions have fuel on three sides. Experiments can be performed using test loops installed in some flux traps with individual flow and temperature control, or in reflector irradiation positions using the primary fluid as coolant. Five of the flux traps are equipped with independent test loops and four are used for drop-in capsules. The ATR also uses a combination of rotational control cylinders (shims), and neck shim rods that withdraw vertically to adjust power while maintaining a constant axial flux profile. The power level (or neutron flux) of the flux trap positions in ATR can be adjusted for irradiation requirements. Maximum total power is 250 MW (thermal) in ATR. Balancing maximum ATR full power distribution results in as much as 50 MW produced in each lobe. Power shifting allows for a maximum and minimum lobe powers of 60 and 17 MW.

2.0 Attila Problem Solving Capabilities

Attila uses the standard first order steady state form of the linear Boltzmann Transport Equation (BTE) [1]:

$$\frac{d}{ds}\psi\left(\vec{r},E,\hat{\Omega}\right)+\sigma_t\left(\vec{r},E\right)\psi\left(\vec{r},E,\hat{\Omega}\right)=Q_S\left(\vec{r},E,\hat{\Omega}\right)+Q_f\left(\vec{r},E,\hat{\Omega}\right)+q\left(\vec{r},E,\hat{\Omega}\right) \quad (1)$$

where

$$Q_S\left(\vec{r},E,\vec{\Omega}\right)=\int_0^\infty\int_{4\pi}\sigma_s\left(\vec{r},E'\rightarrow E,\,\hat{\Omega}\circ\hat{\Omega}'\right)\psi\left(\vec{r},E',\hat{\Omega}'\right)d\hat{\Omega}'dE' \quad (2)$$

and

$$Q_f\left(\vec{r},E,\vec{\Omega}\right)=\frac{\chi(E)}{k}\int_0^\infty\nu\sigma_f\left(\vec{r},E'\right)\int_{4\pi}\psi\left(\vec{r},E',\hat{\Omega}'\right)d\hat{\Omega}'dE' \quad (3)$$

where ψ denotes the angular flux, d/ds is the directional derivative along the particle flight path, $\hat{\Omega}$ is a unit vector denoting the particle direction, σ_t denotes the total macroscopic interaction cross section (absorption plus scattering), σ_s denotes the differential macroscopic scattering cross section, χ is the fission spectrum, σ_f denotes the fission macroscopic cross section, ν is the mean number of fission neutrons produced in a fission and q denotes a fixed source.

This is the basic form of the transport equation solved by Attila. Attila uses multi-group energy, discrete-ordinate angular discretization and linear discontinuous finite-element spatial differencing (LDFEM). The LDFEM spatial discretization is third-order accurate for integral quantities and provides a rigorously defined solution at every point in the computational domain. The general solution technique within Attila is source iteration. Both k-eigenvalue (K_{eff}) and fixed source modes are supported, including coupled neutron-gamma calculations.

Attila also has depletion capability. Attila uses a built in code called Fornax. Fornax solves the fully coupled equations for the production, depletion, and decay of nuclides using a series expansion approximation to the matrix exponential solution. Short time constant products are treated separately using the same algorithm as in the ORIGEN code. Fornax supports an arbitrary number of fissile species. Separate data for up to 99 metastable states are supported for a given nuclide. Default data for 1307 nuclides, including half lives, three group reaction cross sections, and fission product yields are provided in an XML data file (fornax.xml, 30,000 lines) based on an ORIGEN-S data set.

Special DTF cross sections files were developed to support the burn, including detailed KERMA values for power normalization and cross sections for the individual capture reactions. For representative problems Fornax typically solves 20-75 burn zones per second on a single CPU 2.0 GHz Athlon Linux system.

3.0 Cross-Section Libraries

The COMBINE [2] code was used and modified to develop a four group ENDF-5 and ENDF-6 set of cross section (XS) libraries for Attila that gives the cross section libraries in Data Table Format (DTF) for fresh fuel configurations. This avoids having to use translation programs written in C or Fortran for ANISN to DTF data table structures. All data processing with COMBINE used an ATR energy spectrum combining the fast and thermal regions in COMBINE. Resonance treatment was used for those materials that have resonance data in the ENDF-5 and ENDF-6 cross-section sets. Testing was performed on the cross-section libraries for assurance of reasonable values. The Combine XS set was compared to the Hansen-Roach cross-section library using the Venus Reactor test provided with Attila. Transpire® also supplied cross section sets that are being used for comparisons. The Transpire® cross-section sets are based on the ENDF-6 formulation with NJOY for neutrons and gammas with depletion (burn). Additional work is being undertaken by Transpire® using SCALE to develop a collapsed eleven group burn cross section set in AMPX format. This work is based on a two-dimensional ATR core regional model for separate 2D cross section sets for the fuel, reflector, shims and other elements of the ATR reactor core. Transpire® has an SBIR with DOE for fiscal year 2006 to couple the ENDF-6/7 libraries to Attila directly for the generation of 2D/3D regional cross section sets.

4.0 Model Development

This section discusses some of the model development efforts for non-depleted fuel and depleted fuel problem comparisons.

4.1 Attila ATR 3D Model

Geometric and material information for the Attila [1] ATR model, which includes atom mixture densities and atom fractions, were obtained from ATR core calculations using the ATR MCNP [3] model. Additional models discussed in this report also used input from MCNP and MCNPX. Geometry parameters for the Attila calculations were generated using SolidWorks®, (SW), a computer aided CAD design system. The CAD assembly allowed test section modifications and control drum (shim) rotations. The ATR Attila model included the structure of the reactor on the top, bottom and perimeter of the reactor core. In order to compare the Attila ATR model with MCNP, the 19 radial plate fuel elements were homogenized into 3 radial sections. The CAD assembly was exported to Attila through the Parasolid® format. Attila preserves the original CAD component names in the translation, aiding the assignment of region-wise material properties. Attila's graphical user interface (GUI) was used for the full analysis, including mesh generation, material assignments, boundary conditions and the creation of post processing edits. The code can be executed in the GUI setup or separately as a solver. The computational model for the Attila ATR model included approximately six hundred thousand tetrahedral elements with 5 axial layers for the core region and one layer each for the top and bottom. The top and bottom layers were a mixture of aluminum and water, based on the MCNP geometry. The outer regions of the

Attila ATR model use an unstructured mesh while the core, loops and fuel can be modeled using specified layers for the mesh. This recent capability allows finer detail for the fuel, absorber regions (shims) and experiments. Figures 1.0, 2.0 and 3.0 provide VisIt [4] illustrations of the solid geometry for the ATR, the fuel and structured portion of the mesh for the Core Internals Changeout (CIC) configuration used in the data comparison of the Attila ATR 3D model. VisIt has been coupled to Attila for plots by the High Perfromance Computer (HPC) group of the INL.

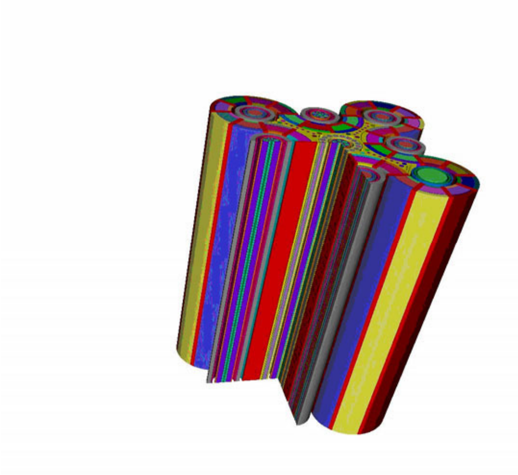


Figure 2.0 3D ATR Core Section

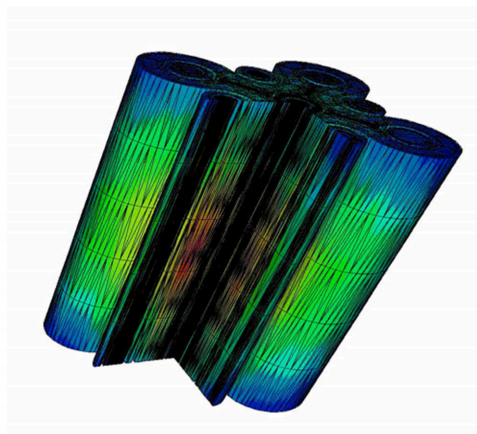


Figure 3.0 ATR Core Layered Mesh

4.2 Attila and MCNP Toy ATR Models

Additional model development was performed for a simplified 3D ATR MCNP model, referred to herein as the Toy ATR model developed by Bruce Schnitzler of the INL. It is also being used for comparisons of the Attila, MCNP-MOCUP [5] and MCNPX [6] codes for depletion analysis. In constructing the Attila Toy ATR model, the same approach was used with Solidworks® and the Attila mesher. The Toy ATR model geometry is illustrated in Figure 5.0. The Toy model consists of an aluminum barrel, a Beryllium core containing the six fuel elements of 93% enriched U-235, shim absorbers, the lower three shims having Hafnium pointed inward, shown in yellow and the upper three shims pointed outward. There are seven interior targets and six outer targets with the same geometrical configurations consisting of Neptunium 237, Np-237. The Toy mesh used in this study consisted of 140 K (thousand) terahedrons (tets). Attila allows fission and depletion of the U-235 and NP-237 in the calculations.

It should be noted that for deterministic codes such as Attila which use the Finite Element Method (FEM) it is important to use a large number of elements in the fuel and absorber regions to approximate the volume correctly. Since the mesh generator places points on the solid model geometric surface the polygons are inscribed. To obtain an exact volume points for the polygons would have to be placed outside the solid geometry surface.

4.3 Attila and MCNPX Godiva Models

A more elementary model used to benchmark the depletion capability was that of the well known Godiva [7] problem. The Godiva facility, shown in Figure 6.0, was one of the experiments performed at Los Alamos in the 1950's to determine the critical mass of a bare

94% enriched U-235 sphere which consisted of two identical sets of nested hemispheres. Figure 7.0 illustrates the solid geometry by VisIt for a half-section of the Godiva model. The

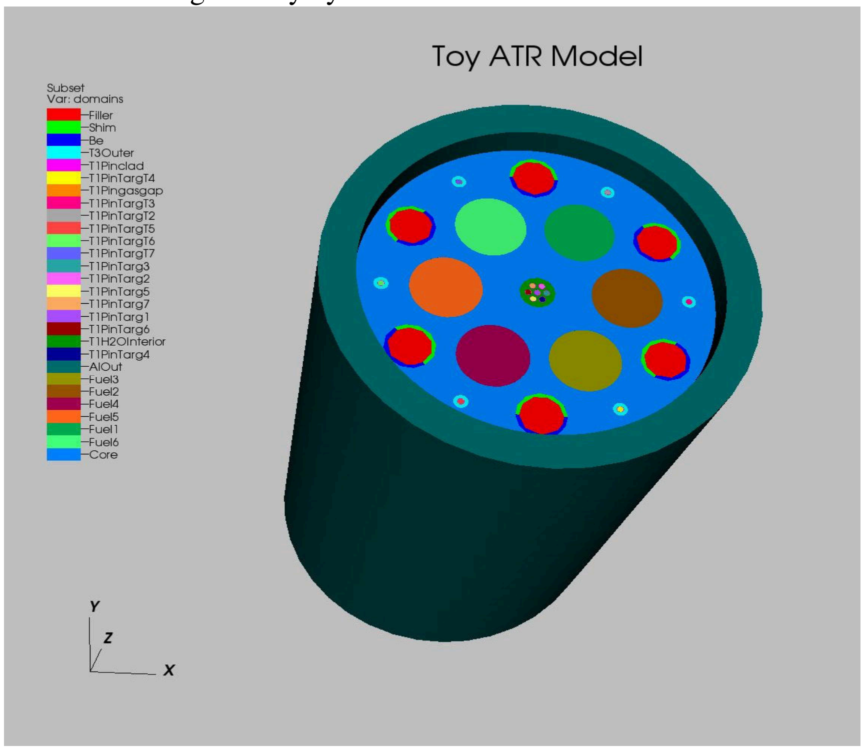


Figure 5.0 Toy ATR Model

MCNPX modified Godiva model problem has a fuel region which consists of two concentric spheres, a larger water region for neutron moderation and a thin iron outer shell. The number of tets used in this model was 70 K. For models such as this which consist of concentric spheres CAD tools normally allow "mating" the surfaces together. However, in some instances the Parasolid or interface file between the CAD program and the mesher utility allows extra numerical "slop" that results in some of the mesh not appearing. This is overcome during the assembly process of the CAD code by placing the concentric bodies at the origin.

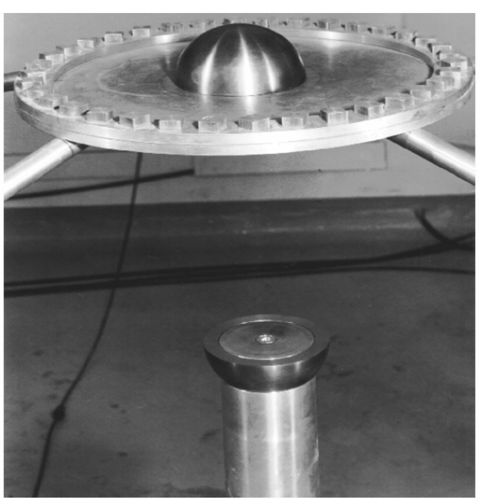


Figure 6.0 Godiva Multiplication Configuration

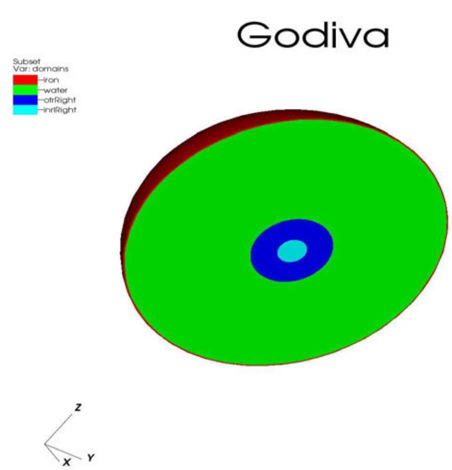


Figure 7.0 Godiva Solid Geometry

4.4 Attila and MCNPX 7 Can HEU Models

The last model discussed in this report is entitled the 7-Can HEU Test Problem by the authors of the MCNPX depletion code, shown in Figure 8.0 and a solid geometry section view in Figure 9.0 for Attila. [5] It consists of seven aluminum cans with 5% enriched U-235 in the lower portions of the can and a void in the upper part of the can. The cans are surrounded by air. The model consists of approximately 50 K mesh elements.

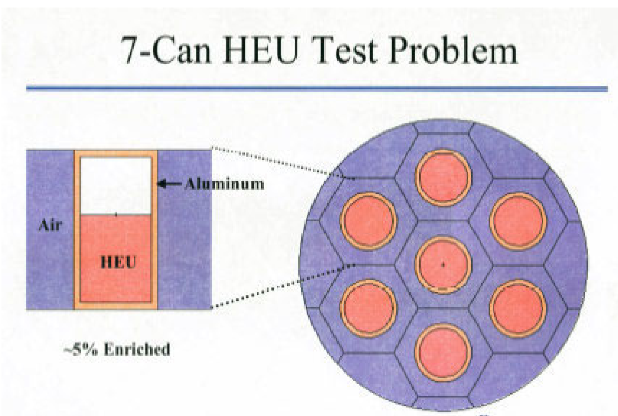


Figure 8.0

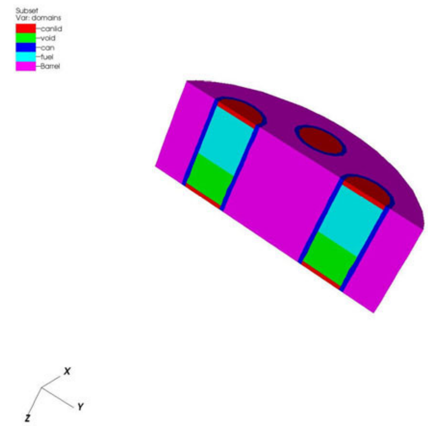


Figure 9.0 7- Can HEU Solid Geometry

5.0 Calculations and Results

This section provides the highlights of the calculations and results obtained for the models discussed in Section 4.0 of this report.

5.1 Comparison of 3D Attila Model to MCNP and Test Data

The first calculation discussed in this section will be for the 3D Attila ATR model, shown in Figure 1.0, compared to the measured data from the 1994 Core Internals Changeout (CIC) [8] performed for the ATR. After the Beryllium reflector block was taken out and replaced with a new reflector block and fresh fuel, measurements were taken using flux wands in the water gaps of the fuel elements. The forty fuel elements are arranged in a serpentine pattern as shown in Figure 1.0. The flux wands were placed in the water gaps between the eighteenth and nineteenth fuel plates. The experiments were also repeated in the ATRC (Advanced Test Reactor Critical Facility), a miniature low-power version of the ATR. MCNP models were compared to the data taken from these tests. Edits were used in the Attila code for fission (n,f) reactions for the power. These edits are also available for plotting using VisIt. This calculation was performed using the original Radion cross-section libraries. The model used was that of Figure 1.0 with 622 K tetrahedral elements. The calculation was performed on a 2CPU Opteron with a locally parallel version of Attila. The run time was approximately 24 hours. The K_{eff} for Attila was 1.015 compared to a K_{eff} computed by MCNP of 1.0012. The results shown in Figure 10.0 are for the ATR Attila model compared to the test data from ATR and ATRC along with comparisons to MCNP. The MCNP results compare well with the

ATR data while Attila compares favorably with the ATRC data. The cross section set used a default fission spectrum from NJOY given by

$$\chi(E) = 0.453 e^{-1.036E} \sinh\sqrt{2.29E} \qquad (4)$$

with the energy E in MeV. In addition, some of the flux wands for the ATR testing were installed incorrectly and "symmetry" was used to obtain data for fuel elements 16 through 21. Additional Attila modeling was performed for quarter core and 2D core comparisons to the CIC 94 data with good results. An advantage of the quarter core and 2D modeling is the significant reduction in runtime due to a smaller number of degrees of freedom in the problem, on the order of minutes for locally parallel computing.

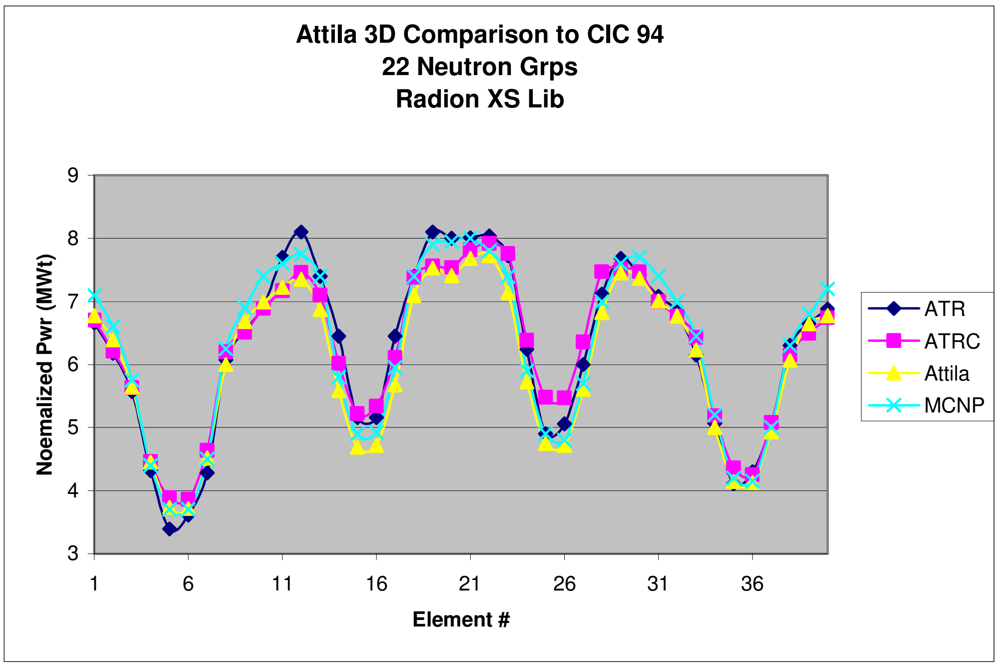
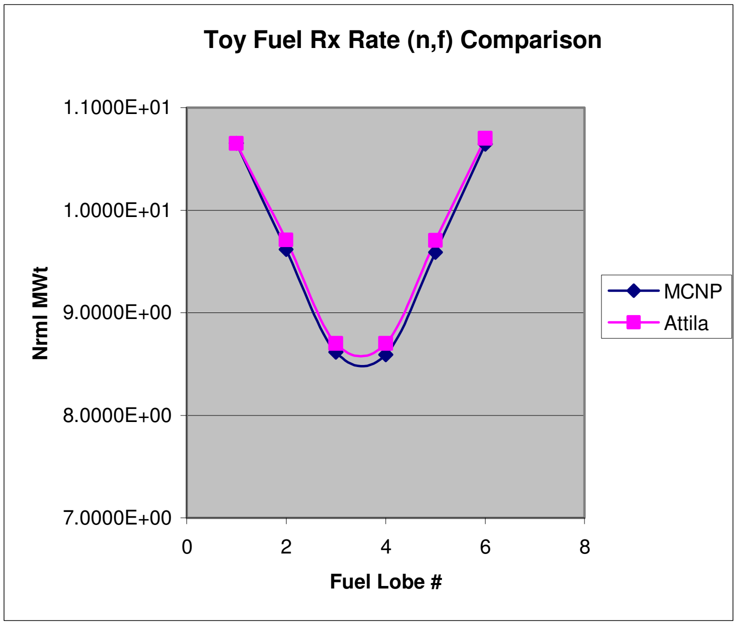


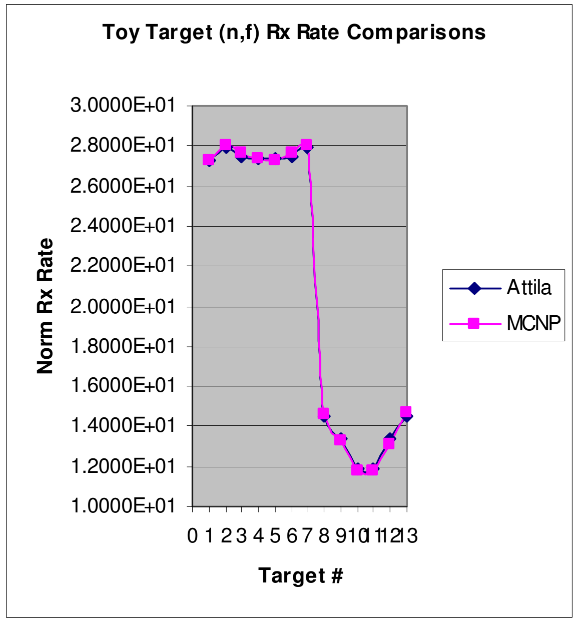
Figure 10.0 Attila, MCNP, ATRC and ATR Data Comparisons

5.2 Attila ATR Toy Model

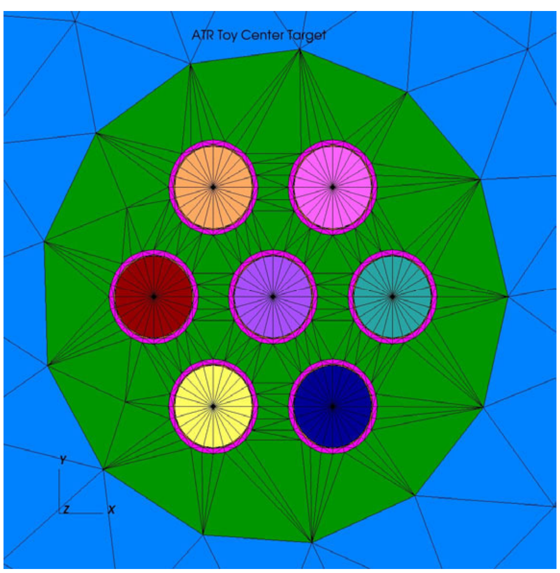
The Attila Toy ATR model was compared to MCNP for a fresh fuel configuration. Attila edits were used for data comparison along with VisIt graphs in this section. The computed K_{eff} for the Attila and MCNP models in this calculation were 1.016 and 1.0103 using the Transpire cross section Library. The first reaction compared was the (n,f) or neutron capture and fission reaction for the U-235 in the fuel. The results are shown in Figure 11.0. The run time for this problem is approximately six hours. The fuel region numbering shown in Figure 5.0 starts with fuel region number one in the northeast and continues clockwise through fuel region number six in the northwest. The connection of the calculation points in the figures of this section is not meant to convey continuity since this is a "discrete" model but is meant to convey visual comparisons between the two sets of data for Attila and MCNP. The reaction rate (power) is shown to be sensitive to the shim positions.

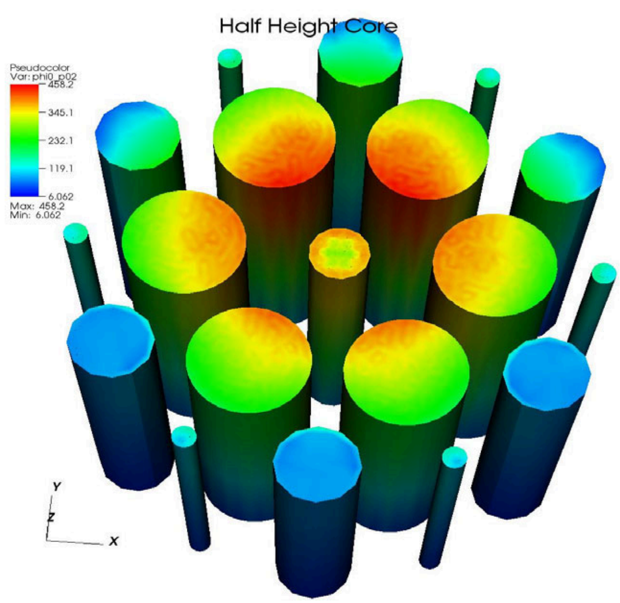
The next comparison is for the target fission rates. The target numbering starts at target number one in the center target of the center target region of Figure 5.0, target number two is in the northeast sector of the center region and continues clockwise through target number seven in the northwest region of the center targets. Outer target number eight commences in the northeast region of the reactor and continues clockwise through outer target thirteen. As discussed earlier the targets use Np-237, a fissionable material. The results for the targets are shown in Figure 12.0. Recently, Attila has been modified to allow a number of angular regions to be used axially in the thin annuli of cylindrical structures. Such thin annuli have challenged the capabilities of mesh generators in the past. This feature is shown in Figure 13.0 for the center targets.





Figures 11.0 & 12.0 Attila-MCNP Toy Model Fuel & Target Reaction Rates





Figures 13.0 & 14.0 Angular Polygon Meshing and Thermal Flux Distribution for Toy ATR Core

This feature is implemented in the Attila GUI and allows a more "exacting" mesh for smaller regions without failure of the mesh generator.

Figure 14.0 shows the correlation between the plots of Figures 11.0 and 12.0 with a half-height core sectional view. One can see the effects of the shim position on flux and power distribution by examination of the VisIt plot. Figure 14.0 also demonstrates the power of VisIt for chopped views of the reactor in 3D.

Attila and MCNP both allow a number of neutron or gamma reactions for comparison. One of interest is the (n,3n) reaction shown in Figure 15.0 for the inner Np-237 targets. The MCNP results approach those of Attila with more cycles and neutrons per cycle. A number of parameters were compared between the two codes which are too voluminous to discuss in this report. At the present time a depletion comparison between the Attila Toy and MCNP-MOCUP and MCNPX code models is being performed.

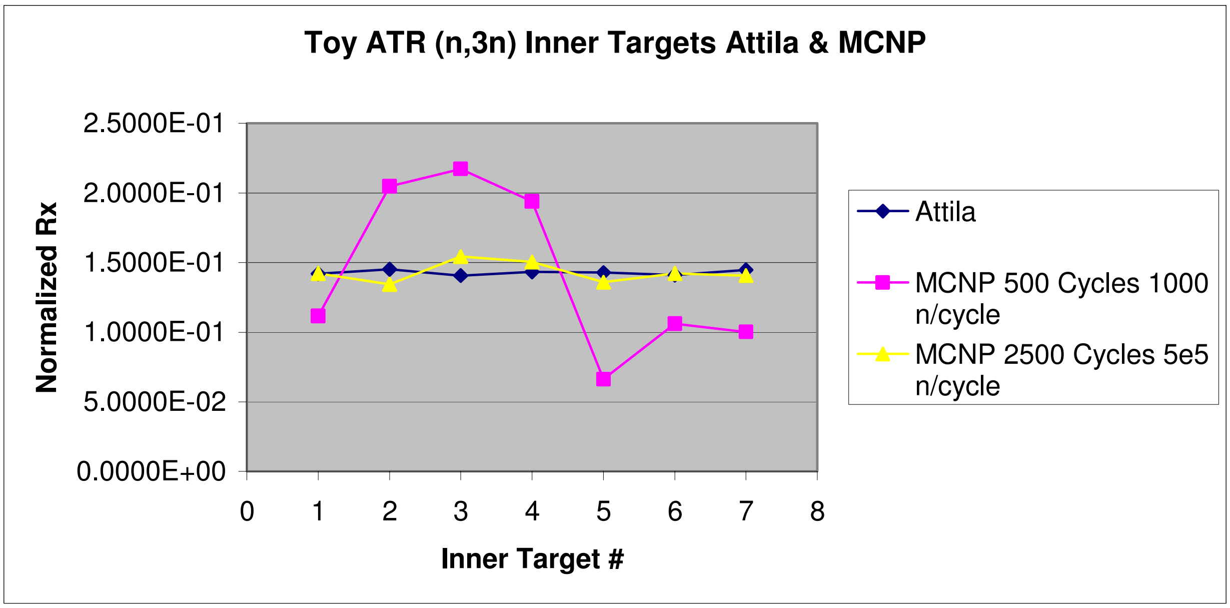


Figure 15.0 Inner Target Reaction (n,3n) Comparison

5.3 MCNPX and Attila Godiva Depletion Comparisons

This comparison uses a Godiva model from the MCNPX depletion code. This version of MCNPX is an alpha test version. The MCNPX Godiva input deck was used to obtain the dimensions and material properties of the Godiva model. The dimensions were used in SolidWorks^{TM} to develop the solid geometry input for Attila. The Attila GUI and mesher were used to build the model which consisted of 44 K tetrahedral elements. The solid geometry outline of the model is shown in Figure 7.0 and was discussed previously in the model development section.

The depletion or burn periods used for this case were time steps of 1.1574, 10.0, 2.31 and 99 days for both models. The power used was 3.26 Megawatts. The power fractions for each cycle were 1.0, 0.0, 1.0 and 0.0. The power fractions used have an interesting effect on the Xe-135 concentration as shown in Figure 16.0. The Xe-135 concentration increases during cycles with power and burns away during cycles without power.

Figure 17.0 shows the K_{eff} comparisons throughout the cycles. Figures 18.0 and 19.0 illustrate the fuel burn for the atom densities (barn-cm) of U-235 and the Pu-239 generation.

5.4 MCNPX and Attila 7 HEU Can Problem Comparisons

The last problem examined for depletion is that of the 7 HEU Can problem discussed in the model development section. MCNPX [5] uses CINDER90 as the depletion and decay part of the code package instead of ORIGEN. CINDER90 is a multi-group depletion code developed at LANL. The solid geometry portion of this calculation was developed from the MCNPX information of Reference [5] and built using SolidWorks,™ Attila and displayed in Figure 20.0 using VisIt. The mesh shown in Figure 20.0 employs 135 K tetrahedrons.

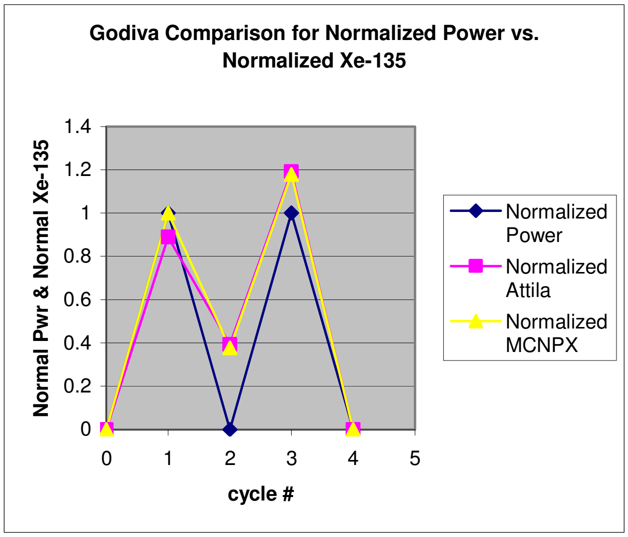


Figure 16.0 Normalized Xe-135 & Power Comparison

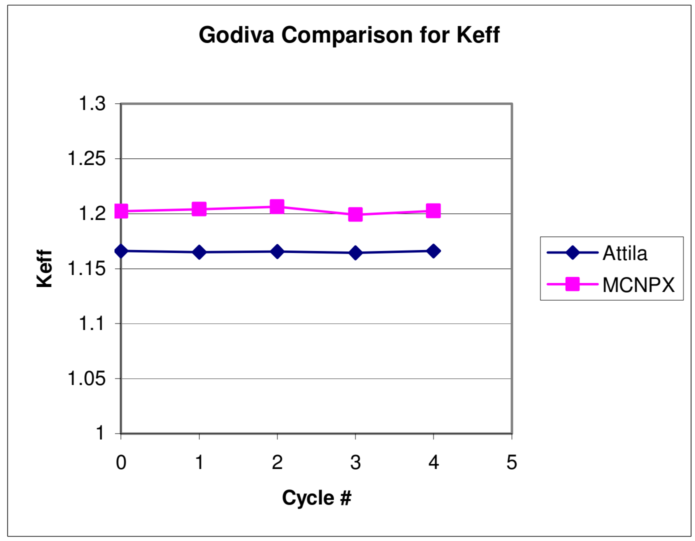


Figure 17.0 Godiva Keff Comparison

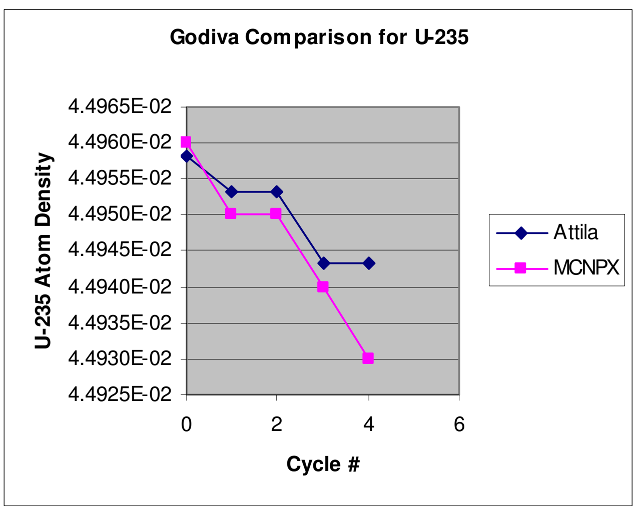


Figure 18.0 U-235 Burn

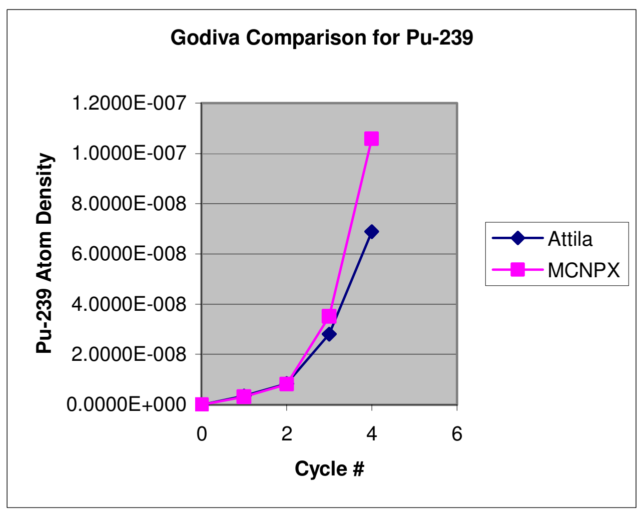


Figure 19.0 Pu-239 Generation

When the model is built in its entirety without the use of symmetry the code defaults to vacuum boundaries. The total power used in this calculation was 1.0 MW. Figure 21.0 shows a sectional view of the KERMA distribution in the fuel. Twelve burn cycles were used in this calculation consisting of 15.22 days for the first burn cycle and 30.44 days for the other eleven cycles. Figure 22.0 shows the calculated K_{eff} comparisons over the cycles and Figure 22.0 illustrates the buildup of Pu-239 in the fuel.

The cross section library used for this calculation was provided by Transpire and is based on the SCALE code in AMPX format.

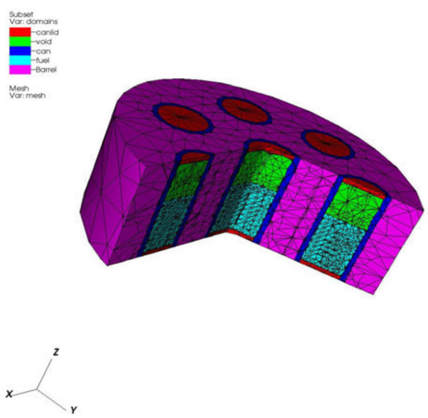


Figure 20.0 7 Can HEU Model & Mesh

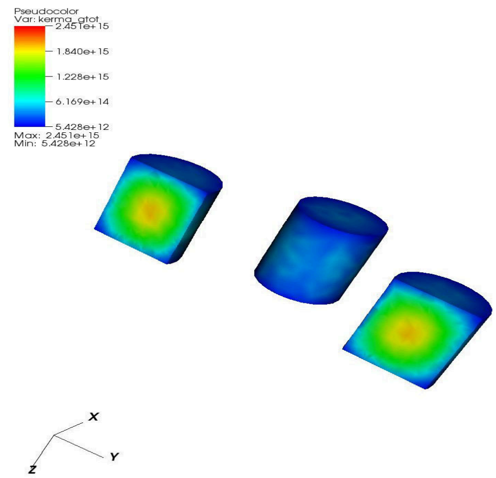


Figure 21.0 KERMA in Fuel Section View

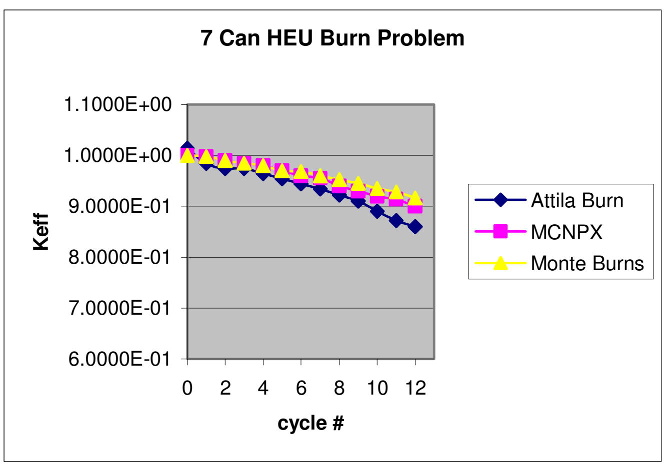


Figure 22.0 Keff Comparison

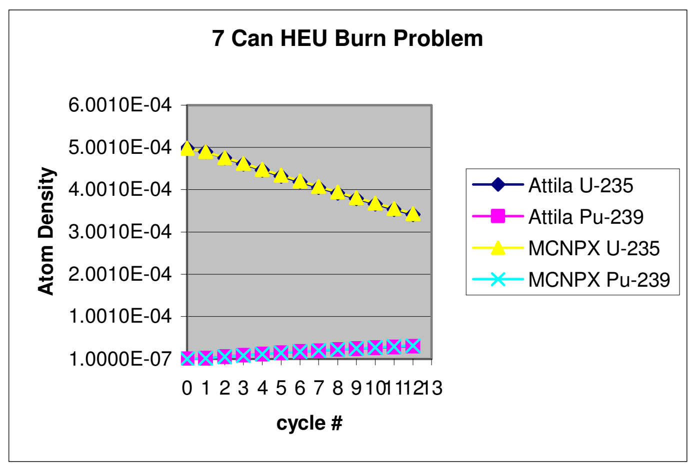


Figure 23.0 Fuel U-235 Burn and Pu-239 Generation

6.0 Summary and Future Work

The analysis performed to date indicates the acceptability of Attila for performing core wide safety analysis for the ATR. Additional work is being performed to validate the Attila ATR 3D and Toy models for depletion. These calculations are being compared to MCNP-MOCUP and MCNPX with depletion. Transpire is assisting INL in the development of a 3D ATR model using a complete 19 plate fuel assembly. Additionally, a number of criticality calculations are being performed as well as comparisons to analytical solutions.

The work on cross section libraries is of great interest and is being performed by both INL and Transpire. Transpire is presently collapsing a 248 group SCALE cross section set down to eleven groups using Attila. INL is also working with Studsvik®Scandpower to use HELIOS for additional cross section generation. We are also purchasing a 4CPU Opteron with 32

Gigabytes of RAM for 3D Attila ATR models with upwards of 5 million elements (tetrahedrons) in the model.

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References

1. T. A. Wareing, J. M. McGhee, J. E. Morel, and S. D. Pautz, "Discontinuous Finite Element Sn Methods on 3-D Unstructured Meshes," Nuclear Science and Engineering, 138:1-13, 2001.

2. R.A. Grimesey, D.W. Nigg and R.L. Curtis, "COMBINE/PC - A Portable ENDF/B Version 5 Neutron Spectrum and Cross-Section Generation Program," EGG-2589, Rev. 1 (February 1991).

3. S. S. Kim and R. B. Nielson, "MCNP Full Core Modeling of the Advanced Test Reactor," NRRT-N-92-021, INEL, EGG Idaho Inc.

4. VisIt, http://www.llnl.gov/visit

5. R.L. Moore, B.G. Schnitzler, C.A. Wemple, R.S. Babcock, D.E.Wessol, "MOCUP: MCNP-ORIGEN2 Coupled Utility Program", INEL-95/0523 (September 1995).

6. G.W. McKinney and H.R. Trellue, "Transmutation Feature Within MCNPX," LA-UR-04-1572.

7. Raphael J. LaBauve, "Bare, Highly Enriched Uranium Sphere (Godiva)," Volume II, NEA/NSC/Doc (95) 03/II.

8. R.T. McCracken et. al, " Results of Nuclear Requalification Testing Following the ATR Reflector V Core Internals Changeout Outage," INEL-94/089, December, 1994.