

UCRL-TR-233310

**ENDF/B-VII.0 Data Testing
for Three Fast Critical Assemblies**

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U.S. Department of Energy

Lawrence
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July 31, 2007

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Work performed under the auspices of the U. S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

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June 31, 2007

Table of Contents

I - Introduction	- 5 -
II - ENDF/B-VII.0 vs. ENDF/B-VI.8	- 5 -
III - Why these Three Fast Three Systems.....	- 5 -
IV - What are we testing?	- 6 -
V - K-eff is NOT Enough	- 7 -
VI - A Pragmatic Standard: Which Code is Right?	- 7 -
VII - Definition of the Three Systems	- 8 -
VIII - Consistency and Accuracy.....	- 8 -
IX - Statistical Accuracy	- 9 -
X - What is Important and What is NOT Important?	- 10 -
XI - Contributions to this comparison	- 13 -
XII - Summary of more Detailed Results	- 14 -
XIII - 8 Code Energy Dependent Flux Comparisons.....	- 17 -
Godiva 8 Code Comparisons	- 18 -
Jezebel 8 Code Flux Comparisons.....	- 20 -
Jezebel23 8 Code Flux Comparisons.....	- 22 -
XIV - First Step Detailed Results: One code/Two Data Libraries.....	- 24 -
MCNP results using VII.0 and VI.8 (one code/two data libraries).....	- 24 -
Godiva MCNP using ENDF/B-VI.8 and VII.0.....	- 25 -
Jezebel MCNP using ENDF/B-VI.8 and VII.0.....	- 27 -
Jezebel23 MCNP using ENDF/B-VI.8 and VII.0.....	- 29 -
XV - Second Step Detailed Results: One data Library/multiple codes	- 32 -
Godiva 8 Code Comparisons using VII.0.....	- 32 -
Jezebel 8 Code Comparisons using VII.0.....	- 35 -
Jezebel23 8 Code Comparisons using VII.0.....	- 38 -
XVI - Recommendations for Improving ENDF/B-VII.0.....	- 41 -
XVII - Differences in delayed neutron spectra	- 42 -
XVIII - Accuracy of ENDF/B-VII.0 Tabulated Fission Spectra	- 43 -
XX - The Godiva “Bump”	- 47 -
XXI - Conclusions	- 48 -
XXII - References	- 49 -
Appendix A: Contact Information	- 51 -
Appendix B: Submitting Code Results.....	- 53 -
Appendix C: Definition of K-eff.....	- 56 -

I - Introduction

In this report we consider three fast critical assemblies, each assembly is dominated by a different nuclear fuel: Godiva (U235), Jezebel (Pu239) and Jezebel23 (U233) [1]. We first show the improvement in results when using the new ENDF/B-VII.0 data [2], rather than the older, now frozen, ENDF/B-VI.8 data [3]. We do this using what we call a one code/ multiple library approach, where results from one code (MCNP) are compared using two different data libraries (ENDF/B-VII.0 and VI.8). Next we show that MCNP results are not specific to this one code by using what we call a one data library/multiple code approach; for this purpose we invited many codes to submit results using the ENDF/B-VII.0 data; the most detailed results presented in this report compare MCNP and TART.

The bottom line is that we have shown that using the new ENDF/B-VII.0 data library with a variety of transport codes, for the first time we are able to reproduce the expected K-eff values for all three assemblies to within the quoted accuracy of the models, namely 1.0 +/- 0.001. This is a BIG improvement compared to the results obtained using the older ENDF/B-VI.8 data library. Another important result of this study is that we have demonstrated that currently there are many computer codes that can accurately use the new ENDF/B-VII.0 data.

II - ENDF/B-VII.0 vs. ENDF/B-VI.8

Recently (December 2006) the much anticipated ENDF/B-VII.0 data library was finally approved by the Cross Section Evaluation Working Group (CSEWG) and generally distributed by the National Nuclear Data Center (NNDC), Brookhaven National Laboratory.

The preceding version of ENDF/B, namely ENDFV/B-VI, Release 8 [3], contained 328 evaluations [R2]; of these 328 evaluations 13 elemental evaluations are not included in ENDF/B-VII.0 (these have been replaced by isotopic evaluations). ENDF/B-VII.0 [2] includes 315 evaluations from ENDF/B-VI (all but the 13 elemental evaluations), and 78 evaluations for new isotopes, for a total of 393 evaluations in ENDF/B-VII.0.

We plan extensive data testing of the new library to: 1) Compare results for VII.0 vs. VI.8, using a single computer code [multiple data libraries/single code] and 2) Compare results for VII.0, using as many computer codes as possible [one data library/multiple codes]. In all cases we will use the internationally available critical assemblies defined in Ref [1].

III - Why these Three Fast Three Systems

As a first step in this data testing here we limited our comparisons to only three fast critical assemblies [1]. These assemblies have been selected as the simplest measured systems; in each case both the composition and the geometry is as simple as possible.

We have selected three homogeneous, spherical systems, each contains primarily one of the three fuels: Godiva (U235), Jezebel (Pu239) and Jezebel23 (U233).

Regardless of what type of critical assembly you are interested in, it is important to understand that all fission systems are driven by a source of fast (MeV) fission neutrons emitted when an atom fissions. Since the results of any calculation can be no more accurate than the definition of the neutron source, we have decided to first insure that we can accurately model the source of fission neutrons in these three systems.

The intent is that after we have verified our results for these three fast systems will we consider progressively slower systems, working our way downward in medium neutron energy from fast to intermediate and ultimately to thermal systems.

IV - What are we testing?

Obviously we are testing the new ENDF/B-VII.0, but we are also testing all of the participating neutron transport codes, and less obvious, we are also testing the nuclear data processing codes used to prepare data for our transport codes. The most important point to understand is that neither our nuclear data, nor our codes are perfect. This and preceding comparisons have led to important improvements in both our data and our codes.

One important step that is often "overlooked" is the **nuclear data processing** step that comes between the basic evaluated data and our neutron transport codes. We should not forget that even though all of the transport codes included in this study say they used the ENDF/B-VII.0 data, there has actually been a lot of assumptions and manipulation of the data done by nuclear data processing codes before our transport codes ever see the data. Often it is the assumptions made by our data processing codes that define and sometimes limit the accuracy of the subsequent use of the data in our applications. Important as this step is trying to explicitly include analysis of all of the nuclear data processing codes was deemed beyond the scope of this paper. However, by comparing the detailed output of our transport codes we can implicitly test our nuclear data processing codes, and at least in the case of NJOY [19] we do explicitly show the influence that this often "overlooked" step can have on our results.

Related to nuclear data processing codes is the approximations used by each code. It was deemed beyond the scope of this paper to go into the detailed of the approximations used by each nuclear data processing code and how it limits our transport codes. I will merely mention a few points: 1) All eight Monte Carlo codes now use continuous energy cross sections (earlier versions of some of these codes only used multi-group data). but the accuracy to which the continuous energy cross sections are defined varies from one code to another, 2) Some of these codes use a unresolved resonance treatment, while others do not; for the three fast critical assemblies the unresolved resonance region is not as important as it is for slower systems, 3) Some of these codes use continuous secondary energy and angular distributions, while others use equally probable bins, 4) There are a variety of methods used to interpolable secondary energy/angle distributions.

These are but a few of the differences used by each code systems. So it would be naïve to assume that saying they all use ENDF/B-VII.0 uniquely defines how they are actually interpreting the data. What is important to us in this study is whether or not all of these approximations result in any important differences in the answers. **To summarize, for this study we are testing both nuclear data processing codes and transport codes, and the results we present must be consider as what is produced due to the each overall system, including both nuclear data processing code and transport codes.**

V - K-eff is NOT Enough

Another important point to understand is that calculating K-eff is necessary, but not sufficient, to guarantee that our data and codes are accurate. In our comparisons we try to go one step further to insure that not only are integral parameters, such as K-eff, accurate, but so are our differential results. Specifically, when we consider the definition,

$$K\text{-eff} = \frac{\text{Pr oduction}}{\text{Absorption} + \text{Leakage}} = \frac{\text{Pr oduction}}{\text{Re moval}}$$

Here neutron production, absorption and leakage, are each one integral parameter, defined by integrating over the entire system in space, direction, and energy. For our comparisons we look at integral parameters, such as K-eff, but we also look in detail at the differential production, absorption and leakage, versus neutron energy. These detailed comparisons often lead to identifying problems with our nuclear data and/or our transport codes, ultimately leading to improvements in both data and codes. For details on how we uniquely define the energy dependent production, absorption and leakage, see appendix B and C.

VI - A Pragmatic Standard: Which Code is Right?

We do not assume that the answers from one code are any better or worse than the answers from any other code. Rather we attempt to establish what I call a pragmatic standard, based on comparing results from as many different codes as possible. As we will see “BEST” may be defined in several different ways, for example, we could define BEST as the most accurate interpretation of the ENDF/B data, or we could define BEST as the most accurate physical models, or in any number of other ways. Here we will present results from as many codes as possible, explain the sources of differences in results, and let users decide what is BEST for their use.

Our Two Step Approach

In our data testing we will use a two step approach.

- 1) **One code/multiple data libraries:** In the first step we want to determine whether or not the new ENDF/B-VII.0 data is an improvement over the old ENDF/B-VI.8 data. To do this we will use one code (MCNP) to compare results for these two data libraries.

- 2) **One data library/multiple codes.** In our second step we verify that our ENDF/B-VII.0 results generally can be obtained from a variety of computer codes, i.e., we want to insure that our results from step one are not specific to only one code.

VII - Definition of the Three Systems

For these comparisons all codes MUST use only ENDF/B-VII.0 data [2]. If you wish to compare to results using other nuclear data, please feel free to do so using the results from this study; but in this case this would have to be a separate study organized by you.

All three models are taken from ref. [1]. Each is a solid sphere with only one uniform spatial zone. Therefore to uniquely define each model we need only specify: radius, density and composition. All systems are at room temperature (293.6 Kelvin). All of these models are designed to produce K-eff close to 1.0. The table below includes parameters exactly as they are quoted in ref. [1].

Model	HMF001-002 Godiva	PMF001-001 Jezebel	UMF001-001 Jezebel23
Radius (cm)	8.7407	6.3849	5.9838
Density (grams/cc)	18.74	15.61	18.424
Composition (atoms/barns-cm)	235U 4.4994d-2 238U 2.4984d-3 234U 4.9184d-4	239Pu 3.7047d-2 240Pu 1.7512d-3 241Pu 1.1674d-4 69Ga 8.26605d-4 71Ga 5.48595d-4	233U 4.6712d-2 234U 5.9026d-4 238U 2.8561d-4 235U 1.4281d-5

Derived Quantities based on the above radius and density

Volume (cc)	2797.224	1090.312	897.4697
Mass (grams)	52419.98	17019.77	16534.98

For PMF001-001 (Jezebel) the original model specification was for natural gallium. For use with ENDF/B-VII.0 data this has been replaced by the isotopes,

69Ga 8.26605d-4
 71Ga 5.48595d-4
 Ga 13.75200d-4 = same as original model Ga total

VIII - Consistency and Accuracy

It wasn't too long ago that when calculating criticality we were pleased if we could calculate K-eff within 0.5%, e.g., any results between 0.995 and 1.005 was considered indistinguishable = 1.0. Today we feel that we can calculate systems to much better precision, but not to infinite precision; we are pleased if we can calculate K-eff to within 0.1%, e.g., any results between 0.999 and 1.001 is considered indistinguishable = 1.0. In ref [1] these models are quoted to produce integral results (K-eff) as follows,

Godiva (U235) = 1.0 +/- 0.001
Jezebel (Pu239) = 1.0 +/- 0.002
Jezebel23 (U233) = 1.0 +/- 0.002

There are many factors that contribute to limiting the accuracy to which we can calculate results, among these factors are: uncertainty in the parameters for the systems we calculate, uncertainties in the nuclear data we use, uncertainties in the computer codes we use, and more... None of these factors are perfect and in the real world we must make allowances for these uncertainties by avoiding assuming we can calculate results to too high precision. As an example, let's take a look at an obvious uncertainty in our models.

Anyone who reads the documentation for these systems in Ref [1] will find pictures of these systems, and can see that they are not "exactly" simple spherical systems completely isolated from the surrounding world. From this you can appreciate that our simplified isolated, homogeneous, spherical three systems are idealized models of the actual measured systems; this is a major contributing factor in the quoted uncertainty of these models.

Naturally nuclear data can be a major contributing factor to uncertainty; that's why we are comparing results for two different data libraries: the new ENDF/B-VII.0 and the old ENDF/B-VI.8 data files.

IX - Statistical Accuracy

We are naturally very interested to know the accuracy of our results. But we must use care to insure that we do not confuse the overall accuracy of our results with the statistical uncertainty reported by our Monte Carlo transport codes. For example, if we run our Monte Carlo codes long enough our results will indicate no significant statistical uncertainty in our answers. **In this case it is incorrect to assume that this means our answers are "perfect". All this really means is that the statistical uncertainty is much less than the overall uncertainty due to other factors.**

For the systems that we are calculating here the uncertainty due to the models are, as defined above, of the order of 1.0 +/- 0.001 in K-eff. Therefore in order to be sure that we are not introducing any significant additional uncertainty, we should insure that the statistical uncertainty from our Monte Carlo calculations is much less than this.

The results presented in this paper are based on 1 billion (10^9) histories for most codes, and 10 billion (10^{10}) histories for TART [4]. **At this level the statistical accuracy of the results are much smaller than the inherent inaccuracies of other factors. Therefore below we do not quote code errors +/- the statistical uncertainty for each result, because they are not a good indicator of the overall accuracy of our results.**

As a guide toward judging the accuracy of the quoted results, the below table presents TART results and their statistical accuracy for each of the three systems, for both

expected (recommended) and analog results, for several different number of histories run. These results are all based on running 100 settle batches, followed by 10,000 active batches (settle batches are only 1% overhead). The total number of histories run is based on changing the number of source neutrons per batch: 10 billion = 1,000,000; 1 billion = 100,000; 100 million = 10,000 per batch.

To help guide you, note that relative to the K-eff values which are all very close to 1.0, an uncertainty of +/-1.0D-5, means an uncertainty of +/-0.00001, or 1 in the last quoted digit of K-eff. So that anything less than this, as with the 10 billion expected results, means less than +/-0.00001 in the quoted K-eff. Conversely, with the 100 million analog results +/-1.0D-4, means +/-0.00010 or more.

From these results we can see that by 10 billion histories the statistical uncertainty is 1 or less in the last quoted digit. Since, based on the uncertainties in the models, this is two orders of magnitude below the +/- 0.001 accuracy we are trying to achieve. **In other words the statistical uncertainties are irrelevant compared to other uncertainties.**

K-eff expected and analog results vs. the number of histories run

	10 billion	1 billion	100 million
Godiva Expected	1.00019+/-7.162D-6	1.00017+/-2.287D-5	0.99997+/-7.311D-5
Analog	1.00018+/-1.319D-5	1.00021+/-4.218D-5	0.99991+/-1.338D-4
Jezebel Expected	1.00010+/-7.215D-6	1.00008+/-2.262D-5	0.99996+/-7.174D-5
Analog	1.00011+/-1.525D-5	1.00011+/-4.793D-5	1.00002+/-1.538D-4
Jezebel23 Expected	0.99983+/-6.919D-6	0.99985+/-2.179D-5	0.99988+/-7.008D-5
Analog	0.99983+/-1.360D-5	0.99986+/-4.302D-5	0.99990+/-1.371D-4

X - What is Important and What is NOT Important?

We will be focusing on K-eff values calculated by a variety of codes. We define,

$$K\text{-eff} = \frac{\text{Pr oduction}}{\text{Absorption} + \text{Leakage}} = \frac{\text{Pr oduction}}{\text{Removal}}$$

Where Production, Absorption and Leakage are integrated over the entire system. Besides the scalar values of Production, Absorption and Leakage, we will also compare the energy dependent spectra for these quantities (see, Appendix B and C for their definitions). These energy dependent spectra are extremely helpful in explaining differences between integral results and also serve to insure that even when we obtain the same integral results, the details of the calculations are correct, i.e., as stated earlier, the correct value of K-eff is necessary, but not sufficient, to insure the accuracy of our results. These spectra are also extremely important because they allow us to determine what energy ranges are important for any systems.

We determine what energies ranges are important by normalizing the integral of all spectra to unity, and then integrating the energy dependent spectra, first starting from zero integral at low energy and working our way up toward unity integral at high energy,

and then starting from zero integral at high energy and working our way down toward unity integral at low energy.

These three fast critical systems are so similar that it is sufficient for us to illustrate results of these integrals for only one system; the following page shows plots of these integrals for Godiva.

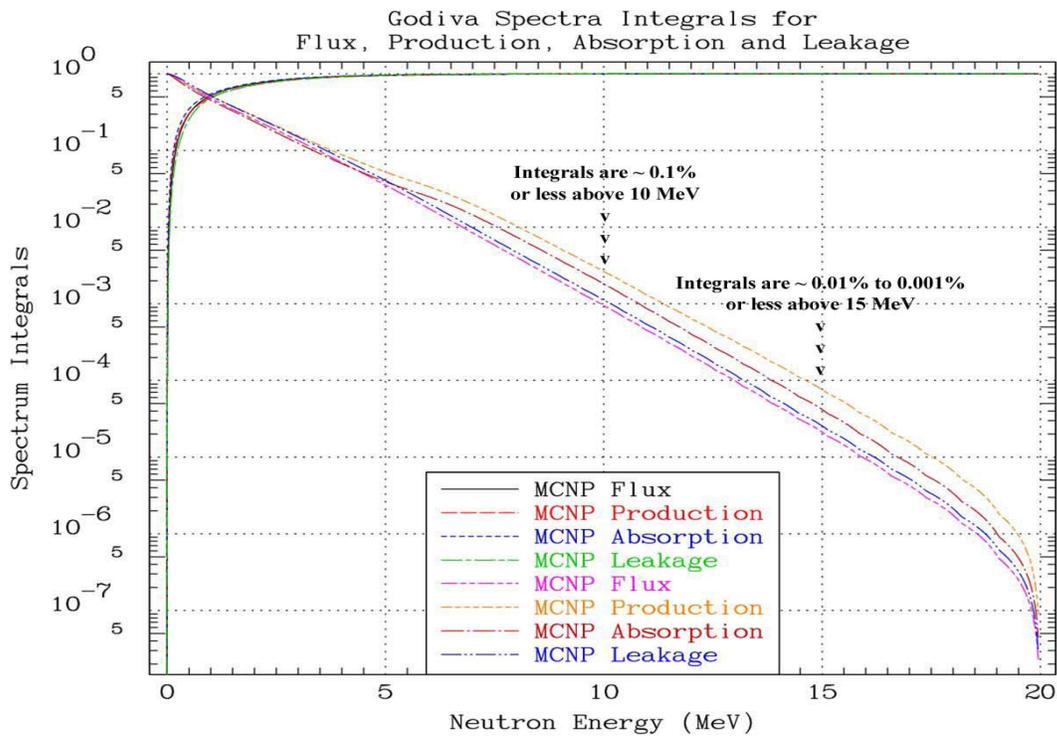
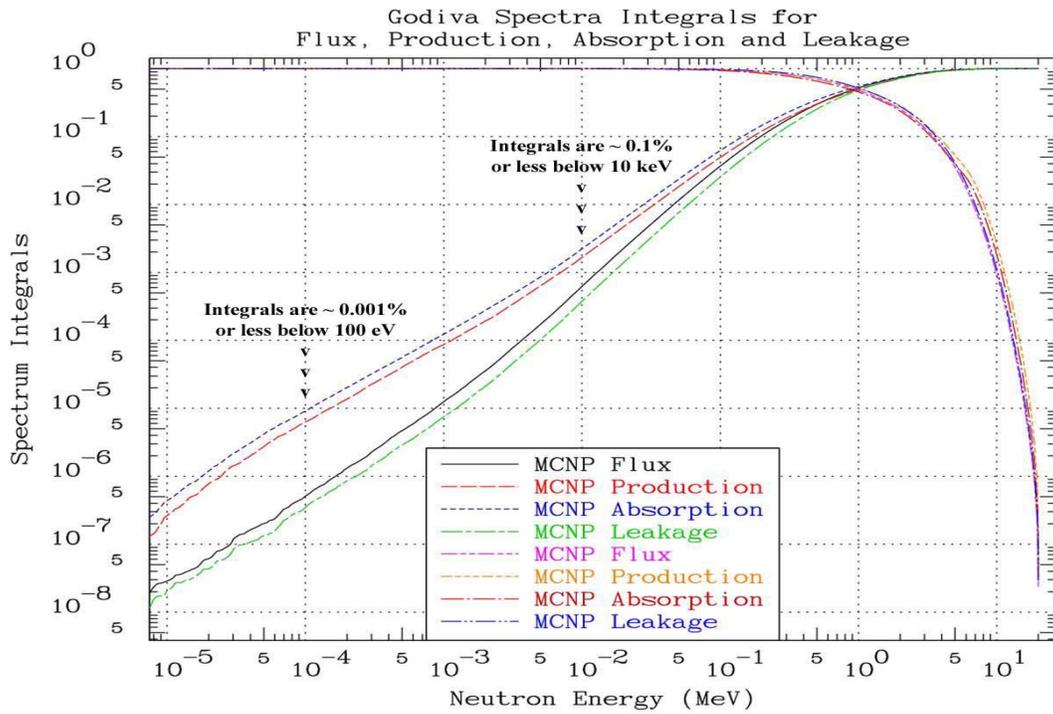
From the below plots we can see the median energies for these systems, which is the point where the two integrals cross at 50%. Here we can see that the media energy for flux, production, absorption and leakage are all very close to 1 MeV, as they are for all three of these systems. This is a clear indication of how truly “fast” these critical systems are. For comparison, when we look at well thermalized system we find median energies close to $(3/2)KT$, at a fraction of 1 eV, more than a million times slower than the fast systems we are focusing on here.

We can see from the integral from low energy to high is that the integrals up to about 10 keV are only roughly 0.1% of the total integrals. Similarly, we can see from the integral from high energy to low is that the integrals above about 10 MeV are only roughly 0.1% of the total integrals. We can summarize these results as,

Below 10 keV ~ 0.1%
Above 10 MeV ~ 0.1%
10 keV to 10 MeV ~ 99.8%

What this means is that as far as K-eff is concerned, results will be very insensitive to how accurately we calculate results below 10 keV and above 10 MeV, so that in our comparisons we will concentrate on the important energy range 10 keV to 10 MeV. We will also discuss differences we see outside of this energy range, but only to explain the sources of these differences, not because they will have any major impact on K-eff.

But a word of caution here: K-eff is not the only parameter of interest. For example, if you are interested in reaction rates, such as $(n,2n)$, then the high energy range will be very important for your application. So please do not make the mistake of assuming that what we are saying is that the low and higher energies are generally not important; **we are only saying that as far as these fast critical systems to define K-eff the lower and higher energy ranges are not important.**



XI - Contributions to this comparison

Many codes were invited to participate in this code comparison. The below list shows a complete list of all codes that were invited, as well as results received from codes by the time this report was issued; hopefully in the future additional results will be received from other codes, and these will be included in revisions of this report. To date in alphabetical order contributions were received from,

Code	Contributors
CE-KENO	Sedat Goluoglu, ORNL [7]
COG	Edward Lent, LLNL [8]
MCNP	Robert MacFarlane, LANL [9]
MERCURY	Scott McKinley, LLNL [10]
MONK	Christopher Dean, Serco Assurance [11]
TART	Ernest Plechaty, LLNL and Dermott Cullen, LLNL [4]
TRIPOLI	Yi-Kang Lee, CEA and Jean-Christophe Sublet, CEA [12]
VIM	Roger Blomquist, ANL [13]

Summary of K-eff Results using ENDF/B-VII.0 data and Many Transport Codes

	Godiva	Jezebel	Jezebel23
MCNP	0.99985	0.99986	0.99964
TART	1.00019	1.00010	0.99983
COG	1.00057	1.00010	0.99986
TRIPOLI (Sublet)	1.00024	0.99991	0.99979
TRIPOLI (Lee 1)	1.00015	1.00003	0.99978
TRIPOLI (Lee 2)	1.00023	1.00006	0.99981
CE-KENO	0.99971	0.99960	0.99938
VIM	1.00032	1.00011	0.99981
MERCURY	1.00024	1.00071	1.00048
MONK	1.00056	1.00066	1.00086
AMTRAN (Sn)			
ARDRA (Sn)			
MC2000			
MCU			
MVP			
WIMS			

TRIPOLI (Lee 1) is based on K-eff collisions.

TRIPOLI (Lee 2) is based on K-eff = Production/Removal.

Results were received for eight Monte Carlo codes. **The most important point to note from the above results is that ALL of the Monte Carlo reported K-eff results are within what we consider to be the acceptable range 1.0 +/- 0.001.** This illustrates that these codes are already able to use ENDF/B-VII.0 data, and that they produce reliable results, at least for K-eff.

XII - Summary of more Detailed Results

First we compare MCNP results using the new ENDF/B-VII.0 data library [2] and the older ENDF/B-VI.8 data library [3] (one code/two data library results). The important point to note here is big improvement in K-eff results using VII.0 compared to VI.8. Using the older VI.8 data K-eff is in all three cases underestimated by much more than what we consider to be the acceptable range of 1 ± 0.001 . In contrast, using the new VII.0 data K-eff is in all cases well within this range.

MCNP results using VII.0 and VI.8 (one code/two data libraries)

	Godiva VII.0	Godiva VI.8	Jezebel VII.0	Jezebel VI.8	Jezebel23 VII.0	Jezebel23 VI.8
Flux	6.74192	6.76161	4.68642	4.69703	4.12318	4.10447
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.43009	0.43042	0.32795	0.32803	0.38792	0.38730
Leakage	0.57005	0.57315	0.67219	0.67458	0.61244	0.61988
Removal	1.00014	1.00357	1.00014	1.00261	1.00036	1.00718
K-eff	0.99985	0.99644	0.99986	0.99740	0.99964	0.99287
Removal Time nanoseconds	6.21699	6.18135	3.72886	3.73463	3.20374	3.15053

To demonstrate that the above results are not specific to only MCNP, below we present comparisons between MCNP and TART both using the same VII.0 data (one data library/two codes). Here we see that both MCNP and TART produce results well within our acceptable range of 1 ± 0.001 for all three systems.

MCNP and TART using VII.0 (one data library/two codes)

	Godiva MCNP	Godiva TART	Jezebel MCNP	Jezebel TART	Jezebel23 MCNP	Jezebel23 TART
Flux	6.74192	6.74039	4.68642	4.68691	4.12318	4.12237
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.43009	0.43012	0.32795	0.32790	0.38792	0.38799
Leakage	0.57005	0.56969	0.67219	0.67200	0.61244	0.61218
Removal	1.00014	0.99981	1.00014	0.99990	1.00036	1.00017
K-eff	0.99985	1.00019	0.99986	1.00010	0.99964	0.99983
Removal Time nanoseconds	6.21699	6.21765	3.72886	3.72938	3.20374	3.20556

Finally, integral test results are shown below, where we compare results from eight different codes, all using the same VII.0 data. Here we see that all eight codes produce results well within our acceptable range of 1 ± 0.001 for all three systems.

Godiva 8 Code Comparisons using VII.0

	MCNP	CE-KENO	COG	Mercury	MONK	TART	Tripoli	VIM
Flux	6.74192	6.77669	6.78467	6.73976	6.73125	6.74039	6.74048	6.75933
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.43009	0.42832	0.43022	0.42969	0.42970	0.43012	0.43017	0.42864
Leakage	0.57005	0.57209	0.56921	0.57007	0.56973	0.56969	0.56958	0.57104
Removal	1.00014	1.00041	0.99943	0.99976	0.99943	0.99981	0.99976	0.99968
K-eff	0.99985	0.99959	1.00057	1.00024	1.00056	1.00019	1.00024	1.00032
Removal Time nanoseconds	6.21699	6.21401	6.24093	6.18991	6.17658	6.21765	6.22675	6.23371

Jezebel 8 Code Comparisons using VII.0

	MCNP	CE-KENO	COG	Mercury	MONK	TART	Tripoli	VIM
Flux	4.68642	4.69200	4.69669	4.68307	4.68415	4.68691	4.68639	4.68955
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.32795	0.32731	0.32792	0.32778	0.32787	0.32790	0.32798	0.32732
Leakage	0.67219	0.67299	0.67198	0.67151	0.67147	0.67200	0.67211	0.67257
Removal	1.00014	1.00030	0.99990	0.99929	0.99934	0.99990	1.00009	0.99989
K-eff	0.99986	0.99970	1.00010	1.00071	1.00066	1.00010	0.99991	1.00011
Removal Time nanoseconds	3.72886	3.72023	3.73901	3.71855	3.71715	3.72938	3.73398	3.72361

Jezebel23 8 Code Comparisons using VII.0

	MCNP	CE-KENO	COG	Mercury	MONK	TART	Tripoli	VIM
Flux	4.12318	4.12735	4.11889	4.11874	4.12217	4.12237	4.12278	4.12624
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.38792	0.38737	0.38793	0.38750	0.38781	0.38799	0.38795	0.38741
Leakage	0.61244	0.61326	0.61221	0.61202	0.61133	0.61218	0.61226	0.61278
Removal	1.00036	1.00063	1.00014	0.99952	0.99914	1.00017	1.00021	1.00019
K-eff	0.99964	0.99937	0.99986	1.00048	1.00086	0.99983	0.99979	0.99981
Removal Time nanoseconds	3.20374	3.19927	3.20874	3.19033	3.19598	3.20556	3.20658	3.19885

A lot has changed since 1965 when Keepin published his estimates of removal times for these systems, but his 1965 values are reasonable close to what we calculate today; his values are: Godiva 6.04, Jezebel 3.00, Jezebel (Skidoo) 2.82 nanoseconds [14]. This is admittedly not great agreement, but not bad after 40 years.

The bottom line is that these results demonstrate at least two important points,

- 1) For these systems ENDF/B-VII.0 produced much better results than VI.8.**
- 2) We now have at least these eight codes that can accurately use the VII.0 data.**

Deterministic results (Sn)

It is unfortunate that we do not have any Sn results available at publication time; we are still hoping that even after the initial publication of this report, we receive Sn results from other codes, in the hope that we can obtain a clearer picture of Monte Carlo vs. Sn results.

Until additional Sn results are available, we provide references to a few other reports [15, 16], that show comparisons between Monte Carlo and Sn results; see,

[15] Intercomparison of Calculations for Godiva and Jezebel, JEFF Report 16 (December 1999), currently on-line at http://www.nea.fr/html/dbdata/nds_jefreports/jefreport-16.pdf

[16] JEFF3.1 Benchmarking against Critical Integral Experiments, JEF/DOC-1187, June 2007, by Isabelle Duhamel, Institute for Radioprotection and Nuclear Safety.

XIII - 8 Code Energy Dependent Flux Comparisons

Below we compare the scalar flux (actually fluence) from 8 codes for these 3 fast critical systems. Here we defined the flux integrated over the entire system per neutron produced; this is simply the pathlength traveled by neutrons in cm.

The below figures contain a lot of data and you may not be able to follow the energy dependent variation of the flux from any one code. That's o.k. **These plots indicate that a given code has a problem only if it stands out from the crowd.** So if the flux from a given code does not stand out, its results are sufficiently similar to the results from all other codes and we judge the results to be acceptable.

The below comments are roughly the same for all three systems. Below we show a comparison of the scalar flux over 3 energy ranges:

- 1) 10 keV to 10 MeV, which is roughly 99.8% of the integral of the flux;
- 2) low energy range, 100 eV to 10 keV, 0.1% of integral
- 3) high energy range, 1 to 20 MeV, 0.1% of integral

The number after the code name is in all cases the integral of the flux from 10^{-5} eV to 20 MeV per neutron produced in each system. The top 2/3 of each plot is of the data, and the bottom 1/3 is the ratio of the all sets of data to MCNP.

For simple integral parameters, such as K-eff, they are only sensitive to the flux between 10 keV and 10 MeV.

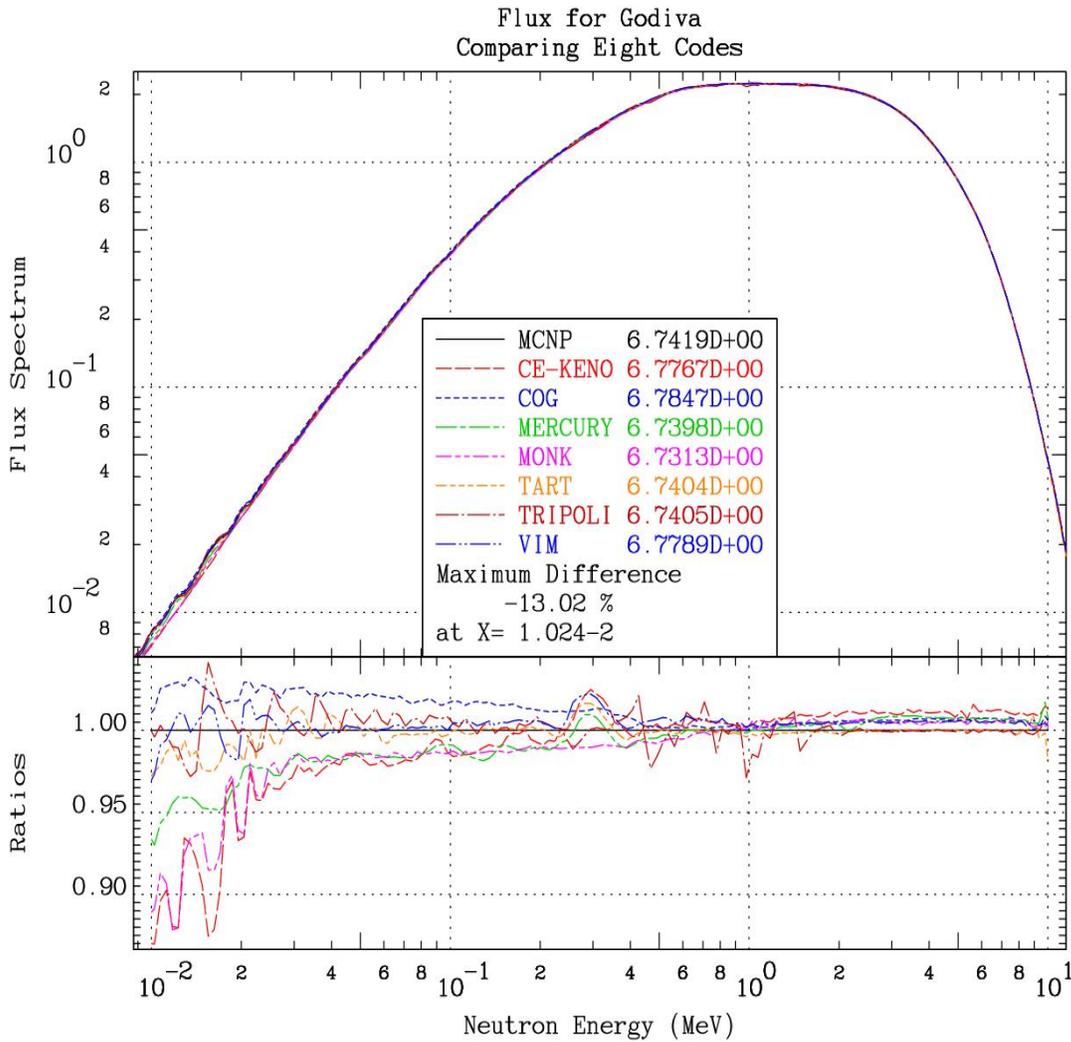
The low probability low and high energy ranges can effect other important parameters, such as (n,2n) reaction rates, which are sensitive to the high energy range.

The overall conclusion is that for all three systems all of the codes agree closely in the important, high probability energy range 10 keV to 10 MeV. At low energy CE-KENO has a “blip” in the 3 to 4v keV range, followed by a drop in the flux at lower energies; this has no apparent effect on integral results. At low and high energy ranges the spread in results is larger; below 10 keV down to 100 eV, up to +/- 50%, and above 10 MeV, up to about +/- 10%, with the exception of MERCURY that shows large differences at high energy; the source of this difference is understood and is being corrected.

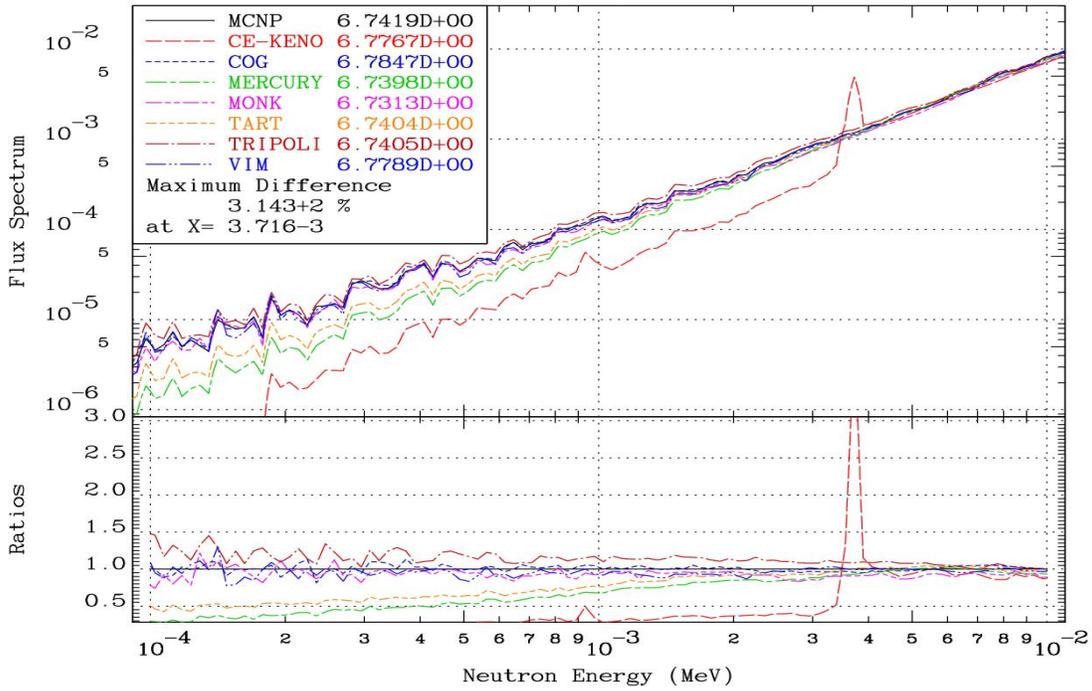
Godiva 8 Code Comparisons

Generally we see very good agreement over the important 10 keV to 10 MeV range, with very close agreement near the peak of the spectra (1 MeV), and agreement to within a few per-cent over the entire range. Below 30 keV down to 10 keV CE-KENO and MONK drift to about 10% below MCNP, but this trend does not continue to lower energy.

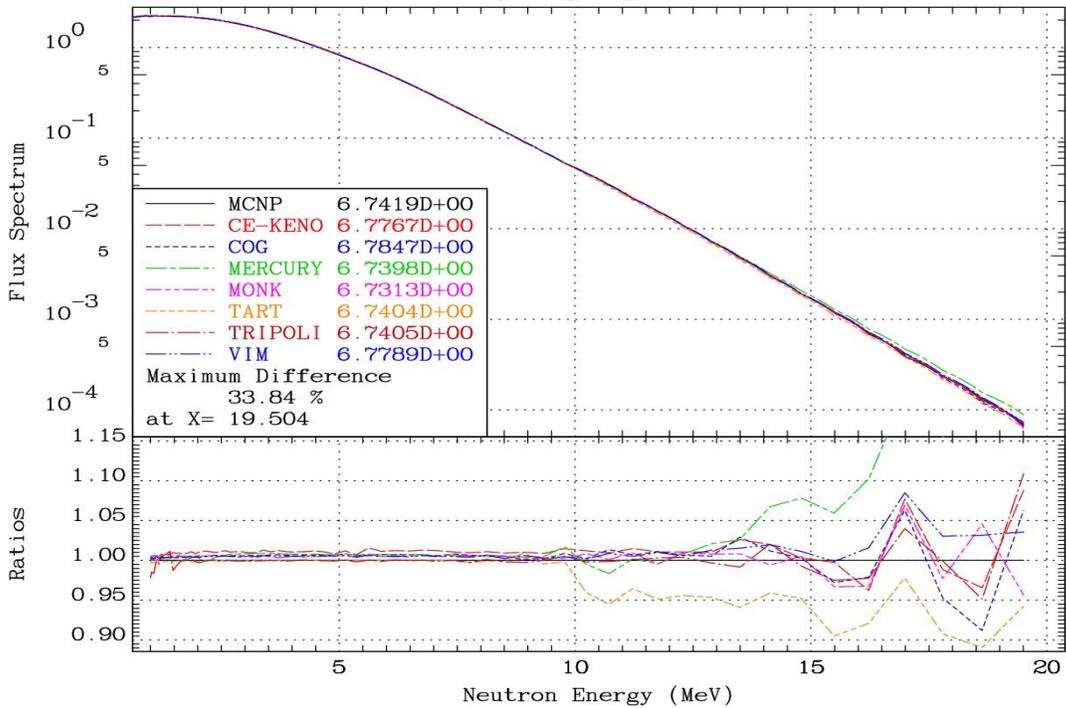
We see larger differences over the lower probability low and high energy ranges. At low and high energy TART differs from MCNP; this is explained later in this paper. At low energy we see a spread of up to +/- 50% by 100 eV. **At low energy CE-KENO has a “blip” in the 3 to 4v keV range, followed by a drop in the flux at lower energies; this has no apparent effect on integral results. At high energy MERCURY is up to 30% too high; this is understood and is being corrected.** At high energy by suppressing the MERCURY results in the ratio, for the other codes we see about 10% differences in this very low probability energy range.



Flux for Godiva
Comparing Eight Codes



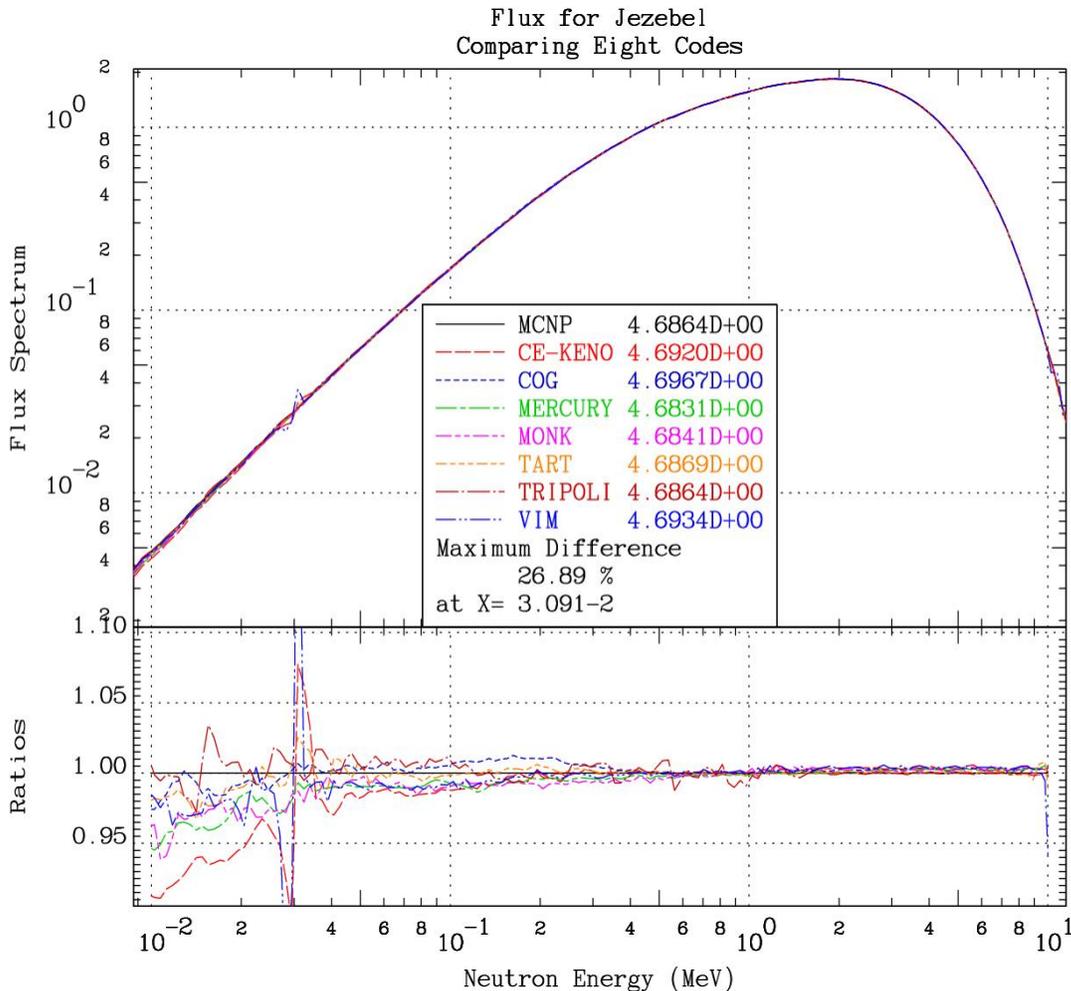
Flux for Godiva
Comparing Eight Codes

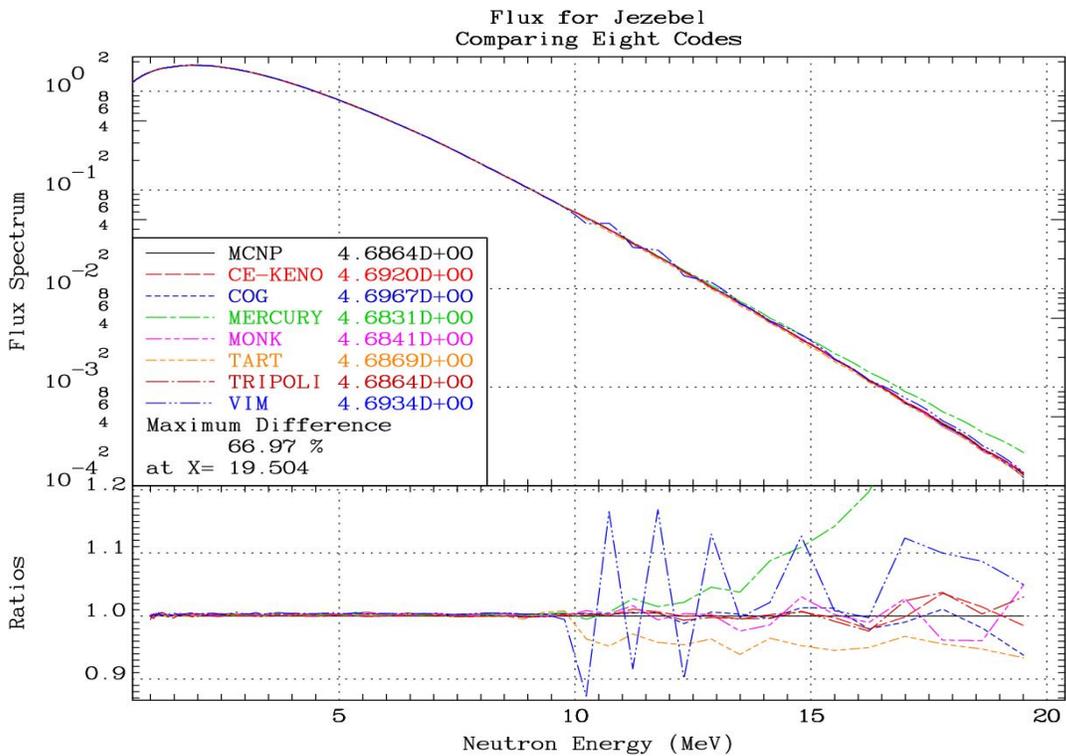
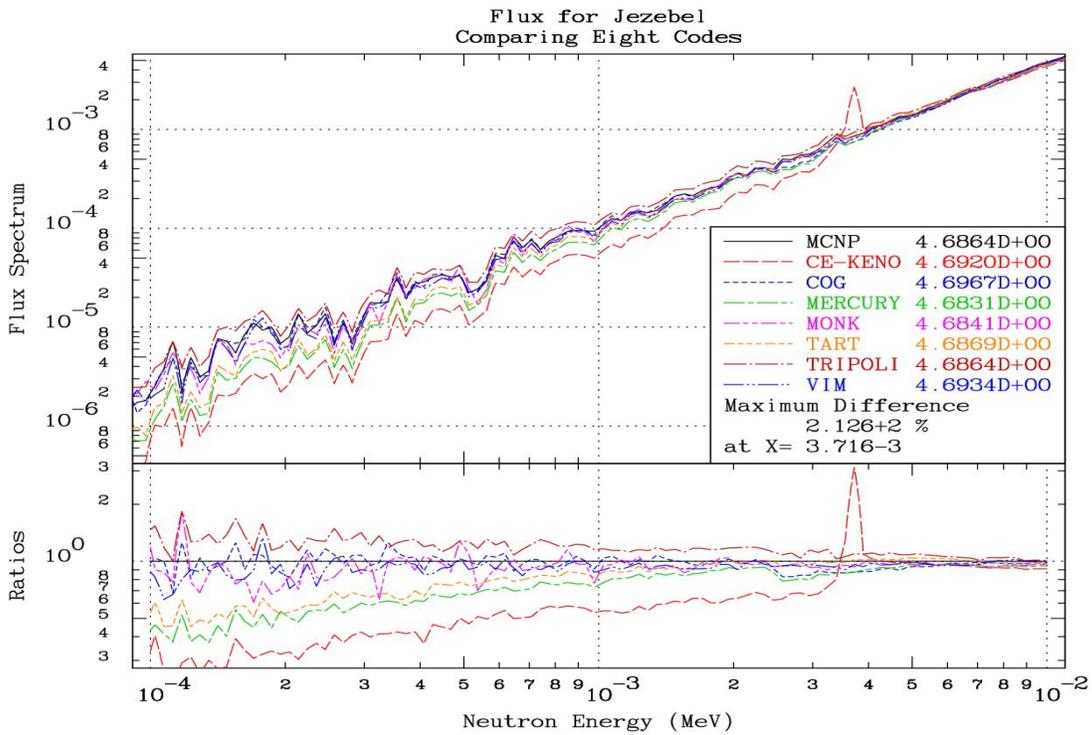


Jezebel 8 Code Flux Comparisons

Generally we see very good agreement over the important 10 keV to 10 MeV range, with very close agreement near the peak of the spectra (1 MeV), and agreement to within a few per-cent over the entire range, except for **CE-KENO (6%)** and **VIM (28%)** have a **problem over a narrow energy range near the unresolved resonance region boundaries near 30 keV**; the source of this problem is understood, and it is being fixed. To see the variation of the other codes the VIM ratio has been suppressed.

We see larger differences over the lower probability low and high energy ranges. At low and high energy TART differs from MCNP; this is explained later in this paper. At low energy we see a spread of up to +/- 50% by 100 eV. **At low energy CE-KENO has a “blip” in the 3 to 4v keV range, followed by a drop in the flux at lower energies; this has no apparent effect on integral results. At high energy MERCURY is up to 60% too high; this is understood and is being corrected.** At high energy by suppressing the MERCURY results in the ratio, for the other codes we see about 10% differences, with some spikes to 20% by VIM, in this very low probability energy range.

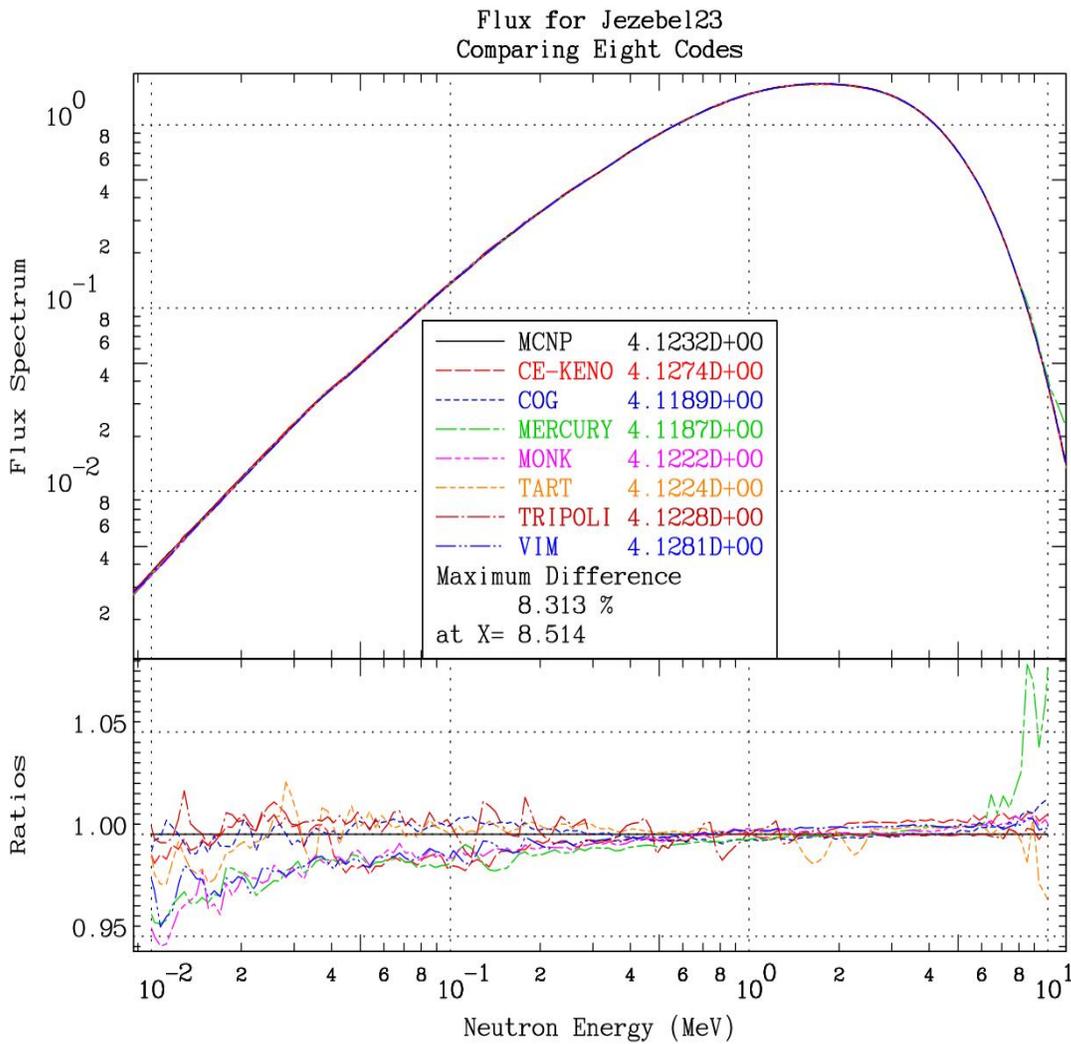


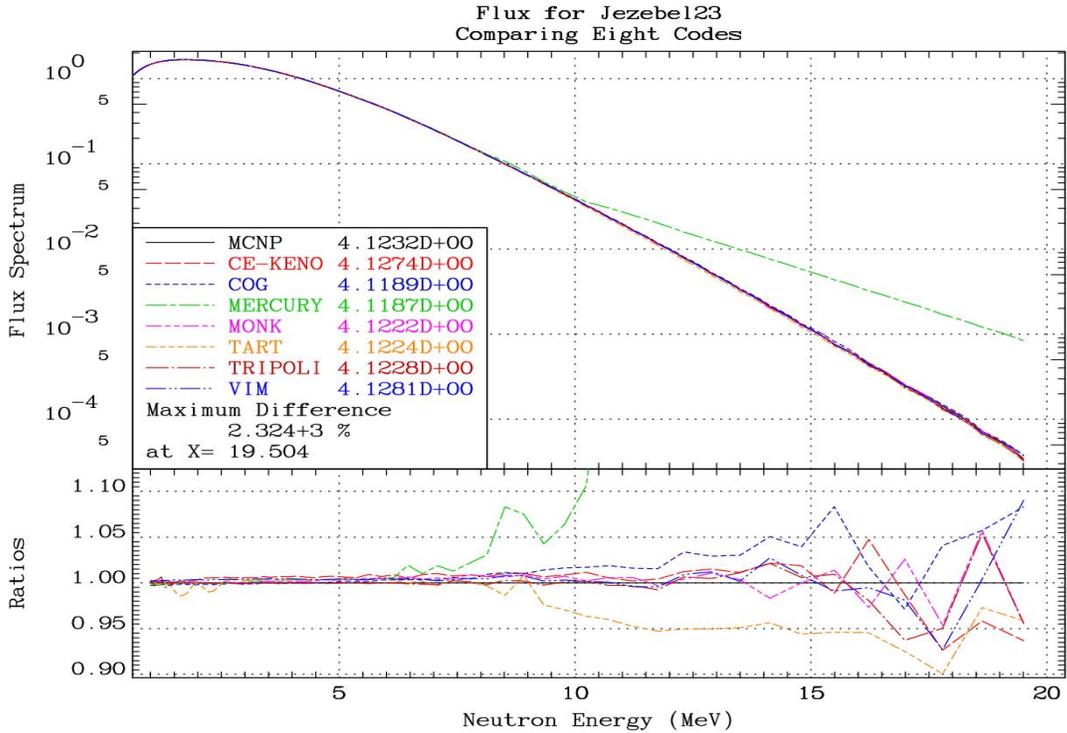
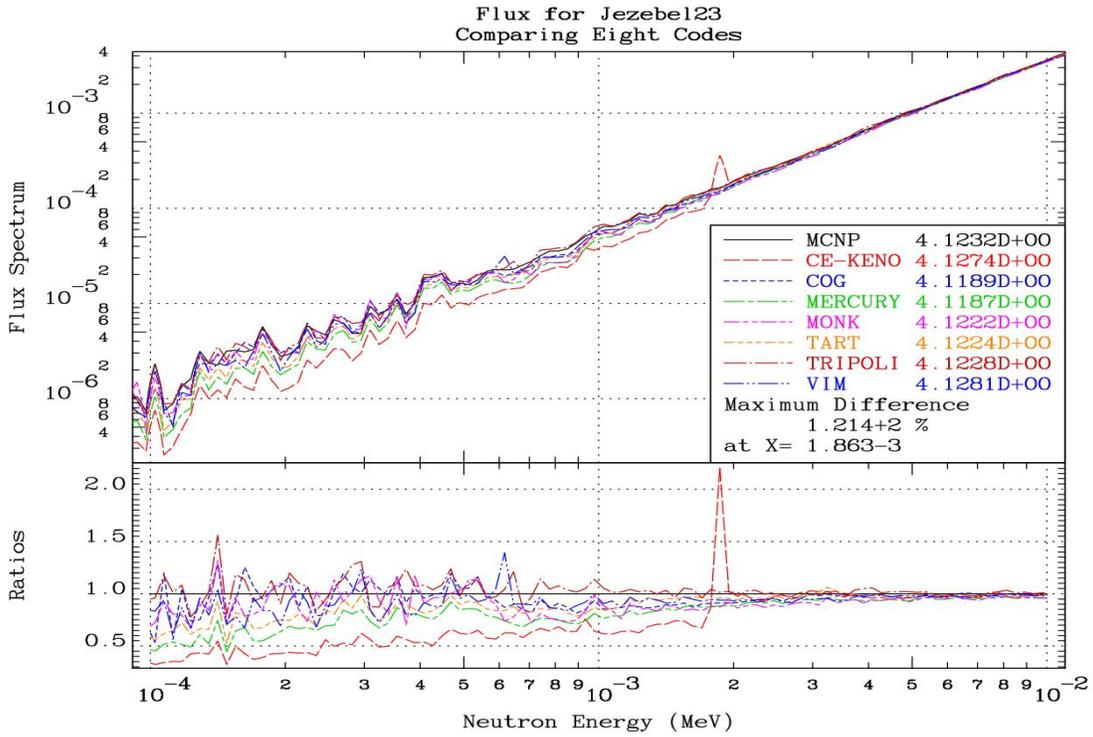


Jezebel23 8 Code Flux Comparisons

Generally we see very good agreement over the important 10 keV to 10 MeV range, with very close agreement near the peak of the spectra (1 MeV), and agreement to within a few per-cent over the entire range, except for MERCURY which is deviating from the other solutions near 10 MeV.

We see larger differences over the lower probability low and high energy ranges, with a spread of up to +/- 50% by 100 eV. At low energy TART and MERCURY differ from MCNP; this is explained later in this paper. **At low energy CE-KENO has a “blip” near 1 keV, followed by a drop in the flux at lower energies; this has no apparent effect on integral results. At high energy MERCURY is up to a factor of 23 to high; this is understood and is being corrected.** At high energy by suppressing the MERCURY results in the ratio, for the other codes we see about 10% differences in this very low probability energy range.





XIV - First Step Detailed Results: One code/Two Data Libraries

Here we present detailed MCNP (one code) results, using ENDF/B-VI.8 and VII.0 (two data libraries). From the below table of integral parameters we can see the improvement in results using VII.0 compared to VI.8. Using VII.0 K-eff for all three systems are well within what we consider to be the acceptable range 1 ± 0.001 . In comparison VI.8 underestimates K-eff for all three systems by much more than 0.001: Godiva -0.003; Jezebel -0.0026; Jezebel23 -0.007.

MCNP results using VII.0 and VI.8 (one code/two data libraries)

	Godiva VII.0	Godiva VI.8	Jezebel VII.0	Jezebel VI.8	Jezebel23 VII.0	Jezebel23 VI.8
Flux	6.74192	6.76161	4.68642	4.69703	4.12318	4.10447
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.43009	0.43042	0.32795	0.32803	0.38792	0.38730
Leakage	0.57005	0.57315	0.67219	0.67458	0.61244	0.61988
Removal	1.00014	1.00357	1.00014	1.00261	1.00036	1.00718
K-eff	0.99985	0.99644	0.99986	0.99740	0.99964	0.99287
Removal Time nanoseconds	6.21699	6.18135	3.72886	3.73463	3.20374	3.15053

There are many differences between the VII.0 [2] and VI.8 [3] evaluations that effect these results; this includes changes in fission cross sections, neutrons emitted per fission (ν), fission spectra, etc., for details see [17]. The below plots of flux, production, absorption and leakage for these three systems show the cumulative effect of all of these changes.

Godiva

The most striking difference we see is softer spectrum using VII.0, e.g. at very high energy the VII.0 results are up to 36% less than the VI.8 results.

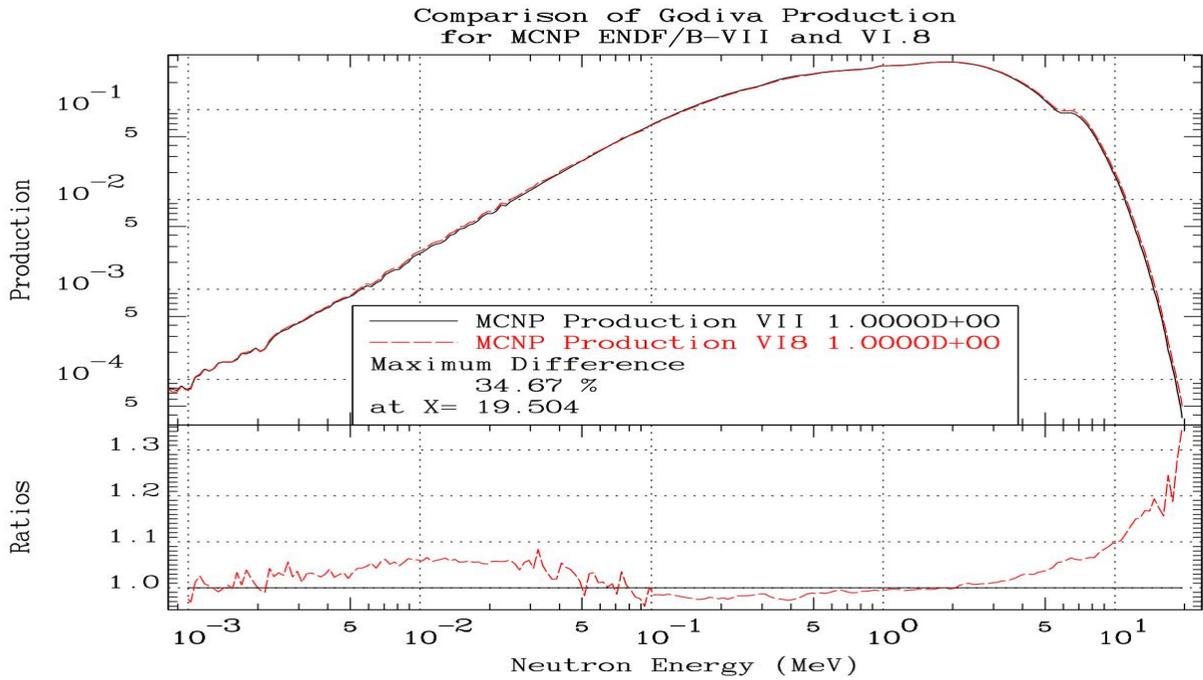
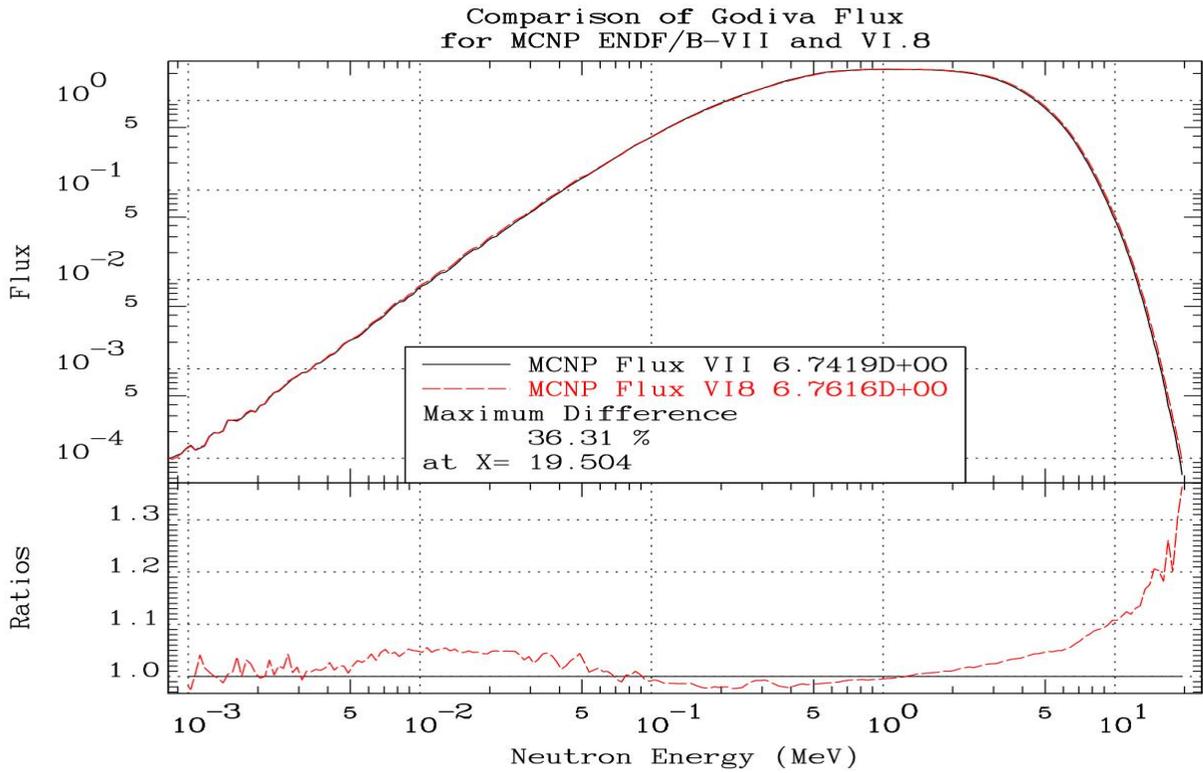
Jezebel

In contrast to Godiva, the Jezebel spectrum is harder using VII.0, e.g., at very high energy the VII.0 results are up to 35% greater than the VI.8 results. At lower energy we can also see “spikey” differences of up to about 10%, as explained below this is due to the difference between the continuous VII.0 and histogram VI.8, fission spectra.

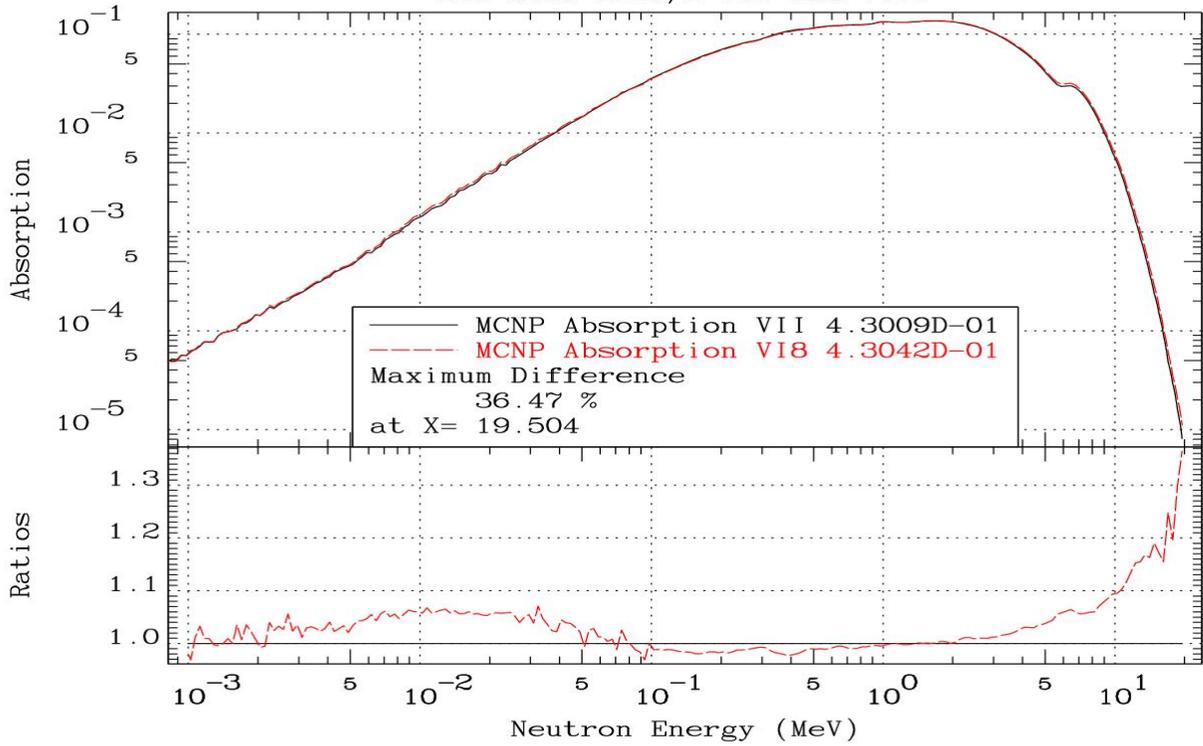
Jezebel23

Compared to the other two systems, we do not see such large per-cent differences, but we do see important differences near the peak of the spectra (1 Mev), which causes such a large discrepancy in K-eff.

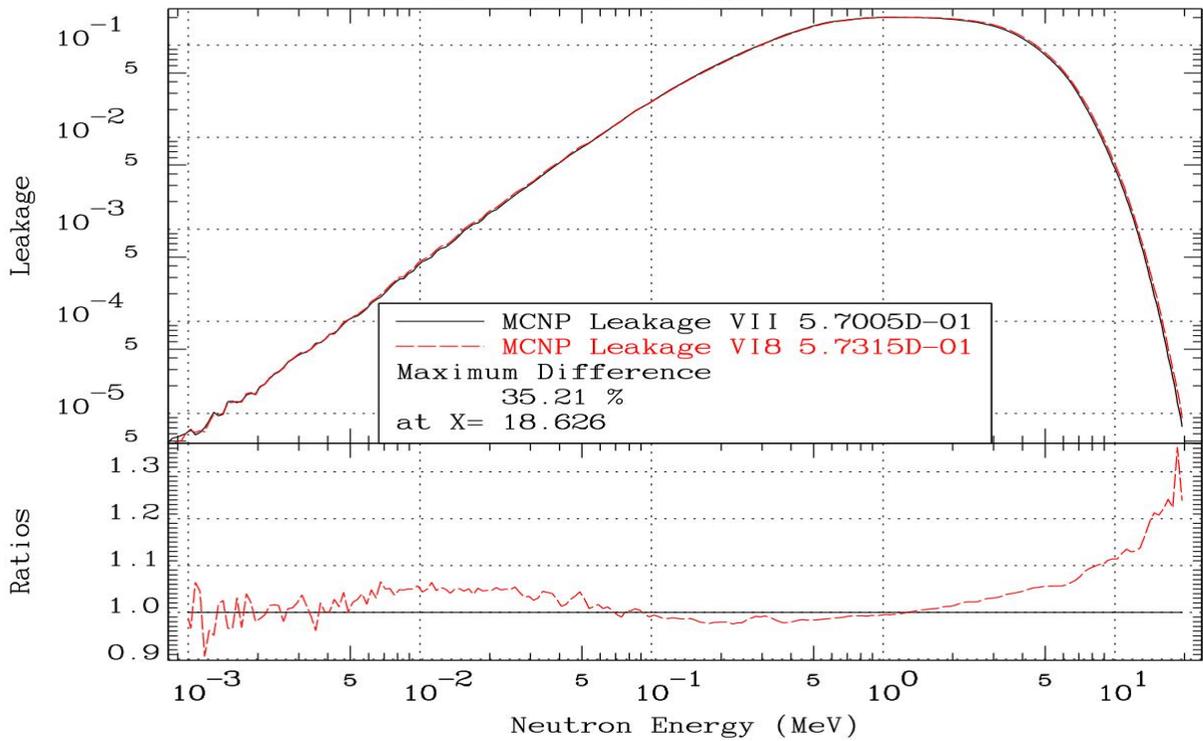
Godiva MCNP using ENDF/B-VI.8 and VII.0



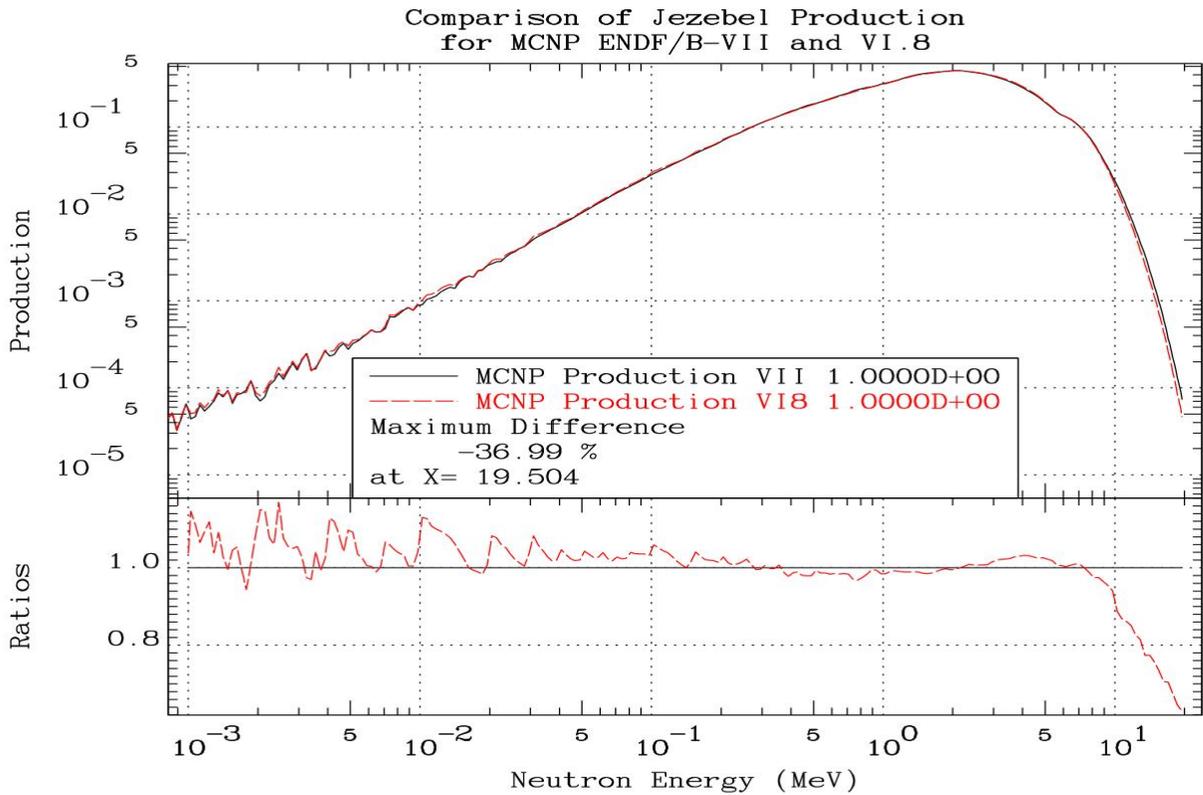
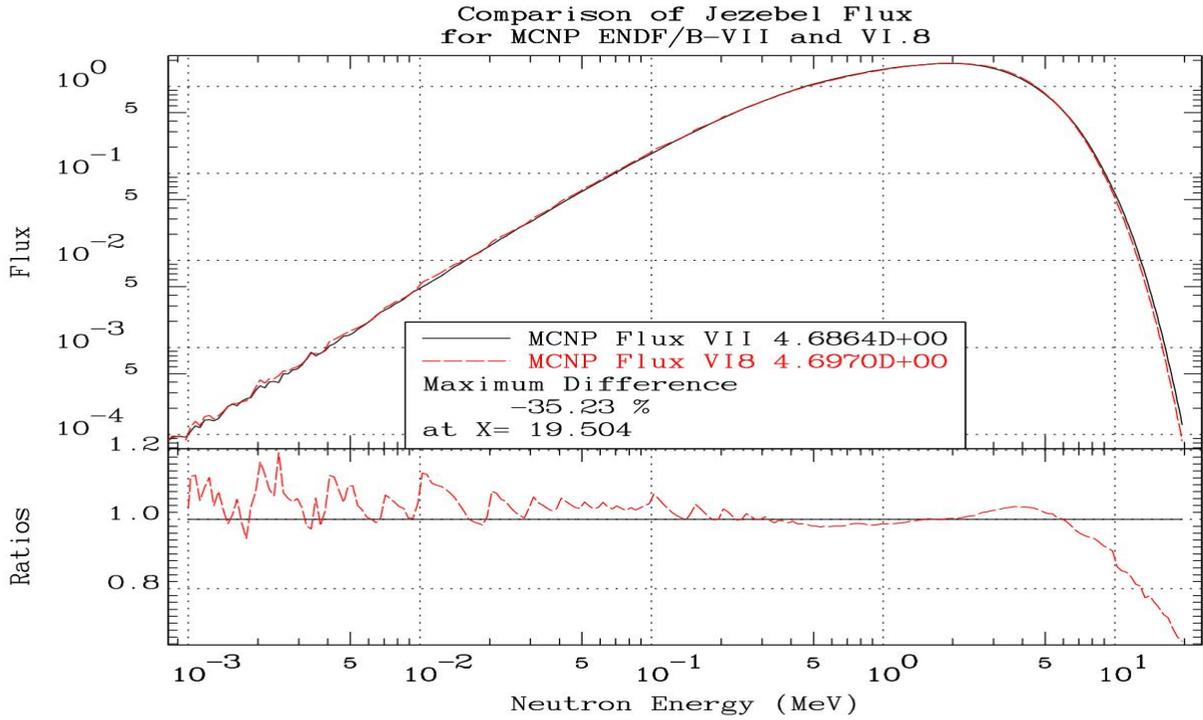
Comparison of Godiva Absorption
for MCNP ENDF/B-VII and VI.8



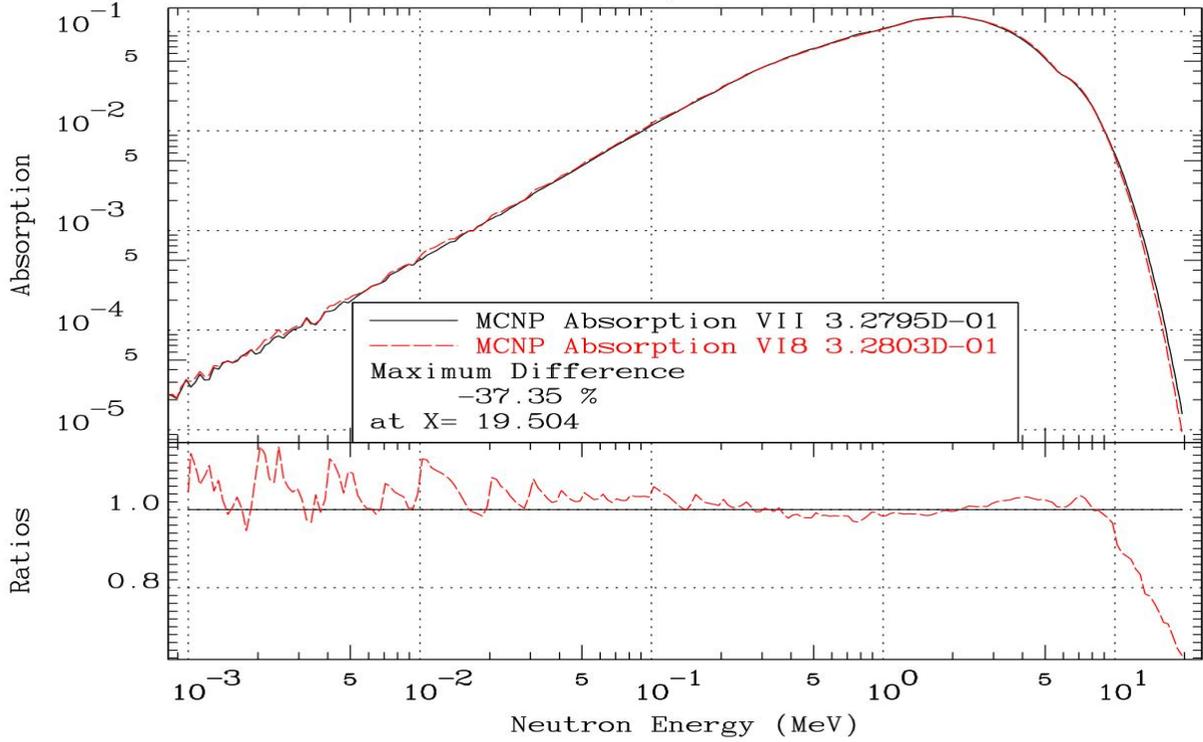
Comparison of Godiva Leakage
Comparison of Godiva Absorption



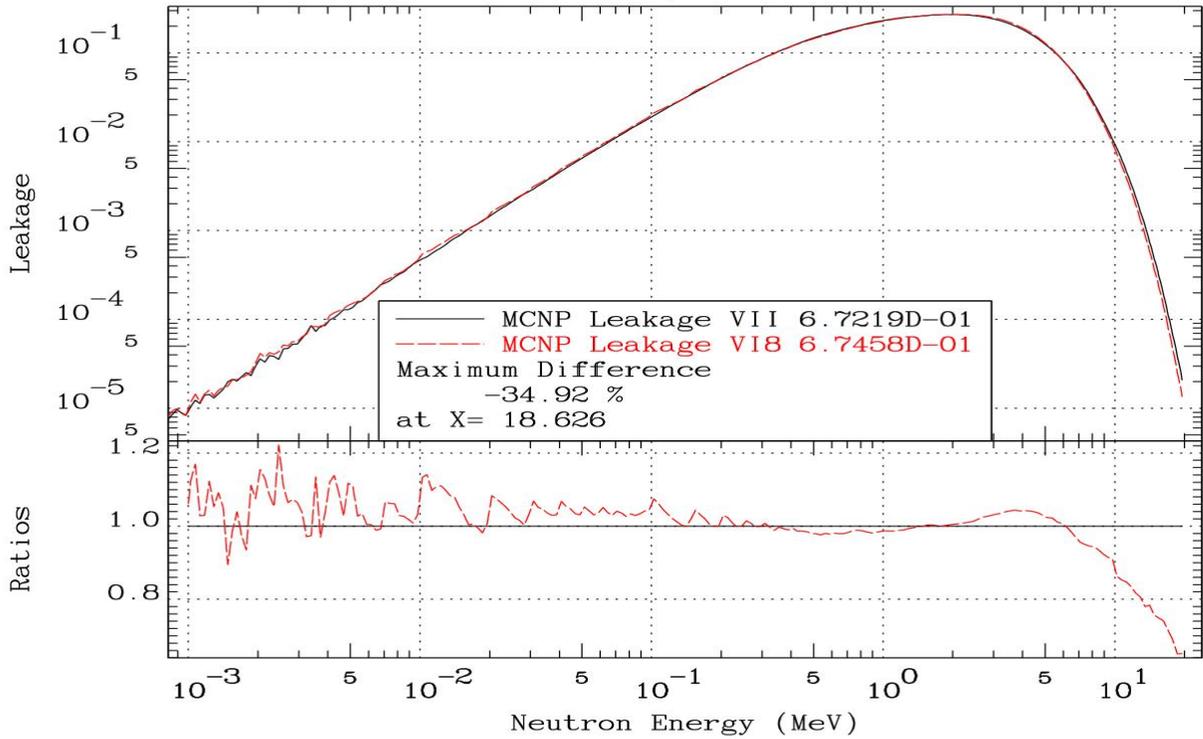
Jezebel MCNP using ENDF/B-VI.8 and VII.0



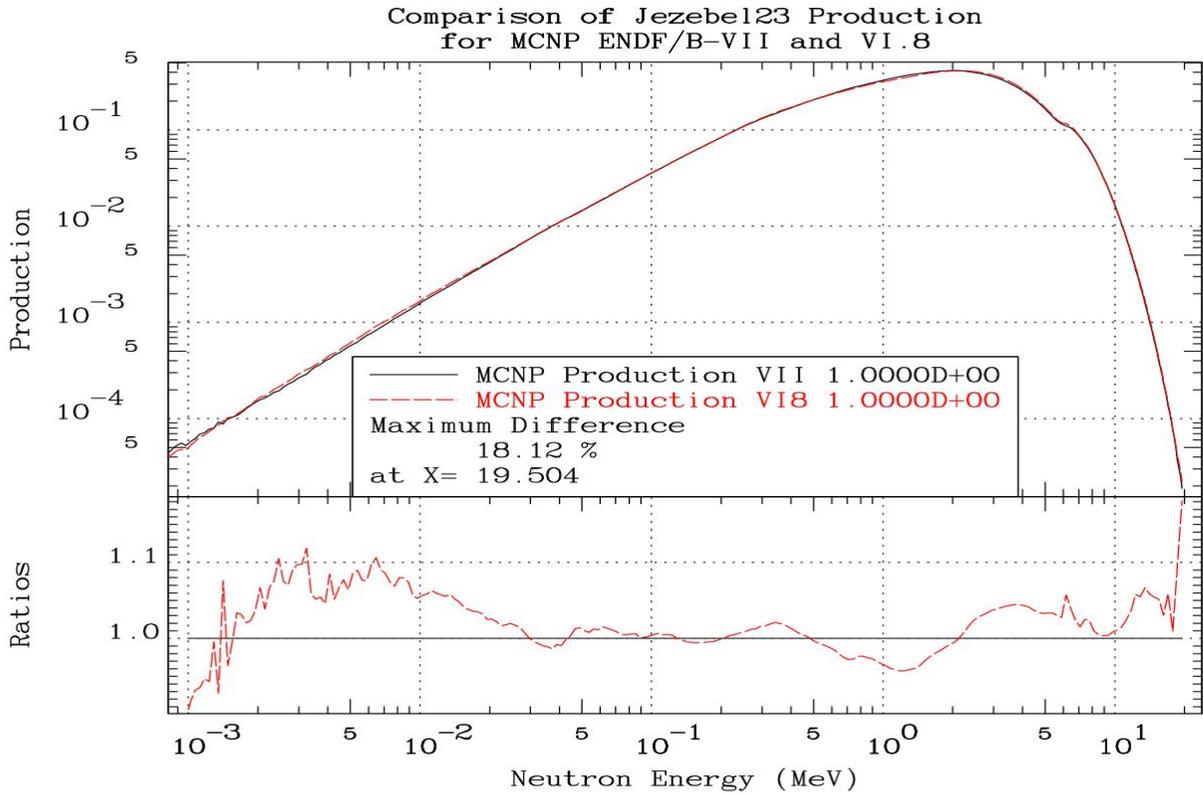
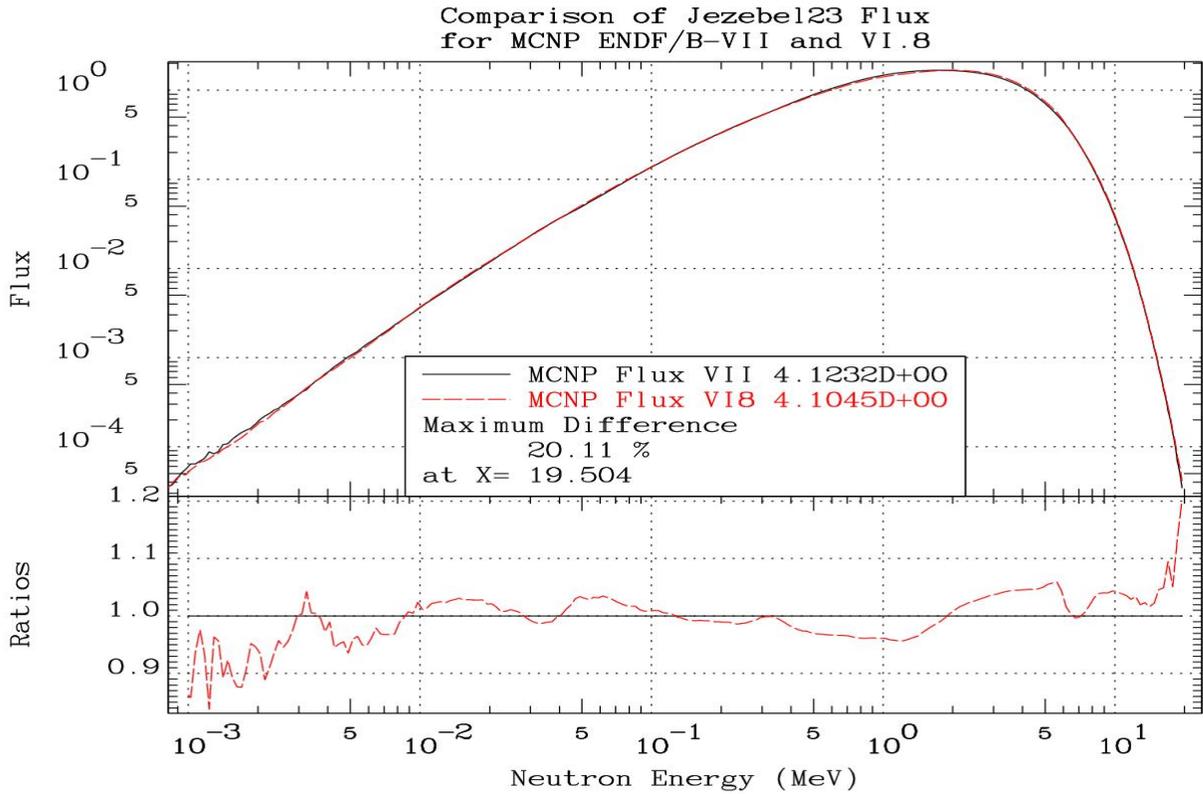
Comparison of Jezebel Absorption
for MCNP ENDF/B-VII and VI.8



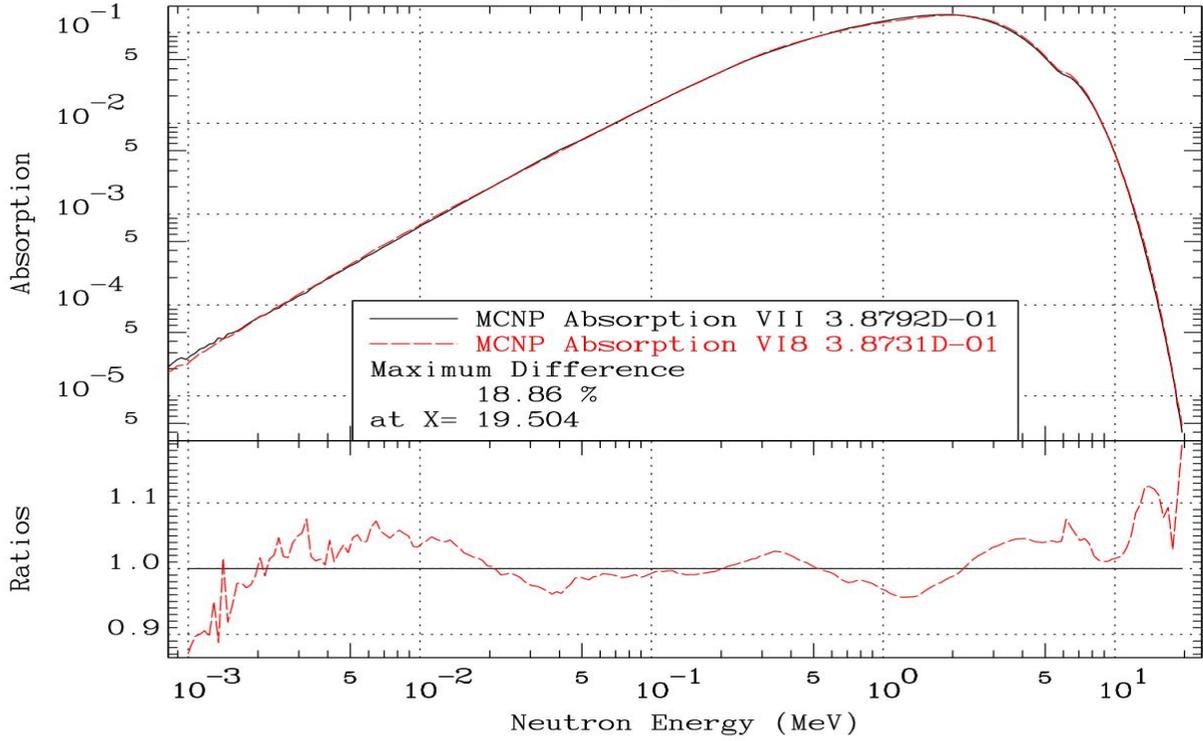
Comparison of Jezebel Leakage
for MCNP ENDF/B-VII and VI.8



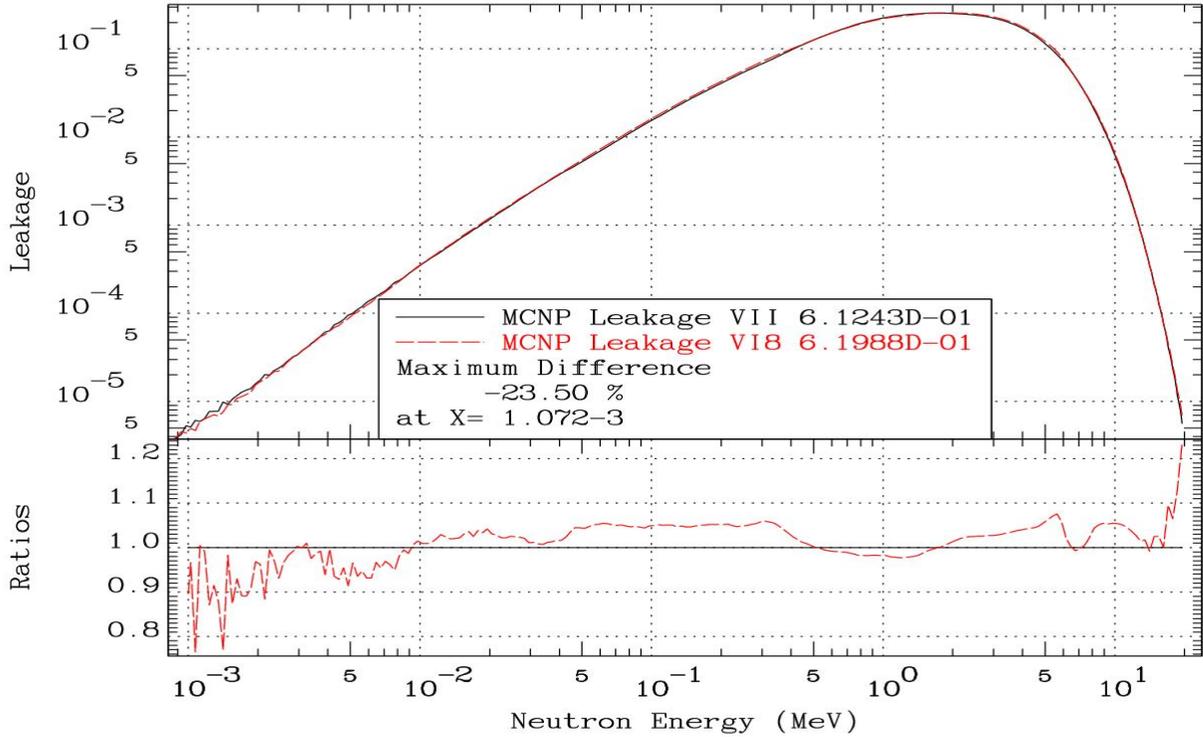
Jezebel23 MCNP using ENDF/B-VI.8 and VII.0



Comparison of Jezebel23 Absorption
for MCNP ENDF/B-VII and VI.8

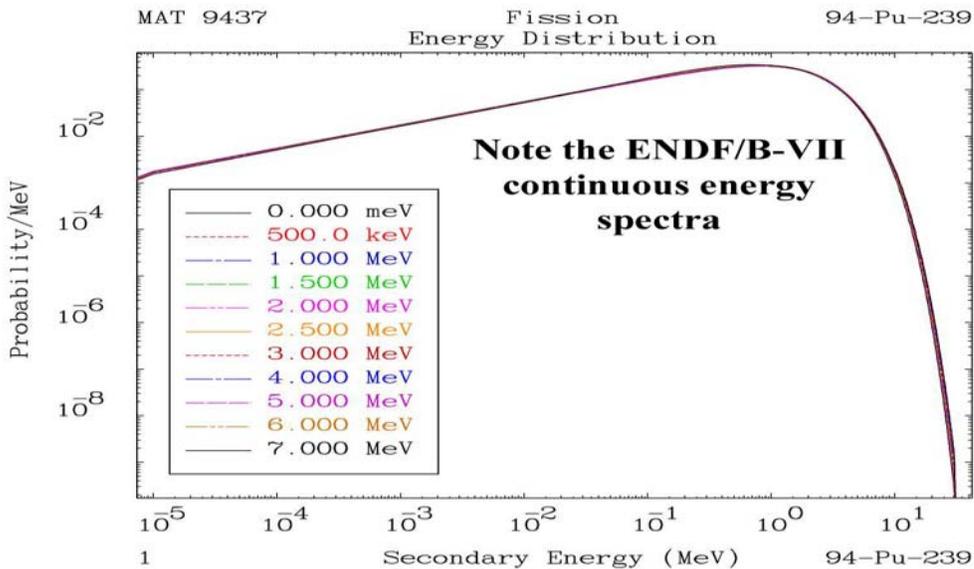
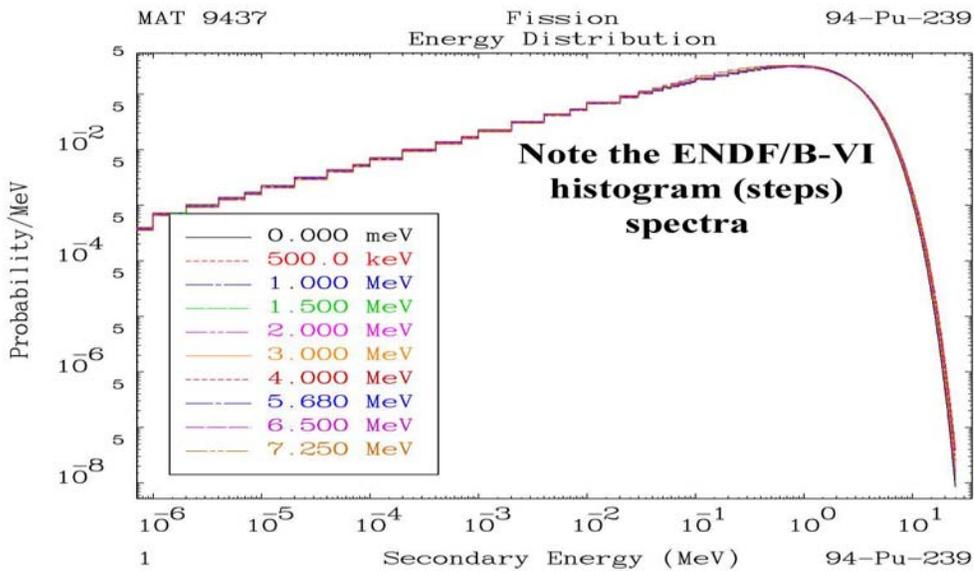


Comparison of Jezebel23 Leakage
for MCNP ENDF/B-VII and VI.8



Explanation of Jezebel Results

From the plots of the Jezebel results comparing VII.0 [2] and VI.8 [3] data we can see jagged edges in the low energy spectra. These have been traced to differences in the Pu-239 fission spectra as defined in ENDF/B-VI and VII. Specifically, as we can see from the figures below, for ENDF/B-VI the fission spectra are defined by a series of histograms, whereas for ENDF/B-VII they are defined more physically acceptable continuous energy distributions. When we take the ratio of these different representations we find the jagged edges as seen in the Jezebel results; these are significant $\sim 10\%$ differences in the energy dependent fission spectra. **ENDF/B-VII continuous energy spectra are a definite improvement over the older VI spectra.**



XV - Second Step Detailed Results: One data Library/multiple codes

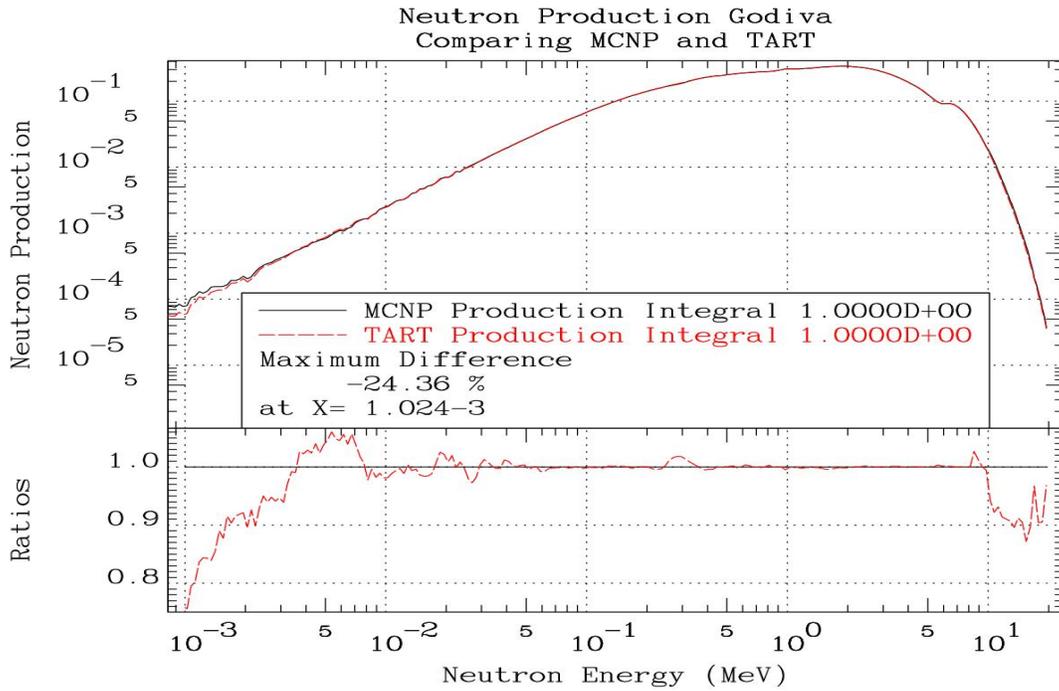
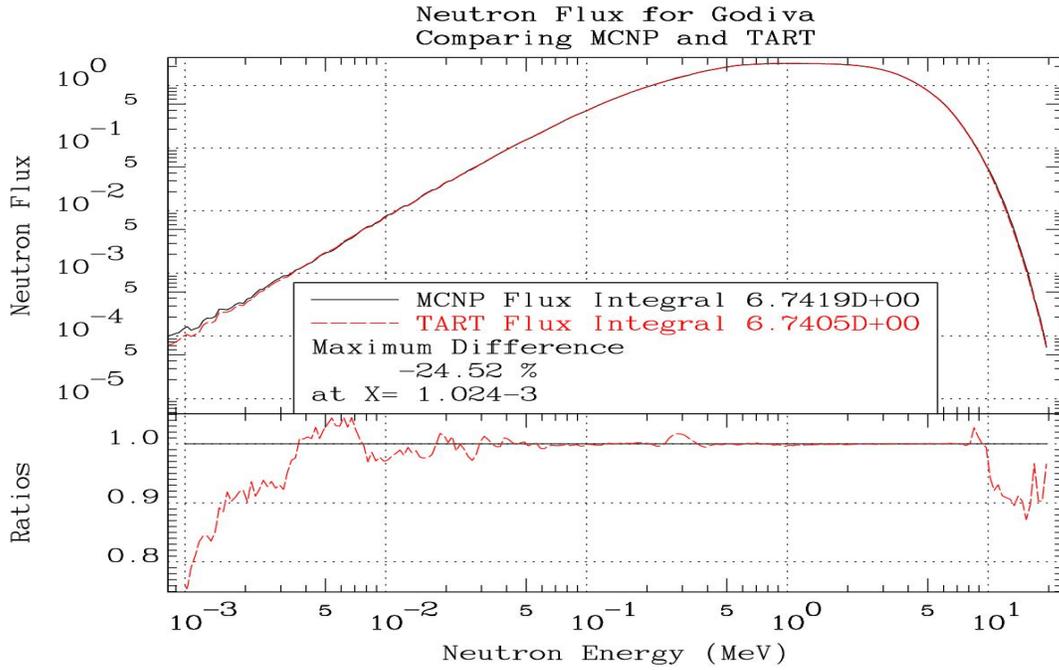
Godiva 8 Code Comparisons using VII.0

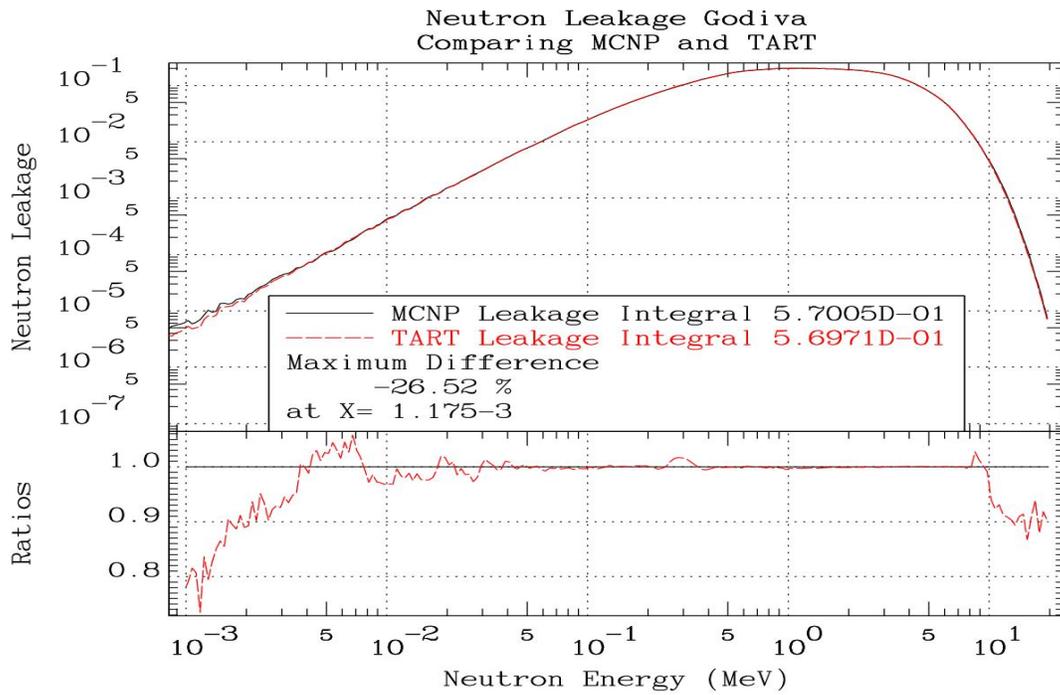
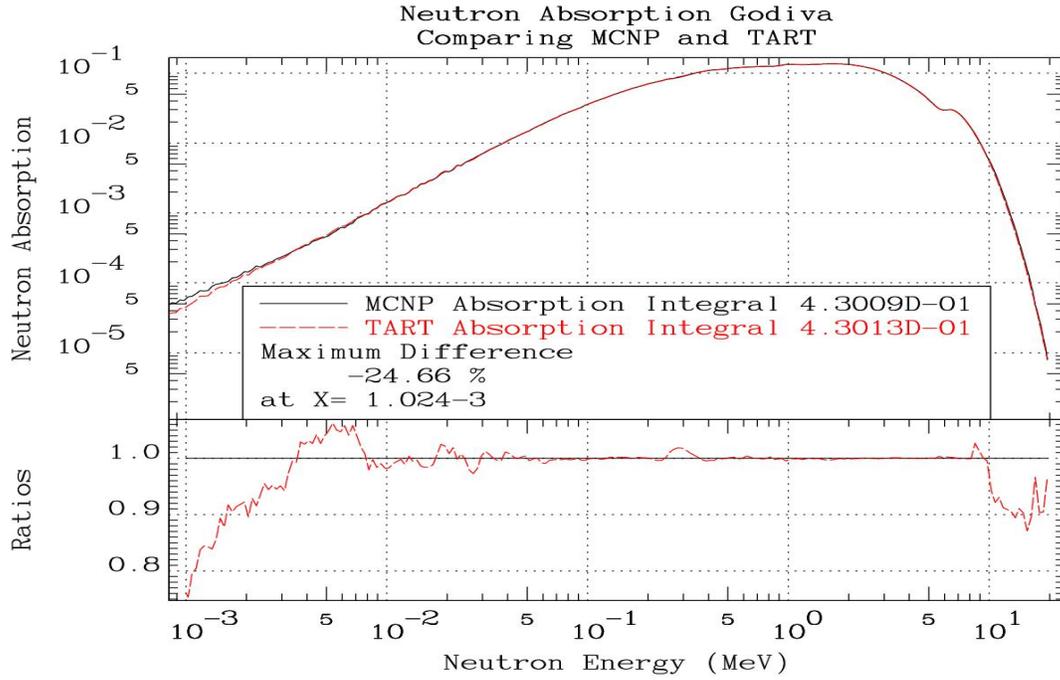
	MCNP	CE-KENO	COG	Mercury	MONK	TART	Tripoli	VIM
Flux	6.74192	6.77669	6.78467	6.73976	6.73125	6.74039	6.74048	6.75933
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.43009	0.42832	0.43022	0.42969	0.42970	0.43012	0.43017	0.42864
Leakage	0.57005	0.57209	0.56921	0.57007	0.56973	0.56969	0.56958	0.57104
Removal	1.00014	1.00041	0.99943	0.99976	0.99943	0.99981	0.99976	0.99968
K-eff	0.99985	0.99959	1.00057	1.00024	1.00056	1.00019	1.00024	1.00032
Removal Time nanoseconds	6.21699	6.21401	6.24093	6.18991	6.17658	6.21765	6.22675	6.23371

When we compare the MCNP and TART results shown below,

- 1) Integral results look Fantastic!!! For example, when we look at K-eff = 1.00019 – 0.99985 = 0.00034, well within the 0.001 we are shooting for.
- 2) Differential results show differences at high and low energy, as well as a “bump” near 300 keV.
- 3) The high energy, above 10 MeV we understand is due to an approximation TART is using as explained later in this report.
- 4) The low energy difference is because MCNP uses the ENDF/B-VII histogram data, while TART uses a low energy \sqrt{E} model, again explained later in this report.
- 5) The “bump” near 300 keV is the only difference we have not been able to explain; more about this later in this report.

Godiva MCNP and TART results using ENDF/B-VII





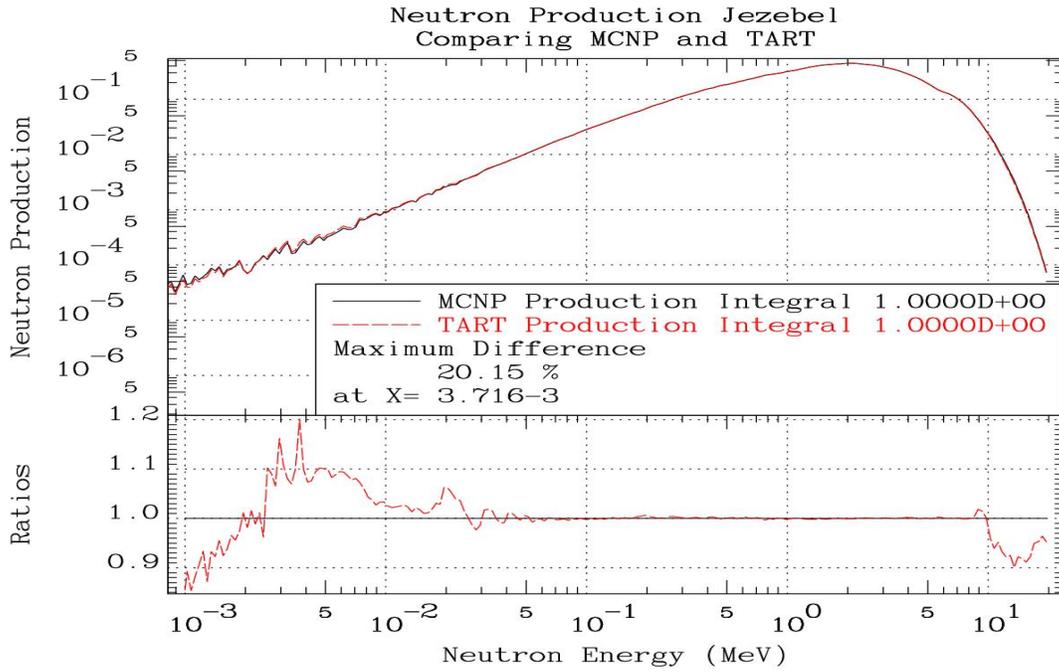
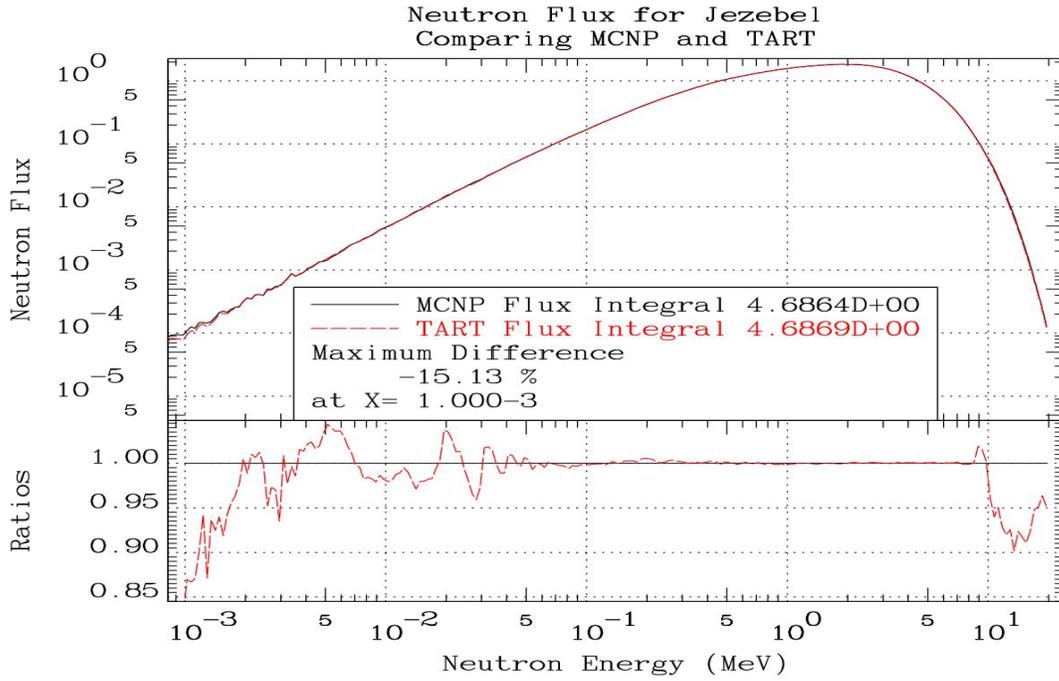
Jezebel 8 Code Comparisons using VII.0

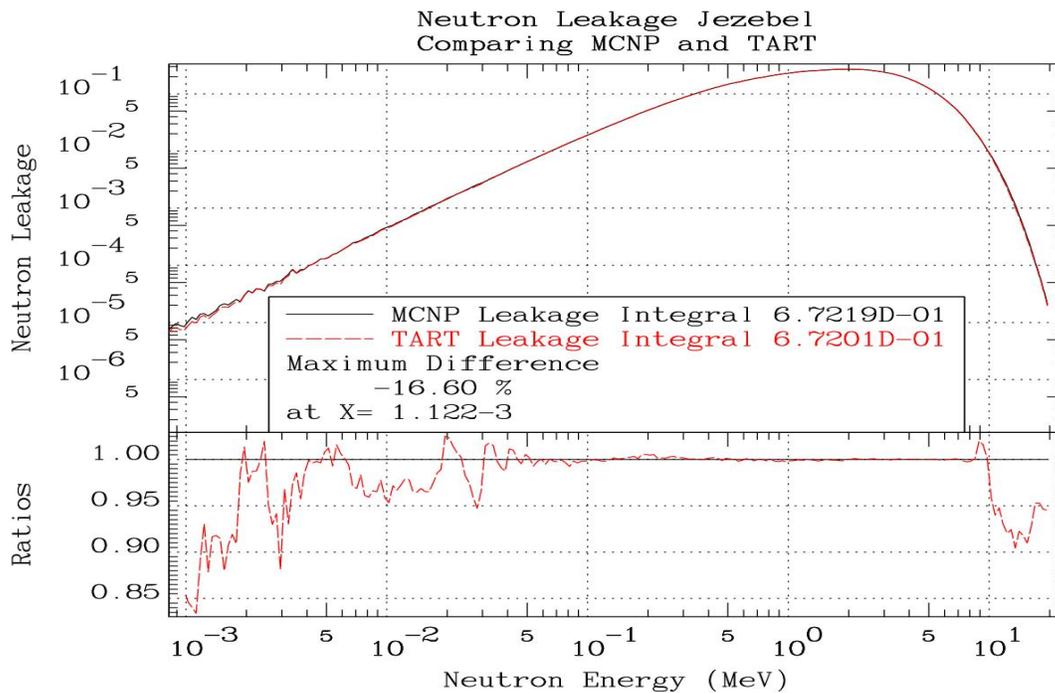
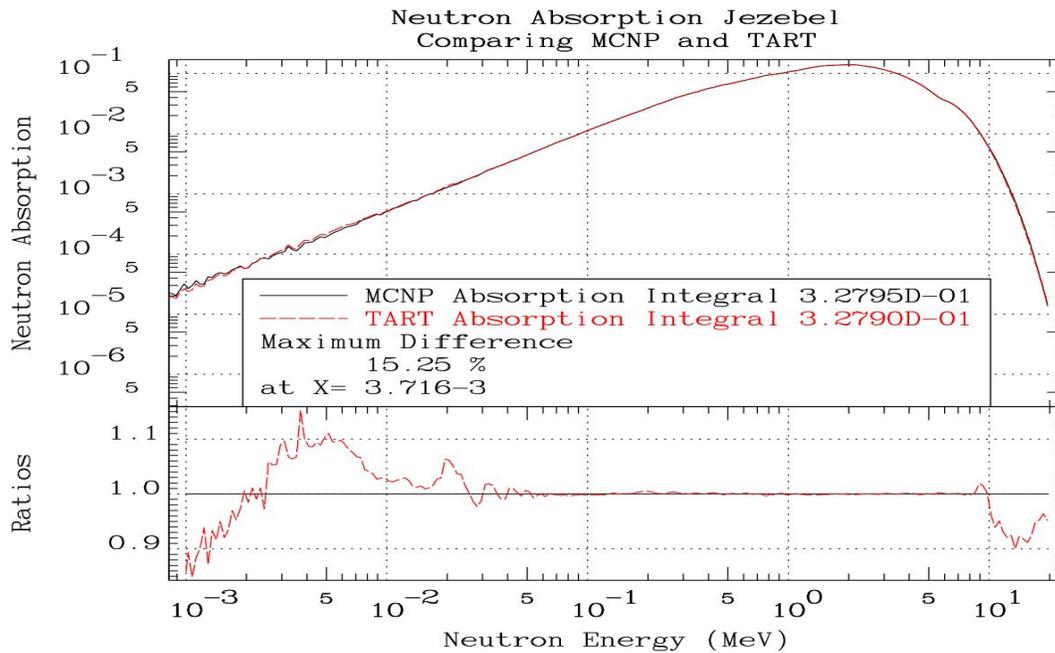
	MCNP	CE-KENO	COG	Mercury	MONK	TART	Tripoli	VIM
Flux	4.68642	4.69200	4.69669	4.68307	4.68415	4.68691	4.68639	4.68955
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.32795	0.32731	0.32792	0.32778	0.32787	0.32790	0.32798	0.32732
Leakage	0.67219	0.67299	0.67198	0.67151	0.67147	0.67200	0.67211	0.67257
Removal	1.00014	1.00030	0.99990	0.99929	0.99934	0.99990	1.00009	0.99989
K-eff	0.99986	0.99970	1.00010	1.00071	1.00066	1.00010	0.99991	1.00011
Removal Time nanoseconds	3.72886	3.72023	3.73901	3.71855	3.71715	3.72938	3.73398	3.72361

When we compare the MCNP and TART results shown below,

- 1) Integral results look Fantastic!!! For example, when we look at $K\text{-eff} = 1.00010 - 0.99986 = 0.00024$, well within the 0.001 we are shooting for.
- 2) Differential results show differences at high and low energy. I looked in detail in the middle energy range and the agreement is very good (no “bump” as seen for Godiva).
- 3) The high energy, above 10 MeV we understand is due to an approximation TART is using, as explained later in this report.
- 4) The low energy difference is because MCNP uses the ENDF/B-VII histogram data, while TART uses a low energy \sqrt{E} model, gain explained later in this report.

Jezebel MCNP and TART results using ENDF/B-VII





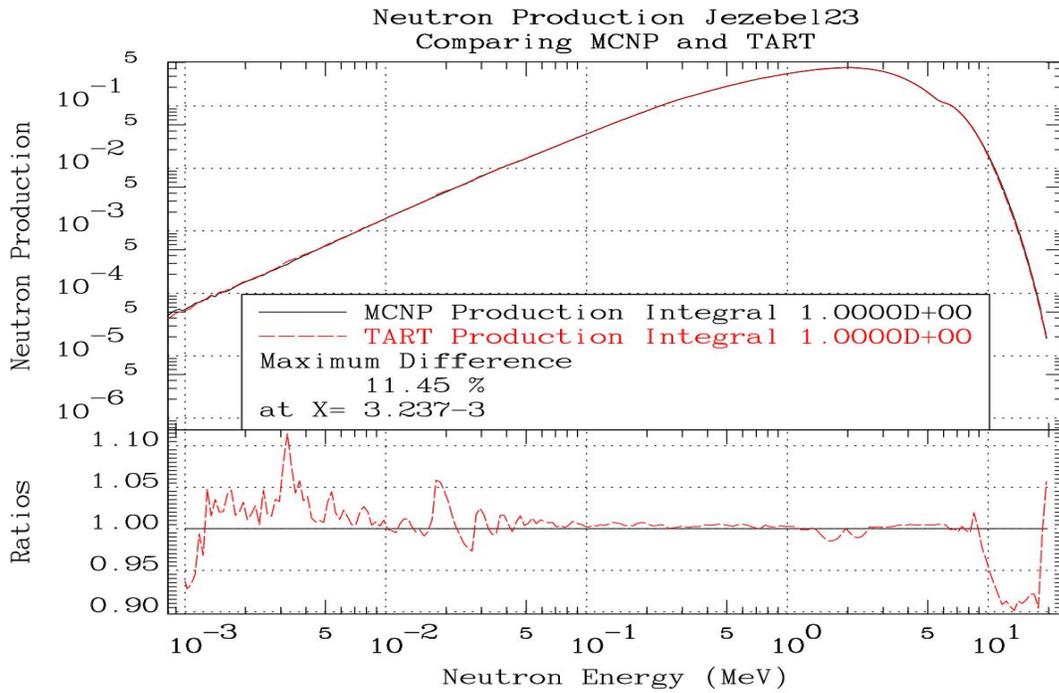
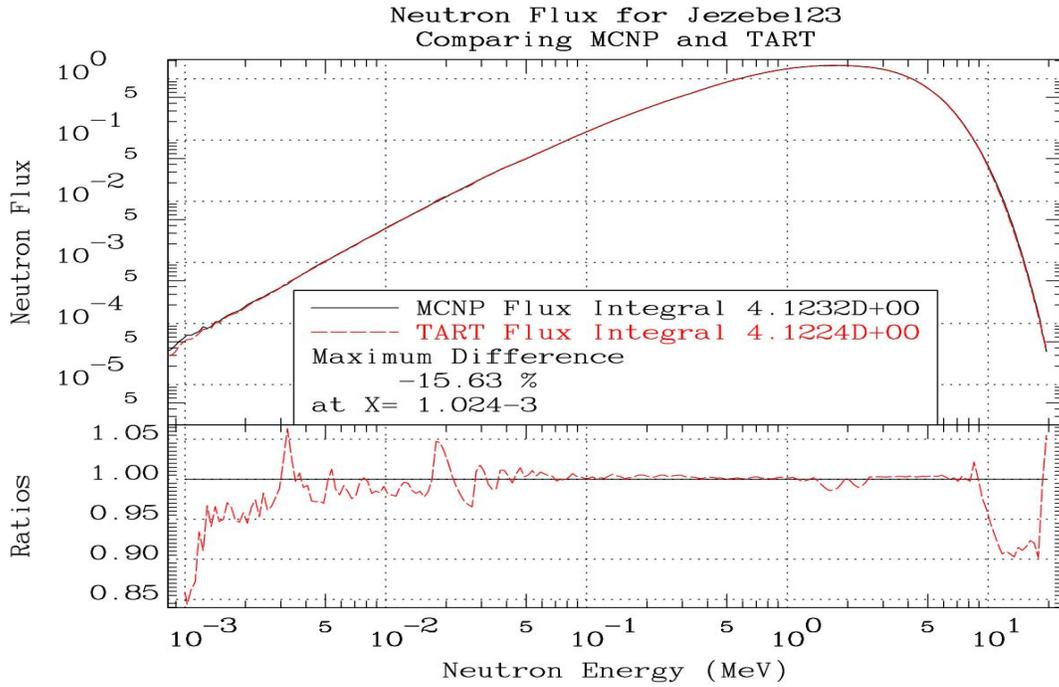
Jezebel23 8 Code Comparisons using VII.0

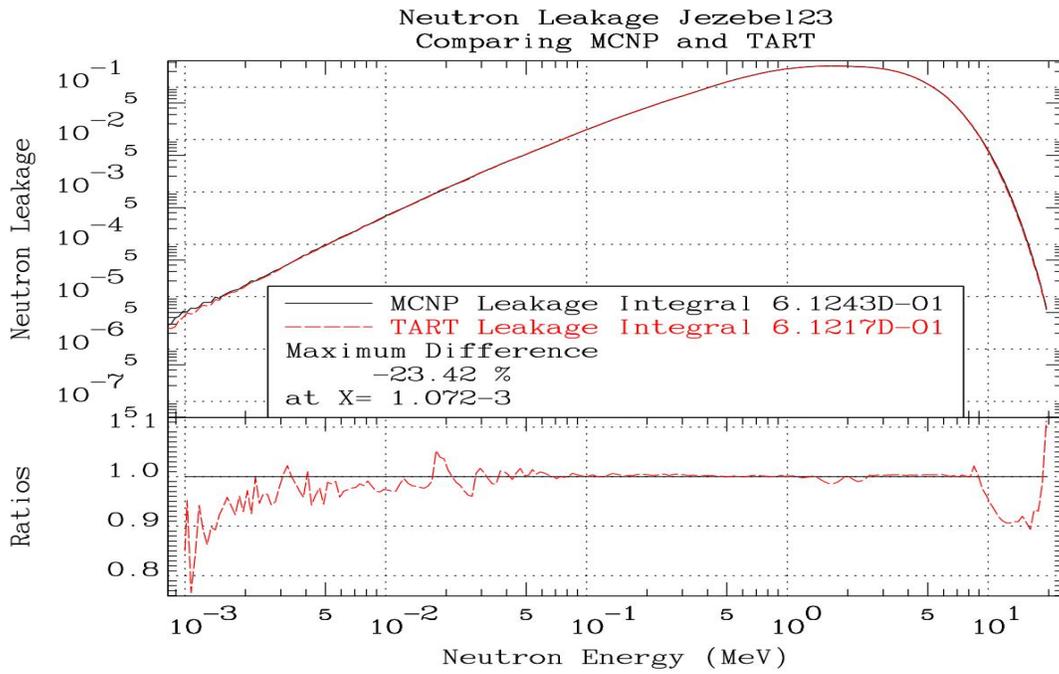
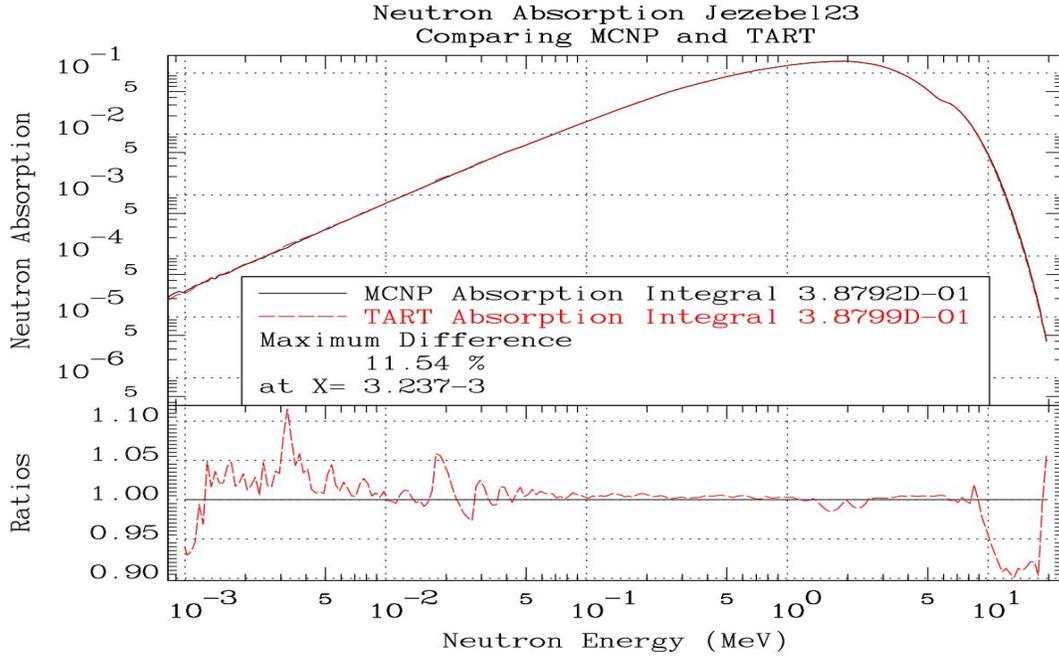
	MCNP	CE-KENO	COG	Mercury	MONK	TART	Tripoli	VIM
Flux	4.12318	4.12735	4.11889	4.11874	4.12217	4.12237	4.12278	4.12624
Production	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
Absorption	0.38792	0.38737	0.38793	0.38750	0.38781	0.38799	0.38795	0.38741
Leakage	0.61244	0.61326	0.61221	0.61202	0.61133	0.61218	0.61226	0.61278
Removal	1.00036	1.00063	1.00014	0.99952	0.99914	1.00017	1.00021	1.00019
K-eff	0.99964	0.99937	0.99986	1.00048	1.00086	0.99983	0.99979	0.99981
Removal Time nanoseconds	3.20374	3.19927	3.20874	3.19033	3.19598	3.20556	3.20658	3.19885

When we compare the MCNP and TART results shown below,

- 1) Integral results look very good. For example, when we look at $K\text{-eff} = 0.99983 - 0.99964 = 0.00019$, well within the 0.001 we are shooting for.
- 2) Differential results show differences at high and low energy.
- 3) The high energy, above 10 MeV we understand is due to an approximation TART is using, as explained later in this report.
- 4) The low energy difference is because MCNP uses the ENDF/B-VII histogram data, while TART uses a low energy \sqrt{E} model, explained later in his report.

Jezebel23 MCNP and TART results using ENDF/B-VII





XVI - Recommendations for Improving ENDF/B-VII.0

Based on comparisons for this study we found some differences between MCNP and TART results. Most of these can be traced to how these codes interpret ENDF/B data. A major difference is that the standard NJOY/MCNP treatment is to provide the “best” literal interpretation of all ENDF/B data; this is very important for data testing. In contrast TART treatment is to provide the “best” physical interpretation of data for use in TART’s applications; obviously very important for applications. These differences in interpretation are reflected in the below recommendations.

As we can see from the above results comparing ENDF/B-VII.0 and VI.8, the new VII.0 data library is a big improvement over the older VI.8 library. However, our tests indicate that VII.0 is not yet perfect, and here we mention a few points where we feel it could be even further improved, these include,

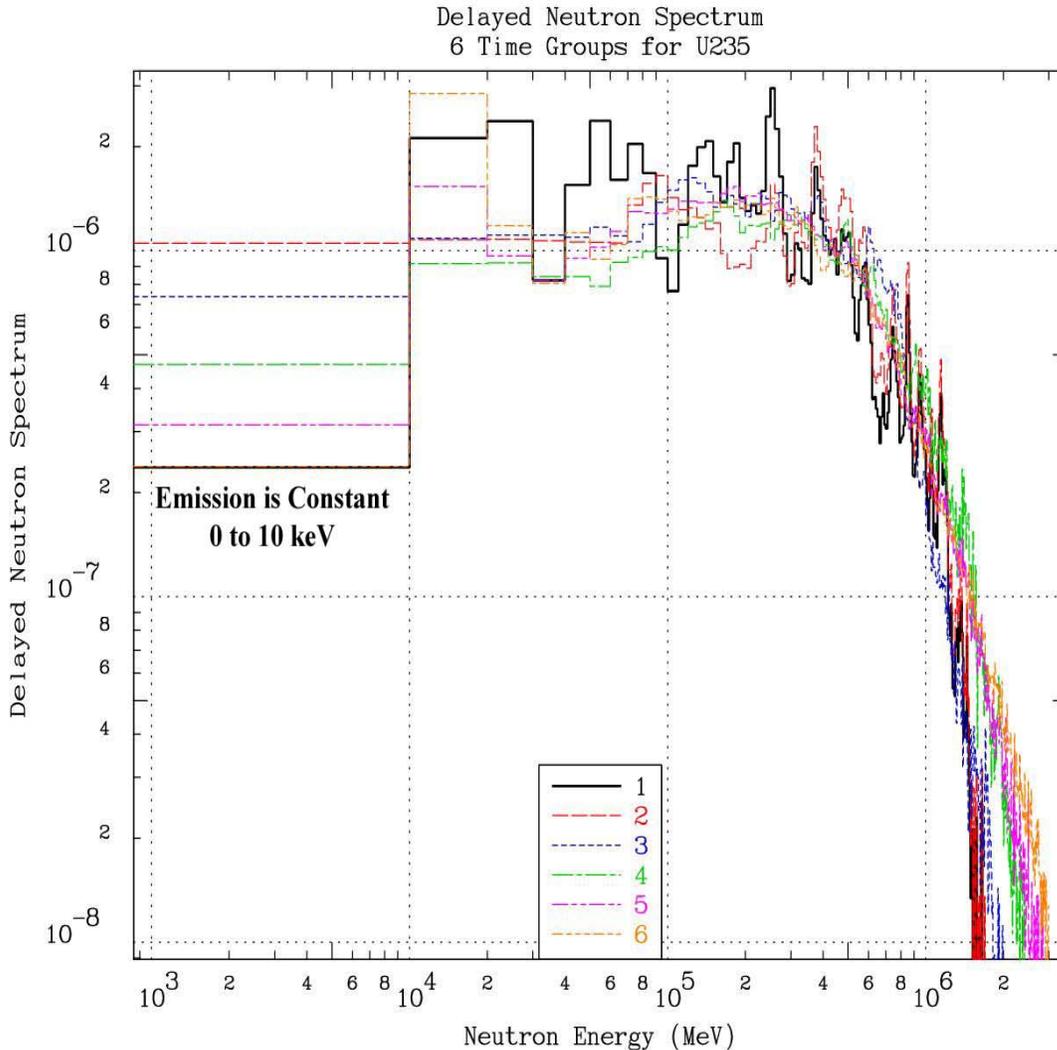
- 1) Improved delayed neutron spectra, i.e., no histograms
- 2) More precision in tabulated fission spectra.
- 3) Improvement reaction spectra, i.e., no histograms and \sqrt{E} low E variation

When ENDF/B-VII.0 was released in December 2006 the Cross Section Evaluation Working Group (CSEWG) declared that the library would be frozen for three years. If true, there is nothing we can do to improve the basic evaluated data until December 2009, but in the meantime we can take some actions to improve the interpretation of the data by our processing and transport codes.

XVII - Differences in delayed neutron spectra

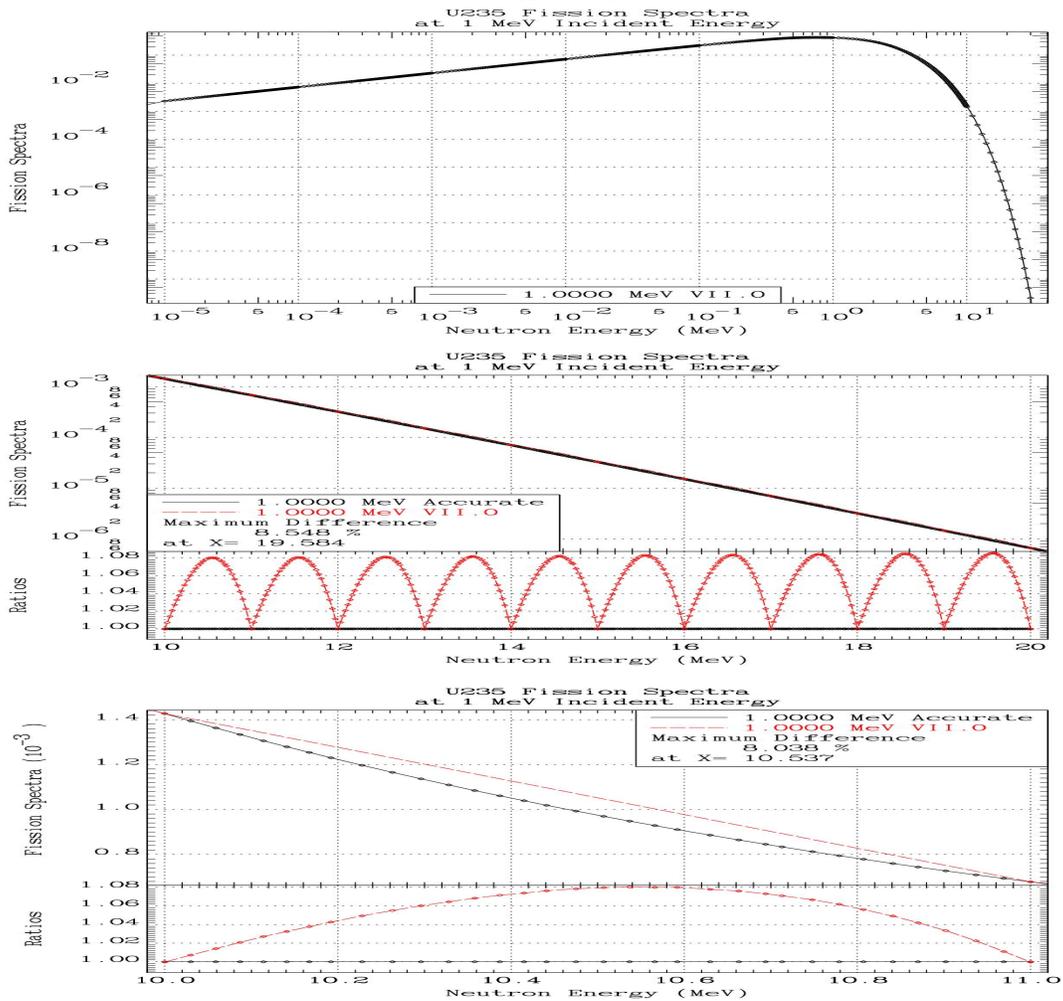
ENDF/B delayed neutron spectra are defined by nuclear model code output, where the spectra are given by a series of histograms, each step of the histogram being about 10 keV wide. This 10 keV width seems reasonable at high energy in the MeV, but is totally unrealistic at low energy to define the delayed neutron emission as a constant step between 0 and 10 keV, as shown in the below figures. MCNP interprets this exactly as given, whereas TART replaces the low energy shape by a more physically acceptable Maxwellian; see ref. [18] for details.

These histograms that come directly out of nuclear model codes should be improved to define more physically acceptable energy variation before they are used in ENDF/B evaluations. Since ENDF/B-VII.0 is frozen until December 2009 this obviously cannot be done today. However, until this is done TART [18] and NJOY [19] with its “smoothing” option (see the below example), attempt to improve this data for use today.



XVIII - Accuracy of ENDF/B-VII.0 Tabulated Fission Spectra

At high energy the ENDF/B-VII.0 are not tabulated to a fine enough energy grid. We illustrate this point below where we first show the U235 fission spectrum tabulated at 1 MeV incident neutron energy. Over most of the energy range the tabulated secondary energy points (small circles on plots) are closely enough spaced to accurately define the fission spectrum. But above 10 MeV the spectrum is changing so rapidly that more energy points are needed to accurately define it. The first figure shows the tabulated VII.0 spectrum which between 10 and 30 MeV changes by 7 orders of magnitude, and there are far too few points to accurately define this variation. The second plot shows the 10 to 20 MeV energy range where compared to an accurately tabulated spectrum, the VII.0 overestimates the value by up to over 8%. Finally the third figure shows the 10 to 11 MeV energy range where the VII.0 evaluation only includes tabulated energy points at 10 and 11 MeV; obviously too few points to accurately define the shape. **The fission spectra are so important that we recommend they always be tabulated to high accuracy over the entire secondary energy range.**

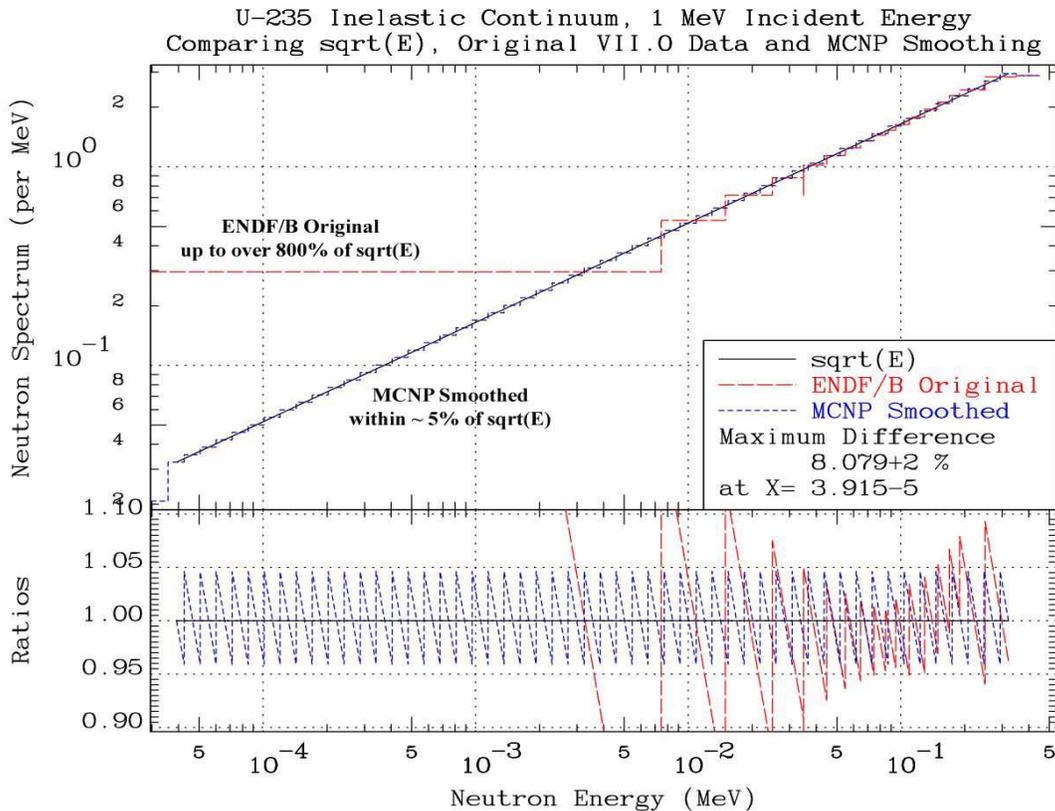


XIX - Effect of low energy spectra smoothing

Many ENDF/B spectra now use histograms. As stated earlier MCNP and TART results differ at very low energies because the two codes are interpreting the VII.0 data differently: MCNP results are based on its BEST literal interpretation of the VII.0 low energy histogram data, whereas TART results are based on smoothing the VII.0 results assuming what it considers to be a more physically acceptable \sqrt{E} low energy variation (rather than histogram). NJOY [19] now includes a “smoothing” option to approximate the low energy \sqrt{E} variation in a manner similar to TART.

The below plot illustrates the effect of NJOY smoothing on the U235 inelastic continuum (MT=91) spectrum for 1 MeV incident neutrons. Physically the low energy spectra should have \sqrt{E} variation, but what is output by nuclear model codes and used in ENDF/B-VII.0 is a series of histograms steps each about 10 keV wide; this is adequate at higher energies, but it is a very poor approximation at very low energy. The NJOY “smoothing” option improves histogram spectra by replacing the original ENDF/B 10 keV histogram intervals by smaller energy steps to better approximate the \sqrt{E} variation.

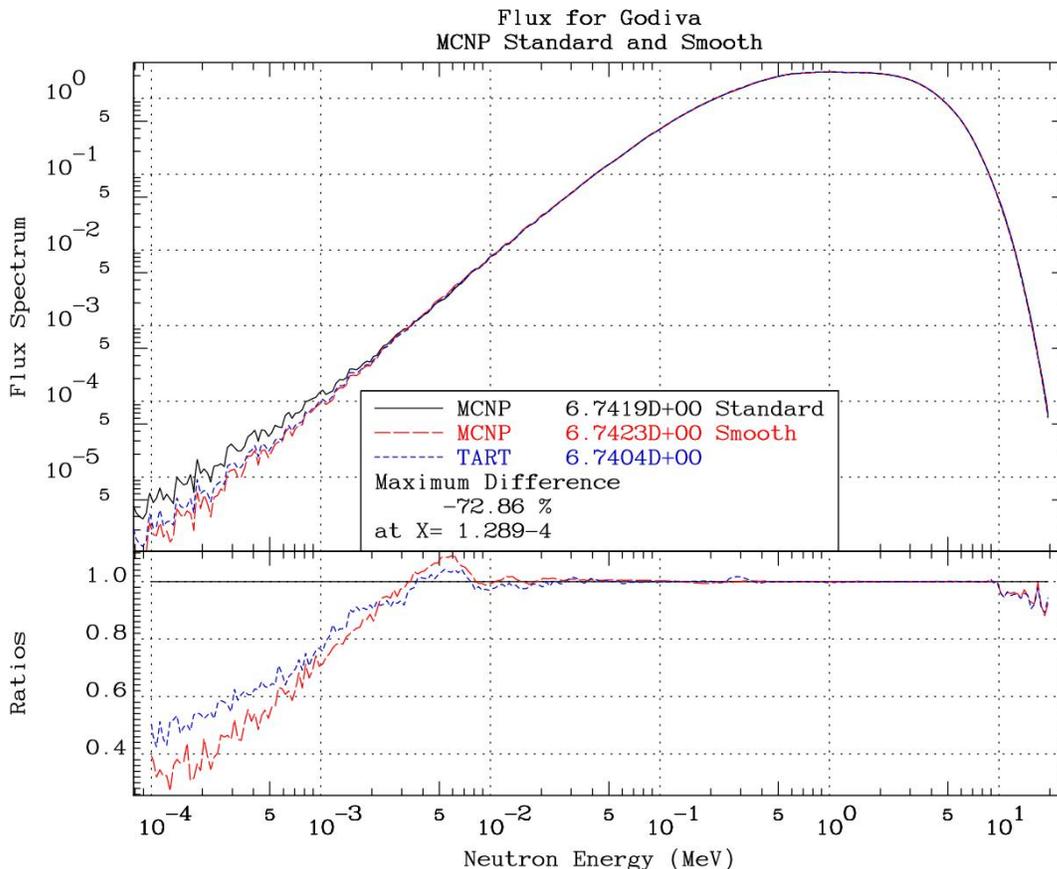
Hopefully in the future this histogram output from nuclear model codes can be improved to more realistically define a continuous energy variation of spectra, which will improve the ENDF/B data.

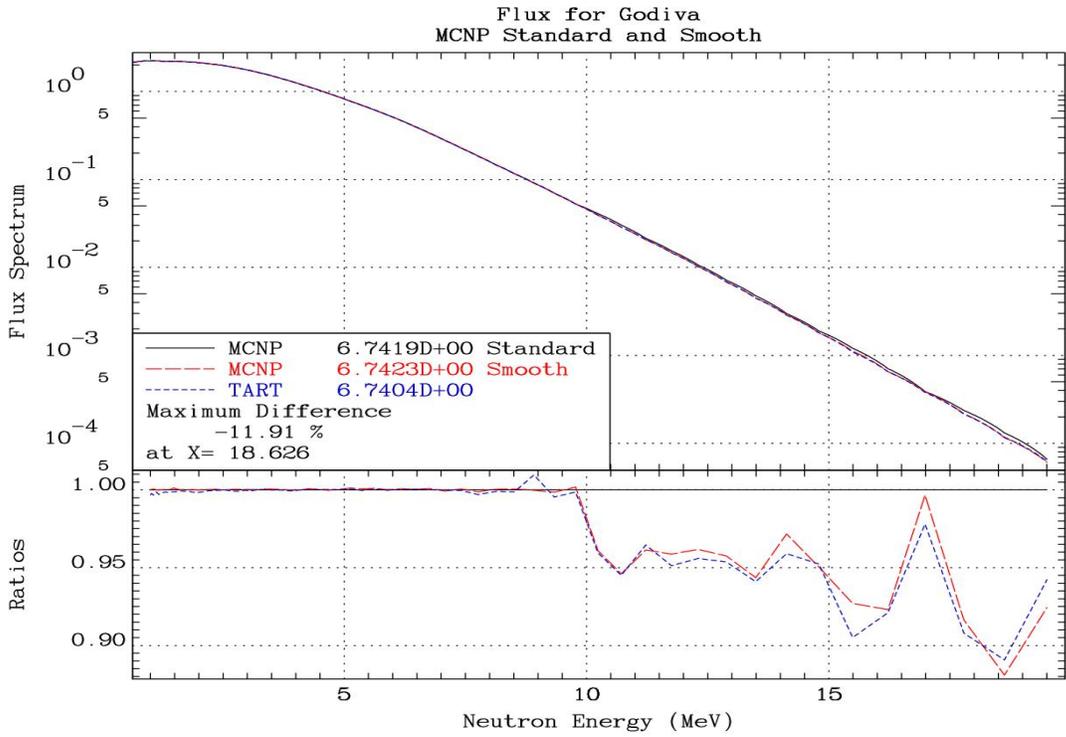
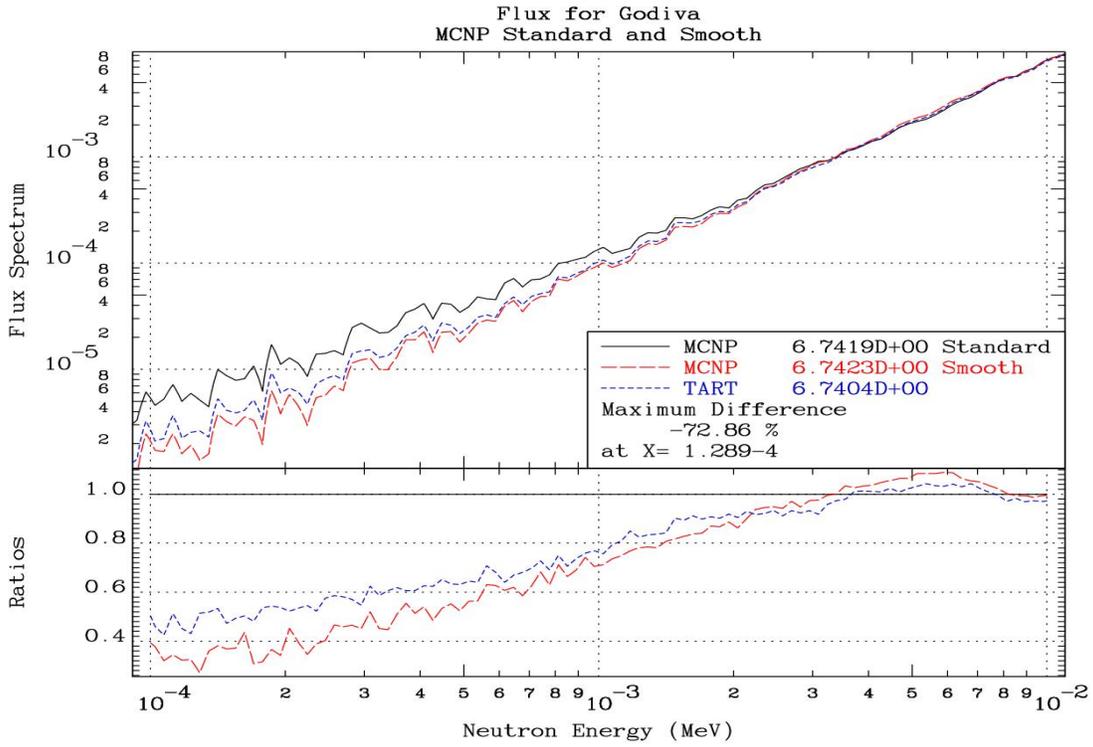


NJOY's "smoothing" Option

To illustrate the source of the differences at low and high energy, we can use NJOY's "smoothing" option, and the TART data used by TART and MERCURY. The figure below presents original MCNP results, as well as both MCNP and TART results, both using the same low energy \sqrt{E} and high energy improved fission spectra "smoothing". From this figure it seems clear that this "smoothing" is the source of the differences. Comparing the MCNP Original and Smooth results, we can see from the below plot that in this case there is very little effect on the integral of the flux: 6.7419 vs. 6.7423, differing only by 0.0004. Comparing the MCNP Original and Smooth results for K-eff we find: 0.99986 vs. 0.99977, differing only by 0.00009, well below the +/- 0.001 we consider acceptable. In principle both TART and MCNP "smooth" are using the same low and high energy approximations, but we can see from the below results that although the agreement is good it is not exact, showing that the actual details differ as to what each code is doing.

To repeat what was said earlier: for the three fast critical systems we are examining, these lower and higher energy ranges are not important when defining K-eff., but this may not be generally true. Here we explain the sources of the differences to insure that we understand them, which in turn can lead to better general agreement between our codes and wider applicability of our codes to other problems.



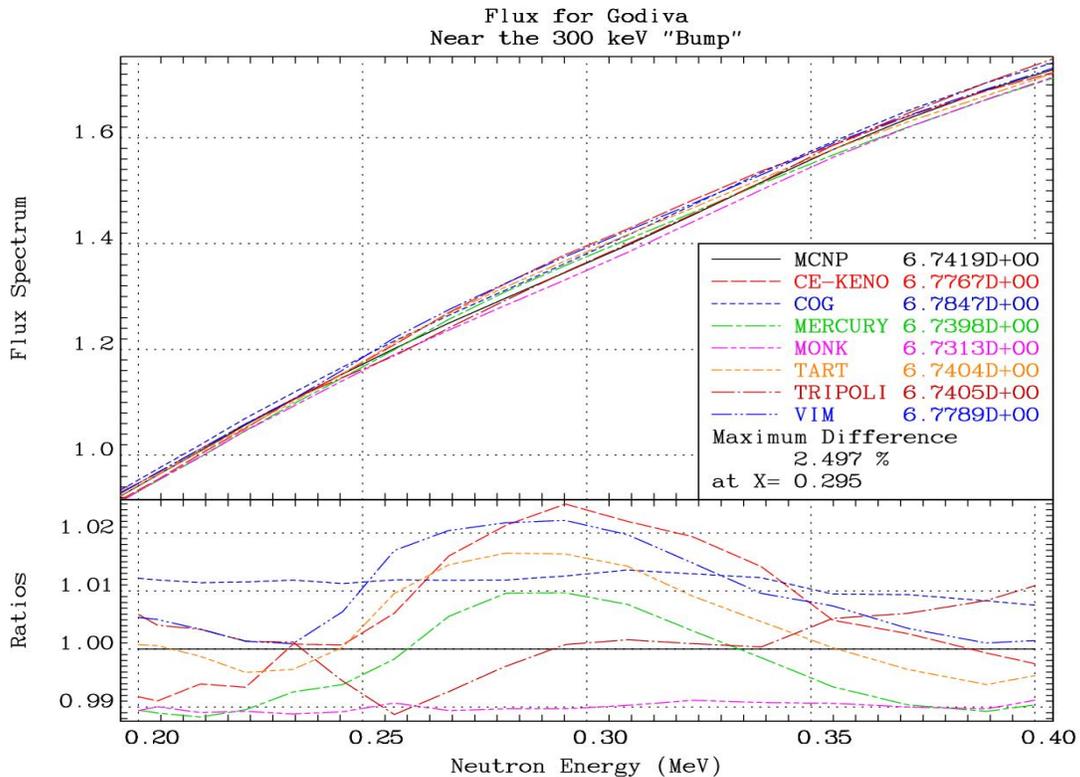


XX - The Godiva “Bump”

Usually one of the big advantages of code comparisons is that when we see a difference between two codes by comparing results from many codes we can easily explain the source of the difference, see that one code does not agree with all of the other codes, and correct the code. This approach has led to many improvements in our codes – and often also in our data.

During this study we identified the sources of differences we saw at low and high energies, presented methods for how we can handle these differences today and we made recommendations as to how the evaluated data can be improved to generally address these problems in the future.

The one difference we have at yet not been able to explain is what we call the 300 keV “bump” in the Godiva results. We can now compare results from a variety of different Monte Carlo codes. Using MCNP as a standard to ratio everything to, four codes show a “bump” (CE-KENO, MERCURY, TART, VIM) and four codes do not (MCNP, MONK, COG, TRIPOLI). Keeping an open mind as to which codes are correct, either four independent codes produce a minimum near 400 keV following by a maximum near 300 keV, or else MCNP produces a maximum near 400 keV followed by a minimum near 300 keV. We have tested many features of the codes but we still cannot explain this behavior. So our parting word will just have to be: **obviously still more works needs to be done.**



XXI - Conclusions

In this report we considered three fast critical assemblies, each assembly is dominated by a different nuclear fuel: Godiva (U235), Jezebel (Pu239) and Jezebel23 (U233) [1]. We first showed the improvement in results when using the new ENDF/B-VII.0 data [2], rather than the older, now frozen, ENDF/B-VI.8 data [3]. We did this using what we call a one code/multiple library approach, where results from one code (MCNP) are compared using two different data libraries (ENDF/B-VII.0 and VI.8). Next we showed that MCNP results are not specific to this one code by using what we call a one data library/multiple code approach; for this purpose we invited many codes to submit results using the ENDF/B-VII.0 data; the most detailed results presented in this report compare MCNP and TART.

The bottom line is that we have shown that using the new ENDF/B-VII.0 data library with a variety of transport codes, for the first time we are able to reproduce the expected K-eff values for all three assemblies to within the quoted accuracy of the models, namely 1.0 +/- 0.001. This is a BIG improvement compared to the results obtained using the older ENDF/B-VI.8 data library. Another important result of this study is that we have demonstrated that currently there are many computer codes that can accurately use the new ENDF/B-VII.0 data.

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Appendix A: Contact Information

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Appendix B: Submitting Code Results

This is an ongoing study that will not end with the initial publication of this report. Therefore if you, a reader, would like to submit results please feel free to do so; and your results will be included in the next published version of this report.

In order to minimize the amount of work done by everyone, I ask you to submit results **ONLY** for **EXACTLY** the systems defined above. **Please do not try to be creative and change (“improve”) the systems in any way.** If you submit results for any other systems ore for modified versions of these three systems, I will not be able to use them, and you will end up merely wasting your time.

You can submit results to Red Cullen by e.mail in any computer readable text format, as long as you adequately define the format; please, only submit text files, no spreadsheets, documents or anything else.

As a minimum you are asked to provide K-eff. If available the neutron production, absorption and leakage integral values and/or spectra would be very useful in attempting to explain any differences that we see between code results (see, appendix C for the definition of these terms). We define,

$$K\text{-eff} = \frac{\text{Pr oduction}}{\text{Absorption} + \text{Leakage}} = \frac{\text{Pr oduction}}{\text{Re moval}}$$

Where Production, Absorption and Leakage are defined as integrated over the entire system. For comparisons we need to use unique definitions of production, absorption and leakage (see Appendix C for details of definitions). Here we state the rules to use in an analog Monte Carlo calculation. For Leakage tally 1 for each neutron that leaks. Production and Absorption should be defined based on the number of neutrons resulting for each reaction,

- 0 - tally 1 neutron absorbed
- 1 - no tally, e.g., scatter does not contribute to either production or absorption
- < 1 – tally 1 neutron absorbed AND the number of neutrons resulting

For example, for capture tally 1 neutron absorbed and 0 neutrons produced; for fission tally 1 neutron absorbed and $\langle \nu \rangle$ neutrons produced; for (n,2n) tally 1 neutron absorbed and 2 neutrons produced; for elastic or inelastic scatter there is no tally.

Most convenient would be if you provide the production, absorption and leakage spectra using 50 tally bins per energy decade, with the bins equally spaced in the log of energy between, 10^{-5} eV and 20 MeV (616 bins). It is very easy to define the group index using this equal lethargy groups,

$$\text{Group \#} = 1 + 50 * \text{Log}_{10} [E/10^{-5}] = 616 \text{ group bins, } 10^{-5} \text{ eV to } 20 \text{ MeV}$$

For the convenience of MCNP users, below I include these 616 energies that can be used as a part of an MCNP input deck.

```

e1  1.00000E-11  1.04713E-11  1.09648E-11  1.14815E-11  1.20226E-11
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    1.58489E-11  1.65959E-11  1.73780E-11  1.81970E-11  1.90546E-11
    1.99526E-11  2.08930E-11  2.18776E-11  2.29087E-11  2.39883E-11
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    2.51189E-05  2.63027E-05  2.75423E-05  2.88403E-05  3.01995E-05

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3.16228E-05 3.31131E-05 3.46737E-05 3.63078E-05 3.80189E-05
3.98107E-05 4.16869E-05 4.36516E-05 4.57088E-05 4.78630E-05
5.01187E-05 5.24807E-05 5.49541E-05 5.75440E-05 6.02560E-05
6.30957E-05 6.60693E-05 6.91831E-05 7.24436E-05 7.58578E-05
7.94328E-05 8.31764E-05 8.70964E-05 9.12011E-05 9.54993E-05
1.00000E-04 1.04713E-04 1.09648E-04 1.14815E-04 1.20226E-04
1.25893E-04 1.31826E-04 1.38038E-04 1.44544E-04 1.51356E-04
1.58489E-04 1.65959E-04 1.73780E-04 1.81970E-04 1.90546E-04
1.99526E-04 2.08930E-04 2.18776E-04 2.29087E-04 2.39883E-04
2.51189E-04 2.63027E-04 2.75423E-04 2.88403E-04 3.01995E-04
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5.01187E-04 5.24807E-04 5.49541E-04 5.75440E-04 6.02560E-04
6.30957E-04 6.60693E-04 6.91831E-04 7.24436E-04 7.58578E-04
7.94328E-04 8.31764E-04 8.70964E-04 9.12011E-04 9.54993E-04
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1.58489E-03 1.65959E-03 1.73780E-03 1.81970E-03 1.90546E-03
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2.51189E-03 2.63027E-03 2.75423E-03 2.88403E-03 3.01995E-03
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6.30957E-03 6.60693E-03 6.91831E-03 7.24436E-03 7.58578E-03
7.94328E-03 8.31764E-03 8.70964E-03 9.12011E-03 9.54993E-03
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1.25893E-02 1.31826E-02 1.38038E-02 1.44544E-02 1.51356E-02
1.58489E-02 1.65959E-02 1.73780E-02 1.81970E-02 1.90546E-02
1.99526E-02 2.08930E-02 2.18776E-02 2.29087E-02 2.39883E-02
2.51189E-02 2.63027E-02 2.75423E-02 2.88403E-02 3.01995E-02
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5.01187E-02 5.24807E-02 5.49541E-02 5.75440E-02 6.02560E-02
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1.25893E-01 1.31826E-01 1.38038E-01 1.44544E-01 1.51356E-01
1.58489E-01 1.65959E-01 1.73780E-01 1.81970E-01 1.90546E-01
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3.16228E-01 3.31131E-01 3.46737E-01 3.63078E-01 3.80189E-01
3.98107E-01 4.16869E-01 4.36516E-01 4.57088E-01 4.78630E-01
5.01187E-01 5.24807E-01 5.49541E-01 5.75440E-01 6.02560E-01
6.30957E-01 6.60693E-01 6.91831E-01 7.24436E-01 7.58578E-01
7.94328E-01 8.31764E-01 8.70964E-01 9.12011E-01 9.54993E-01
1.00000E+00 1.04713E+00 1.09648E+00 1.14815E+00 1.20226E+00
1.25893E+00 1.31826E+00 1.38038E+00 1.44544E+00 1.51356E+00
1.58489E+00 1.65959E+00 1.73780E+00 1.81970E+00 1.90546E+00
1.99526E+00 2.08930E+00 2.18776E+00 2.29087E+00 2.39883E+00
2.51189E+00 2.63027E+00 2.75423E+00 2.88403E+00 3.01995E+00
3.16228E+00 3.31131E+00 3.46737E+00 3.63078E+00 3.80189E+00
3.98107E+00 4.16869E+00 4.36516E+00 4.57088E+00 4.78630E+00
5.01187E+00 5.24807E+00 5.49541E+00 5.75440E+00 6.02560E+00
6.30957E+00 6.60693E+00 6.91831E+00 7.24436E+00 7.58578E+00
7.94328E+00 8.31764E+00 8.70964E+00 9.12011E+00 9.54993E+00
1.00000E+01 1.04713E+01 1.09648E+01 1.14815E+01 1.20226E+01
1.25893E+01 1.31826E+01 1.38038E+01 1.44544E+01 1.51356E+01
1.58489E+01 1.65959E+01 1.73780E+01 1.81970E+01 1.90546E+01
1.99526E+01 2.00000E+01

c

Appendix C: Definition of K-eff

The first point to mention is that nothing in this section is new; the ideas presented here have been known for many years, but we repeat these ideas here because definitions can effect the interpretation of the results presented in this report. When we discuss the sources of differences between results from a variety of computer codes, one thing we must consider is that all codes do not use exactly the same definitions. Even if two codes do the same calculation and neutron history by history get the same answers, how these results are interpreted using different definitions can impact even simple integral quantities, such as K-eff.

It might come as a surprise to readers to be told that the definition of K-eff and the terms that contribute to it (production, absorption, and leakage) are not the same in all codes. In particular, it is important for readers of this report to understand that MCNP and TART do not use the same definitions. The differences are due to how each code treats (n,2n), (n,3n), etc. Either the MCNP or TART definitions can be used and both have been used for many years; there is nothing intrinsically wrong with either. The difference between their definitions only becomes important when we wish to compare results. To compare results we must adopt one standard set of definitions to interpret the results from all codes. For this report all of the comparison results presented earlier in this report are based on TART's definitions. With that said, let me derive the definitions used by each code.

Time Independent (Static) Formulation

For time independent codes there is what seems like a very simple textbook definition that can be used to define K-eff. It is the ratio of the number of neutrons produced in one generation to the number produced in the preceding generation; sounds simple and unique. Unfortunately, all textbooks and codes do not use the same definition of a "generation" and/or neutrons "produced". The time independent problem is a classic eigenvalue problem that can be written in several different forms – in all of these forms we have the same left hand side of the equation,

$$A N = \Omega * \nabla N + \Sigma_t * N$$

- 1) $A N = \lambda T N$
- 2) $A N = \lambda F N + O N$
- 3) $A N = \lambda [F N + M N] + S N$

In all case the eigenvalue $\lambda = 1/K$. Here in 1) T N is the Total (T) transfer; in 2) F N is the fission, and O N is all other transfer; in 3) F N is the fission, M N is multiple neutron transfer, e.g., (n,2n), and S N is scatter, i.e., one neutron transfer. The actual value of the calculated eigenvalue, λ , depends on which form is used, and therefore so does K. Many textbooks on particle transport will use the simplest form 1), where all secondary particles are multiplied by λ (1/K); I do not know of any computer codes that use this form. The difference between 2) and 3) is how multiple neutron transfer, e.g., (n,2n), is

handled. Most textbook assume all neutron multiplication is only due to fission and use form 2). This is for historical reasons back many years ago when the original transport codes were written (actually diffusion, then Sn). These codes did not include (n, 2n), etc. and fission was defined by a single secondary distribution, $\chi(E, E')$. Later when (n,2n) was included it was difficult to include it similar to fission as a neutron production term, and mathematically the simplest way to include (n,2n) was as a **negative absorption** term. But these leads to some strange results in order to define our all important neutron balance; I'll illustrate this point below where we see **negative absorption**.

Time Dependent (Dynamic) Formulation

For time dependent codes or codes that define K-eff in terms of a balance between neutrons produced and removed this is more complicated, because fission is not the only process that can produce neutrons during a generation; there is also (n,2n), (n,3n), etc., and how codes handle these lead to different definition of K-eff. Below I'll explain the differences.

Starting from the time dependent, linear Boltzmann equation in general geometry,

$$\frac{1}{v} \frac{\partial N}{\partial t} + \Omega * \nabla N + \Sigma t * N = \iint (\langle v \rangle \Sigma f + \Sigma_{scatter} + 2\Sigma_{n,2n} + 3\Sigma_{n,3n} + \dots) N d\Omega' dE'$$

Where $N(r, \Omega, E, t)$ is the neutron flux, $v * n(r, \Omega, E, t)$, $n(r, \Omega, E, t)$ is the neutron density, v is the neutron speed, Σt is the macroscopic total cross section, $\langle v \rangle$ is the average number of neutrons emitted per fission, Σf , $\Sigma_{scatter}$, $\Sigma_{n,2n}$, $\Sigma_{n,3n}$, etc., are the macroscopic cross sections for each type of event. For simplicity I will use neutron density $n(r, \Omega, E, t)$ in the following,

Integrate over all space, energy, and direction

$$\frac{\partial n}{\partial t} + [L * v * n] + [\Sigma t * v * n] = [(\langle v \rangle \Sigma f + \Sigma_{scatter} + 2\Sigma_{n,2n} + 3\Sigma_{n,3n} + \dots) v * n]$$

Collecting terms together we find a simple equation defining the time dependent behavior of the neutron density in the system,

$$\frac{\partial n}{\partial t} = \alpha * n$$

$$\begin{aligned} \alpha &= [(\langle v \rangle \Sigma f + \Sigma_{scatter} + 2\Sigma_{n,2n} + 3\Sigma_{n,3n} + \dots) v] - [L * v] - [\Sigma t * v] \\ &= [\text{Production rate}] - [\text{Removal Rate}] \end{aligned}$$

The time constant (α) is a physical observable and as such has a unique value that we can determine. The non-uniqueness of K-eff and related terms is because exactly the same

terms appear in this definition of α as positive and negative terms that we can completely cancel (scatter), or are simply related terms that we can partially cancel (n,2n).

I will divide the total cross section by events according to how many neutrons result from each type of event: **none** – capture, (n,p), (n,a), etc., **one** – scatter, (n,np), (n,na), etc., **more than one** – fission, (n,2n), (n,3n), etc.. All of those events that result in one neutron do not directly effect the neutron balance of the system (they effect it indirectly through the leakage), and appear in exactly the same form in this definition as positive and negative terms, so that we can cancel them. Upon cancelling all scatter, and all other reactions with one neutron emitted, (n,np), (n,na), etc.,

$$\alpha = [(\langle \nu \rangle \Sigma_f + 2\Sigma_{n,2n} + 3\Sigma_{n,3n} + \dots)\nu] - [L * \nu] - [(\Sigma_{n,0} + \Sigma_f + \Sigma_{n,2n} + \Sigma_{n,3n} + \dots) * \nu]$$

Up to this point all or least most of the codes use the same definitions. Let me stress this point: both MCNP and TART calculate roughly the same values for each of the terms in the above definition of α ; there is no difference up to this point. As we will see below, the difference arises only because MCNP and TART use different definitions of neutron production and absorption.

TART defined neutron production and absorption without any further cross cancellation of terms in the above definition of α . In other words, any event that introduces additional neutrons into the system is considered production, and any event that produces neutrons also removes neutrons, etc., (n,2n) removes one neutron and produces two neutrons,

$$\text{Production rate} = [(\langle \nu \rangle \Sigma_f + 2\Sigma_{n,2n} + 3\Sigma_{n,3n} + \dots)\nu]$$

$$\text{Removal Rate} = \text{Leakage} + \text{Absorption} = [L * \nu] + [(\Sigma_{n,0} + \Sigma_f + \Sigma_{n,2n} + \Sigma_{n,3n} + \dots) * \nu]$$

Other codes, such as MCNP, change this to agree with the textbook definition of K-eff where production is only due to fission. This requires that they subtract $2\Sigma_{n,2n} + 3\Sigma_{n,3n} + \dots$ from the production and removal resulting in the definitions,

$$\text{Production rate} = [(\langle \nu \rangle \Sigma_f)\nu]$$

$$\text{Removal Rate} = [L * \nu] + [(\Sigma_{n,0} + \Sigma_f) * \nu] - [(\Sigma_{n,2n} + 2\Sigma_{n,3n} + 3\Sigma_{n,4n} + \dots) * \nu]$$

Note, that we still have exactly the same definition of the physically observable time constant (α), and for an exactly critical system K-eff remains unity using any of these definitions. Regardless of how they define production and removal, the codes define,

$$\alpha = [\text{Production Rate}] - [\text{Removal Rate}] = \left[\frac{\text{Pr oduction}}{\text{Re moval}} - 1 \right] * [\text{Removal Rate}]$$

$$= [\text{K-eff} - 1] / Tr \quad Tr = \text{Removal Time}$$

$$\text{K-eff} = \frac{\text{Pr oduction}}{\text{Re moval}} \quad \text{Removal Time} = 1 / [\text{Removal Rate}]$$

Here we can see that even though the time constant (α) has a unique definition, K-eff and the removal time, do not; again let me stress that this is only because all codes do not define production and removal the same way. With the TART definition any event that produces more than one neutron ends a generation, and adds to the removal $\Sigma f + \Sigma n,2n + \Sigma n,3n + \dots$ and adds to the production $\langle \nu \rangle \Sigma f + 2\Sigma n,2n + 3\Sigma n,3n + \dots$. Codes that do not consider that $(n,2n), (n,3n)$, etc., end a generation (e.g., MCNP), they add nothing to production for these events and **subtract** from the removal $\Sigma n,2n + 2\Sigma n,3n + 3\Sigma n,4n + \dots$.

For exactly critical systems, (K-eff=1) the production and removal exactly balance regardless of which definition we use, but even in this case the individual terms, production, absorption and leakage can be quite different. I will define,

$$\begin{aligned}
 P &= [(\langle \nu \rangle \Sigma f + 2\Sigma n,2n + 3\Sigma n,3n + \dots)\nu] \\
 R &= [L * \nu] + [(\Sigma n,0 + \Sigma f + \Sigma n,2n + \Sigma n,3n + \dots) * \nu] \\
 M &= [(2\Sigma n,2n + 3\Sigma n,3n + \dots)\nu]
 \end{aligned}$$

$$\text{TART K-eff} = \frac{P}{R} \qquad \text{MCNP K-eff} = \frac{P - M}{R - M}$$

In this form we can see that,

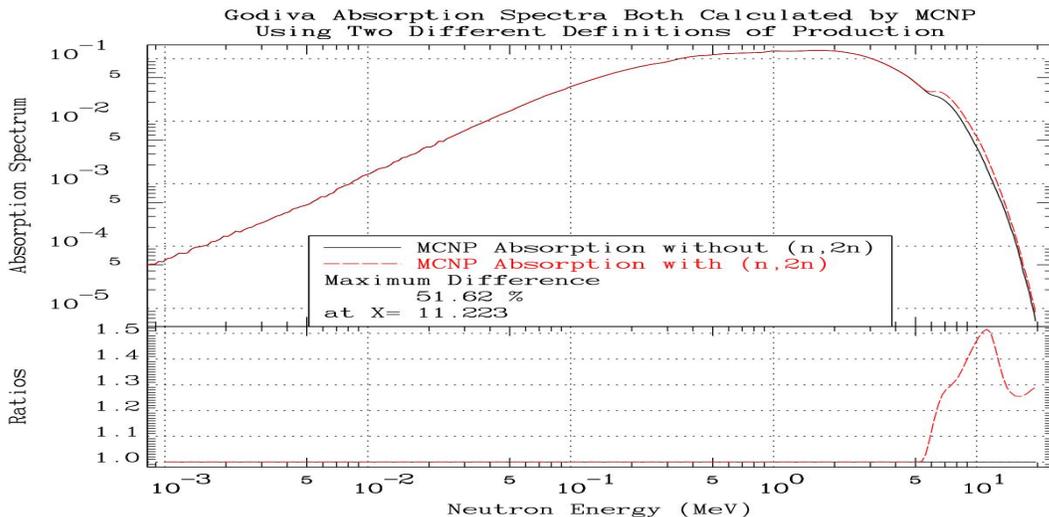
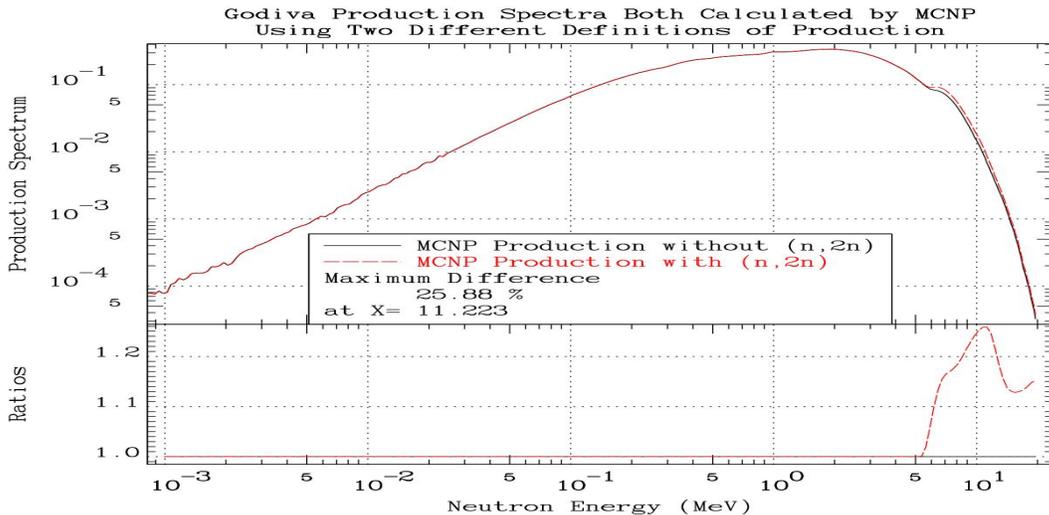
- Super-critical: $P > R$: MCNP K-eff > TART K-eff
- Exactly critical: $P = R$: MCNP K-eff = TART K-eff = 1
- Sub-Critical: $P < R$: MCNP K-eff < TART K-eff

Earlier in this report we showed comparisons of energy dependent production, absorption and leakage. Even for an exactly critical system, K-eff = 1, it would have been impossible to obtain agreement when comparing results unless we used a single consistent set of definitions for production, absorption, and leakage. For example, if for production we compared the energy dependent production as defined by MCNP to the production defined by TART, we would not expect to obtain agreement, because the TART results would include the effect of (n,2n), etc., and MCNP would not. Let us stress that either MCNP or TART definitions are perfectly acceptable, but for the comparisons shown in this report we had to adopt one set of definitions; in this report I arbitrarily adopted the TART conventions to define production, absorption and leakage. The importance of using unique definitions is illustrated below using only MCNP results, but two different definitions of production and absorption.

Godiva Production and Absorption Spectra Using Two Different Definitions

In order to illustrate the importance of using unique definitions when performing comparisons, below we use MCNP Godiva results to illustrate the energy dependent production and absorption spectra using two different definitions: first MCNP's standard definition without including (n,2n), and next TART's standard definition including (n,2n). **It is important to understand that both results are based on exactly the same MCNP calculation, and they differ only in how we interpret the MCNP results.**

What we see is that the spectra are identical up to the (n,2n) threshold; above this energy point the production and absorption spectra including (n,2n) will obviously exceed the spectra without (n,2n). **The important point to note is that had we compared MCNP results using its standard definition without including (n,2n) to TART results using its standard definition including (n,2n), we would have been misled into thinking that the codes disagree in their transport of high energy neutrons, where in fact they agree quite well WHEN WE USE UNIQUE DEFINITIONS.**



Critical Godiva

To illustrate the difference in results due to definitions the standard TART output includes K-eff defined using both TART's definition and MCNP's definition. Below is an example portion of a TART output listing for Godiva: after tracking N neutrons to determine which lead to leakage, absorption and/or production, the results are arbitrarily normalized per neutron removed.

First, I use TART's definition, where (n,2n), (n,3n), etc., are included in absorption, and 2(n,2n), 3(n,3n), etc., are included in production. Because this is a very fast system we see that (n,2n) produces about 0.5% of the neutrons, compared to 99.5% produced by fission.

Next, I use MCNP's definition where only fission contributes to production; not (n,2n), (n,3n), etc. In this case (n,2n), etc., are treated as **negative absorption**; from the below table we can see that physically this assumption is unrealistic, but here it is merely a mathematical convenience. I haven't changed the normalization in order to maintain the same definition of Leakage (in principle this is a physical observable that could be measured directly). The removal is reduced by about 0.5%, but so is production. The net result is that in both cases we get the same value for K-eff (**1.00025**), even though how we define **production** and **removal** are quite different.

----- Analog Removal and Production vs. Reaction C Number per Removed Neutron -----

C Number	Reaction	Removal	Production	Events
10	Elastic	0.00000D+00	0.00000D+00	1.64320D+00
11	(n,n')	0.00000D+00	0.00000D+00	5.60583D-01
12	(n,2n)	2.54982D-03	5.09963D-03	2.54982D-03
13	(n,3n)	2.51910D-06	7.55730D-06	2.51910D-06
14	(n,4n)	3.00000D-10	1.20000D-09	3.00000D-10
15	Fission	3.82883D-01	9.95144D-01	3.82883D-01
46	(n,g)	4.47771D-02	0.00000D+00	4.47771D-02
	Leakage	5.69789D-01	0.00000D+00	

	Totals	1.00000D+00	1.00025D+00	2.63400D+00
	K-eff		1.00025D+00	

----- Alternate Definition of K-eff using ONLY Fission Production -----

C Number	Reaction	Removal	Production
12	(n,2n)	-2.54982D-03	0.00000D+00
13	(n,3n)	-5.03820D-06	0.00000D+00
14	(n,4n)	-9.00000D-10	0.00000D+00
15	Fission	3.82883D-01	9.95144D-01
46	(n,g)	4.47771D-02	0.00000D+00
	Leakage	5.69789D-01	0.00000D+00

	Totals	9.94894D-01	9.95144D-01
	K-eff		1.00025D+00

HMF066-9

Now let's look at a system that contains beryllium and has many (n,2n) reactions; below are results for HMF006-9, where over 10% of the neutrons produced are due to (n,2n). As we move away from criticality the results become more sensitive to the definition we use. Now we see a difference even in K-eff: TART (0.9865) and MCNP (0.9853), for a difference of 0.0012, which exceeds the 0.1% agreement we are trying to achieve.

Note, that the difference is still quite small, near 0.1%; the important point to understand is that both MCNP and TART do the same calculations and generally get the same results. The differences we see here are based strictly on how we interpret the results – in particular, how we define production and absorption. This makes it difficult to blindly comparing results from different codes, without considering the definitions they use.

Analog Removal and Production vs. Reaction C Number per Removed Neutron				
C Number	Reaction	Removal	Production	Events
10	Elastic	0.00000D+00	0.00000D+00	8.46671D+00
11	(n,n')	0.00000D+00	0.00000D+00	3.77274D-01
12	(n,2n)	4.62875D-02	9.25749D-02	4.62875D-02
15	Fission	3.51294D-01	8.94127D-01	3.51294D-01
42	(n,t)	3.05810D-06	0.00000D+00	3.05810D-06
45	(n,a)	3.33150D-02	0.00000D+00	3.33150D-02
46	(n,g)	6.70535D-02	0.00000D+00	6.70535D-02
	Leakage	5.02047D-01	0.00000D+00	
Totals		1.00000D+00	9.86702D-01	9.34193D+00
K-eff			9.86702D-01	
Alternate Definition of K-eff using ONLY Fission Production				
C Number	Reaction	Removal	Production	
12	(n,2n)	-4.62875D-02	0.00000D+00	
15	Fission	3.51294D-01	8.94127D-01	
42	(n,t)	3.05810D-06	0.00000D+00	
45	(n,a)	3.33150D-02	0.00000D+00	
46	(n,g)	6.70535D-02	0.00000D+00	
	Leakage	5.02047D-01	0.00000D+00	
Totals		9.07425D-01	8.94127D-01	
K-eff			9.85345D-01	

HMF066-9 Sub and Super Critical

The above HMF066-9 results are what we expect for K-eff close to 1.0. Merely to illustrate differences in defined K-eff when we are further from critical, below I present results for completely hypothetical sub and super critical systems. I first decreased and then increased the density of the fuel in HMF066-9 to make it first sub critical and then super critical

Sub Critical

Analog Removal and Production vs. Reaction C Number **per Removed Neutron**

C Number	Reaction	Removal	Production	Events
10	Elastic	0.00000D+00	0.00000D+00	8.86549D+00
11	(n,n')	0.00000D+00	0.00000D+00	3.01481D-01
12	(n,2n)	5.00123D-02	1.00025D-01	5.00123D-02
15	Fission	2.97755D-01	7.56188D-01	2.97755D-01
40	(n,p)	4.62963D-06	0.00000D+00	4.62963D-06
42	(n,t)	1.54321D-06	0.00000D+00	1.54321D-06
45	(n,a)	3.63827D-02	0.00000D+00	3.63827D-02
46	(n,g)	5.98256D-02	0.00000D+00	5.98256D-02
	Leakage	5.56019D-01	0.00000D+00	

	Totals	1.00000D+00	8.56213D-01	9.61095D+00
	K-eff		8.56213D-01	

Alternate Definition of K-eff using ONLY Fission Production

C Number	Reaction	Removal	Production
12	(n,2n)	-5.00123D-02	0.00000D+00
15	Fission	2.97755D-01	7.56188D-01
40	(n,p)	4.62963D-06	0.00000D+00
42	(n,t)	1.54321D-06	0.00000D+00
45	(n,a)	3.63827D-02	0.00000D+00
46	(n,g)	5.98256D-02	0.00000D+00
	Leakage	5.56019D-01	0.00000D+00

	Totals	8.99975D-01	7.56188D-01
	K-eff		8.40232D-01

Super Critical

Analog Removal and Production vs. Reaction C Number **per Removed Neutron**

C Number	Reaction	Removal	Production	Events
10	Elastic	0.00000D+00	0.00000D+00	7.99639D+00
11	(n,n')	0.00000D+00	0.00000D+00	4.72933D-01
12	(n,2n)	4.23259D-02	8.46519D-02	4.23259D-02
13	(n,3n)	1.62963D-05	4.88889D-05	1.62963D-05
15	Fission	4.20087D-01	1.07184D+00	4.20087D-01
40	(n,p)	2.96296D-06	0.00000D+00	2.96296D-06
42	(n,t)	1.18519D-05	0.00000D+00	1.18519D-05
45	(n,a)	2.96622D-02	0.00000D+00	2.96622D-02
46	(n,g)	7.59896D-02	0.00000D+00	7.59896D-02
	Leakage	4.31908D-01	0.00000D+00	

	Totals	1.00000D+00	1.15654D+00	9.03742D+00
	K-eff		1.15654D+00	

Alternate Definition of K-eff using ONLY Fission Production

C Number	Reaction	Removal	Production
12	(n,2n)	-4.23259D-02	0.00000D+00
13	(n,3n)	-3.25926D-05	0.00000D+00
15	Fission	4.20087D-01	1.07184D+00
40	(n,p)	2.96296D-06	0.00000D+00
42	(n,t)	1.18519D-05	0.00000D+00
45	(n,a)	2.96622D-02	0.00000D+00
46	(n,g)	7.59896D-02	0.00000D+00
	Leakage	4.31908D-01	0.00000D+00

	Totals	9.15304D-01	1.07184D+00
	K-eff		1.17102D+00

Compared to HMF066-9 close to critical, now we see larger differences:
Sub-critical: TART (0.8562) and MCNP (0.8402); 0.0160 difference
Super-critical: TART (1.1565) and MCNP (1.1712); 0.0147 difference

Here the differences are well over 1%, at least an order of magnitude more than the 0.1% agreement we are hoping to achieve. Note that these differences are as predicted, where for sub-critical systems, MCNP K-eff < TART K-eff, and for super-critical systems MCNP K-eff > TART K-eff. The magnitude of the difference between the definitions of K-eff depend both on how far the system is from criticality and how much n,2n, etc., reactions occur in the system.

In these cases which value of K-eff is correct? The answer is that they both are, based on the definitions that TART and MCNP use.

Bottom line: With all that said, let me repeat what was said at the beginning of this section defining K-eff. MCNP and TART use different definitions of production and absorption. The differences are due to how each code treat (n,2n), (n,3n), etc. Either the MCNP or TART definitions can be used and both have been used for many years; there is nothing intrinsically wrong with either. The difference between their definitions only becomes important when we wish to compare results. To compare results we must adopt one standard set of definitions to interpret the results from all codes. For this report all of the comparison results presented earlier in this report are based on TART's definitions.

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