TRISO Homogenization

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Abstract

We present a method that allows us to simplify our geometric models by **homogenizing** portions of our geometry, while still simulating the same **reaction rates** in our homogenized system as we calculate in our detailed **heterogeneous** system. This model is illustrated here as applied for use with a sub-critical system driven by a high energy external neutron source. This sub-critical system differs significantly from critical systems, so that we cannot use the standard methods used for nuclear reactors. We define our proposed method in detail and then demonstrate that it can actually be used to correctly model **reaction rates** in our **homogenized** system that reproduce the **reaction rates** we calculate in our detailed **heterogeneous** system.

Overview

Example Sub-Critical System

Here we illustrate our model as applied to a sub-critical assembly driven by a nominally 14.1 MeV neutron source; the source is created by laser induced fusion. This system is designed to burn-up fissionable materials and the products of fission, and in the process to produce considerable amounts of energy.
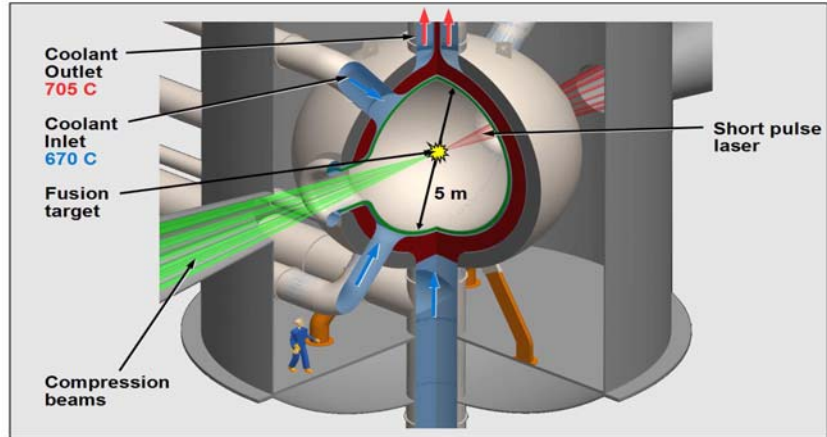
The fission material and products inside our system are contained in a typical pebble/TRISO design.
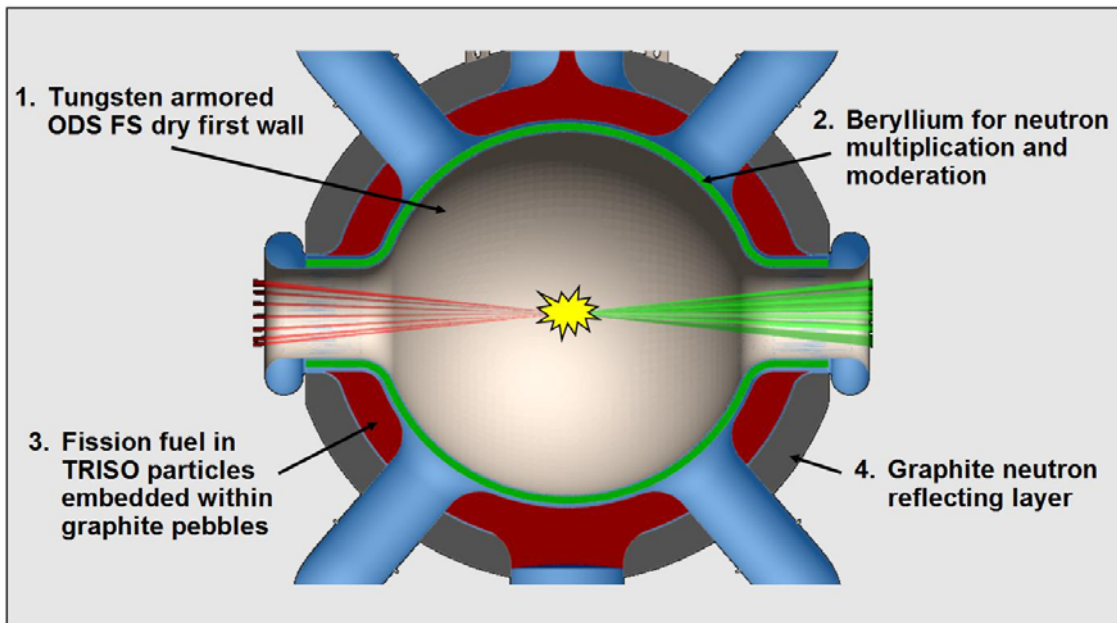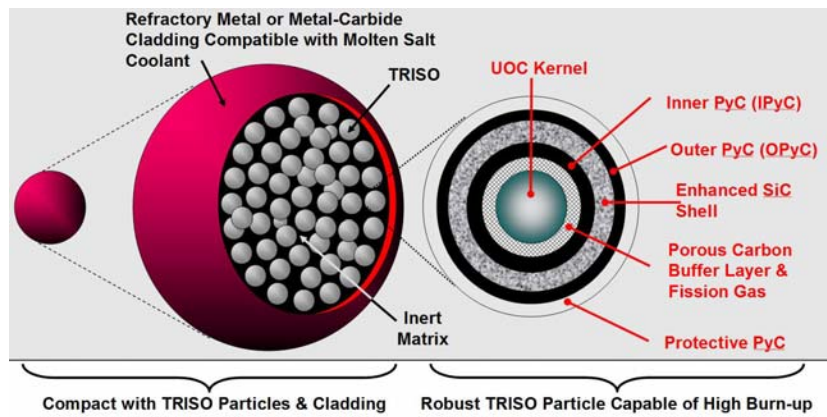
This system differs from a typical fission reactor assembly in a number of significant features, one of the most important difference is that because it is a sub-critical assembly, driven by an external fast neutron source, **there are inherently rather large neutron flux gradients and currents throughout the**

system. Unlike a typical thermal reactor which is designed to "flatten" the flux distribution throughout the reactor to minimize leakage, with this system large gradients are inherent, due to the external neutron source and sub-critical condition. This makes some of the methods used in reactor design inappropriate for use with this system; this point will be discussed in detail below.

The pebble/TRISO problem addressed here is similar to the problems addressed in other studies for critical reactors [4, 5, 6, 7, 8], where similar differences due to heterogeneity and the random positioning of TRISO were found. These earlier studies clearly illustrate the importance of accounting for heterogeneity and random positioning effects. In particular note that **reference [8] mentions that resonance self-shielding can decrease K-eff by up to 11%, and TRISO size and position can further significantly affect K-eff**. The solution to this problem suggested here is different, primarily because, our system is not a critical reactor. But it should be mentioned that the approaches presented in refs. [4, 5, 6, 7, 8] and the method proposed here are somewhat complementary, and indeed could be used to good advantage in combination; however, brevity forces us to only focus on the one method proposed here. We will mention that **here we limit discussion to only one example system, whereas reference [8] considers a variety of variations in the system based on TRISO size and position; we strongly recommend that anyone dealing with systems containing TRISO read reference [8].**

Contents of This Paper

This paper will be concerned with neutron transport calculations as they apply to a typical sub-critical system. The primary, time dependent calculation for our system are presently being perform using the MCNP continuous energy Monte Carlo code [2]. The studies described in this paper, to handle homogenization and self-shielding, were performed using the TART continuous energy Monte Carlo code [3]. These two Monte Carlo codes can be used in parallel to meet the needs of our system.

The system we are presently investigating contains about 31 million pebbles, and each pebble contains about 2,445 TRISO, corresponding to 30% TRISO packing within each pebble, and each TRISO contains four spatial zones. This means a fully defined system would require about 31 million x 2,445 or over 74 billion TRISO, and about 300 billion spatial zones. We judge this to be beyond our present calculational capabilities. However, million of zones are within our capability today. By taking advantage of the spatial symmetry of our system, we could model all of the pebbles in this system. **Therefore this paper investigates how we can accurately homogenize the contents of each pebble, to reduce the number of spatial zones required from many billions to several million.**

Specifically we consider,
1) How many Monte Carlo **sampled neutrons** are needed for converged results? In our calculations we will be taking differences between results, so each result must be as accurate as possible. To determine how many neutrons are required we used a brute force approach by running problems with progressively more neutrons until we achieve convergence.
2) Is self-shielding **qualitatively** important in our system? This is the major concern when we attempt to homogenize the TRISO within each pebble. To determine how important an effect this is we present results using a variety of cross section models: including continuous energy cross sections, multiband cross sections, and multigroup cross sections.
3) **Quantitatively** how important is self-shielding in our system? To determine this we performed calculations for a variety of spatial models, including:

a) full detailed (4 zone) TRISO, randomly positioned within each pebble,
b) full detailed TRISO, regularly positioned within each pebble,
c) homogenized (1 zone) TRISO within a pebble as separate TRISO and pebble zones; and
d) finally completely homogenized TRISO and pebble as one combined spatial zone.
4) Finally we present a model that we can use to homogenize our geometry and yet reproduce **the same reaction rates in the homogenized geometry that we calculate in our detailed geometry**.

One Example Problem

During its lifetime our system can contain many variations in the contents of the TRISO, and will include temperatures between cold, room temperature, startup, and hot, operating temperatures. In this paper as an example of the methods that can be used to handle any of these conditions, we illustrate results for only one condition. All of the following results are for a cold, room temperature, where the system contains depleted uranium. **What is important to focus on is that the results and methods presented here are typical and the methods can be applied to any other system conditions**.

Here we define enough information to uniquely define the system we consider, with sufficient details to allow anyone else to reproduce these results.

Heterogeneous versus Homogeneous Systems

Even by the early 1940's it was understood that from a neutronics viewpoint there is a significant advantage to heterogeneous uranium fueled systems. In these systems fast neutrons created within the fuel by fission could leak from the fuel, slow down within a surrounding moderating system, **avoiding parasitic absorption in the U238 resonance energy range**, and re-enter the fuel at lower energies creating the next generation of fission neutrons. This was so well understood that even Fermi's first reactor (1942) was a heterogeneous system of uranium rods in a graphite pile.

Since we understand this difference between heterogeneous and homogeneous system, this means that when we attempt to simplify geometry by homogenizing a portion of it, if we wish to insure that the homogenized system is equivalent to our heterogeneous system, we must be insure that **the reaction rates in the two systems are equivalent**, by mimicking the heterogeneous resonance self-shielding in the homogeneous system. This is not a new problem unique to our system; throughout the lifetime of the nuclear industry we have been faced with the same problem for nuclear reactors. For many years our solution has been to perform **cell calculations**: first we perform detailed heterogeneous calculations to define **the true reaction rates,** we then define multi-group constant for use in our homogeneous system to produce **the same reaction rates**. All this requires is that we define these **"equivalent" multi-group constants** to account for the resonance self-shielding that occurs in the heterogeneous system.

For our system we propose to do the same type of cell equivalence, self-shielding calculations, but rather than producing multi-group cross sections, we will produce **self-shielded continuous energy cross sections**, so that we will still be able to use our continuous energy Monte Carlo codes, MCNP and TART. We want to still be able to use continuous energy cross sections, because our system is a sub-critical system driven by an external high energy neutron source. It has large spatial gradients in the flux, and currents, which do not occur in critical nuclear reactors. Using multigroup methods would make it more difficult to account for the higher moments of the flux that we expect to encounter in our

system, whereas this is an ideal problem for the use of continuous energy cross sections. **To make sure the reaction rates are the same in both systems all we need insure is that the correct self-shielded cross sections are used in the homogeneous system.**

What happens if we do not account for self-shielding?

Obviously even by the 1940's Fermi and others knew the answer to this question: In a homogenized system containing the same constituents (atoms of each material) the reaction rate (particularly absorption) in the resonance region will be higher than in an "equivalent" heterogeneous system. In the case of Fermi's reactor the difference was so large that an "equivalent" homogeneous system would not have gone critical. An alternative way to say this is that we know the results for heterogeneous and homogeneous systems differ. So that if one naively homogenizes geometry based solely on atoms of each constituent, they can accurately calculate results for this homogenized system, but these results will have nothing to do with the results that one would accurately calculate for a heterogeneous system.

If Fermi knew this over 60 years ago, surely anyone doing calculations today should understand: **You cannot expect to simply homogenize a system based on only its constituents, and calculate results that are "equivalent" to what happens in a heterogeneous system**. If you try this everyone knows that you will overestimate the reaction rates in the resonance region, and your homogeneous results will have no relationship to the ACTUAL results of the heterogeneous system that we are actually interested in, i.e., you are wasting your time and will obtain misleading results.

Here we MUST focus on the fact that we want results for the **heterogeneous** system, not the **homogenized** system; we use the homogenized system only in an attempt to simplify our calculations. But the results of our simplified homogeneous model will be applicable to our heterogeneous model ONLY if both have **the same reaction rates**. The entire focus of this paper is to present a method that will allow us to conserve the reaction rates, thereby allowing us to use a simplified homogeneous model to simulate a heterogeneous system and allowing us to continue using our continuous energy (not multi-group) Monte Carlo codes, such as MCNP [2] and TART [3]. The method we present here is quite simple: **We will self-shield the cross sections that we use in our homogeneous calculation, so that the reaction rates are the same in both heterogeneous and homogeneous systems**.

An important point to consider is that we know that the reaction rates in the heterogeneous system differs from that in the "equivalent" homogeneous system, and at least in the case of a classic reactor-like problem involving uranium (as in our example problem), the result is that the calculated K-eff for the homogeneous system is generally lower than in heterogeneous system. The example system described in this paper is very sub-critical, so that minor differences in K-eff generally will not be too misleading, but for systems near critical this can lead to **dangerously misleading results**, where our homogeneous calculations predict the system to be safely sub-critical, whereas the heterogeneous system with a higher K-eff may actually be critical, i.e., hardly a conservative, safe approximation. Depending on how you intend to use your results this fact should lead you to consider more closely the question we ask in this section: **What Happens if we do not account for self-shielding?**

Cell Calculations

We performed cell calculations for arrays of TRISO inside a pebble. We assume there are so many TRISO in each pebble that any one particular TRISO "sees" itself as inside an array of TRISO extending in all directions to infinity, i.e., an infinitely repeating array. We defined each cell as a cube containing a TRISO, and performed criticality and source calculations for arrays of one or more cells with perfectly reflecting outer boundary, for the array in planar (x, y, z) geometry. For the regularly positioned TRISO it is sufficient to perform calculations using only one cell. For the randomly positioned TRISO many cells are used to properly sample the possible random positions of the TRISO; for this case an array of cells was used, specifically up to, 101 x 101 x 101 = over 1 million cells, each containing a randomly position TRISO; each cell includes a four zone TRISO and a fifth zone is the surround pebble, so that for the calculation of randomly positioned TRISO the Monte Carlo model uses over five million spatial zones, which is well within the capability of TART on one of today's personal computers. We have found that using significantly fewer randomly positioned TRISO does not give an adequate statistical sample representing the effect of the random positioning.

Our sub-critical system versus a critical reactor

Cell calculations have historically worked very well to model fission reactors; over the last fifty years an entire class of computer code systems has been developed to address exactly this problem, so that in principle there is nothing new about what we are proposing. In a thermal reactor cell calculation the reactor is close to critical and all of the neutrons are due to sources of fission neutrons within the cell; in this type of calculation it is assumed that the system has relaxed into its fundamental mode, so that a standard criticality calculation can be used to model it. Our system differs in that it is very sub-critical and driven by a external source of neutrons; in this case the system is not in its fundamental mode, and a significant fraction of the neutron multiplication is not due to fission, e.g., Be (n,2n). This makes completely standard cell calculations inappropriate for use with our system. To model a cell with TART we have run both source problems and criticality problems with no settle cycles (to include non-fundamental mode contributions) and neutron generation scaling by the multiplication. **Using TART both of these approaches give the same answer**. To illustrate how different the results of a "standard" fundamental mode cell calculation are, we also include results for this model.

Geometry and Composition

Each cell includes a spherical TRISO 0.0497 cm in outer radius, surrounded by the pebble which is sized to correspond to 30% packing, i.e., of the total volume of the cell 30% is inside the TRISO, and 70% is outside the TRISO, inside the pebble. Based on the 0.0497 cm radius of the TRISO, for 30% packing the cubic cell is defined to have a side length of 0.1196774078 cm. For the cases we consider here each cell includes somewhere between five and one spatial region:
1) The fully defined TRISO includes 4 spatial zones plus the pebble (5 zones),
2) The homogenized TRISO includes 1 spatial zone plus the pebble (2 zones), and
3) the homogenized TRISO and pebble (only 1 spatial zone).
We define the composition for each of these models to conserve the number of atoms, and therefore grams, of each material, in the fully defined TRISO.

Note, that in all three compositions listed below, the mass of 92238, 92235 and 14028 is exactly the same, because each of these only appear in one zone; the mass of 6000 and 8016 is the sum of the masses in the zones being mixed. Therefore in all cases we have conserved the mass of all constituents.

Fully detailed TRISO (5 zones)

Zone #	Radius (cm)	Density (grams/cc)	Volume (cc)	Composition (weight fraction)	Mass (grams)
1	0.03	10.5	1.130973d-4	92238 0.8925 92235 0.0023 8016 0.0601 6000 0.0451	1.059864d-3 2.731302d-6 7.137020d-5 5.355656d-5
2	0.0402	1.1	1.590266d-4	6000 1.0	1.749293d-4
3	0.0407	1.95	1.028069d-5	6000 1.0	2.004735d-5
4	0.0497	3.217	2.318258d-4	14028 0.8004 6000 0.2996	5.223488d-4 2.234348d-4
	Side (cm)				
5	0.1196774078	1.7	1.199871d-3	6000 1.0	2.039781d-3

Homogenized TRISO (2 zones)

Zone #	Radius (cm)	Density (grams/cc)	Volume (cc)	Composition (weight fraction)	Mass (grams)
1	0.0497	4.13877141	5.142304d-4	92238 0.497990069 92235 0.00128333575 6000 0.221761299 14028 0.245431175 8016 0.0335341212	1.059864d-3 2.731302d-6 4.719658d-4 5.223488d-4 7.137020d-5
	Side (cm)				
2	0.1196774078	1.7	1.199871d-3	6000 1.0	2.039781d-3

Homogenized pebble/TRISO (1 zone)

Zone #	Side (cm)	Density (grams/cc)	Volume (cc)	Composition (weight fraction)	Mass (grams)
1	0.1196774078	2.43163142	1.714101d-3	92238 0.254282007 92235 0.000655292566 6000 0.602618384 14028 0.125321237 8016 0.0171230797	1.059864d-3 2.731302d-6 2.511738d-3 5.223488d-4 7.137055d-5

How many neutrons are needed for converged results?

In our calculations we will be taking differences between results, so each result must be as accurate as possible. To determine how many neutrons are required we used a brute force approach by running problems with progressively more neutrons until we achieve convergence. The following table shows convergence using successively more neutrons.

Results are based on in all cases 100 settle cycles followed by,
1/10 M =   100 batches of   1,000 each (1/10 of 1 million)
   1 M = 1000 batches of   1,000 each (1 million)
  10 M =   "   10,000 each (10 million)

Geometry versus K-eff	1/10 M	1 M	10 M
Full Details/Regular Position	0.2700	0.2715	0.2713
Full Details/Random Position	0.2703	0.2710	0.2711
Homogenized TRISO	0.2582	0.2586	0.2584
Homogenized pebble/TRISO	0.2551	0.2544	0.2546

The 10 M results were run a number times using different random number sequences and in all cases the results were identical to the number of digits quoted here, i.e., to within 0.01%. Using fewer neutrons results in small, but significant differences from the converged 10 M results. For example, the difference between the converged full details regular and random position results is less than the difference between 1/10M and 10 M random results. Indeed the 1/10 M results show that the full details/regular results are less than the random results, whereas the converged 10 M results show the opposite effect, i.e., the 1/10M results are completely misleading.

Based on the above results 10 M neutrons are needed to insure convergence, so that ALL of the following results used 10 M neutrons.

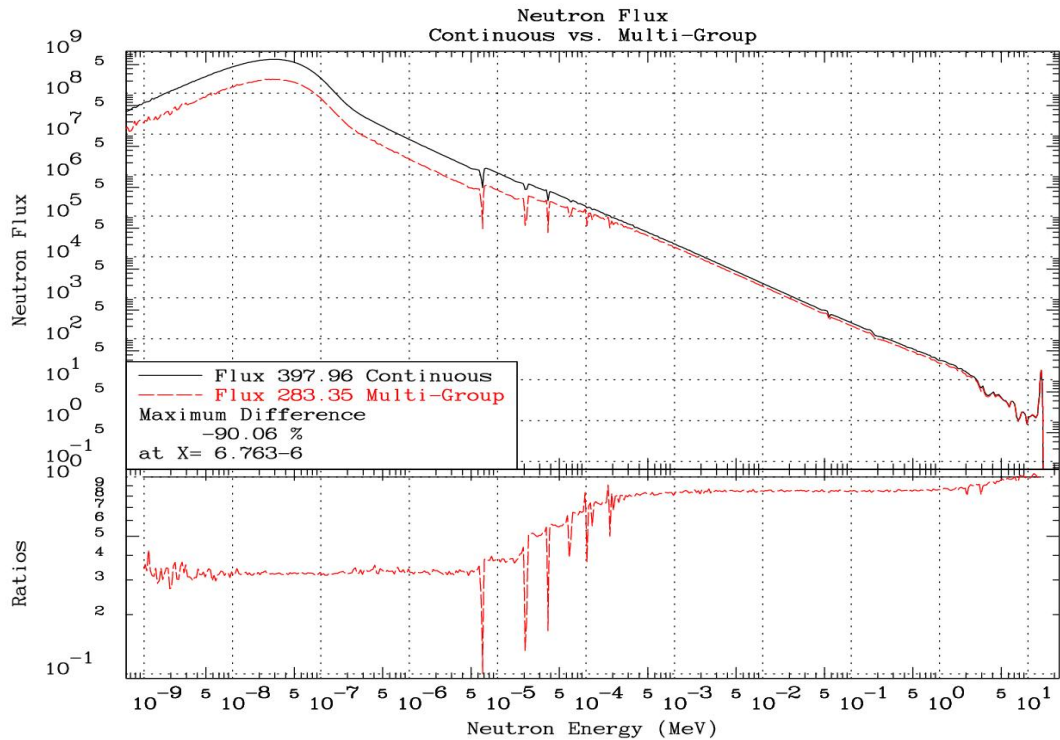**Is self-shielding qualitatively important in Our System?**

This is the major concern when we attempt to homogenize the TRISO within each pebble. To determine how important an effect this is we present results using a variety of cross section models: including continuous energy cross sections, multiband cross sections, and unshielded multigroup cross sections. The multiband and multigroup results are based on using 616 groups. The following tables shows the effect of self-shielding by comparing methods,

| Geometry	Continuous	Multiband	Multigroup
Full Details/Regular Position	0.2713	0.2785	0.1436
Full Details/Random Position	0.2711	0.2781	0.1432
Homogenized TRISO	0.2584	0.2650	0.1331
Homogenized pebble/TRISO	0.2546	0.2612	0.1307

The first point to note is the ENORMOUS difference between the continuous energy and multigroup results, which demonstrates that self-shielding is important in our system. See the below comparison of the continuous and multi-group flux, showing the enormous difference between the two, particularly at

low energy below the resonance energy region where the multi-group flux is only about 30% of the continuous energy flux. This also illustrates that **the 616 groups used here are far too few to eliminate the effects of self-shielding**. A common error is to assume one can eliminate self-shielding by using on the order of a thousand or so groups; hopefully these results demonstrate that this is not true. In this calculation for the continuous energy cross section calculation over 227,000 energy points were needed to represent the U238 cross sections, and a different set of over 70,000 to represent the U235, plus a smaller number of energy points to represent the other constituents. Using significantly fewer energy points makes it impossible to accurately reproduce the above continuous energy results.

Neutron Flux
Continuous vs. Multi-Group

Flux 397.96 Continuous
Flux 283.35 Multi-Group
Maximum Difference
    -90.06 %
at X= 6.763-6

The below figures illustrate the energy dependent neutron production and absorption. The production has more or less the same energy shape as the flux, but the absorption shows the enormous difference across the resonance energy range, with the multi-group method absorbing far too many neutrons.
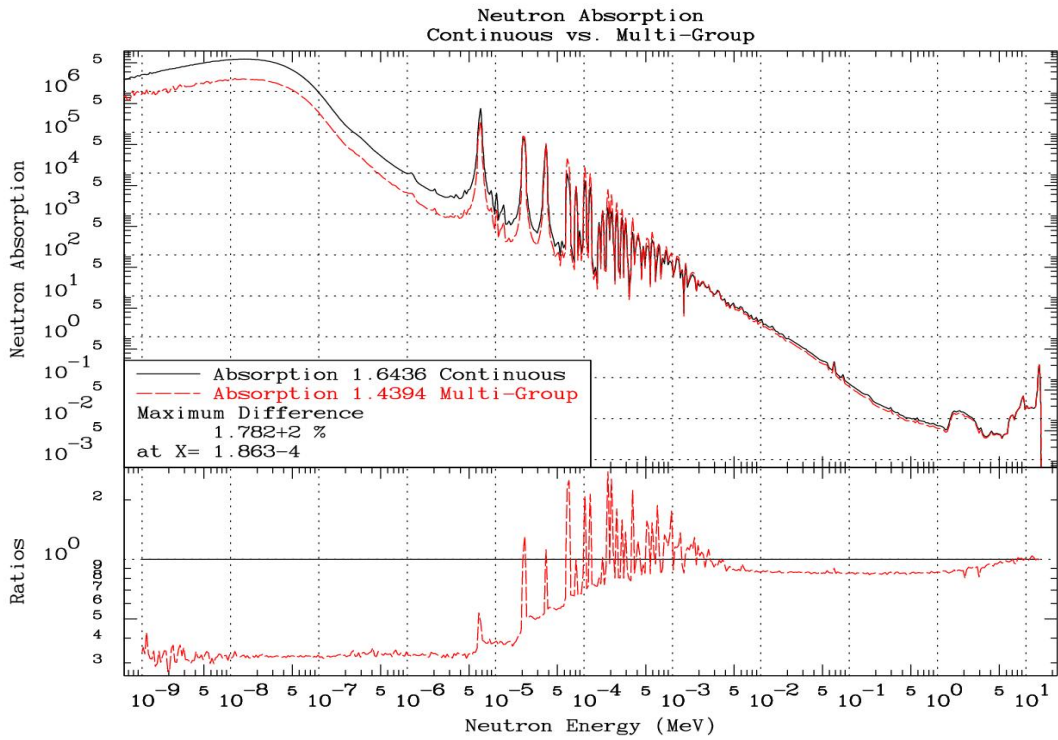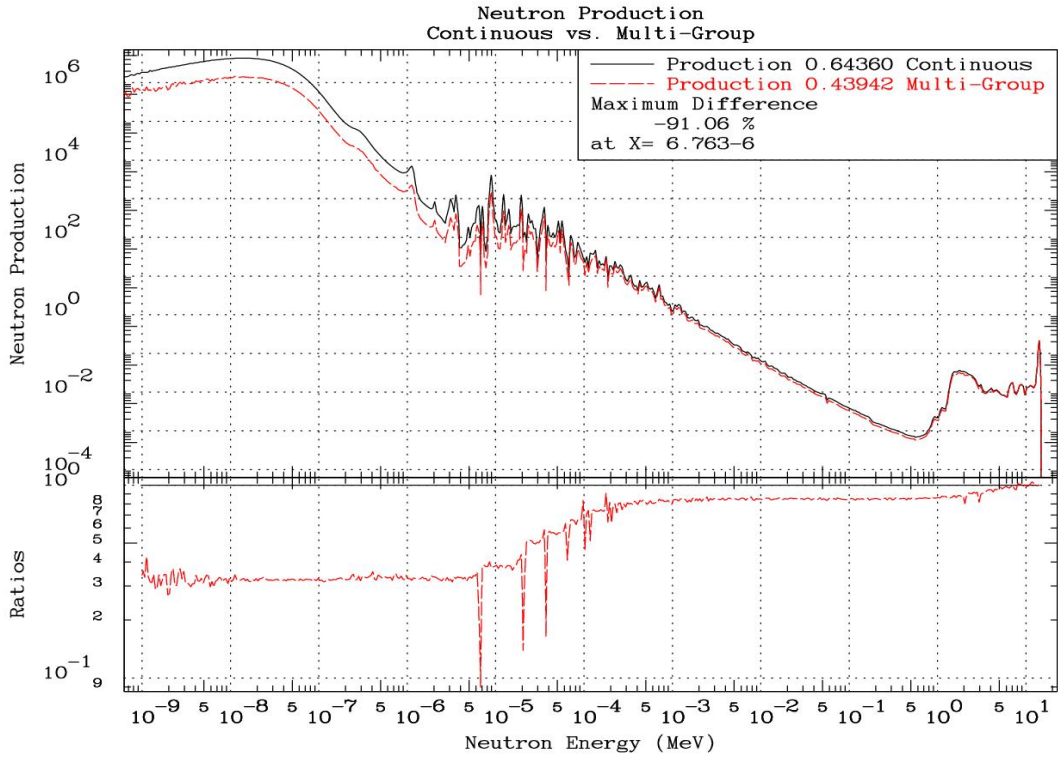
Neutron Production
Continuous vs. Multi-Group

Neutron Absorption
Continuous vs. Multi-Group

Below we show the ratio of the neutron production to the flux and neutron absorption to the flux; these are essentially the spatially average energy dependent cross sections. The fission cross sections differ only in a few strong fission resonances, but the absorption cross sections show large differences across the entire resonance region; here we see differences of up to a factor of eight (8), 800%. It is this enormous difference that prevents multi-group neutrons from reaching lower energies, resulting in the much lower neutron flux at low energy.
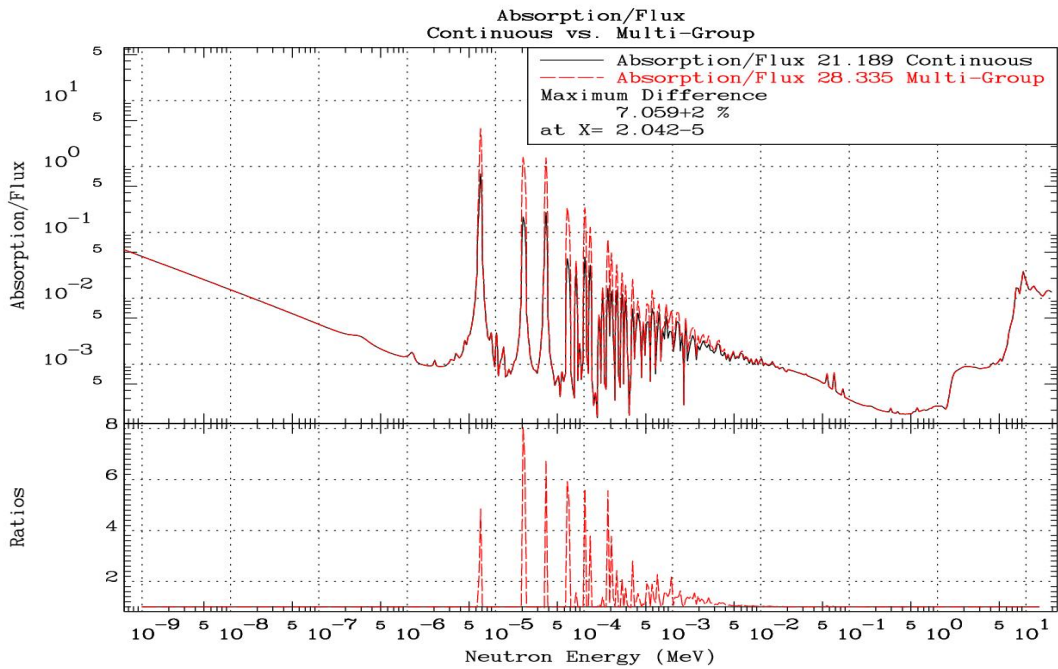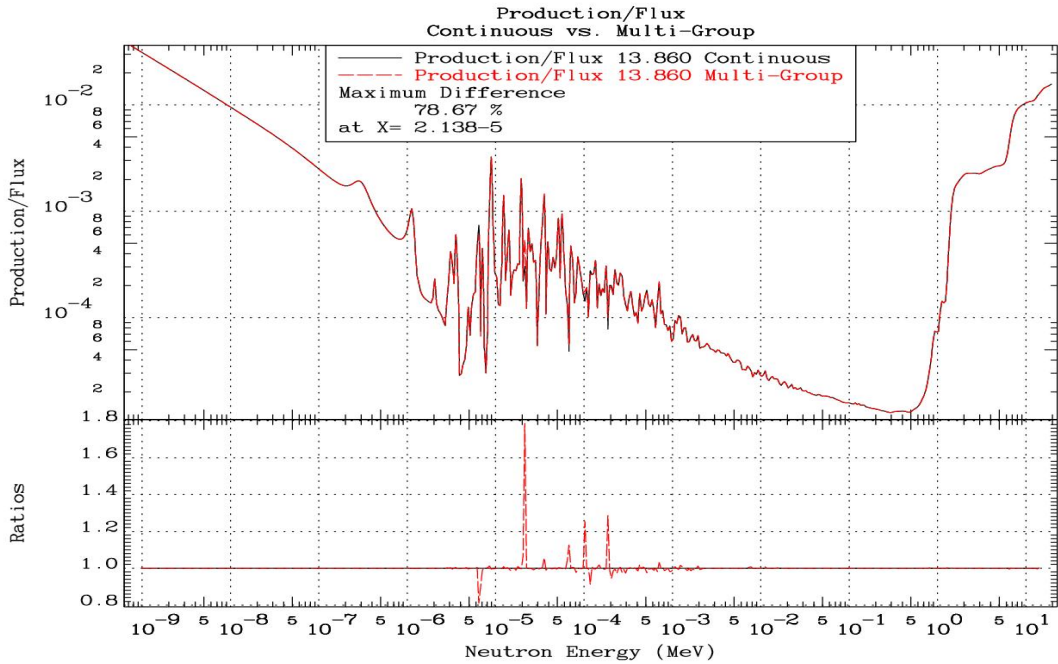
The next point to note is the excellent agreement between the continuous energy and multiband results; here in all cases the results agree to within 0.1%. Normally this would indicate that we could save computer time by using the multiband method. However, in this case where we will be taking differences between results, it is important that we use continuous energy calculations to guarantee that we achieve the 0.01% accuracy shown in the preceding section.

Based on these results ALL of the following results used continuous energy cross sections.

Quantitatively how important is self-shielding in our system?

To determine this we performed calculations for a variety of spatial models, including:
a) full detailed (4 zone) TRISO, randomly positioned within each pebble,
b) full detailed TRISO, regularly positioned within each pebble,
c) homogenized (1 zone) TRISO within a pebble as separate TRISO and pebble zones; and
d) completely homogenized TRISO and pebble as one combined spatial zone.

Lastly we add results obtained using self-shielded continuous energy cross section in case d) homogenized Pebble/TRISO case. The following table shows the effect of homogenization and how these can be corrected for using self-shielded continuous energy cross sections.

To illustrate the difference between our system and a critical reactor, below we present results starting with depleted uranium in the TRISO, for a "standard" fundamental mode reactor type cell calculation and our system cell calculations, driven by an external source, using both sources calculations and a non-fundamental mode criticality calculation. What is important to note here is,

1) The enormous difference between a "standard" and cell calculation for our system; hopefully this demonstrates why our system cannot be treated in the same manner as a critical reactor; here our system is far from critical.
2) Both calculations (source and non-fundamental mode criticality) give the same answer, i.e. mathematically the two calculations are identical.
3) Although for the standard criticality and cell calculations for our system, the percent differences in K-eff may differ, when we look at the detailed energy dependent spectra we find that the difference are strictly in the resonance region, and are actually very similar in terms of changes in resonant absorption and production.
4) Comparison of the two source calculations shows that **as expected** the homogeneous system is more absorbent than the heterogeneous system. We can see this from the average number of elastic collisions by each neutron. In the heterogeneous system on average each neutron has about 138 elastic collisions, whereas in the homogeneous system it has about 132. This means that per collision the probability of absorption is significantly higher in the homogeneous system, e.g., 1/132 vs.1/138; 4.34% higher.
5) Homogenization based strictly on an atom mix without correcting for self-shielding **introduces a BIAS** that reduces K-eff for the normal criticality calculation of over 6% and in the non-fundamental mode or source problem calculation of 2.8%. It is important to understand **that this is a BIAS, not a statistical difference**; in the homogeneous system there is much more absorption, particularly in the U238 resonance region, and this introduces a BIAS in U238 absorption and therefore eventual Pu239 production, as well as a reduction in U235 fission, and therefore burn-up. In a many step time dependent

calculation including burn-up this BIAS can result in an accumulation of error in the quantities calculated.

6) **This BIAS can be easily eliminated by self-shielding the cross sections used in the homogenized system**. The below results demonstrate that by self-shielding the continuous energy cross sections we can calculate the correct scatter, absorption, fission, K-eff, and the entire energy dependent spectra. The results below show that the large BIAS introduced by homogenization can be reduced to less than 0.1% for all of the integral quantities mentioned here, and tabulated below; if we wanted to spend more time on these calculations even this tiny difference could be eliminated.

Bias due to Homogenizing
Normal Criticality – 100 settle cycles

	K-eff	% Regular
Full details/regular position……………….	0.2796	---------
Full details/random position………………	0.2792	-0.1431
Homogenized TRISO/regular position…..	0.2667	-4.6137
Homogenized Pebble/TRISO…………….	0.2628	-6.0086
Eliminate bias by self-shielding		
Homogenized Pebble/TRISO……………..	0.2798	0.0712

Criticality - No Settle and Source Problem (Results are Identical for these two cases)

	K-eff	% Regular
Full details/regular position……………….	0.4029	------------
Full details/random position………………	0.4020	-0.2234
Homogenized TRISO/regular position…..	0.3936	-2.3083
Homogenized Pebble/TRISO……………...	0.3916	-2.8047
Eliminate bias by self-shielding		
Homogenized Pebble/TRISO……….……..	0.4025	0.0993

Below we present more detailed results by each reaction. Since this sub-critical, non-fundamental mode criticality problem and equivalent source problem are time independent, detailed balance tells us that the number of neutrons removed from the system MUST be exactly equal to the neutron source plus all neutrons produced in the system. Per neutron source neutron this is exactly what we see here: Removal = 1 + Production.

Source – full details/regular position – results are per source neutron

```
C Number Reaction    Removal         Production      Events
-----------------------------------------------------------------
    10 Elastic        0.00000D+00     0.00000D+00     1.38501D+02
    11 (n,n')         0.00000D+00     0.00000D+00     1.03416D+00
    12 (n,2n)         3.49973D-02     6.99946D-02     3.49973D-02
    13 (n,3n)         8.79630D-03     2.63889D-02     8.79630D-03
    15 Fission        2.05238D-01     5.78379D-01     2.05238D-01
    20 (n,n'p)        0.00000D+00     0.00000D+00     6.81770D-03
    26 (n,n'a)        0.00000D+00     0.00000D+00     4.35690D-03
    27 (n,n'2a)       0.00000D+00     0.00000D+00     3.48350D-01
    40 (n,p)          4.44996D-02     0.00000D+00     4.44996D-02
    41 (n,d)          2.23290D-03     0.00000D+00     2.23290D-03
    45 (n,a)          1.63087D-01     0.00000D+00     1.63087D-01
    46 (n,g)          1.21591D+00     0.00000D+00     1.21591D+00
       Leakage        0.00000D+00     0.00000D+00
-----------------------------------------------------------------
       Totals         1.67476D+00     6.74762D-01     1.41569D+02
       K-eff                          4.02901D-01
-----------------------------------------------------------------
```

Source – homogenized pebble/TRISO – results are per source neutron

```
C Number Reaction    Removal         Production      Events
-----------------------------------------------------------------
    10 Elastic        0.00000D+00     0.00000D+00     1.32432D+02
    11 (n,n')         0.00000D+00     0.00000D+00     1.02500D+00
    12 (n,2n)         3.50156D-02     7.00312D-02     3.50156D-02
    13 (n,3n)         8.79680D-03     2.63904D-02     8.79680D-03
    15 Fission        1.92450D-01     5.47180D-01     1.92450D-01
    20 (n,n'p)        0.00000D+00     0.00000D+00     6.76670D-03
    26 (n,n'a)        0.00000D+00     0.00000D+00     4.33050D-03
    27 (n,n'2a)       0.00000D+00     0.00000D+00     3.48622D-01
    40 (n,p)          4.45914D-02     0.00000D+00     4.45914D-02
    41 (n,d)          2.19870D-03     0.00000D+00     2.19870D-03
    45 (n,a)          1.62859D-01     0.00000D+00     1.62859D-01
    46 (n,g)          1.19769D+00     0.00000D+00     1.19769D+00
       Leakage        0.00000D+00     0.00000D+00
-----------------------------------------------------------------
       Totals         1.64360D+00     6.43602D-01     1.35460D+02
       K-eff                          3.91581D-01
-----------------------------------------------------------------
```

Source – SHIELDED homogenized pebble/TRISO – results are per source neutron

```
C Number Reaction    Removal         Production      Events
-----------------------------------------------------------------
    10 Elastic        0.00000D+00     0.00000D+00     1.38517D+02
    11 (n,n')         0.00000D+00     0.00000D+00     1.03303D+00
    12 (n,2n)         3.49604D-02     6.99208D-02     3.49604D-02
    13 (n,3n)         8.81010D-03     2.64303D-02     8.81010D-03
    15 Fission        2.04911D-01     5.77305D-01     2.04911D-01
    20 (n,n'p)        0.00000D+00     0.00000D+00     6.79610D-03
    26 (n,n'a)        0.00000D+00     0.00000D+00     4.31820D-03
    27 (n,n'2a)       0.00000D+00     0.00000D+00     3.48302D-01
    40 (n,p)          4.45666D-02     0.00000D+00     4.45666D-02
    41 (n,d)          2.20080D-03     0.00000D+00     2.20080D-03
    45 (n,a)          1.63373D-01     0.00000D+00     1.63373D-01
    46 (n,g)          1.21483D+00     0.00000D+00     1.21483D+00
       Leakage        0.00000D+00     0.00000D+00
-----------------------------------------------------------------
       Totals         1.67365D+00     6.73656D-01     1.41583D+02
       K-eff                          4.02506D-01
-----------------------------------------------------------------
```

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Compared to the above results by reaction, below results are defined in even greater detail, by also defining event by reaction and isotope. Here we can see that the reduction in scatter in the homogeneous system is mostly due to a reduction in the scatter from carbon (ZA = 6000).

Source – full details/regular position – events per source neutron

C Number Reaction	92238	92235	8016	14028	6000
10 Elastic	6.94424D+00	1.70404D-02	2.30857D+00	6.14780D+00	1.23083D+02
11 (n,n')	3.92428D-01	8.06700D-04	1.10686D-02	1.72971D-01	4.56882D-01
12 (n,2n)	3.49424D-02	5.49000D-05	0.00000D+00	0.00000D+00	0.00000D+00
13 (n,3n)	8.79430D-03	2.00000D-06	0.00000D+00	0.00000D+00	0.00000D+00
15 Fission	6.83139D-02	1.36924D-01	0.00000D+00	0.00000D+00	0.00000D+00
20 (n,n'p)	0.00000D+00	0.00000D+00	2.63000D-05	6.79140D-03	0.00000D+00
26 (n,n'a)	0.00000D+00	0.00000D+00	2.70610D-03	1.65080D-03	0.00000D+00
27 (n,n'2a)	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00	3.48350D-01
40 (n,p)	0.00000D+00	0.00000D+00	1.07920D-03	4.34201D-02	3.00000D-07
41 (n,d)	0.00000D+00	0.00000D+00	3.77500D-04	1.85510D-03	3.00000D-07
45 (n,a)	0.00000D+00	0.00000D+00	6.39030D-03	2.61105D-02	1.30586D-01
46 (n,g)	1.10746D+00	2.85385D-02	1.61000D-05	6.53060D-02	1.45890D-02
Totals	8.55617D+00	1.83367D-01	2.33023D+00	6.46591D+00	1.24034D+02

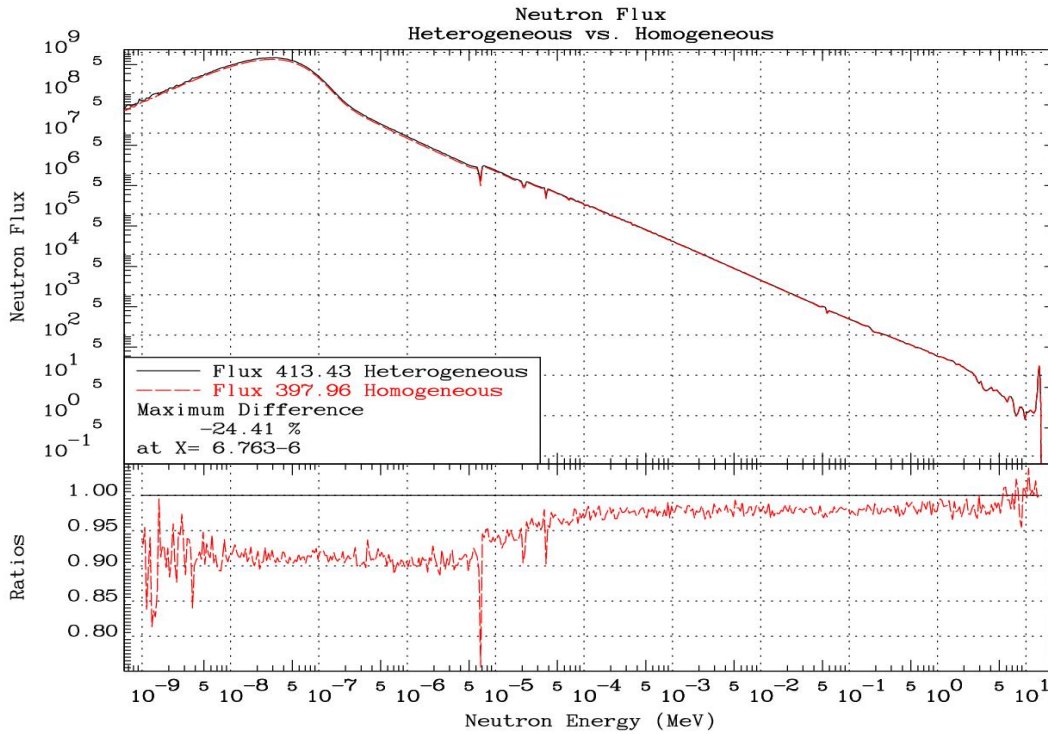## Source – homogenized pebble/TRISO – events per source neutron

C Number Reaction	92238	92235	8016	14028	6000
10 Elastic	6.73042D+00	1.62361D-02	2.20941D+00	5.91550D+00	1.17560D+02
11 (n,n')	3.85051D-01	7.87800D-04	1.10123D-02	1.71900D-01	4.56245D-01
12 (n,2n)	3.49633D-02	5.23000D-05	0.00000D+00	0.00000D+00	0.00000D+00
13 (n,3n)	8.79400D-03	2.80000D-06	0.00000D+00	0.00000D+00	0.00000D+00
15 Fission	6.78721D-02	1.24578D-01	0.00000D+00	0.00000D+00	0.00000D+00
20 (n,n'p)	0.00000D+00	0.00000D+00	2.93000D-05	6.73740D-03	0.00000D+00
26 (n,n'a)	0.00000D+00	0.00000D+00	2.71430D-03	1.61620D-03	0.00000D+00
27 (n,n'2a)	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00	3.48622D-01
40 (n,p)	0.00000D+00	0.00000D+00	1.09530D-03	4.34959D-02	2.00000D-07
41 (n,d)	0.00000D+00	0.00000D+00	3.57400D-04	1.84070D-03	6.00000D-07
45 (n,a)	0.00000D+00	0.00000D+00	6.39350D-03	2.60950D-02	1.30371D-01
46 (n,g)	1.09913D+00	2.61155D-02	1.44000D-05	5.92489D-02	1.31776D-02
Totals	8.32623D+00	1.67773D-01	2.23103D+00	6.22644D+00	1.18509D+02

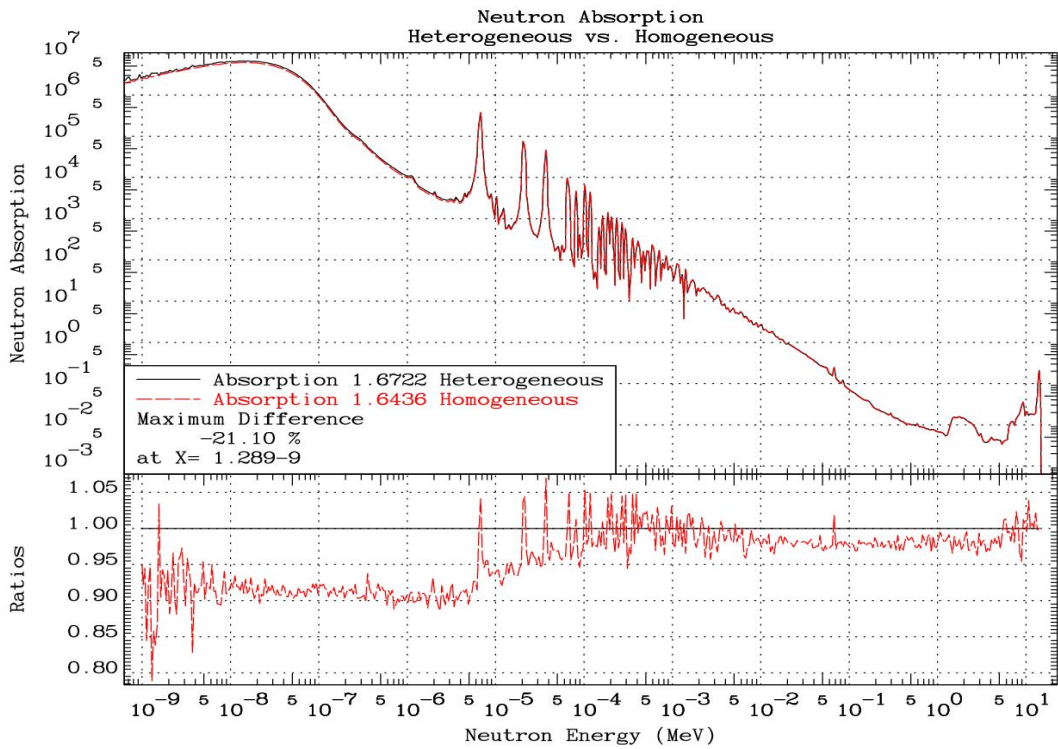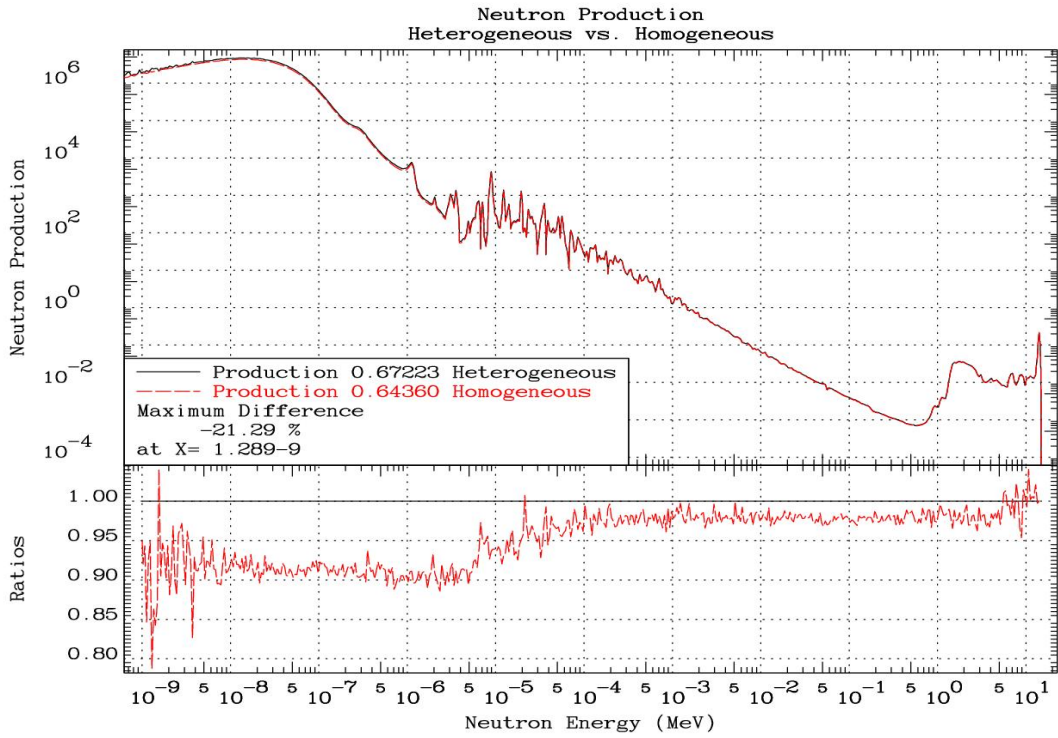## Source – SHIELDED homogenized pebble/TRISO – events per source neutron

C Number Reaction	92238	92235	8016	14028	6000
10 Elastic	6.98645D+00	1.70170D-02	2.30915D+00	6.14803D+00	1.23056D+02
11 (n,n')	3.91567D-01	8.05000D-04	1.10710D-02	1.73075D-01	4.56507D-01
12 (n,2n)	3.49035D-02	5.69000D-05	0.00000D+00	0.00000D+00	0.00000D+00
13 (n,3n)	8.80840D-03	1.70000D-06	0.00000D+00	0.00000D+00	0.00000D+00
15 Fission	6.80874D-02	1.36823D-01	0.00000D+00	0.00000D+00	0.00000D+00
20 (n,n'p)	0.00000D+00	0.00000D+00	2.53000D-05	6.77080D-03	0.00000D+00
26 (n,n'a)	0.00000D+00	0.00000D+00	2.69920D-03	1.61900D-03	0.00000D+00
27 (n,n'2a)	0.00000D+00	0.00000D+00	0.00000D+00	0.00000D+00	3.48302D-01
40 (n,p)	0.00000D+00	0.00000D+00	1.08940D-03	4.34770D-02	2.00000D-07
41 (n,d)	0.00000D+00	0.00000D+00	3.74100D-04	1.82590D-03	8.00000D-07
45 (n,a)	0.00000D+00	0.00000D+00	6.40510D-03	2.61931D-02	1.30774D-01
46 (n,g)	1.10637D+00	2.86239D-02	1.43000D-05	6.53094D-02	1.45173D-02
Totals	8.59618D+00	1.83328D-01	2.33082D+00	6.46630D+00	1.24006D+02

Energy Dependent Neutron Flux, Production and Absorption

In the below figure we can see the effect of the increased absorption in the homogeneous system, compared to the heterogeneous system, where the energy dependent flux is significantly lower; at high energy it is a few percent lower, but through the resonance energy region (keV to eV) it falls to about 10% lower. The following two figures show the effect on the neutron production and absorption, respectively. The production is quite similar in shape to the flux, but the absorption shows the increase in absorption through the resonance energy region; it is of course this increased absorption that results in the 10% lower flux at energies below the resonance energy range, i.e., fewer neutron survive to reach lower energies.


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Neutron Production
Heterogeneous vs. Homogeneous

Production 0.67223 Heterogeneous
Production 0.64360 Homogeneous
Maximum Difference
    −21.29 %
at X= 1.289−9

Neutron Absorption
Heterogeneous vs. Homogeneous

Absorption 1.6722 Heterogeneous
Absorption 1.6436 Homogeneous
Maximum Difference
    −21.10 %
at X= 1.289−9

Energy Dependent Production and Absorption Cross Sections

Below we show the ratio of the neutron production to the flux and neutron absorption to the flux; these are essentially the spatially average energy dependent cross sections. Here we can see that the homogeneous cross sections are higher through the resonance energy range (keV to eV). We can see some effect on the production through a few very strong fission resonances. But we can see much stronger effects on the absorption throughout the resonance energy range. The net effect, relative to the heterogeneous system, is the lower K-eff that we see for the homogeneous system.
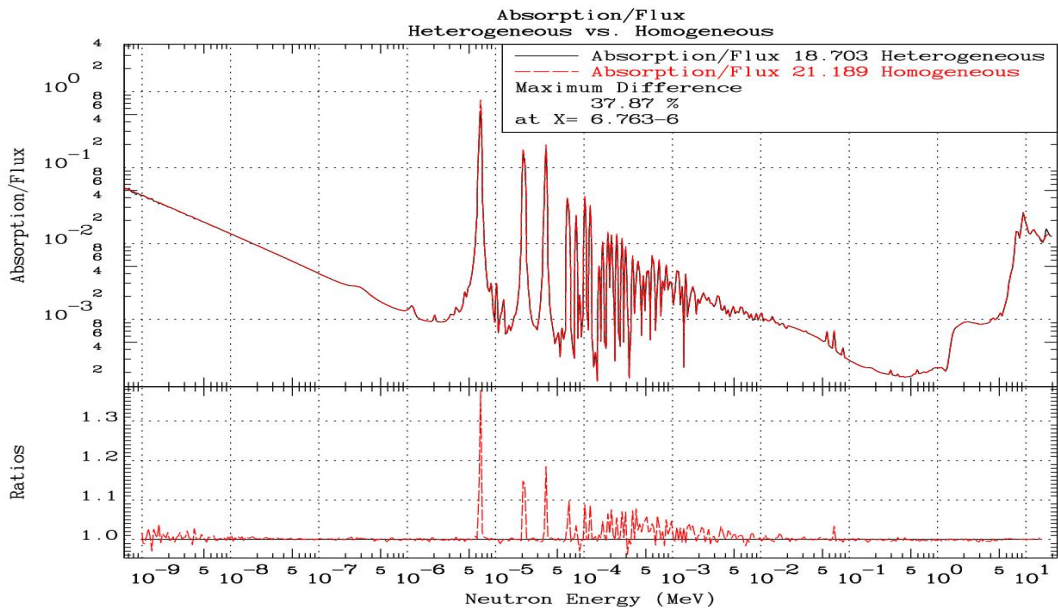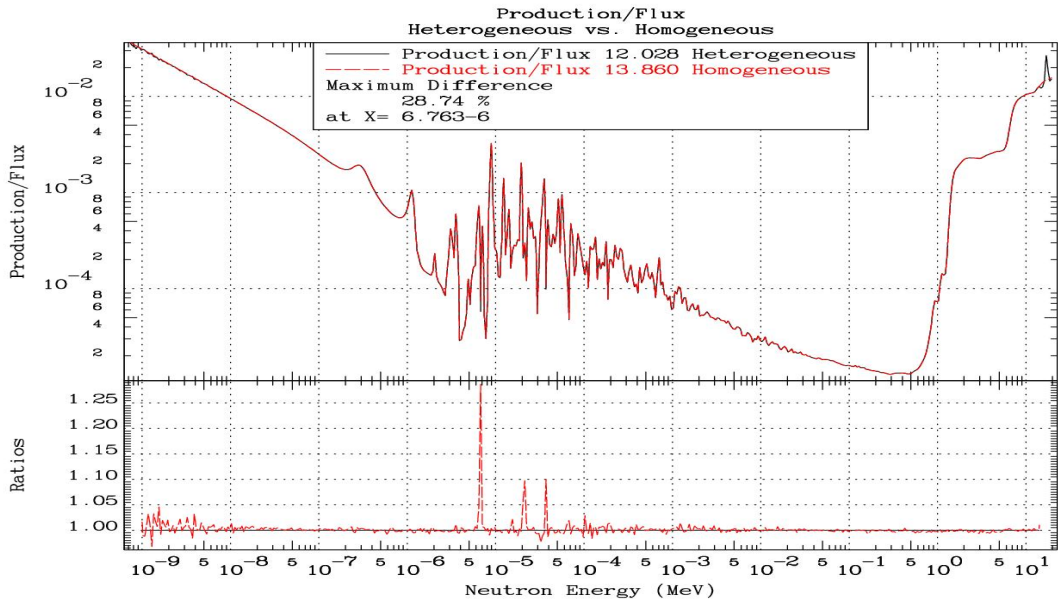
Summary of Difference between Heterogeneous and Homogeneous Systems

From the ratio of the flux in the REAL heterogeneous systems and our APPROXIMATE homogeneous system both using the same, unshielded cross sections, we can see several important effects (see the below figure). Compared to the REAL system the APPROXIMATE system shows the following effects,

1) Increased absorption in the resonance region: eV to keV energy range. This will overestimate capture in materials such as U238 and Pu240, which in turn will overestimate production of materials such as Pu239, results from capture in U238.

2) This increased absorption in the resonance region reduces the probability of neutrons reaching lower energies: thermal to eV. This reduces the flux at lower energy leading to an underestimate of low energy reactions, such as U235 and Pu239 fission, as well of tritium production from Li6(n,t), which is important for our system.
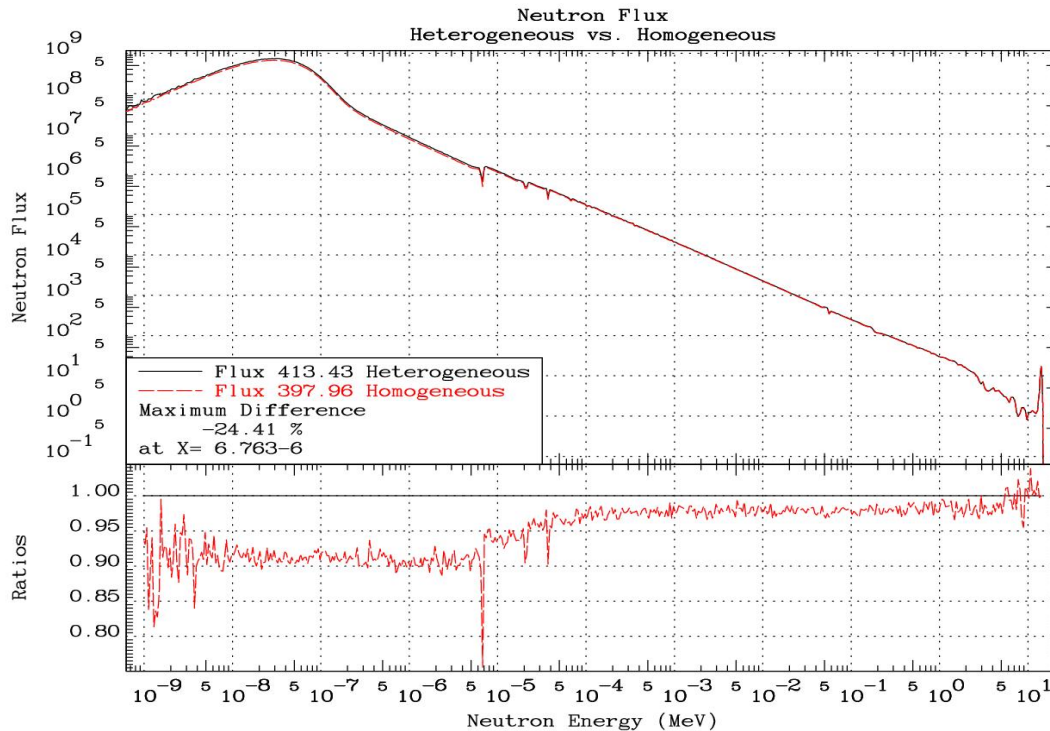
Our proposed method of self-shielding cross sections in the resonance region corrects for both of these problems, i.e., by correcting the absorption in the resonance region we also correct the probability of neutrons reaching lower energy, thereby correcting the low energy reaction rates.

Are these differences important?

Consider the results of the standard criticality problem. Full details/random position are the most accurate, as far as being based on the most accurate model, but the 0.2% difference between regular and random position is here judges to be negligible. However, the 4% to 6% differences due to homogenization are large and cannot be ignored.

Are 6% differences important? The point to understand is that this is **not a statistical uncertainty** in the results that might disappear over a series of time dependent steps in a calculation or identical calculations using different random number sequences. This is **a bias**, where the homogenized results for K-eff always underestimate the full detail results; this is due primarily to the homogenized model overestimating absorption in the U238, but also due to deceasing low energy fission in the U235. Our system calculations involve time dependent tracking of the system over many years, through many time steps. During these time steps any bias can compound, time step by time step, and the REAL material inventory in the heterogeneous system will be progressively different from the APPROXIMATE material inventory we calculate in a homogeneous system that is not corrected for self-shielding. **So if we decide to homogenize we must somehow correct for this self-shielding effect, which is exactly what the method proposed here is designed to do.**

How can our very accurate homogeneous calculation be so far off?

It is important to understand that if we model our homogeneous system using our standard, non-shielded cross sections, we will obtain very accurate results for our homogeneous system. BUT, we are not trying to accurately model the synthetic homogeneous system – **we are trying to model our real heterogeneous system**, and in our real system the reaction rates will be significantly different.

So let us repeat this: **the reaction rates in the two systems differ by about 6%**. If you believe the results from the unshielded homogeneous system for each time step you **will overestimate the reaction rates by 6%**, and compared to using the true reaction rates from the heterogeneous system, this difference can compound over time.

In other words: if you want to model the heterogeneous reaction rates, but only do a simplified homogeneous calculation **you must use the appropriate self-shielded cross section for the homogeneous calculation.**

An Overview of Self-Shielding

Self-shielding theory predicts that the flux will vary inversely to the cross section, and models such as narrow resonance (NR) Bonderenko self-shielding predicts that the flux can be written as the product of,
1) a smoothly varying energy spectrum $S(E)$ (Maxwellian, 1/E, fission, fusion, at progressively higher energy), and
2) a cross section dependent term $W(\Sigma_T)$,

In which case the group averaged cross section is defined as,

$$\Phi_0(E) = S(E)W(\Sigma_T) = S(E)/\Sigma_T = S(E)/[\Sigma_T(E) + \Sigma_0]$$

Where $\Sigma_T(E)$ is the total cross section of one material and Σ_0 is the total cross section of all other materials in a mixture. It is easy to prove that with this definition the self-shielding group averaged total cross section is an increasing function of Σ_0, being minimum for $\Sigma_0 = 0$ and increasing to its unshielded value as Σ_0 approaches infinity. Starting with our general definition of the self-shielded cross section,

$$< \Sigma_T >_k \;=\; \int_{Ek}^{Ek+1} dE \Sigma_T(E) S(E) / [\Sigma_T(E) + \Sigma_0] / \int_{Ek}^{Ek+1} dES(E) / [\Sigma_T(E) + \Sigma_0]$$

We have the limiting values,

$$\Sigma_0 = 0 : \; < \Sigma_T >_k \text{ Minimum} \qquad\qquad \Sigma_0 \to \infty : \; < \Sigma_T >_k \text{ Maximum}$$

$$< \Sigma_T >_k \;=\; \int_{Ek}^{Ek+1} dES(E) / \int_{Ek}^{Ek+1} dES(E) / \Sigma_T(E) \qquad\qquad \int_{Ek}^{Ek+1} dE\Sigma_T(E)S(E) / \int_{Ek}^{Ek+1} dES(E)$$

This helps to explain why our homogenizing geometry results in higher U238 absorption. In the homogenized geometry the equivalent Σ_0 in the entire cell is considerably higher than the U238 containing inner zone in the heterogeneous geometry; hence the higher Σ_0 in the homogenized geometry means a larger U238 absorption cross section.

An important point to understand is that self-shielding is caused by the variation (the range), of the magnitude of the cross section across each group. Once one switches from continuous energy cross sections to multi-group constants, the cross section is defined, or modeled, to be constant across the entire group, so that the self-shielding model is locked in, as far as how you define the self-shielded multi-group cross section, and there can no longer be any variation from this value. In the method that we propose to use this restriction is avoided.

Spatial Self-Shielding

Usually the focus of a discussion of self-shielding is on the energy dependent effect of self-shielding, and it is erroneously thought to be a multi-group effect that can be avoid by using continuous energy cross sections. This is true for detailed heterogeneous geometry, but not when we homogenize geometry. Rather than being an energy dependent effect, **self-shielding should be thought of as an effect due to averaging**, whether the averaging is over energy and/or spatial regions.

Above we discussed self-shielding due to energy averaging, i.e., the multi-group method. Here we also illustrate the effect of spatial self-shielding in heterogeneous geometry. We will consider a typical fuel region surrounded by a moderator. In this case fission will create fast neutrons in the fuel region; these can leak into the moderator and slow down to thermal energies, where they can create the next generation of fission neutrons.

In slowing down the neutrons must transit across the resonance region of the fuel, where they may attempt to penetrate from the moderator back into the fuel. If we assume little or no neutron slowing down in the fuel, neutrons incident from the moderator into the fuel will be exponentially attenuated; this is the so called NRIA model = narrow resonance, infinite absorber model (here "infinite" means infinite weight, so that there is no neutron slowing down). In this case the spatially dependent flux and total reaction rate within the fuel are, respectively,

$$\Phi(E,R) \;=\; \Phi(E,0) * Exp[-\Sigma_T(E) * R]$$

Reaction Rate(E,R) $= \Sigma_t(E) * \Phi(E,0) * Exp[-\Sigma_T(E) * R]$

where,
R $\quad$ = the distance into the fuel from the location of the moderator to fuel interface
$\Phi(E,0)$ $\quad$ = the neutron flux at the moderator to fuel interface
$\Phi(E,R)$ $\quad$ = neutron flux at energy E, and location R into the fuel
$\Sigma_T(E)$ $\quad$ = neutron total cross section at energy E within the fuel

What this predicts is that fuel will have a non-uniform burn-up, with the maximum flux and reaction rates near the surface of the fuel (maximum burn-up), and much lower values deeper into the fuel. In other words the pin will burn-up like the layers of an onion, one layer after the other, from surface toward the interior.

What we are interested in is these quantities integrated over the fuel region,

$$< \Phi(E > \quad = \quad \int_0^{R\max} \Phi(E,0) * Exp[-\Sigma_T(E) * R]dR$$

$$= \quad \Phi(E,0) * \{1 - Exp[-\Sigma_T(E) * R\max]\}/\Sigma_T(E)$$

$$<RR(E)> \quad = \quad \int_0^{R\max} \Phi(E,0) * Exp[-\Sigma_T(E) * R]\Sigma_T(E)dR$$

$$= \quad \Phi(E,0) * \{1 - Exp[-\Sigma_T(E) * R\max]\}$$

If we consider that the fuel region to by optically thick, i.e., $\Sigma_T(E) * R\max$ is large, these reduces to very simple forms,

$$< \Phi(E > \quad = \quad \Phi(E,0)/\Sigma_T(E)$$
$$<RR(E)> \quad = \quad \Phi(E,0)$$

Again, we see the familiar self-shielding of the flux as inversely proportional to $\Sigma_T(E)$. The reaction rate has a very simply interpretation: everything that is incident, $\Phi(E,R0)$ reacts. In a normal cell calculation this is taken one step further by integrating these over the energy range of each group, and using the ratio of reaction rate to flux to define the spatially averaged cross section.

$$< \Sigma_t >_G = < \Phi(E,0) >_G / < \Phi(E,0)/\Sigma_T(E) >_G$$

This is exactly the same as the self-shielding model we discussed above when we consider energy averaging? Here we see exactly the same effect for spatial averaging.

This is an admittedly very simplified model of the transport of neutrons from the moderator into the fuel, but it is fairly accurate near strongly absorbing resonances, and serves to illustrate that spatially heterogeneous effects result in the same self-shielding effect that we saw above when we considered only the energy dependent effect. The actual transport is somewhat more complicated between resonances where absorption vs. scatter may not be as dominant. The net effect is that in order to more

accurately model our system rather than assuming this very simple model we perform cell calculations in order to know the actual reaction rates. But hopefully this simplified description helps to explain why there is spatial self-shielding, and that the actual spatially "averaged" cross sections seen by the neutrons differ from our unshielded cross sections. **Failure to appreciate this effect and properly accounting for it when homogenizing geometry can lead to very inaccurate and misleading results**.

Proposed Method to Correct for Self-Shielding when Homogenizing

Here we present a model that we can use to homogenize our geometry and yet reproduce the same reaction rates in the homogenized geometry that we calculate in our detailed geometry. This is a problem that reactor designers have dealt with for over 50 years, so this is not at all a completely new problem. Basically what has always been done is to modify multigroup homogenized cross sections to obtain the same reaction rates in the detailed and homogenized system. For any reaction the multigroup reaction rate is,

$$\text{Reaction rate} = \int_{Ek}^{Ek+1} dE\,\sigma_{jm}(E)\,n_m\,\Phi_0(E)$$

where,

(E_k,E_{k+1}) - the energy range of the group

$\sigma_{jm}(E)$ - cross section for reaction j in material m (j = total, elastic, capture, etc.)

n_m - the number density of the atoms of material m (m = U235, U238, etc.)

$\Phi_0(E)$ - neutron scalar flux

In this equation we do not want to modify the number density of atoms and we have no control over the scalar flux, so the standard method that has been used for many years is to modify the homogenized multigroup cross section to reproduce the reaction rate in the detailed system,

In macroscopic form,

$$<\Sigma_{jm}>_k = \int_{Ek}^{Ek+1} dE\,\sigma_{jm}(E)\,n_m\,\Phi_0(E)\, / \int_{Ek}^{Ek+1} dE\,\Phi_0(E)$$

Or, microscopic form, which differs only by the atom density,

$$<\sigma_{jm}>_k = \int_{Ek}^{Ek+1} dE\,\sigma_{jm}(E)\,\Phi_0(E)\, / \int_{Ek}^{Ek+1} dE\,\Phi_0(E)$$

What is often overlooked in this procedure is that self-shielding tells us that if we **explicitly** modify cross section we may end up **implicitly** modifying the flux, i.e., the product of cross section time flux tends to remain constant to produce the same reaction rate. To accurately account for this effect may require a few iterations.

The traditional methods of modifying cross sections to produce the same reaction rates in the heterogeneous and homogeneous systems uses multi-group methods; so all we need modify are the multi-group cross sections. For our system calculations we perform Monte Carlo calculations using continuous energy cross sections, using MCNP [2] and TART [3]; we would like to continue using the same methods, even after correcting for homogenization and self-shielding. In order to do this we propose to modify the continuous energy cross sections, rather than multi-group constants. Logically the multi-group or continuous energy approaches are equivalent, but as actually implemented the continuous energy approach is more appropriate for use with our system, because of the large spatial gradients that we expect; these are difficult to model with multi-group cross sections.

The above spatially averaged cross sections defined as the ratio of production to flux and absorption to flux are based on energy binned results, using the TART 616 energy group structure, of 50 groups per energy decade. In the normal multi-group approach we would use the cross section in heterogeneous and homogeneous system to re-normalize the 616 group constants to use in the homogeneous system. For use with our system we propose to logically do the same thing, but instead of re-normalizing only the 616 group constants, we will re-normalize the energy dependent cross sections within each of the 616 groups, to accomplish the same end result on a continuous basis. Again, remember what we said above: self-shielding theory predicts that any **explicit** change in the cross section will result in an **implicit** change in the flux, so this may require a few iterations.

What has to be done with MCNP and TART to use this model?

Historically the need to perform cell calculations to account for self-shielding has required the development of fairly large and complicated computer systems; fortunately the method proposed here is much easier to implement and use.

To actually use this model is very simple; basically all we need do is modify the nuclear data files used for the homogeneous calculations, which does not involve very much programming or computer time. We first use TART to perform heterogeneous and homogeneous cell calculations using our standard nuclear data. We can use the TART output to define the cell averaged 616 group flux and reactions for the heterogeneous and homogeneous cells. Using the ratio of reactions to flux for each of the two systems we define an equivalent cell averaged 616 group cross sections for each reaction. We then use the ratio of cross sections in homogeneous and heterogeneous to define how to modify (self-shield) the cross sections to produce the same reaction rates in the homogeneous system that we have in the heterogeneous system.

Up to this point this sounds like a standard multi-group cell calculation. Where this method differs is that rather than only changing the 616 multi-group averaged cross sections we change the actual energy dependent cross sections, energy point by energy point, within each group to produce the group average change that we need. Then we need merely replace the original data in the MCNP and TART nuclear data files by these modified self-shielded energy dependent cross sections, e.g., for MCNP using the character formatted nuclear data files, we merely replace each original data point by one with the self-shielded cross section value, and use the modified data file for our homogeneous calculations. No additional transport or other complicated codes are required and no new nuclear data file formats are required; we basically just piggy-back on our existing code systems using a minimum of effort.
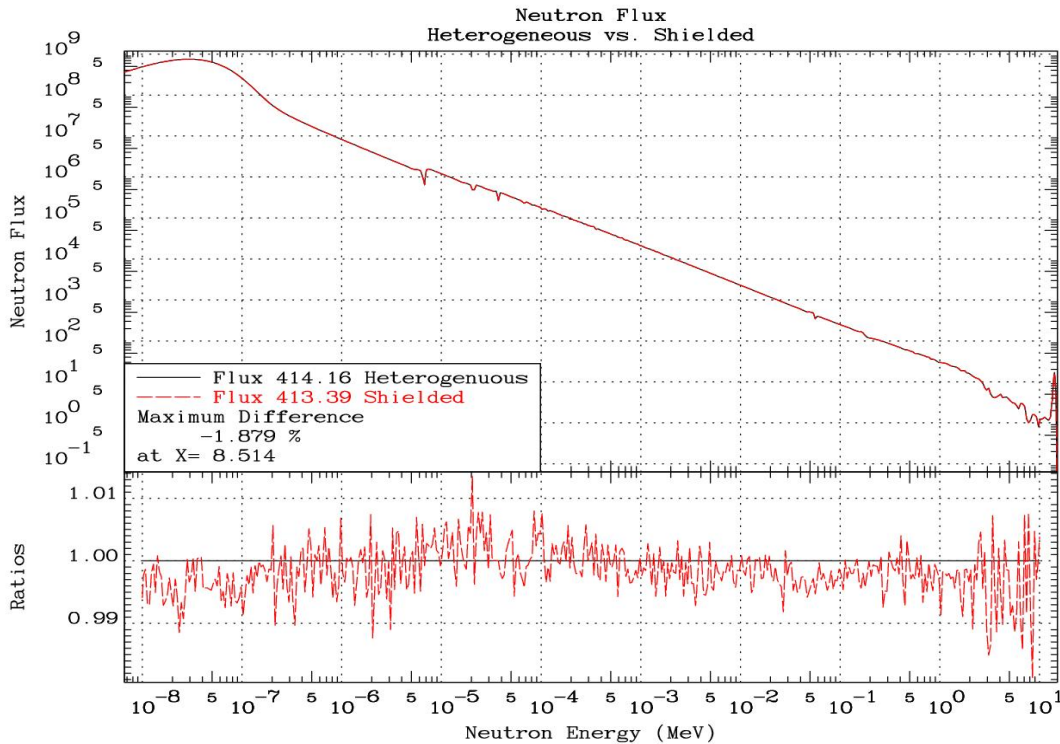
Lastly we have re-run the homogeneous cell calculation using these self-shielded cross sections. As mentioned above, this may take a few iterations, because any change in the cross section will tend to also change the flux (an effect often overlooked in cell calculations). Fortunately, this is a very rapidly converging iteration where all of our tests indicate that the differences are reduced by an order of magnitude or more by each iteration, so that if we consider the starting difference to be 100%, successive iterations reduce this to 10%, 1%, 0.1%, or for the 6% differences that we calculated in our example problem this would be reduced to 0.6%, 0.06%, etc. Remembering that this is an approximate method usually two (2) iterations are all that are necessary to eliminate all significant differences. TART is a very fast running code and the cell calculations we run using TART are so much simpler and faster than the time dependent whole system calculations we run using MCNP. So that there is no problem or delay when we run a series of TART cell calculations for each MCNP time step, to prepare self-shielded cross sections for use by MCNP during its next time step.
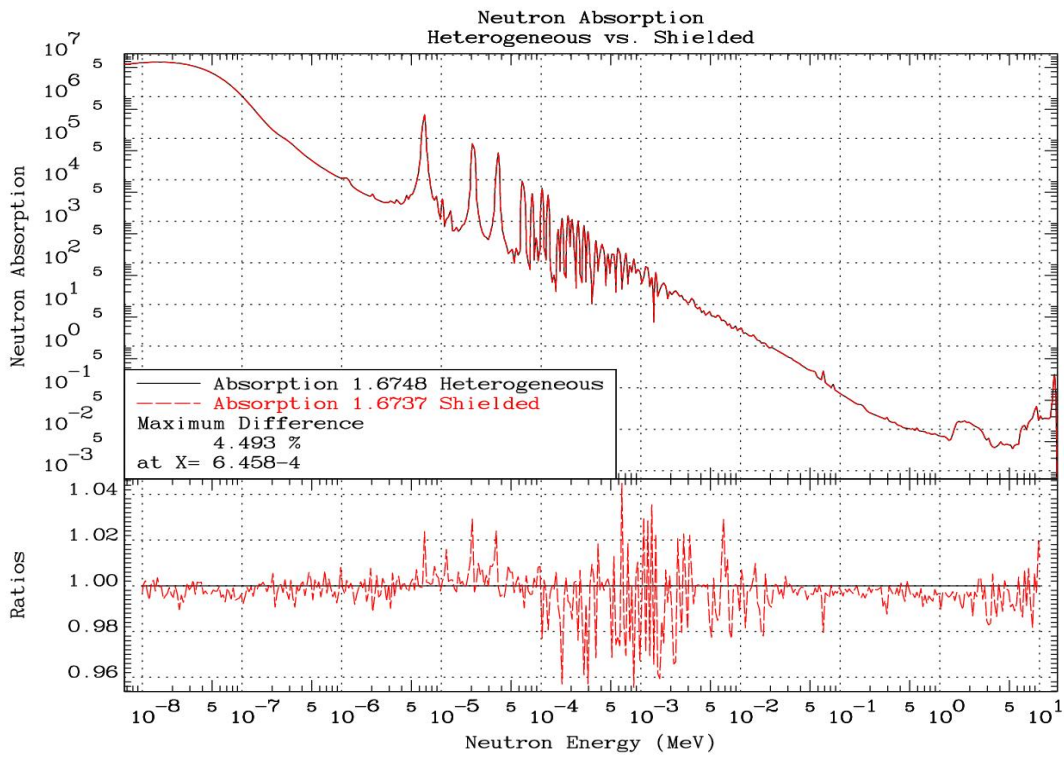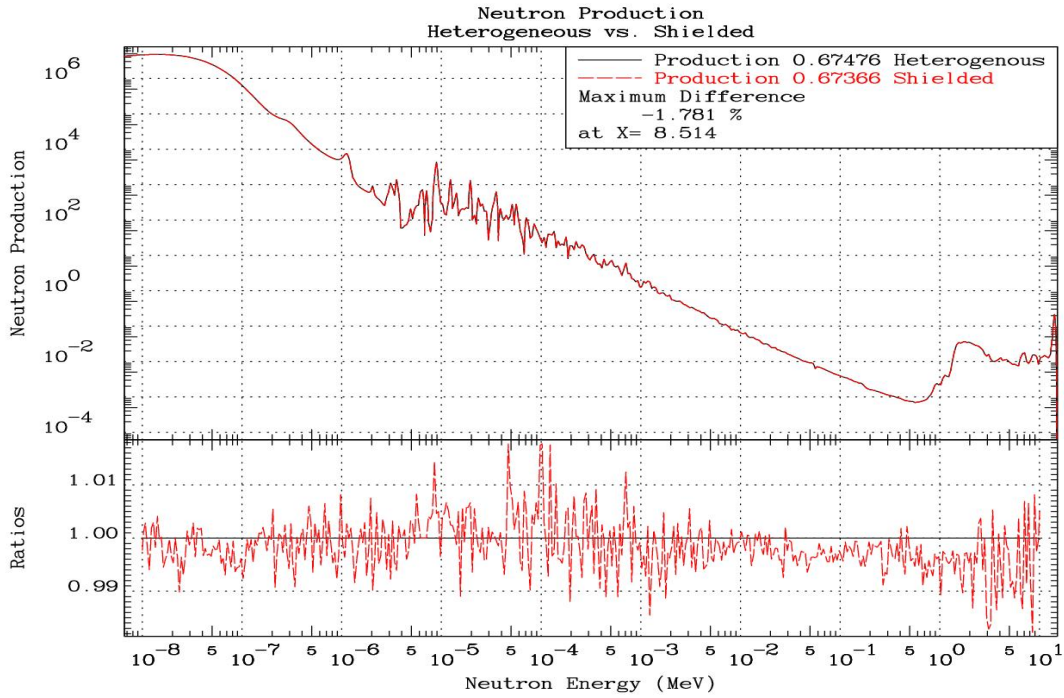
Proof of the Pudding: Results

Below we show energy dependent spectra for flux, production and absorption, comparing the detailed heterogeneous and shielded homogeneous cases. In the above comparison of heterogeneous and unshielded homogeneous cases we saw the BIAS introduced, where the homogeneous case had considerable more absorption, causing the flux through the uranium resonance region to decrease to only about 90% of the flux at lower energies for the heterogeneous case.

The below results show that self-shielding the continuous energy cross sections used for the homogenized case completely eliminates the **BIAS**; for flux, production and absorption we still see small differences, but these are now **all statistical**. For example, note the agreement between the integrals of the flux show on each plot; compare these to the above integrals without self-shielding.

Heterogeneous:	414.16	
Homogeneous:	413.39	
Difference:	0.77	$< 0.2\%$ of 414.16

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Neutron Production
Heterogeneous vs. Shielded

Production 0.67476 Heterogenous
Production 0.67366 Shielded
Maximum Difference
-1.781 %
at X= 8.514

Neutron Absorption
Heterogeneous vs. Shielded

Absorption 1.6748 Heterogeneous
Absorption 1.6737 Shielded
Maximum Difference
4.493 %
at X= 6.458-4

What's Next?

One might think that after successfully using the method proposed here to reduce the geometry from billions of spatial zones to millions, by homogenizing the TRISO in each Pebble, it would be only natural and straightforward to next homogenize the Pebble with the surrounding material, to reduce the number of spatial zones from millions to just a handful. Unfortunately, this is not as easy a task as it sounds. In nuclear reactors where we use cell calculations to homogenize portions of the geometry we generally have a highly absorbing fuel surrounded by a lightly absorbing moderator/coolant. In this case cell calculations can be quite accurate and usually can account for percent like differences in reactions that can be corrected for by self-shielding the cross sections to be used in the homogenized geometry. The same is true when we homogenize the highly absorbing TRISO containing fuel into the surrounding material inside each Pebble, which is basically carbon, a weakly absorbing material. Here we found differences of about 6% in the reaction rates, which we can easily account for by self-shielding the cross sections.

Unfortunately, this is not the situation with our system's pebbles and the material surrounding them. Surrounding the Pebbles is FLiBe, a fairly strong neutron absorber. If we try homogenizing the Pebbles and FLiBe rather than small differences in reaction rates we find very large differences. In the case of homogenizing the TRISO within each Pebble we found a difference of about 2% in K-eff, with the homogenized system less reactive mostly due to absorption in the U238 resonance region. In contrast if we try homogenizing the Pebbles into the FLiBe by running cell calculations we find that K-eff can decrease by an order of magnitude, resulting in very little multiplication, so little multiplication that we cannot establish an accurate estimate of the slowing down spectrum. The end result is that the results based on criticality and source calculations are so different that we obviously are not accurately calculating a representative spectrum that we could use for self-shielding. So **that the bottom line is that to accurately model our system we should maintain the separation of Pebbles and FLiBe, which is still doable on today's computers.**

Conclusions

We have presented a method that allows us to simplify our geometric models by homogenizing portions of our geometry, while still simulating the **same reaction rates** in our **homogenized system** as we calculate in our detailed **heterogeneous system**. This model is designed specifically for use with our system, which is a sub-critical system driven by a high energy external neutron source. This sub-critical system differs significantly from critical systems, so that we cannot use the standard multi-group methods normally used for nuclear reactors. We defined our proposed method in detail and then demonstrated that it can actually be used to correctly model **reaction rates** in our **homogenized system** that reproduce the reaction rates we calculate in our detailed **heterogeneous system**.
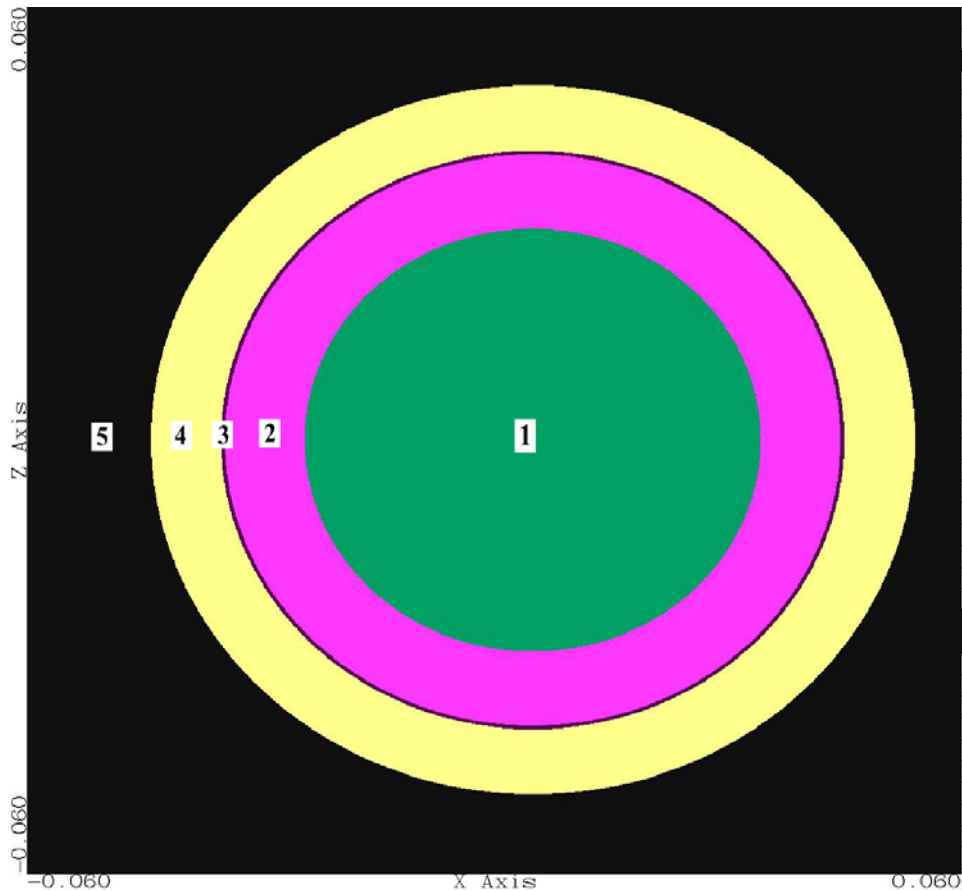
References

[1] The example system illustrated here although similar to a number of systems currently being investigated, does not correspond exactly to any of them. However, the method proposed in this paper is applicable to all similar systems sub-critical systems. Indeed although not strictly required for critical systems, this method could also be applied to critical systems.

[2] **MCNP** - A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory, X-5 Monte Carlo Team, Los Alamos National Laboratory report LA-UR-03-1987 (April 24, 2003). Portions of the MCNP manual are available on-line at,
 http://www-xdiv.lanl.gov/x5/MCNP/themanual.html

[3] **TART 2005**: A Coupled Neutron-Photon 3-D, Time Dependent, Combinatorial Geometry Monte Carlo Transport Code, by Dermott E. Cullen, Lawrence Livermore National Laboratory, UCRL-SM-218009, November 22, 2005.

 [4] F.B. Brown & W.R. Martin, "Stochastic Geometry Capability in MCNP5 for the Analysis of Particle Fuel", Annals of Nuclear Energy, Vol 31, Issue 17, pp 2039-2047 [also LA-UR-04-5362] (Nov, 2004).

 [5] F.B. Brown, W.R. Martin, W. Ji, J.L. Conlin, & J.C. Lee, "Stochastic Geometry and HTGR Modeling for MCNP5", ANS Monte Carlo 2005 Topical Meeting, Chattanooga TN, April 17-21, 2005, [also LA-UR-04-8668] (April, 2005).

[6] F.B. Brown & W.R. Martin, "Stochastic Geometry for MCNP5", Trans. Am. Nucl. Soc. 91 [also LA-UR-04-4432] (Nov, 2004).

[7] L. Snoj and M. Ravnik, "Effect of packing fraction variation on the multiplication factor in Pebble-bed nuclear reactors", Kerntechnik 71 (2006) 208

[8] L. Snoj and M. Ravnik, "Effect of fuel particles' size and position variations on multiplication factor in pebble-bred nuclear reactors", Kerntechnik 72 (2007) 5-6

Appendix

Fully detailed TRISO (5 zones)

Below is an illustration of a single detailed TRISO/pebble; for convenience we also list the composition. Note, that here the TRISO is randomly positioned within the cubic pebble, rather than being centered, e.g. the shift of the TRISO to the right of the center of the cube is clear.

Zone #	Radius (cm)	Density (grams/cc)	Volume (cc)	Composition (weight fraction)		Mass (grams)
1	0.03	10.5	1.130973d-4	92238	0.8925	1.059864d-3
				92235	0.0023	2.731302d-6
				8016	0.0601	7.137020d-5
				6000	0.0451	5.355656d-5
2	0.0402	1.1	1.590266d-4	6000	1.0	1.749293d-4
3	0.0407	1.95	1.028069d-5	6000	1.0	2.004735d-5
4	0.0497	3.217	2.318258d-4	14028	0.8004	5.223488d-4
				6000	0.2996	2.234348d-4
	Side (cm)					
5	0.1196774078	1.7	1.199871d-3	6000	1.0	2.039781d-3

Multiple TRISO/pebbles

Below is an illustration of multiple detailed TRISO/pebbles. Note, that here each TRISO is randomly positioned within a cubic pebble, rather than being centered. This illustration is a small portion of a much larger array of TRISO/pebbles; see the following page. Here we show a slice through an array of 11 x 11 x 11 TRISO, or 1,331 TRISO; this 2-D slice shows a plane containing 11 x 11 = 121 TRISO.
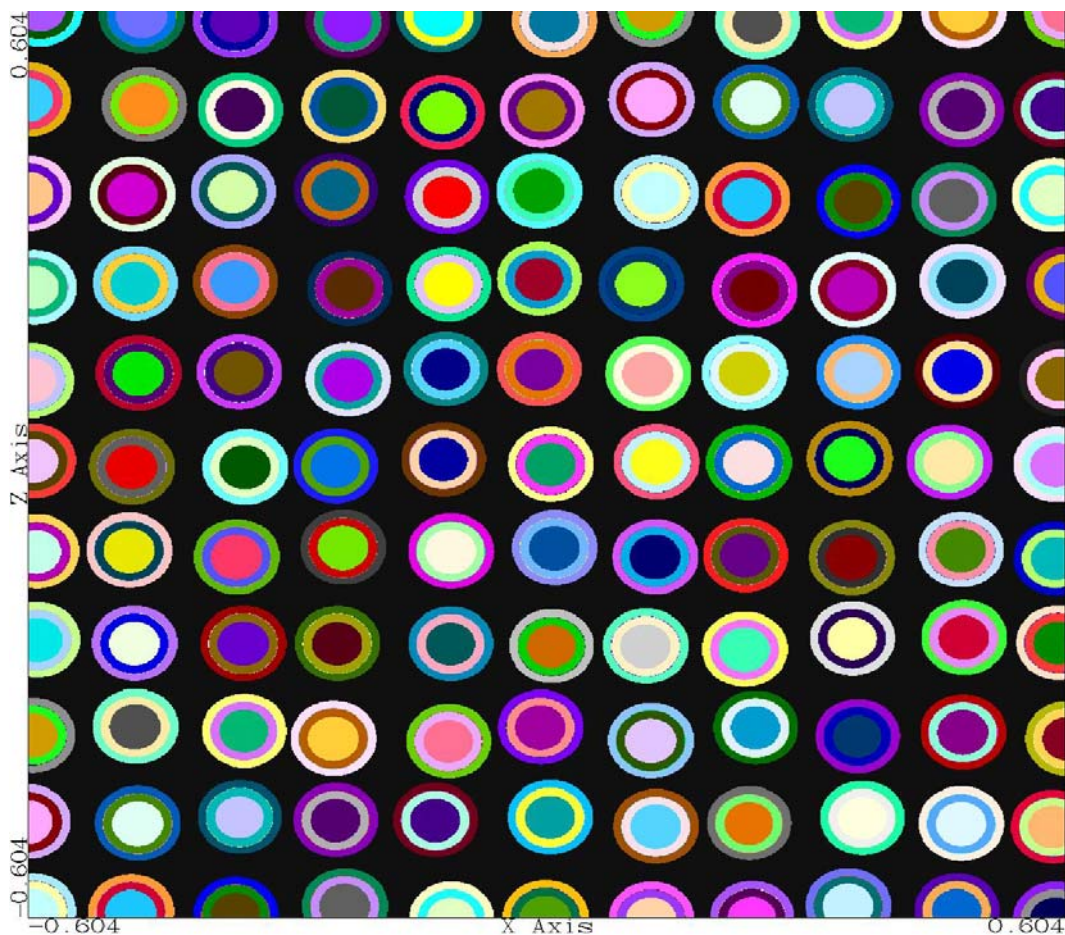
Complete Array of TRISO/pebbles

Below is an illustration of the complete array of detailed TRISO/pebbles used in our calculations for randomly positioned TRISO; here each TRISO is randomly positioned within a cubic pebble, rather than being centered. Here we show a slice through an array of 101 x 101 x 101 TRISO, or 1,030,031 (over 1 million) TRISO; this 2-D slice shows a plane containing 101 x 101 = 10,201 TRISO.