INL/CON-10-18012
PREPRINT

Deterministic Modeling of the High Temperature Test Reactor with DRAGON-HEXPEDITE

HTR 2010

Javier Ortensi
Joshua J. Cogliati
Michael A. Pope
John D. Bess
Rodolfo M. Ferrer
Avery Bingham
Abderrafi M. Ougouag

October 2010

The INL is a
U.S. Department of Energy
National Laboratory
operated by
Battelle Energy Alliance

Proceedings of HTR 2010
Prague, Czech Republic, October 18-20, 2010
Paper 178

Deterministic Modeling of the High Temperature Test Reactor with DRAGON-HEXPEDITE

Javier Ortensi, Joshua J. Cogliati, Michael A. Pope, John D. Bess,
Rodolfo M. Ferrer, Avery Bingham, Abderrafi M. Ougouag
Idaho National Laboratory
P.O. Box 1625, Idaho Falls, Idaho 83415, USA
phone: +1-208-5264256, javier.ortensi@inl.gov

Abstract – *The Idaho National Laboratory (INL) is tasked with the development of reactor physics analysis capability of the Next Generation Nuclear Power (NGNP) project. In order to examine the INL's current prismatic reactor analysis tools, the project is conducting a benchmark exercise based on modeling the High Temperature Test Reactor (HTTR). This exercise entails the development of a model for the initial criticality, a 19 fuel column thin annular core, and the fully loaded core critical condition with 30 fuel columns. Special emphasis is devoted to physical phenomena and artifacts in HTTR that are similar to phenomena and artifacts in the NGNP base design. The DRAGON code is used in this study since it offers significant ease and versatility in modeling prismatic designs. DRAGON can generate transport solutions via Collision Probability (CP), Method of Characteristics (MOC) and Discrete Ordinates (Sn). A fine group cross-section library based on the SHEM 281 energy structure is used in the DRAGON calculations. The results from this study show reasonable agreement in the calculation of the core multiplication factor with the MC methods, but a consistent bias of 2–3% with the experimental values is obtained. This systematic error has also been observed in other HTTR benchmark efforts and is well documented in the literature. The ENDF/B VII graphite and U_{235} cross sections appear to be the main source of the error. The isothermal temperature coefficients calculated with the fully loaded core configuration agree well with other benchmark participants but are 40% higher than the experimental values. This discrepancy with the measurement partially stems from the fact that during the experiments the control rods were adjusted to maintain criticality, whereas in the model, the rod positions were fixed. In addition, this work includes a brief study of a cross section generation approach that seeks to decouple the domain in order to account for neighbor effects. This spectral interpenetration is a dominant effect in annular HTR physics. This analysis methodology should be further explored in order to reduce the error that is systematically propagated in the traditional generation of cross sections.*

I. INTRODUCTION

Idaho National Laboratory (INL) is tasked with the improvement of current calculation methods and analysis approaches in support of the licensing of the NGNP. In this function the INL seeks to 1) determine the current state of the methods available to analyze prismatic HTRs and 2) find any significant gaps in the computation technology that could hinder NGNP deployment. V&V of current computational methods will provide the necessary information to ascertain their state of readiness and the location areas that need further development. The verification of nuclear codes is commonly performed by developers and it has become the main focus area in the research community. The validation of the codes requires experimental data, which is scarce and has become extremely difficult to generate in recent years. A previous assessment [1] suggested that the experiments conducted at the

High Temperature Test Reactor (HTTR) constitute some of the best reactor physics measurements currently available in the open literature applicable to the prismatic NGNP.

Presently, this work must rely on publicly available data that might not contain all the necessary specifications or quality to produce accurate comparisons to the experiments. Better quality data might become available in the future as more emphasis is placed on the validation efforts for NGNP. The three central sources of information used in this work are the International Atomic Energy Agency (IAEA) working group report [2], the Japan Atomic Energy Research Institute (JAERI) benchmark definition memorandum [3], and the International Reactor Physics Experiment Evaluation Project (IRPhEP) reports [4,5]. This latter work represents the modeling task performed at the INL with probabilistic tools, i.e. Monte Carlo. The INL reports conclude that there are still significant questions regarding the quality of the HTTR data available in the public domain, especially in reaction rate distribution and rod worth measurements. Nevertheless, it is still useful to compare computational model results to experimental measurements, since the data can be used to validate some of the calculations that are necessary in the licensing application process. The first stage in the validation of neutronic codes, and the primary focus of this report, is the calculation of the core multiplication factor.

The generation of cross sections for annular HTRs is an active area of research. Previous studies [2,6,7,8] have shown that the neutronic characteristics of these cores complicate this essential step in the calculation process. This work attempts to address some of the areas previously identified as problematic, but significant challenges still remain. These challenges are further discussed in the cross section generation section.

II. METHODS

II.A. DRAGON 4

DRAGON 4 [9] solves the linearized version of the Boltzmann transport equation and includes cross-section generation capabilities. One of the great advantages of the DRAGON 4 code is in its simplicity for modeling, which allows the user to become proficient with the code in a short period of time. The variety of solution methodologies is another great asset of the code. The collision probability (CP), method of characteristics (MOC), and discrete ordinates (Sn) methods were used in during the performance of this work. In addition, the DRAGON code includes a 3-D capability by projection of the third dimension onto a 2-D plane with an MOC solution. The DRAGON 4 calculation options used in cross-section preparation include:

1. A transport correction based on the linearly anisotropic (P1) within group scattering used to correct the library cross sections
2. A self shielding calculation based on the subgroup method
3. The Hebert double heterogeneity treatment in the fuel compacts
4. Use of the CP method with a P_1 leakage model provides the flux solution in 281 groups
5. Spatial homogenization and the energy condensation into 26 groups
6. The 26 group structure was identical used by the German group in the IAEA benchmark [2].

The main limitation of the current version of the code is the geometric specification of a hexagonal block. The 2-D block geometry is built based on a smaller hexagonal unit cell leading to the presence of jagged edges at the block periphery. This introduces small errors with the boundary condition and additional moderator into the block calculation. In order to conserve the graphite mass in the model, the peripheral graphite density is adjusted.

The DRAGON 4 code has been successfully used in high temperature reactor (HTR) applications [10], and it is a well established nuclear analysis tool.

II.B. HEXPEDITE

In hexagonal-z or prismatic geometry, the 3-D flux solution over a prismatic node is split into four 1-D transverse averaged flux equations that are coupled by a leakage source term. These equations are formed by integrating over the nodal flux solution separately in each of the four directions perpendicular to the faces of a prismatic node. The transverse integrated flux is then scaled by the surface area of each face perpendicular to a given directionally dependent transverse integrated flux to get the equations in terms of averaged flux values. A Green's function solution is then applied to the resulting one-dimensional, transverse averaged ODE. The Green's function solution to transverse averaged diffusion equation (equivalently the Sturm-Liouville Operator) can be expressed in an integral form in terms of a source integral and boundary values of the net current on each node. The spatial coupling between two adjacent nodes is formed by requiring that the transverse averaged flux from one node be equal to the transverse averaged flux of an adjacent node. Additionally, the net currents at adjacent nodal interfaces are also assumed equivalent, which is a physically accurate assumption. The result of these two spatial couplings is a tri-diagonal matrix system that can be solved for the net currents at the nodal interfaces.

Despite the analytical nature of the Green's function solution for the transverse averaged flux, the flux solution from the previous iteration must be expanded over a polynomial in order to generate a shape approximation for the fission/scattering source term. Additionally, the net current solutions adjacent to a node of interest are used to approximate a second order polynomial expansion for the leakage source term. The problem domain is split into coupled 1-D problems that can be solved in parallel, and the leakage and fission sources are solved iteratively.

Unlike in Cartesian geometry, the transverse integration procedure applied to hexagonal geometry introduces discontinuous terms in the sources, which are non-physical and purely mathematical in nature. The solution in HEXPEDITE is formed by first assuming that the discontinuous terms are negligible. The flux solution is then corrected by enforcing the node average neutron balance equation on the flux solution. For each directional sweep, the node balance is used to update the flux moments for the other sweeping directions across a given node.

Previous work on the HEXPEDITE methodology [11,12,13] has tested the approach against other spatial discretizations for the neutron diffusion equation in hexagonal and triangular geometry, such as the nodal expansion method (NEM) and finite difference method (FDM). These studies have established HEXPEDITE's superiority in terms of accuracy and runtime over NEM and FDM.

II.C. Monte Carlo

Two Monte Carlo codes are used for benchmarking purposed, MCNP5 [14] and SERPENT [15]. Both use continuous energy treatments with libraries based on ENDF/B-VII.

III. CROSS SECTION PREPARATION

The European benchmark analysis group report [17] concluded that in order to better approach the experimental HTTR results, several effects had to be considered:

- The detailed heterogeneity of the BPs and the fuel region in the whole-core calculation. INL has developed a new method to model the BP heterogeneity in the whole-core diffusion solver. This new technique is currently under testing within the HEXPEDITE code and has not been used in this report.
- Using fine group structure in the whole-core diffusion calculation proposed by the German team or considering the neighbor effects in the transport calculation, proposed by the French team. Following the suggestion of the German team, the DRAGON 4 cross section used in this analysis will be generated in 26 groups based on the FZJ structure [2]. New cross-section generation approaches that take into account neighbor effects were initiated and a summary included in Section V.
- Modeling axial effects of the BP heterogeneity. This effect was quantified in the European benchmark report [17] to be 1.5% $\Delta k/k$ for the annular 19-column core and 2.2% $\Delta k/k$ for the full core. For the DRAGON 4 models this effect was quantified with MCNP5 to be much larger in magnitude. The results show 2.38% and 2.94% Δk for the annular and fully loaded cores, respectively. Since no NGNP design has currently been selected, it is uncertain whether this will be an important issue in the future. The 3-D capabilities of the DRAGON 4 code are currently under testing to determine if these effects can be accurately modeled.
- Treatment of the axial streaming in CR channels. This was quantified to be -1.8% $\Delta k/k$ for the annular core and -1.3% $\Delta k/k$ for the full core [17]. These effects can be modeled in the future with DRAGON 4, but might require some modifications to the source code in order to accurately describe the axial streaming effects in the large CR holes.

Since the current capabilities of the codes are limited, both the axial BP heterogeneity and axial streaming are corrected using the values provided in this section. Studies continue to improve the capabilities of INL codes when required for the NGNP.

The annular core cross sections were all generated at 300 K. Cross sections for the fully loaded core configuration were generated at 300, 340, 380, 420, 460, and 480 K.

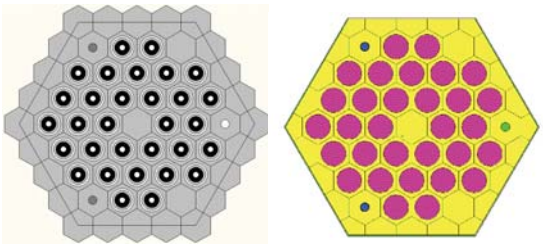
III.A. Fuel blocks

The DRAGON 4 energy and spatial flux calculations are performed with the full-block geometry in order to maximize the fidelity of the calculation. The model includes the annular compact with the double heterogeneity (DH) treatment in the fuel region, the gap between the compact and graphite sleeve, the graphite sleeve, and the cooling channel gap. The description of the microstructure comprises five layers including kernel, porous graphite, IPyC, SiC, and OPyC imbedded in the graphite matrix with the as-built specifications delineated in the JAERI memo [3].

The fuel handling positions, dowels, and sockets were not included in the model. The size of the small hexagons is determined based on the fuel pitch. This approach introduces an error since the location of

the BP rod is closer to the fuel than in the actual design (from a pitch of 5.45 cm to 5.15 cm). This effect was quantified in MCNP5 and shown to be insignificant—just a few pcm. In addition, the fuel-handling hole is not modeled explicitly; instead, the region is treated as a lower graphite density region. The geometry is closed with a white boundary condition at the periphery.

The main error introduced in the fuel model has to do with the jagged edges as seen in Figure 1(a). This geometric approximation changes the fuel-to-graphite ratio, which affects the neutron energy spectrum and, consequently, the microscopic cross sections generated. This issue can be circumvented by decreasing the graphite density in the peripheral region in an effort to conserve the graphite content in the model. Unfortunately, this approach generates incorrect homogenized number densities in the DRAGON 4 code, because the graphite-to-block area is inconsistent with the design.



(a) (b)

Figure 1. DRAGON 4 (left) and MCNP5 models

An MCNP5 model, shown in Figure 1(b), and DRAGON 4 fuel-block model with 31 pins were developed for benchmarking purposes. A set of calculations was used to compare the two transport solutions. The DRAGON 4 models used in this study were spatially converged and solved via a CP solution with linear anisotropic current coupling.

The first case, which contains homogeneous fuel without burnable poison (BP) pins, shows good agreement, while the presence of BP pins more than doubles the difference as shown in Table 1. Significant discrepancies in the solution appear with the double heterogeneity treatment. These differences are exacerbated in the presence of the BP pins. These calculations show that the DRAGON 4 model under-predicts MCNP5 by approximately 1% in the multiplication factor when modeling the full-block details. This 1% difference versus MCNP5 in the calculation of infinite fuel-block multiplication factor is expected to propagate into the whole-core calculation via the cross sections. This does not mean that the DRAGON 4 results should be considered inadequate, since great uncertainty remains in the capability of all the codes to model this type of fuel accurately, and better benchmark data is not readily available.

Model	Δk (pcm)
Homogeneous fuel no BP	84
Homogeneous Fuel with BP	190
DH treatment no BP	-518
DH treatment with BP	-1,034

Table 1: Benchmarking results from DRAGON 4 vs. MCNP5.

The differences in the DRAGON 4 modeling approach at the block level had to be further investigated to determine the effect on the cross sections generated. The difference between the DRAGON 4 generic (reference design density) and corrected (modified peripheral graphite density) models were quantified, and the results are included in Figure 2 and Table 2.

The graphite-adjusted model yields a harder neutron spectrum due to the reduction of the moderator content in the infinite lattice calculation. The generic model produces a softer neutron spectrum that leads to neutron production cross sections with a 3–8% error in the thermal range. Based on these results, it was decided to compute the macroscopic properties externally in order to obtain both the spectral effect from the graphite-density-adjusted calculation and retain number densities that are more consistent with the design. These macroscopic diffusion parameters were computed from the DRAGON 4 microscopic properties and the separately calculated homogenized number densities.

The geometric constraints in DRAGON 4 are impractical but still can be eluded. The DRAGON team has been working on the development of a flat-side hexagon configuration that will remove this limitation in the code. In addition, the new DRAGON 4 version will allow the precise positioning of various geometric features within the block, i.e.control rods.

Results from the DRAGON 4 calculations with both the reference design graphite density and the graphite density reduced at the periphery of the model are shown in Table 3. In addition, some of the APOLLO 2 and TOTMOS-DORT [2] results from the French and German programs are included for comparison.

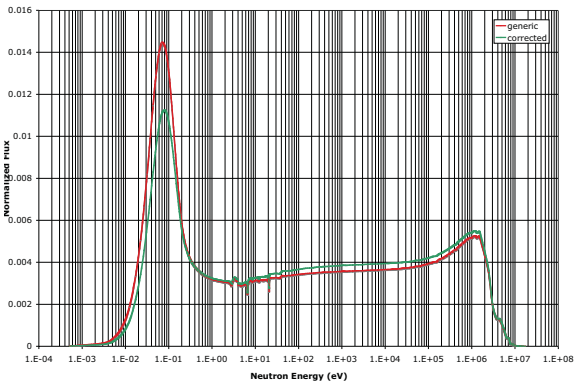


Figure 2: Change Change in the neutron energy spectrum with and without adjustment of the peripheral graphite

Group	Generic Peripheral ρ	Adjusted Peripheral ρ	% Difference
1	1.18E-03	1.07E-03	-10.6
2	5.94E-04	5.38E-04	-10.5
3	2.01E-04	1.83E-04	-9.8
4	3.89E-05	3.72E-05	-4.6
5	5.18E-05	5.07E-05	-2.1
6	9.01E-05	8.94E-05	-0.8
7	1.55E-04	1.55E-04	-0.4
8	2.30E-04	2.30E-04	-0.2
9	3.85E-04	3.85E-04	0.0
10	5.31E-04	5.32E-04	0.2
11	7.18E-04	7.21E-04	0.4
12	1.10E-03	1.11E-03	0.7
13	1.11E-03	1.12E-03	1.0
14	1.80E-03	1.82E-03	1.1
15	4.59E-04	4.67E-04	1.5
16	4.41E-04	4.49E-04	1.7
17	4.24E-04	4.30E-04	1.4
18	1.65E-03	1.68E-03	1.3
19	2.65E-03	2.68E-03	1.2
20	4.51E-03	4.59E-03	1.7
21	4.83E-03	4.94E-03	2.1
22	6.25E-03	6.42E-03	2.7
23	8.14E-03	8.44E-03	3.5
24	1.16E-02	1.22E-02	4.4
25	1.84E-02	1.96E-02	6.0
26	2.66E-02	2.90E-02	8.2

Table 2: Percent differences in νσf with and without adjustment of the peripheral graphite.

The 2-D APOLLO 2 model used a 172 group structure with homogenized fuel region cross sections obtained from an initial 1-D cell calculation to treat the self-shielding. The German team used a TOTMOS 1-D cell calculation to generate homogenized fuel region cross sections. A 2-D R-Z DORT calculation was used to treat the BP axial heterogeneity. In contrast, The DRAGON 4 and APOLLO 2 models use an axial BP homogenized representation. Both DRAGON 4 models yield higher values of k_{inf} when compared to APOLLO 2. These differences can be attributed to a variety of reasons: fuel representation, leakage model, and fine group data, among others. The DORT results lie in between the two DRAGON 4 calculations.

III.B. Permanent Reflector

During the generation of the cross sections for non-multiplying media (i.e., regions with no fissile or fissionable material) participants of the CRP-5 benchmark used various techniques. The French approach used a 1-D cylindrical core solution to generate permanent reflector cross sections with a single, representative fuel spectrum in a source-driven problem [2]. This study expands this technique for the analysis of the annular core in order to better account for the strong coupling between the various core regions. An R-Z solution of the annular core problem with homogenized regions is used for two purposes: (1) generate permanent reflector cross sections, and (2) obtain neutron spectra in various core regions. These spectra are subsequently used as a surface source in a source-driven problem in order to better approximate the neutron spectrum and the cross sections in the regions outside the active core.

The schematic of the R-Z cylindrical annular core used in the calculation is depicted in Figure 3. The model only includes 18 fuel columns in order to avoid the azimuthal homogenization of the 19th fuel column. Therefore, the results should yield lower eigenvalues than a model with all of the fuel columns, but the spectra should still be well represented. The absorber regions are modeled as a ring with the equivalent surface area and volume as the design rods. The fuel region cross section used in the annular R-Z model was generated from a 2-D fuel block model with the average fuel isotopic concentrations pertinent to that axial level. The fuel block was homogenized, but the energy structure was not collapsed in order to carry forward as much spectral information as possible. The model used a void boundary condition at the top and bottom regions and reflected at the center.

Fuel Block	Enrichment [$^{w}/_{o}$]	DRAGON 4 K_{inf}	DRAGON 4 K_{inf} adjusted	APOLLO2 K_{inf}	2-D DORT K_{inf}
f343320	3.4	1.15789	1.11406	1.1065	1.1598
f393320	3.9	1.21318	1.16999	1.14991	1.2068
f433120	4.3	1.24450	1.20505	1.18391	1.2415
f433325	4.3	1.22372	1.17739	1.15656	1.2181
f483120	4.8	1.27936	1.23850	1.21366	1.2728
f523325	5.2	1.28021	1.23141	1.2038	1.2677
f593125	5.9	1.31702	1.27250	1.24481	1.3083
f633125	6.3	1.33291	1.28772	1.25798	1.3217
f633325	6.3	1.33334	1.28266	1.24962	1.3143
f673320	6.7	1.37305	1.32263	1.28423	1.3464
f723125	7.2	1.36883	1.32238	1.28937	1.3529
f793125	7.9	1.39189	1.34412	1.30862	1.3782
f793320	7.9	1.41127	1.35907	1.31733	1.3712
f943120	9.4	1.43421	1.38568	1.36335	1.4216
f993120	9.9	1.44483	1.39570	1.37213	1.4297

Table 3: Results for the HTTR fuel blocks.

		9.13	10.5	18	19	54	55	90	90.5	126	127	127.5	162.0	178.5	195	212.5
		9.13	1.37	7.5	0.5	35.5	0.5	35.5	0.5	35.5	1.0	0.5	34.5	16.5	16.5	17.5
58	58	CRU	ABS1	CRU	1	DB	4	CRUDB	8	RR	ABS2	15	CRU	PR	PR	PR
116	58	CRU	ABS1	CRU	1	DB	4	CRUDB	8	RR	ABS2	15	CRU	PR	PR	PR
174	58	CRU	ABS1	CRU	1	DB	4	CRUDB	9	F1	GAS	15	CRU	PR	PR	PR
232	58	CRU	ABS1	CRU	2	DB	5	CRUDB	10	F2	GAS	16	CRU	PR	PR	PR
290	58	CRU	GAS	CRU	2	DB	5	CRUDB	11	F3	GAS	16	CRU	PR	PR	PR
348	58	CRU	GAS	CRU	2	DB	5	CRUDB	12	F45	GAS	16	CRU	PR	PR	PR
406	58	CRU	GAS	CRU	3	DB	5	CRUDB	13	F45	CRU	16	CRU	PR	PR	PR
464	58	CRU8	GAS	CR8	3	DB	6	CRUDB8	14	RR	CRU8	17	CRU8	PR	PR	PR
522	58	CR9	CR9	CR9	3	DB	7	CRUDB9	14	RR	CR9	18	CR9	PR	PR	PR

Where the following regions are defined.

CRU	Control Rod Guide Block - unroded
CRU8	Control Rod Guide Block 8th level - unroded
CR8	Control Rod Guide Block 8th level
CR9	Control Rod Guide Block 9th level
DB	Dummy Block
CRUDB	Mixed CRU and Dummy Block
CRUDB8	Mixed CRU8 and Dummy Block
CRUDB9	Mixed CRU9 and Dummy Block
ABS1/2	Neutron Absorber Region
GAS	Empty CR Position
RR	Replaceable Reflector Block
FX	Fuel Level X Block
PR	Permanent Reflector Block
X	Spectrum Tally Position

Figure 3: R-Z model of HTTR.

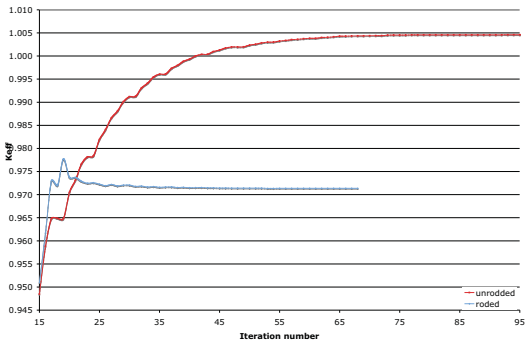


Figure 4. Solutions to the R-Z core problem.

An Sn solution of the R-Z annular core model was obtained with DRAGON 4 using a 281-group structure and 14 discrete angles. A linear anisotropic representation was used for the scattering source. The result from Figure 4 shows that the solution for the unrodded case converges at k_{eff} = 1.005, whereas the rodded configuration converges at k_{eff} = 0.97. This is a good result if one takes into account the fact that this model is missing 1 fuel column, which would generate a near-critical reactor.

Since no leakage model was used in the R-Z transport calculation, the diffusion coefficients for the permanent reflector region were calculated from the available data using

$$D = \frac{1}{3\left(\Sigma_T - \bar{\mu}_0 \Sigma_s\right)} \qquad \text{(eq. 1)}$$

The average scattering angle cosines used in the calculation were determined from a permanent reflector block calculation with reflective boundary conditions.

The spectra obtained from the full-core unrodded model are used in the generation of cross sections for the dummy, replaceable reflector, and CR detailed 2-D models. Figure 5 shows some of the spectra from various regions in the core for the unrodded solution. The regions near the active core (9 and 15) are characterized by a low thermal peak and a high fast peak, whereas regions with considerable moderation (6 and 7) include a high thermal peak and a relatively flat epithermal and fast regions.

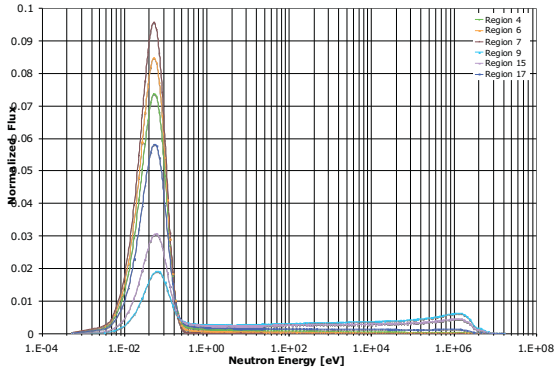


Figure 5. Neutron spectra in various core locations.

Two sets of permanent reflector cross sections for the 30-column core are produced in this study. The first set (referred as PR-I) is based on the 19-fuel column 2-D calculation with the annular core configuration at the various temperatures of interest. This model assumes that the neutron energy spectrum obtained at the reactor periphery is insensitive to the fuel located in the inner rings of the core. A second set of cross sections (referred as PR-II) is developed using a single block configuration with a source on two consecutive sides of the block, and a representative fuel spectrum of the average core enrichment. This last geometry was closed with a reflective boundary condition.

III.C. Dummy, Replaceable reflector, and Control Blocks

The generation of the cross sections for the replaceable reflectors, dummy, and control blocks employs two consecutive calculations in DRAGON 4. The first calculation places an isotropic surface source, based on the spectrum calculated from the R-Z model for that specific core location, at the periphery of the block. A void boundary condition is specified and the flux solution is obtained by solving a source-driven problem. This first computation generates the bulk of the cross sections used in the HEXPEDITE runs. The second calculation is intended only for the generation of the diffusion coefficients. This computation uses a surface source specified with a trace amount of fissile material with a modified neutron spectrum that is consistent with the first calculation. This second model is closed with a reflected boundary condition, and the flux solution is obtained via a k-eigenvalue problem with a P_1 leakage model.

The JAERI memo [3] contains the specific differences in each block design, which include variations in the number, diameter, and length of the holes, as well as the block height. Due to geometric limitations of DRAGON 4, the large insertion holes of 6.15 cm were limited to 5.6 cm, effectively eliminating the gap between the CR and the CR hole. The graphite mass was conserved by reducing the block graphite density.

IV. RESULTS

The results from both critical configurations are included in Table 4. Two HEXPEDITE results are included for the fully loaded core (30 columns) with the two permanent reflector calculation methods (PR-I and PR-II). The first method is based on the R-Z annular core calculation and the second on the single block with a surface source. MCNP5 and SERPENT results are also included for comparison.

All results show a 2–3% bias that is consistent with the MC results. It is noteworthy to mention that similar runs with other MC codes also show significant deviations in the core multiplication factor. This 2–3% bias is believed to be an issue with the continuous energy data libraries for graphite and U235 [4,5,18]. In addition, the resonance scattering models included in the MCNP codes, and potentially SERPENT, are in question [19].

In the annular 19-fuel column core there is very good agreement between HEXPEDITE and MCNP5, but it is coincidental in nature. The MCNP5 models use the same evaluated data files, but geometrically, they are not identical and the material properties are not exactly the same. This discrepancy stems from the fact that the reference design document [3] was not available to INL when the MCNP5 models were built [4,5].

The HEXPEDITE model contains the as-built atomic densities and a better geometric description of the DB design used in the 19-column core critical. This effect was approximately quantified with a DRAGON-HEXPEDITE calculation to be 0.3% Δk. In addition, if a 0.1% Δk correction is applied to account for the fact that HEXPEDITE cannot accurately model the cylindrical periphery of the permanent reflector, the multiplication factor increases to 1.0302. This result is still in good agreement with the MCNP5 model and is more representative of what is expected in diffusion to transport comparisons. The SERPENT model, which is based on the MCNP5 model, also uses continuous energy ENDF/B-VII data and yields roughly 900-pcm higher eigenvalue than the MCNP5.

Number of Fuel Columns	Experiment k[(a)]	DRAGON 4 HEXPEDITE	DRAGON 4 HEXPEDITE[(b)]	MCNP5[(c)]	SERPENT
19	1.0048 ± (>?)	1.0212	1.0262	1.0276 ± 0.0001	1.0370 ± 0.00003
30 (PR-I)	1.0025 ± (>3.6%)	1.0230	1.0394	1.0229 ± 0.0001	N/A
30 (PR-II)	1.0025 ± (>3.6%)	1.0179	1.0343	N/A	N/A

(a) Corrected for instrumentation bias [4,5].
(b) Corrected for axial streaming and BP homogenization effects.
(c) From the IRPHEP reports [4,5].

Table 4: Multiplication factor results for the annular and fully loaded critical core configurations.

Temp. [K]	WIMS-D/4 JAR	DELIGHT CITATION	APOLLO2 CRONOS2	DRAGON 4 HEXPEDITE PR-I	DRAGON 4 HEXPEDITE PR-II
300	1.0023	1.01696	1.00395	1.02303	1.01789
340	0.9930	1.01199	0.99724	1.01588	1.01061
380	0.9844	1.00653	0.99088	1.00878	1.00321
420	0.9768	1.00110	0.98455	1.00172	0.99592
460	0.9699	0.99570	0.97823	0.99486	0.98890
480	0.9665	0.99015	0.97525	0.99149	0.98544

Table 5: Eigenvalue calculation results for the fully loaded core at various temperatures.

Temp. [K]	Experiment	WIMS-D/4 JAR	DELIGHT CITATION	APOLLO2 CRONOS2	DRAGON HEXPEDITE PR-I	DRAGON HEXPEDITE PR-II
320	—	-2.33E-4	-1.19E-4*	-1.68E-4	-1.72E-04	-1.77E-04
345.55	-1.23E-4	—	—	—	—	—
360	—	-2.19E-4	-1.32E-4	-1.61E-4	-1.73E-04	-1.82E-04
400	—	-1.97E-4	-1.33E-4	-1.62E-4	-1.75E-04	-1.82E-04
406.65	-1.32E-4	—	—	—	—	—
440	—	-1.82E-4	-1.34E-4	-1.64E-4	-1.72E-04	-1.78E-04
470	—	-1.81E-4	-1.39E-4	-1.56E-4	-1.72E-04	-1.78E-04

Table 6: Isothermal temperature coefficients of reactivity for HTTR.

The full-core loading results show a significant departure from MCNP5. This core configuration does not contain dummy fuel blocks, which removes that uncertainty from the calculation. Unfortunately, the axial BP correction becomes quite large (3% Δk). The two HEXPEDITE results (I and II) also show a significant sensitivity to the approach used in the generation of permanent reflector cross sections (500 pcm). Only the second approach falls within the uncertainty of the experiment.

The multiplication factors at several isothermal fully loaded core temperatures are listed in Table 5. In addition, some results from the CRP-5 benchmark [2] are also included for comparison. The DRAGON-HEXPEDITE results (PR-I) with the R-Z annular solution for the permanent reflector cross sections are significantly higher than the rest. The other set of DRAGON-HEXPEDITE (PR-II) results are similar to those generated with DELIGHT-CITATION, but are still significantly higher than the other codes.

The isothermal temperature coefficients included in Table 6 are calculated with the data from Table 5 and using

$$\rho = \frac{k_{T_1} - k_{T_2}}{k_{T_1} k_{T_2}} \frac{1}{(T_1 - T_2)} \qquad \text{(eq. 2)}$$

The HEXPEDITE results are over 40% higher than the experimental results, but these were measured at different CR positions, which in this reactor have significant effects on the entire core. Alternatively, the HEXPEDITE results show reasonable agreement with the majority of the CRP-5 calculations. Only the Japanese results with the DELIGHT-CITATION system agree well with the experimental data.

V. ADVANCED CONCEPTS IN HTR CROSS SECTION PREPARATION

One of the main issues with the generation of cross section in HTRs is the strong coupling between the blocks. This strong coupling invalidates the assumption made in the lattice physics calculation (identical neighbors in an infinite domain). In order to better incorporate the neighbor effects into the cross section generation process, a set of DRAGON 4 calculations were performed to determine the decoupling distance in HTTR. Figure 6 shows the variation in the neutron energy spectrum as the domain size increases. The four ring model is equivalent to one single block. The 12 ring block is a two block model, which with reflective boundary conditions constitutes an even larger domain.

The decoupled domain in HTTR is more than two rings of blocks beyond the domain of interest, i.e., cross section generation domain. In some regions this extends beyond the permanent reflector. In an ideal situation one would attempt to generate the cross sections from a 12th, 6th, or full core calculation that would consider all neighbor effects. This is no easy task for the cross section generator currently available. Alternatively, one could use an improved coarse energy structure and a much reduced calculation domain that allows capturing the majority of the spectral effects, which seem to occur in the first few blocks.

Therefore, in order to obtain better estimates of the energy flux, a supercell must include at least 19 blocks. This issue is specific to graphite moderated reactors, which contain fuel and reflector blocks with long migration areas. Table 7 shows the impact of the domain size on the one group macroscopic cross sections.

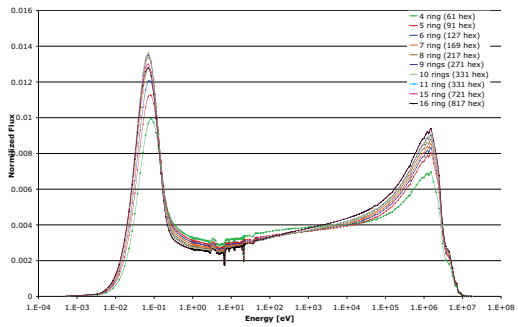


Figure 6: Change in the neutron spectrum as the domain size increases.

	Total	Absorption	NUSIGF	Scattering
Block	3.473E-01	2.697E-03	3.827E-03	3.446E-01
Decoupled	3.445E-01	3.123E-03	4.630E-03	3.414E-01
% Difference	−0.8%	13.6%	17.4%	−0.9%

Table 7: Domain decoupling effects on one group macroscopic cross sections.

VI. CONCLUSIONS

The analysis of the HTTR is a significant challenge for current deterministic methods since they were developed for the analysis of light water reactor (LWR) and fast reactor designs. HTR reactors exhibit neutron physics characteristics that lay between those of light water and fast reactors. In HTRs, especially in annular designs, neutrons travel significant distances. This creates a strong coupling between neighbors and, consequently, invalidates the assumptions made in traditional infinite lattice calculations during the generation of cross sections.

This "spectral interpenetration" can be approximated by using a finer group structure in the full-core calculation, as performed in this work, but the question of accuracy remains unresolved. A preliminary domain de-coupling study included in this work has shown that there can be significant errors if the neighbor effects are not considered in the cross-section generation step for a one group structure. These errors are somewhat alleviated by using the finer group structure, but a comprehensive study is needed to determine if combining a larger domain at the lattice level with a fine group structure in the condensation step can provide high fidelity cross sections for the full core solver.

In addition to the complexities of HTR physics, the HTTR exhibits some special characteristics that further complicate the analysis of the reactor with deterministic methods. The major challenges are the presence of axial heterogeneities in the BP regions and the strong axial streaming in CR channels. There was no attempt in this study to directly address these effects, because they are not significant in the current NGNP design and there is uncertainty with regard to the fidelity of the data currently available from the HTTR experiment. Instead, a correction was applied to the final calculations. The use of these large corrections obscures the comparisons to other methods of analysis and the experimental data. If better HTTR data is available in the future to validate NGNP neutronic codes these two effects need to be addressed. To better model the axial heterogeneities in this reactor two potential options are available: 1) decompose the block in axially homogeneous regions, or 2) perform a 3-D calculation for the BP

region. The first option can be conducted with most cross section generators available, but DRAGON 4 is the only lattice physics code known to the author that includes 3-D capability. Unfortunately, it is still experimental in nature and requires future development. Various lattice physics codes, including DRAGON 4, feature some capability to treat axial streaming effects via generation anisotropic diffusion coefficients. The method might need to be improved to accurately model the large diameter CR holes in the HTTR, since it was initially developed for smaller diameters holes.

This paper shows that there are significant discrepancies between the MCNP5 and the DRAGON 4 results at the block level when the coated particles and BPs are modeled. These discrepancies can be resolved with comparisons to other cross section generators. Nevertheless, the values of the multiplication factor obtained in this report show reasonable agreement with MCNP5 for the two critical configurations analyzed. Unfortunately, there seems to be a systematic bias of 2–3% common to all methods of solution, when compared to the experimental values, which is believed to stem from the cross-section data. Furthermore, the generation of cross sections for the permanent reflector region of HTRs is an area that requires some investigation due to its significant impact of 0.5% Δk in HTTR.

These results from the deterministic codes can be further improved with more accurate modeling of the axial heterogeneity, axial streaming, radial positioning of the BP pins in the whole core model, and the use of more advanced cross section generation techniques applicable to these reactors.

ACKNOWLEDGEMENTS

Work supported by the U.S. Department of Energy, Office of Nuclear Energy, under DOE Idaho Operations Office Contract DE-AC07-05ID14517.

REFERENCES

[1] Terry, W.K., et. al., Preliminary Assessment of Existing Experimental Data for Validation of Reactor Physics Codes and Data for NGNP Design and Analysis, ANL-05/05, September 2004.

[2] IAEA, 2003, Evaluation of High Temperature Gas Cooled Reactor Performance: Benchmark Analysis Related to Initial Testing of the HTTR and HTR-10, IAEA-TECDOC-1382.

[3] Nojiri, N., et al., 1998, Benchmark Problems' Data for the HTTR's Start-up Core Physics Experiments, JAERI memo 10-005, January 1998.

[4] Bess, J. D., and N. Fujimoto, "Evaluation of the Start-Up Core Physics Tests at Japan's High Temperature Engineering Test Reactor (Fully Loaded Core)," HTTR-GCR-RESR-001, *International Handbook of Evaluated Reactor Physics Benchmark Experiments*, NEA/NSC/DOC(2006)1, OECD- NEA, March 2009.

[5] Bess, J. D., and N. Fujimoto, "Evaluation of the Start-Up Core Physics Tests at Japan's High Temperature Engineering Test Reactor (Annular Core Loadings)," HTTR-GCR-RESR-002, *International Handbook of Evaluated Reactor Physics Benchmark Experiments*, NEA/NSC/DOC(2006)1, OECD- NEA, March 2009.

[6] Kim, T.K., et al., "Whole-Core Depletion Studies in Support of Fuel Specification for the Next Generation Nuclear Plant (NGNP) Core," July 2004.

[7] Lee, C.H., et al., "Status of Reactor Physics Activites on Cross Section Generation and Functionalization for the Prismatic Very High Temperature Reactor, and Development of Spatially-Heterogeneous Codes,"ANL-GenIV-075, August 2006.

[8] Kim, K.S., et al., "Development of a physics analysis procedure for the prismatic very high temperature gas-cooled reactors," *Annals of Nuclear Energy*, Vol. 34, pp. 849, (2007).

[9] Marleau, G., A. Hébert, and R. Roy, 2010, "A User Guide for Dragon Version4," Technical Report IGE–294, École Polytechnique de Montréal.

[10] Taiwo, T. A., and T. K. Kim, 2005, Evaluation of the DRAGON code for VHTR Design and Analysis, ANL-GenIV-060, September 2005.

[11] Fitzpatrick, W. E. and Ougouag, A. M., "HEXPEDITE: A Net Current Multigroup Nodal Diffusion Method for Hexagonal-z Geometry", *Trans. Am. Nucl. Soc.,* Vol. 66, 1992.

[12] Ougouag, A. M. and Fitzpatrick, W. E., "An Inherently Parallel Multigroup Nodal Diffusion Method for Hexagonal-Z Geometry", *Fourth International Conference on Simulation Methods in Nuclear Engineering,* June 2-4, Montreal, Canada. (1993).

[13] Fitzpatrick, W. E., "Developments in Nodal Reactor Analysis Tools for Hexagonal Geometry," Ph.D. Dissertation, University of Illinois at Urbana-Champaign. (1995).

[14] Brown, F. B., et al., 2002, MCNP Version 5, LA-UR-02-3935, Los Alamos National Laboratory.

[15] Leppänen, J., 2007, Randomly Dispersed Particle Fuel Model in the PSG Monte Carlo Neutron Transport Code, In *Proc. M&C + SNA 2007, Monterey, California, April 15–19, 2007*.

[16] Leppänen, J., 2007, Development of a New Monte Carlo Reactor Physics Code, D.Sc. Thesis, Helsinki University of Technology, VTT Publications 640.

[17] Raepsaet, X., et al., Analysis of the European Results on the HTTR's Core Physics Benchmarks, *Nucl. Eng. and Design*, Vol. 222, pp. 173–187 (2003).

[18] Goto, Minoru, et al., 2006, Neutronics Calculations of HTTR with Several Nuclear Data Libraries, *J. Nuc. Scien. Tech.*, Vol. 43, N. 10, pp. 1237–1244.

[19] Becker, et al., 2009, Improvements of the Resonance Scattering Treatment in MCNP in View of HTR Calculations, *Ann. Nucl. Energy*, Vol. 36, pp. 281–285.