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Benchmarking of CASMO-5 ENDF/B-VII Nuclear Data Against Critical Experiments

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ABSTRACT

This paper presents results from the critical experiment portion of the validation process for the Studsvik Scandpower CASMO-5 lattice physics code and its ENDF/B-VII neutron data library. One major advantage of comparing to criticals is that they provide a direct method of comparison for code and library evaluation. However, one drawback of comparing to critical experiments is that they are typically only performed at room temperature (cold conditions). This paper presents not only room temperature criticals, i.e., two sets of B&W criticals: the 1810 Series which covers a wide range of burnable absorbers, and the 1484 Series (which helps verify the accuracy of radial leakage calculations), the DIMPLE criticals S06A, and S06B (which helps validate PWR reflector/baffle calculations), but also results for the Kritz-4 BWR criticals which were performed at both cold and hot conditions, with and without gadolinia, and which help to validate the CASMO-5 isothermal temperature coefficient and gadolinium worth.

1. INTRODUCTION

The benchmarking of a lattice physics code and its cross section library typically involves several phases:

(1) Comparison against critical experiments,

(2) Comparison against actual measured isotopics,

(3) Comparison against detailed continuous energy Monte Carlo assembly calculations (including Monte Carlo depletions)[1],

(4) Comparison to standard international benchmarks, e.g. C5G7[2,3].

Each part of this approach is used to validate a different aspect of the library and lattice code methodology.

This paper presents results for Studsvik's next generation lattice physics code CASMO-5[4] and its ENDF/B-VII data library for the first tier of this benchmarking effort: comparison against critical experiments.

2. CASMO-5 LATTICE PHYSICS CODE

CASMO-5 is Studsvik's next generation LWR (both PWR and BWR) lattice physics specifically designed to handle next generation heterogeneous fuel designs and extended cycle lengths.

As the next major release of the CASMO code series, CASMO-5 shares some common methodology heritage with CASMO-4[5]:

- Equivalence theorem based resonance calculation.
- 1D collision probability based pincell calculations performed in the library group structure.
- 2D heterogeneous Method of Characteristics (MoC) based transport calculation (typically performed in 19 groups for UO2 lattices and 35 groups for MOX lattices).
- Predictor/corrector based depletion (with optional azimuthal depletion).
- Optional 18 group gamma calculation (with ENDF/B-VII.0 based gamma data).
- Automated case matrix generation capability for SIMULATE-3 and SIMULATE-5[6] library generation.

However, CASMO-5 also has many advanced numerical models/features not present in CASMO-4:

- Optimum 3 polar angle numerical quadrature (T-Y quadrature)[7].
- Characteristics based Dancoff factor calculation (square geometry with reflective boundary conditions).
- Quadratic Gd-depletion model[8].
- Enhanced BWR cruciform control rod geometries.
- Greatly extended depletion chains.
- Monte Carlo based resonance upscatter model to overcome deficiencies in NJOY modeling[9].
- Explicit energy release per fission mode based on problem specific capture rates[10].

The evolution from CASMO-3 to CASMO-4, was primarily a change in spatial detail (changing from a 2D transport solution based upon homogeneous pincells to a 2D transport solution with full heterogeneous geometry). Likewise, the transition from CASMO-4 to CASMO-5 included not only additional spatial detail in the 2D transport solution, but more importantly it added significantly more detail in the energy dimension (increasing from 70 energy groups to 586 energy groups) and at the same time updating to a state-of-the-art cross section data evaluation.

3. ENDF/B-VII DATA LIBRAY

An important feature of CASMO-5 is the associated 586 group ENDF/B-VII.0 data library. Because the underlying neutron data library is extremely important to a lattice physics code, the recent (Dec. 2006) release of the ENDF/B-VII.0 evaluation[11] provided an opportunity to generate a neutron data library for CASMO-5 based upon the latest available data.

NJOY99.245 was used to process the ENDF/B-VII.0 data to generate a 586 group library for CASMO-5. This library has 128 fast groups (20 MeV to 9.118 keV), 41 resonance groups with shielded data (9.118 keV to 10 eV), 375 narrow groups (10 eV to 0.625 eV) and 42 thermal groups (below 0.625 eV). This energy structure allows the U-238 resonance at 6.67 eV, and the Pu-240 resonance at ~1.0 eV, to be explicitly treated and reduce reliance on resonance self-shielding models in this energy range.

The CASMO-5 ENDF/B-VII.0 library has 446 nuclides/materials with shielded data for 112 nuclides including major fission products. The library has 51 heavy nuclides as well as 234 explicit fission products. Pn-scattering data up to order 5 is present for nuclides where anisotropic scattering effects are important. Note, this is the standard CASMO-5 production library and is not a special library that was created just for testing.

Resonance self-shielding data is tabulated at up to 18 background cross sections (requiring NJOY99 code modifications) and up to 10 temperatures spanning 293 K to 2700 K. No ad-hoc adjustment to U-238 resonance absorption was made to this library as had been necessary in the past for ENDF/B-VI data. This alone represents a significant improvement in ENDF/B-VII.0 data evaluation over ENDF/B-VI.

4. CASMO-5 CALCULATION AND MODELING DETAILS

For the results presented in Sections 5 through.8, CASMO-5 was run in 95 energy groups (to help capture high energy leakage effects), using the default quadrature in the 2D transport solution (64 azimuthal angles, 3 polar angles and a ray spacing of 0.05 cm). In all cases, the number of mesh (flat source regions) in the coolant regions surrounding the fuel pins was increased from the default 3 rings to a value of 5 (to help capture the steep flux gradient near the surface of pins at cold conditions). All results are P0 transport corrected unless otherwise noted in the text. As CASMO-5 is a 2D transport code, axial bucklings were part of the CASMO-5 input. Also, the CASMO-5 default thermal expansion model was active for all cases (important for cores at hot conditions).

5. B&W 1810 SERIES CRITICALS

One of the most widely analyzed series of criticals is the Babcock & Wilcox (B&W) 1810 Series[12]. These critical experiments represent realistic core configurations and consist of a 5x5 array of either 15x15 PWR or 16x16 PWR assemblies. The central “assembly” was modified from one experiment to the next. Some cores contained gadolinium fuel pins, Ag-In-Cd (AIC), B4C control rods, or hollow rods. All core configurations from this set were analyzed, with the exception of Core 11, which was explicitly designed to measure resonance parameters.

The geometry of Cores 1 through 17 was representative of B&W, and Westinghouse type reactors. These cores consisted of a 5x5 array of pseudo-assemblies (individual pins without spacers), each containing a 15x15 pin array. Cores 1 through 10 consisted of a uniform fuel enrichment distribution. Cores 12 through 17 consisted of a high enrichment central area surrounded by a low enriched zone (split zone enrichments).

The geometry of Cores 18 through 20 was representative of a Combustion Engineering type of reactor design. These cores consisted of a 5x5 array of pseudo-assemblies, each containing a 16x16 pin array. All of these cores contained a high enrichment central area surrounded by a low enriched zone. These cores differed only in the number of gadolinium fuel pins present.

Table 1 presents the critical eigenvalues (and fission rate RMS for cores where measured fission rate data exists) for the B&W 1810 series of criticals from CASMO-5 with the 2D transport solution run with a P0 scattering order and in 95 energy groups and using the CASMO-5 ENDF/B-VII.0 library.

Table 1. CASMO-5 ENDF/B-VII.0 Results B&W 1810 Criticals (95 groups, P0)

Core	Boron (PPM)	# 4% Gd Pins	# of AIC Rods	CASMO-5 k-eff	Fission Rate Total RMS (%)
01	1337.9	--	--	1.00083	0.51
02	1250.0	--	16	1.00027	
03	1239.3	20	--	1.00047	
04	1171.7	20	16	1.00106	
05	1208.0	28	--	1.00018	
05A	1191.3	32	--	1.00008	0.57
05B	1207.1	28	--	1.00025	
06	1155.8	28	16	1.00037	
06A	1135.6	32	16	1.00031	
07	1208.8	28	--	1.00019	
08	1170.7	36	--	1.00028	
09	1130.5	36	16	1.00015	
10	1177.1	36	16	1.00010	
12	1899.3	--	--	1.00114	0.69
13	1635.4	--	16	1.00156	
14	1653.8	28	16	1.00084	0.79
15	1479.7	28	16	1.00140	
16	1579.4	36	---	1.00081	
17	1432.1	36	16	1.00098	
18	1776.8	--	--	1.00268	0.86
19	1628.3	16	--	1.00235	
20	1499.0	32	--	1.00214	
Average (Cores 01-17)				1.00059	
Standard Dev. (Cores 01-17)				**0.00047**	
Average (Cores 18-20)				1.00239	
Standard Dev. (Cores 18-20)				**0.00027**	
Average (All Cores)				1.00084	
Standard Dev (All Cores)				**0.00077**	

These results show excellent agreement over a wide range of burnable absorber types and loadings and well within the expected experimental error.

Figure 1 shows the CASMO-5 fission rate comparison to measurements made for B&W 1810 Core 01, again which demonstrates excellent agreement between code and library, and experiment.

Calc. Meas. Diff %							
----- ----- ----- -----	1.021 1.018 0.003 0.310	1.007 1.011 -0.004 -0.360	0.992 0.987 0.005 0.490	0.988 0.981 0.007 0.680	0.989 0.997 -0.008 -0.810	0.965 0.966 -0.001 -0.070	0.944 0.945 -0.001 -0.110
1.021 1.018 0.003 0.310	1.023 1.019 0.004 0.430	1.063 1.067 -0.004 -0.410	1.019 1.012 0.007 0.670	1.015 1.009 0.006 0.630	1.047 1.058 -0.011 -1.030	0.987 0.999 -0.012 -1.210	0.949 0.945 0.004 0.410
1.007 1.011 -0.004 -0.360	1.063 1.067 -0.004 -0.410	----- ----- ----- -----	1.083 1.081 0.002 0.170	1.084 1.090 -0.006 -0.540	----- ----- ----- -----	1.036 1.032 0.004 0.360	0.956 0.953 0.003 0.270
0.992 0.987 0.005 0.490	1.019 1.012 0.007 0.670	1.083 1.081 0.002 0.170	1.063 1.054 0.009 0.890	1.101 1.104 -0.003 -0.290	1.081 1.086 -0.005 -0.440	0.992 0.989 0.003 0.320	0.947 0.945 0.002 0.220
0.988 0.981 0.007 0.680	1.015 1.009 0.006 0.630	1.084 1.090 -0.006 -0.540	1.101 1.104 -0.003 -0.290	----- ----- ----- -----	1.054 1.059 -0.005 -0.450	0.966 0.965 0.001 0.090	0.935 0.934 0.001 0.150
0.989 0.997 -0.008 -0.810	1.047 1.058 -0.011 -1.030	----- ----- ----- -----	1.081 1.086 -0.005 -0.440	1.054 1.059 -0.005 -0.450	0.985 0.988 -0.003 -0.340	0.943 0.938 0.005 0.550	0.924 0.923 0.001 0.080
0.965 0.966 -0.001 -0.070	0.987 0.999 -0.012 -1.210	1.036 1.032 0.004 0.360	0.992 0.989 0.003 0.320	0.966 0.965 0.001 0.090	0.943 0.938 0.005 0.550	0.926 0.925 0.001 0.150	0.914 0.914 0.000 -0.050
0.944 0.945 -0.001 -0.110	0.949 0.945 0.004 0.410	0.956 0.953 0.003 0.270	0.947 0.945 0.002 0.220	0.935 0.934 0.001 0.150	0.924 0.923 0.001 0.080	0.914 0.914 0.000 -0.050	0.904 0.903 0.001 0.120

Figure 1. CASMO-5 Fission Rate Comparison for Core 01 of the B&W 1810 Criticals. Total RMS error : 0.51%

6. B&W Series 1484 (Simple B&W Criticals)

The Babcock & Wilcox (B&W) critical experiments analyzed in this section consists of two very simple cores, one circular and one square[13]. These cores contain no heterogeneities (e.g., water holes, absorber rods, enrichment splits) but since the cores differ in size and shape, they present a wide range of radial leakage. Core I consists of 458 identical fuel pins (2.459 wt%) arranged in a circular shape. The axial leakage represents 2% of the total reactivity of the core; however, the radial leakage represents nearly 35%, so this core is a very high leakage core. Core II consists of 1764 identical fuel pins (2.459 wt%) arranged in a square shape. The axial leakage represents 2% of the total reactivity of the core and the radial leakage represents roughly 15%, so this core is a relatively low leakage core. Fig. 2 shows the geometry of these two cores.

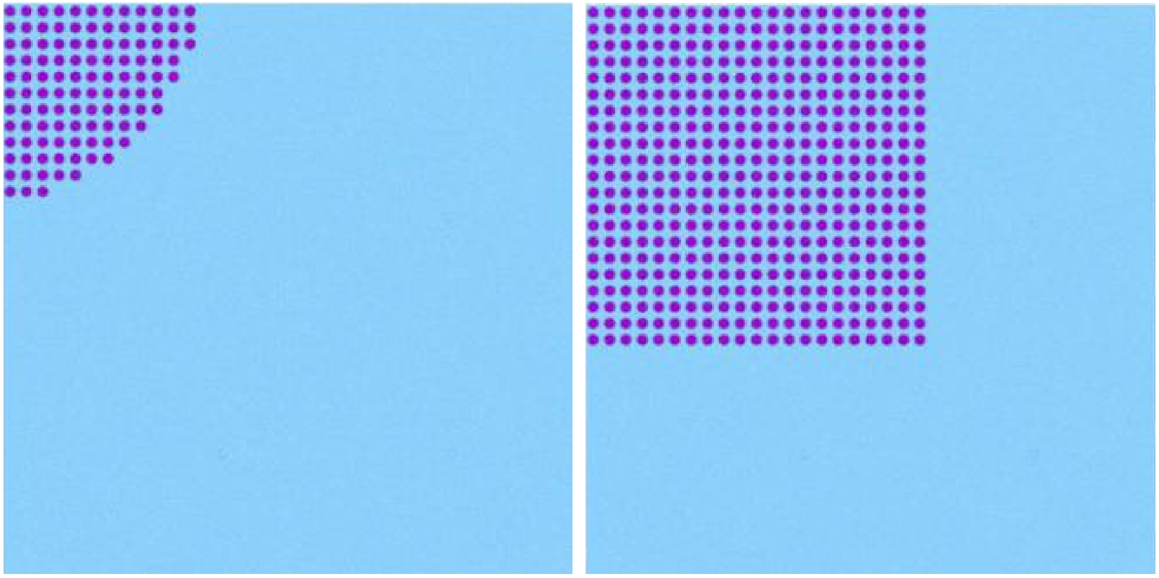

Figure 2. B&W Simple Cores I and II

The two cores when taken together, provide a very good indication of the accuracy with which CASMO-5 predicts radial leakage and they also provide validation of the CASMO-5 transport cross section (which is critical in determining the overall leakage in whole core systems). In CASMO-5, anisotropic scattering effects are normally included by transport correcting the self-scattering term in each group. However, in addition, CASMO-5M (an extended capability version of CASMO-5) can optionally perform a detailed, higher order Pn-scattering calculation instead of using a simple transport corrected total cross section. Table 2 presents three sets of CASMO-5/5M results for these two criticals: P0 non-transport corrected (which will be wildly inaccurate), standard CASMO-5 P0 results, and finally CASMO-5M results with a Pn-scattering order of 3.

Table 2. CASMO-5 ENDF/B-VII.0 Results B&W 1484 Simple Criticals (95 groups)

Core	**Boron (PPM)**	**# Pins**	**Geometry**	**CASMO-5 k-eff (P0 Non-Transport Corrected)**	**CASMO-5 k-eff (P0 Transport Corrected)**	**CASMO-5M k-eff (Pn=3)**
I	0.0	458	Circular	1.10190	0.99957	0.99998
II	1037.0	1764	Square	1.04041	0.99923	1.00044
Average (All Cores)					0.99940	1.00021
Standard Dev (All Cores)					**0.00023**	0.00033

From the P0, transport corrected CASMO-5 results presented in Table 2, one can observe that the eigenvalue agreement between the two cores is excellent (~34 pcm).

Furthermore the above comparison demonstrates just exactly how well the CASMO-5 transport cross section is performing as the transport cross section has to account for almost 10200 pcm in Core I and approximately 4000 pcm in Core II.

7. DIMPLE Criticals S06A and S06B

This section presents results of the calculations for two core configurations from the AEA Winfrith DIMPLE criticals S06A and S06B. The fuel assembly is a PWR type with 16x16 uniform fuel rods at 3.0% U-235 enrichment. The core layout consists of five assemblies forming a cruciform core, both with and without a surrounding 2.67 cm thick stainless steel baffle. The significant amount of Fe in the stainless steel baffle is known to have a fairly large transport effect. No special treatment for iron transport cross section was performed when generating the CASMO-5 ENDF/B-VII cross section library.

The two cores taken together indicate how well CASMO-5 is performing for the baffle/reflector calculation such as that found in a typical PWR. No excess reactivity was reported for these two cores. Fig. 3 shows the geometry of these two cores.

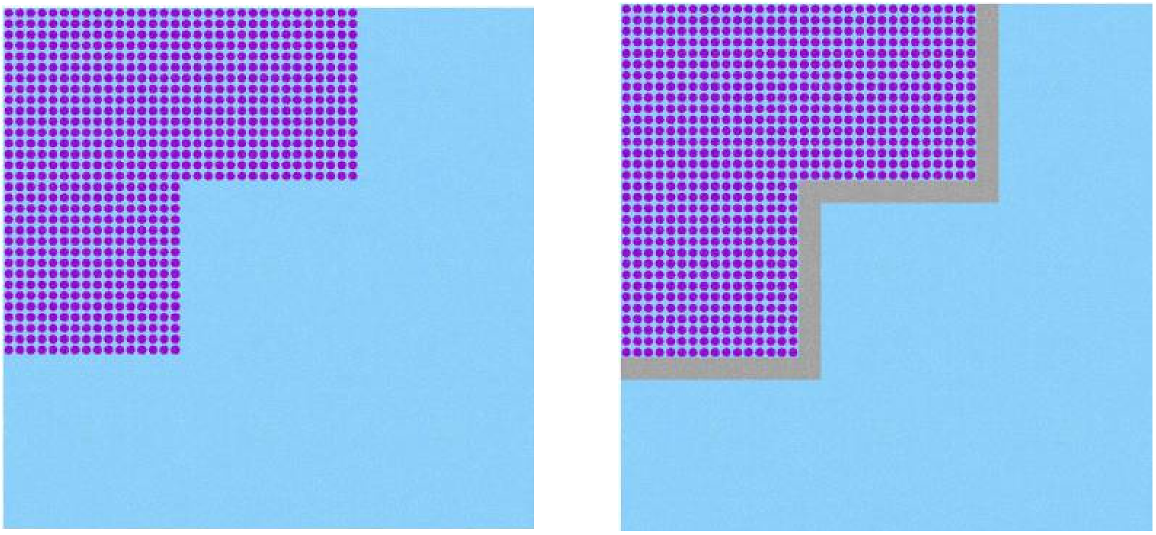

Figure 3. DIMPLE Cores S06A (no baffle) and S06B (with baffle)

Table 3. CASMO-5 ENDF/B-VII.0 Results Dimple Criticals (95 groups, P0)

Core	Boron (PPM)	Geometry	CASMO-5 k-eff
S06A	0.0	Without Baffle	1.00126
S06B	0.0	With Baffle	1.00099
Average (All Cores)			1.00113
Standard Dev (All Cores)			**0.00019**

As can be seen in Table 3, the two DIMPLE cores agree quite well (27 pcm). Furthermore, the 95 group energy structure for these calculations is the exact same group structure used in the standard CASMO-5 reflector calculation for single assembly cross section generation. The accuracy of this baffle/reflector calculation is very important in the modeling of next generation advanced PWRs with large steel block reflectors and this test helps demonstrate that CASMO-5 is performing this calculation very well.

8. Kritz-4 Criticals

In the 1970s, Studsvik in Sweden operated a research facility known as Kritz. This facility was unique in that it could support critical experiments at temperatures ranging from 20^o C to 245^o C (essentially spanning cold to hot zero-power conditions).

The Kritz-4 BWR critical experiments represent realistic core configurations consisting of a 4x4 array of 8x8 BWR assemblies (the details of which are still proprietary) including the channel box[14]. Two separate core designs were modeled at both cold and hot-zero-power operating conditions. In the first set, the wide water gap was centrally located, whereas in the second set the narrow water gap was centrally located. There were a total of seven different assembly types available from which to design each core. The enrichment distribution was common among all assemblies; however, each assembly contained a different number of Gd_2O_3 pins. Note that two cores were brought to critical both with and without the cruciform control blade present in the wide water gap (i.e., Cores 2:1/2:2 and Cores 2:3/2:4). In addition, Cores 3:3 and 3:4 contained different strength gray gadolinium rods (i.e., P06 and P08), while Core 3:2 contained black gadolinium rods and Core 3:1 contained no gadolinium rods, enabling a direct comparison of the Gd worth for black and gray designs.

In Table 4 below, “Cold” indicates temperatures near 293 K, “Warm” indicates near 360 K, and “Hot” indicates temperatures near 516 K. Some cores were measured multiple times with various boron concentrations and critical water levels.

Table 4. CASMO-5 ENDF/B-VII Results Kritz-4 BWR Criticals (95 groups, P0)

Core	Condition	Total No. of Gd Pins	CASMO-5 k-eff
2:1	Cold	0	0.99879
2:1	Cold	0	0.99855
2:2	Cold	0	0.99897
2:2	Cold	0	0.99884
2:3	Cold	8	0.99910
2:3	Cold	8	0.99892
2:3	Warm	8	0.99880
2:3	Warm	8	0.99823
2:3	Hot	8	0.99791
2:3	Hot	8	0.99798
2:4	Cold	8	0.99865
2:4	Cold	8	0.99868
2:5	Cold	28	0.99927
2:5	Cold	28	0.99900
3:1	Cold	0	0.99909
3:1	Warm	0	0.99857

3:1	Hot	0	0.99798
3:1	Hot	0	0.99777
3:2	Cold	20	0.99984
3:2	Cold	20	0.99965
3:2	Warm	20	0.99935
3:2	Warm	20	0.99891
3:2	Hot	20	0.99853
3:2	Hot	20	0.99857
3:2	Hot	20	0.99880
3:3	Cold	20	1.00027
3:3	Cold	20	1.00082
3:3	Cold	20	1.00045
3:3	Warm	20	0.99914
3:3	Warm	20	0.99915
3:3	Hot	20	0.99832
3:4	Cold	20	0.99953
3:4	Cold	20	1.00058
3:4	Cold	20	1.00066
3:4	Warm	20	0.99920
3:4	Hot	20	0.99866
3:4	Hot	20	0.99845
3:5	Cold	12	0.99933
3:5	Cold	12	0.99974
3:5	Cold	12	0.99985
3:5	Warm	12	0.99889
3:5	Warm	12	0.99898
3:5	Hot	12	0.99848
3:5	Hot	12	0.99831
4:1	Cold	40	1.00039
4:1	Cold	40	1.00021
4:1	Hot	40	0.99939
4:1	Hot	40	0.99886
4:2	Cold	24	1.00046
4:2	Cold	24	1.00032
4:2	Cold	24	0.99988
4:2	Cold	24	1.00009
4:2	Cold	24	0.99997
5	Cold	48	0.99952
5	Cold	48	0.99937
5	Warm	48	0.99888
5	Hot	48	0.99837

Average Cold Cores	0.99964
Standard Dev.	**0.00067**
Average Warm Cores	0.99892
Standard Dev.	**0.00031**
Average Hot Core	0.99843
Standard Dev.	**0.00042**
Average All Cores	0.99918
Standard Dev.	**0.00077**

For the purposes of verifying isothermal temperature coefficient (ITC) it is the standard deviation with temperature that is of the most interest and one can see that the spread here is very small. However, there is a very small bias of approximately -0.5 pcm/K in going from cold to hot conditions. As can be seen in Table 4, CASMO-5 also does a very good job in calculating, Gd-worth by comparing core 3:1 to cores 3:N with various Gd loadings, even for the technically challenging gray gadolinium pins.

9. SUMMARY AND CONCLUSIONS

CASMO-5 is Studsvik Scandpower's next generation lattice physics code for LWR analysis. An important part of the CASMO-5 neutron library validation is comparison against critical experiments. Comparisons of CASMO-5 calculations performed with the ENDF/B-VII.0 data library to the series of critical experiments presented here demonstrate excellent agreement with no obvious significant bias versus the number of Gd pins, number of AIC rods, or boron concentration, geometry, presence of reflector/baffle. There is a small bias with respect to temperature.

Table 5. CASMO-5 ENDF/B-VII.0 Results all criticals (95 groups, P0)

Average (All Cores)	0.99967
Stand. Dev (All Cores)	**0.00107**

Table 5 shows the results from all 83 criticals presented in this paper and demonstrates that CASMO-5 with the ENDF/B-VII.0 library produces a very good average critical level with a standard deviation of approximately 100 pcm. Radial leakage calculations, baffle/reflector reflector calculations and ITC calculations similarly all look very good with CASMO-5. This comparison of CASMO-5 to critical experiments helps validate the overall accuracy of the CASMO-5 lattice physics code and its associated ENDF/B-VII.0 neutron data library.

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