# CASMO-5 Development and Applications

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## Abstract

CASMO-5 is the latest code version in the Studsvik Scandpower series of lattice physics codes for general LWR analysis and has capabilities, features and numerical models not previously available in CASMO-4. Among the new capabilities of CASMO-5 are a "quadratic gadolinium depletion model" and the ability to perform 2D transport calculations in hundreds of energy groups. This paper briefly describes CASMO-5 capabilities and the role of CASMO-5 in generating cross section and discontinuity factor data for SIMULATE-4. This paper also describes the new CASMO-5 data libraries (586 group neutron and 18 group gamma), and details recent work to validate CASMO-5 2D transport calculations for several simple criticals.

***KEYWORDS: Lattice physics, assembly calculations, depletion, criticals***

## 1. Introduction

CASMO-5 is the most recent version in a long line of lattice physics codes sharing the name CASMO and has been under development for some time. Previous versions of CASMO were limited to calculations in a maximum of 70 energy groups (the standard CASMO library group structure). As many other lattice codes have data libraries typically containing approximately 200 energy groups, e.g., HELIOS [1] with 190 energy groups, there has been significant interest from the user community in generating a CASMO data library with several hundred energy groups.

As computer speeds and capabilities increase, the trend in lattice physics codes has been to reduce numerical or modeling approximations, and add more detail directly into the calculation. The move from CASMO-3 [2] to CASMO-4 [3], entailed mainly a change in spatial modeling detail, i.e., 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 involves adding additional detail into the 2D transport solution but entails adding the detail in energy instead of in the spatial dimension. In response to interest in new data libraries for CASMO, a neutron data library has been recently generated with 586 energy groups. This paper details some of the initial calculations with CASMO-5 for this new data library.

## 2. CASMO-5 Description and Development

Much of the motivation for developing CASMO-5 was the additional data requirements of the

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SIMULATE-4 [4, 5] nodal code compared to the previous generation SIMULATE-3 [6] nodal code. An advanced nodal code such as SIMULATE-4 has sophisticated data requirements, and CASMO-5 was specifically designed with to fulfill that particular role. For SIMULATE-4, CASMO-5 must generate: generalized assembly averaged multigroup data, (discontinuity factors, and macroscopic and microscopic cross sections) and detailed submesh data, (discontinuity factors, and cross sections) and pin form factors for use in pin power reconstruction at the nodal level. Along with the additional coding to support SIMULATE-4, there was also the desire to update the CASMO code package into a modern programming language (Fortran 95) to facilitate future development.

The CASMO-5 lattice code can be used for both BWR and PWR analysis and shares many common methods heritage with CASMO-4:

- Equivalence theorem based resonance calculation.
- 1D collision probability based pincell calculations (in the library group structure).
- 2D homogenized pincell macrogroup calculation (library or intermediate group structure).
- 2D heterogeneous Method of Characteristics (MoC) transport calculation (performed typically in a few group energy group structure).
- Predictor/corrector based depletion (CASMO-5 performs azimuthal depletion of Gd-bearing fuel pins).

The CASMO-5 lattice physics code has several different numerical models not available in CASMO-4:

- **Quadratic gadolinium depletion** where Gd-absorption rates are assumed to vary over the depletion step (CASMO-4 used a sub-stepping method where the 2D transport calculation was skipped on the shorter depletion step submesh). This model will be described in more detail in the next section as it provides several accuracy and performance benefits.
- **Characterisitics based Dancoff factors** for a square pincell with reflective boundary conditions (CASMO-4 used circularized pincells with collision probabilities and a white boundary condition). This modeling change, which is more faithful to the underlying physical model, typically increases reactivity by 200-400 pcm.
- **Gauss-Legendre polar integration** in the 2D transport solution (CASMO-4 used cosine-squared weighting as outlined in the original CACTUS code specification [7]). The use of Gauss-Legendre weighting functions provide much better convergence in polar angle integration.
- **Explicit black boundary condition** (important for reflector calculations).
- **Enhanced BWR cruciform control rod modeling** (increased spatial detail, e.g., explicit cladding on absorber rods).
- **JEF 2.2 and ENDF/B-VI 586 group neutron and 18 group gamma libraries** (ENDF/B-VII and JEFF 3.1 libraries are currently under development).

Additionally, the CASMO-5 code has been split into two separate versions, one optimized for single assembly cross section generation (CASMO-5) and another (CASMO-5M) for more general, multi-assembly transport analysis, and detailed transport analysis beyond the scope of

general cross section generation. The purpose of this split was to delineate between the two distinct tasks for which CASMO is used. Some users run CASMO strictly to generate cross sections for their nodal code, and other users run CASMO to perform detailed transport analysis for applications like fuel assembly design, fuel storage rack calculations, etc. For the purposes of this discussion, the phrase "CASMO-5" refers to both versions (-5 and -5M) unless otherwise noted.

CASMO-5M contains the following additional enhancements not available in the base CASMO-5:

- **Higher order Pn-scattering** (up to order 7) (CASMO-4 is limited to P0 transport corrected calculations).
- **Generalized multi-assembly calculations** allowing full-core transport calculations (CASMO-4 was limited to 2x2 colorset geometries). This capability allows the user to explore complicated multi-assembly depletion effects including reflector and baffle/barrel interactions.
- **Generalized fuel storage rack geometries** (CASMO-4 had only a very limited geometrical capability in this area).
- **Gamma energy deposition calculations.**

CASMO-5M is capable of multi-cycle, full-core, 2D, PWR and BWR calculations complete with fuel shuffling, assembly rotations, and depletion. It should be noted that CASMO-5M in multi-assembly problems performs the ray-tracing over the entire problem rather than applying the Direct Neutron Path Linking (DNPL) methodology employed by some characteristics codes. [8] The direct approach provides convergence benefits in large problems over DNPL, but increases memory usage.

In addition to numerical modeling enhancements, CASMO-5 contains many programming advancements and enhancements over the original CASMO-4:

- Written entirely in Fortran 95 (CASMO-4 was written in Fortran 77).
- 64-bit capable which allows for very large calculations (8 byte integers where appropriate).

CASMO-5 is not restricted to any particular hardware and has been coded to work on a wide variety of platforms and operating systems.

## 3. CASMO-5 Quadratic Gadolinium Depletion Model

The isotopes Gd-155 and Gd-157 commonly used as integral burnable absorbers in LWR fuel are notoriously "black" and special measures must be implemented in order to deplete these isotopes correctly using reasonably sized depletion steps. CASMO-5 automatically sub-divides Gd-bearing fuel pins into 10 radial rings and further sub-divides these rings into azimuthal quadrants, but experience has proven that even more must be done in order to achieve accurate Gd depletion results.

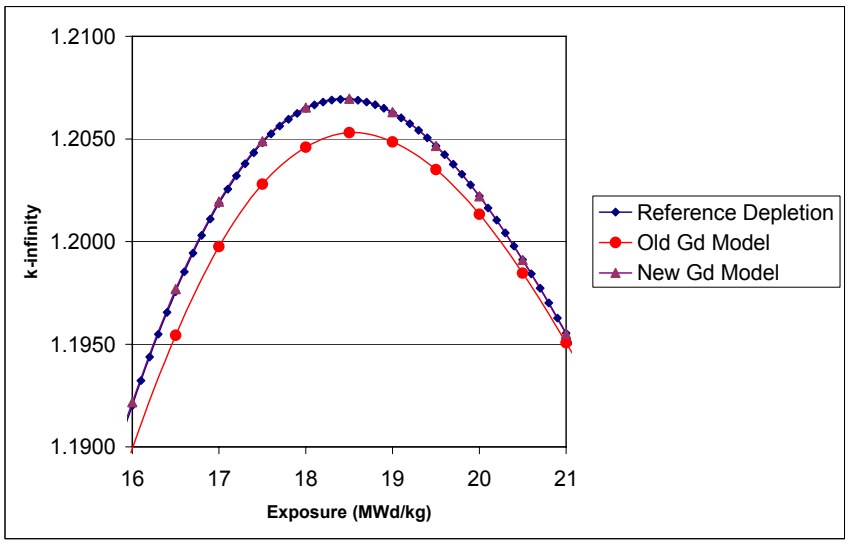
The CASMO-4 code used a computational scheme where the code "sub-stepped" on a depletion mesh finer than that used by the 2D transport solution. The code performed resonance calculations, pincell calculations, and burnup calculations typically with a step size of 0.125

MWd/kg, but would only update the computationally expensive 2D transport calculation every 0.5 MWd/kg. This procedure allows the gadolinium number densities to advance on a shorter time scale (incorporating spectral and spatial flux changes from the pincell calculations) and the global flux shape to change less frequently. This sub-stepping approach provides roughly the same accuracy as a 0.25 MWd/kg direct depletion and eliminates half the 2D transport calculations in favor of twice as many pincell/depletion calculations. This "sub-stepping" approach has worked fairly well over the years, but CASMO-5 uses a more direct approach to provide a specialized scheme that directly addresses the root of the problem, namely the correct depletion of Gd-155 and Gd-157.

The classical predictor/corrector approach assumes that the absorption rate (per atom) is constant in each of the predictor and corrector steps. However, the reality of the situation is that self-shielding and gross thermal flux depression combine such that Gd-155 and Gd-157 absorption rates vary strongly with depletion. The CASMO-5 approach to this problem is to make the assumption that Gd-155 and Gd-157 absorption rates vary smoothly during the depletion step with a "quadratic" dependence on Gd number density. The advantage of this approach over the "sub-stepping" model is that either larger depletion steps can be taken to obtain the same accuracy (relative to a fine-step depletion) or enhanced accuracy can be obtained if the same depletion step size is maintained. This higher order Gd depletion model eliminates the necessity of the CASMO-4 sub-stepping model and decreases runtime while increasing accuracy.

Fig. 1 presents typical CASMO-5 depletion results for a standard GE14 assembly loaded with 17 pins of 7wt% Gd. The quadratic Gd depletion results demonstrate an increase in reactivity on the order of 200 pcm and show excellent agreement with the fine step (step-size=0.1 MWd/kg) reference solution.

**Figure 1:** CASMO-5 quadratic Gd-depletion (New) model versus CASMO-4 sub-stepping model (Old).



## 4. CASMO-5 586 Group Neutron Library -Motivation

While CASMO-5 has many capabilities of a standard transport code, e.g., able to perform large scale, full-core transport calculations, the primary purpose of CASMO-5 is to generate cross section data for 3D nodal codes, e.g., SIMULATE-3 and SIMULATE-4, using single assembly depletions and a case matrix containing 1000's of statepoints. In order to improve results at the core level, the approximations used in the various calculations of the lattice physics code are reviewed periodically to see what improvements can be realized. This periodic methods review is particularly crucial as modern fuel designs evolve beyond the very analysis tools that created them.

The CASMO-5 characteristics based 2D transport solver is capable of high fidelity, heterogeneous solutions [9] and has been the focus of much work and many improvements over the years. From the initial implementation of the base methodology, the 2D transport solver has seen a number of enhancements [10, 11] and has been highly optimized. Utilizing a two-level Coarse Mesh Finite Difference (CMFD) acceleration scheme, the performance of CASMO has been vastly improved over earlier versions. It is now believed that future improvements in results will likely come from updating other computational areas of the code, e.g., the resonance calculation, or the depletion calculation.

Although there has been some recent work in using continuous energy Monte-Carlo depletions to generate data libraries for nodal codes [12], the computational burden is still quite large for current generation workstations and deterministic multi-group methods will likely be the preferred method in the near future for cross section generation for core calculations.

A more direct approach is to simply increase the number of energy groups to explicitly map out more of the detailed resonance structure. Although clearly, 10,000's of groups would be required to map all the resonances, moving to 100's of energy groups will reduce the dependence and computational burden on the CASMO resonance treatment to some degree.

The CASMO-5 hierarchal energy approach (where energy detail is traded off at the expense of increasing spatial detail) provides an interesting opportunity to generate solutions where the initial pincell spectrum calculations are performed in hundreds of energy groups before collapsing to the few group group-structure of the 2D transport calculation. By delaying the group collapsing to as late as possible in the calculational sequence, the collapsing spectrum used is more problem specific and hence realistic to the underlying physical model. However, it is only with the availability of large memory workstations on the desktop, that it is now possible to extend the capabilities of CASMO to perform 2D calculations in hundreds of energy groups.

To enable CASMO to perform such large calculations, several programming challenges had to be overcome, most notably the fixed memory allocation scheme of CASMO-4 (coded in Fortran77) simply did not scale well with large data libraries. To this end, the code was rewritten in Fortran 95 to fully take advantage of features such as dynamic memory, data modules, array operations, and new intrinsics. The resulting code is not only more compact and structured, but more amenable to future code growth and development.

The end result is that CASMO-5 is a lattice physics code written in a modern programming language, and is now capable of calculations limited only by the underlying hardware. However, one critical design restriction is that CASMO-5 remains practical enough to run on current generation workstations, and it has not been designed with the requirements of supercomputers in mind.

## 4.1 CASMO-5 586 Group Neutron Library Description

A new CASMO-5 neutron data library has been generated with a special version of NJOY-94.105 from ENDF/B-VI data for 337 nuclides/materials with the following group structure:

**Table 1**: 586 group CASMO-5 library group structure

| | Upper-Lower Energy Boundaries | # of Energy Groups | Comments |
|---|---|---|---|
| **Fast Groups** | 20 MeV-9118.8 eV | 128 | Similar to LANL VITAMIN-B6 |
| **Res. 1 Groups** | 9118.8 eV-10.0 eV | 41 | Similar to LANL-187 (with shielded data) |
| **Res. 2 Groups** | 10.0 eV - 0.625 eV | 375 | (without shielded data) |
| **Thermal Groups** | 0.625 eV -0.0 eV | 42 | Approx. # of groups as C-4 but over a smaller range |
| **Total** | **586** | | |

For this library, the resonance region has been split into two regions with the upper region having standard shielded resonance data, and the lower region having relatively narrow energy groups and no shielded data.

The library group structure was constructed with two major design constraints:

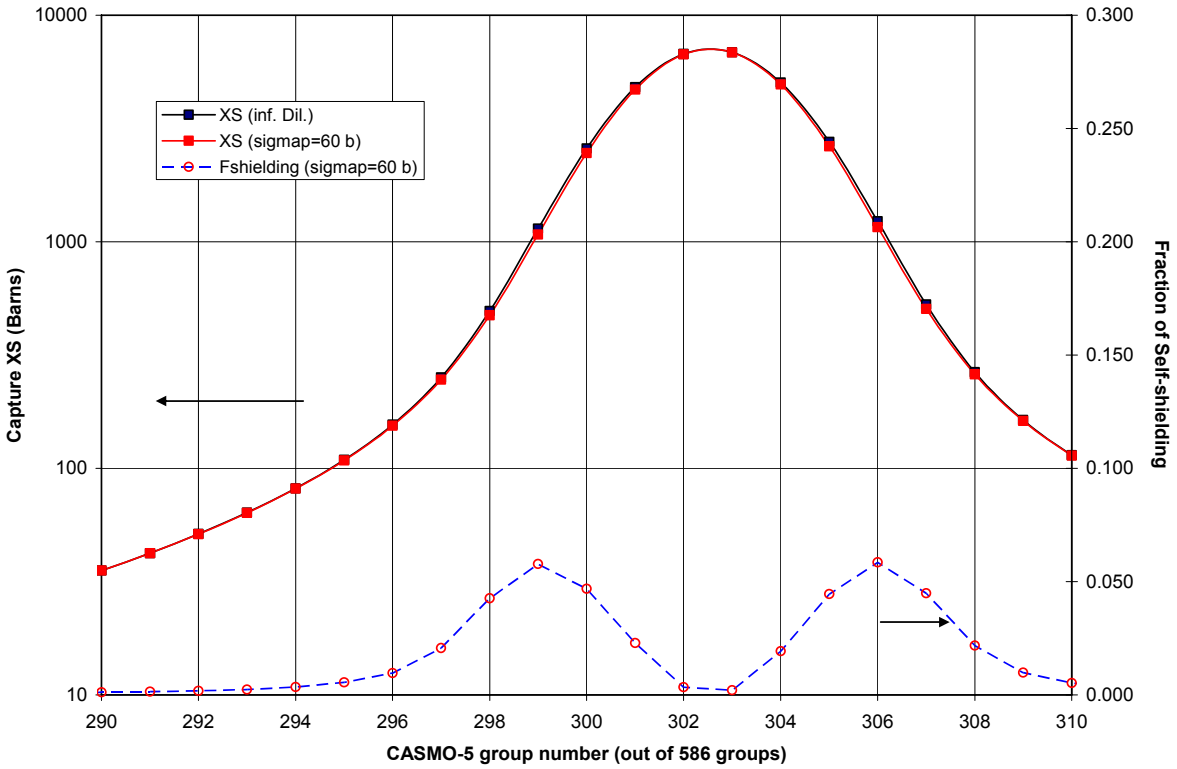
1. The large U-238 resonance at ~6.6 eV is well covered (see Fig. 2).

2. The large Pu-240 resonance at ~1 eV is well covered.

Fig. 2 shows that there is approximately 5-6% self-shielding fraction in the wings of the U-238 resonance with the new 586 group library (where the self-shielding fraction is defined as: s.s. frac=$1.0 - \sigma_{pot}/ \sigma_{(inf. dil.)}$ ). This degree of detail should prove adequate for most LWR analysis of standard UO2 and MOX fuel.

The 586 group library structure has some other advantages over previous CASMO data libraries, e.g., extending the upper range from 10 MeV to 20 MeV, and the addition of additional energy groups in the thermal range. This library also provides great flexibility as it allows one to run the 2D transport solution in any subset of the 586 group library structure, e.g., 290 groups, 180 groups, etc.

**Figure 2:** U-238 capture cross section around 6.6 eV for two dilutions

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## 5. CASMO-5 18 Group, 214 Nuclide, Gamma Library Description

For CASMO-5, a new gamma data library has been generated from JEF 2.2 and ENDF/B-VI data for 214 nuclides/materials. This library maintains the 18 energy groups of the previous CASMO-4 gamma data library, but the gamma production matrices are now present in 70 groups instead of 25 groups. The motivation in developing this new gamma library was not driven by performance of the CASMO-4 gamma library, but rather to exercise an opportunity to update the gamma data with recent, industry standard data.

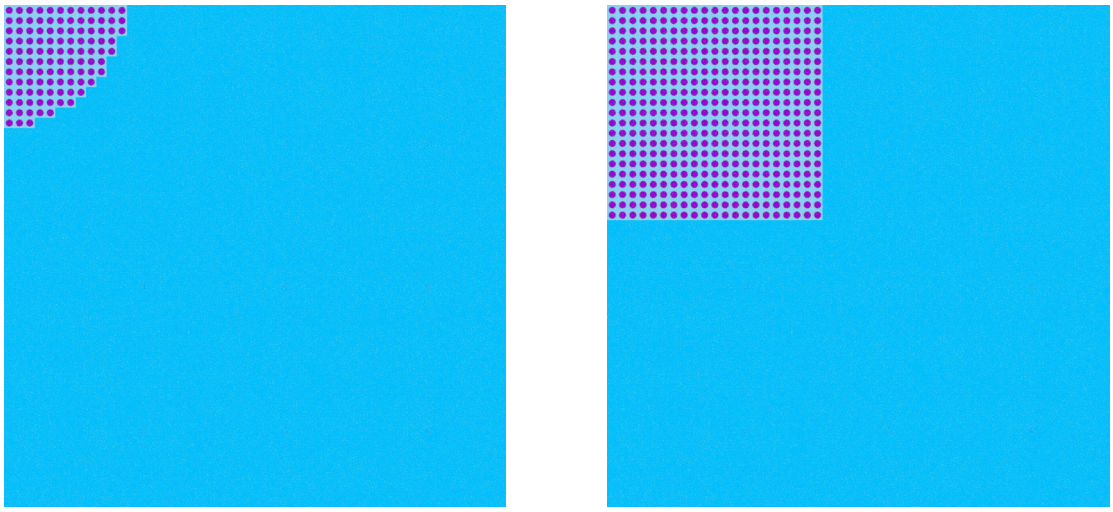
## 6. CASMO-5 586 Group Library Applications and Results

Although comparisons to continuous energy Monte Carlo calculations are often performed for lattice physics code comparisons, comparison to experimental criticals provides a more direct evaluation without the inherent problems of inter-code comparisons, e.g., consistent library data, temperature dependence of libraries, etc. Towards that end, CASMO-5 has been benchmarked against several simple critical experiments and the results presented below.

## 6.1 B&W 3674 Series

A common set of experimental criticals are the Babcock & Wilcox series 3674 [13] which are very simple circular and square cores, containing no perturbations (e.g., water holes, absorber rods, or enrichment splits). The cores are different in shape and size and present a wide range of radial leakage. Illustrated in Fig. 3, Core I consists of 458 identical fuel pins 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 considered a very high leakage core. Core II consists of 1764 identical fuel pins 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 considered a low leakage core.

**Figure 3:** Babcock & Wilcox Core I and Core II (3674 Series)



The two cores together - Core I and Core II - provide a very good indication of the accuracy with which CASMO-5 predicts the radial leakage. Table 2 presents results for these two criticals, with the new 586 group, CASMO ENDF/B-VI library where the 2D transport solution has been run in several energy group structures ranging from 8 to 280 groups.

**Table 2**: ENDF/B-VI CASMO-5 k-effective results for BAW Cores I and II (3674 Series)

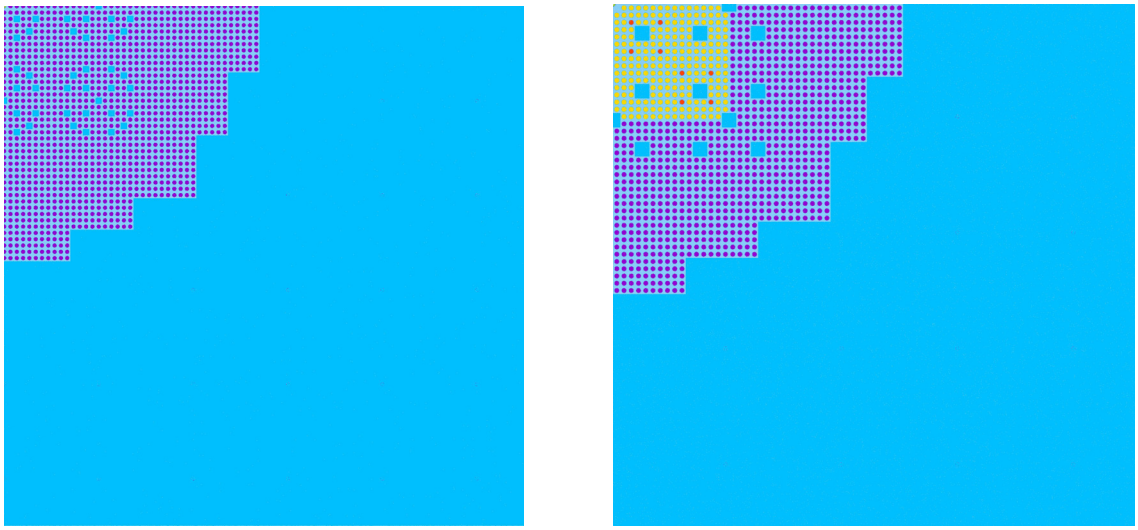
| | 8 Grps | 40 Grps | 70 Grps | 108 Grps | 229 Grps | 280 Grps |
|---|---|---|---|---|---|---|
| **Core I** | 0.99787 | 0.99833 | 0.99830 | 0.99919 | 0.99967 | 0.99995 |
| **Core II** | 0.99828 | 0.99758 | 0.99754 | 0.99848 | 0.99884 | 0.99913 |
| **Average** | **0.99808** | **0.99795** | **0.99792** | **0.99883** | **0.99926** | **0.99954** |
| **Std. Dev.** | **0.00029** | **0.00053** | **0.00054** | **0.00050** | **0.00059** | **0.00058** |

These results demonstrate general good agreement between the two cores under vastly different leakage conditions.

## 6.2 B&W 1810 Series

Another common set of B&W criticals used to verify the modeling accuracy of Gd bearing fuel is the 1810 series [14].

**Figure 4:** Babcock & Wilcox Cores 01-17 (excl. Core 11) and Cores 18-20 (1810 Series).



The geometry of Cores 1 through 17, is illustrated in Fig. 4 in ¼ core symmetry. This configuration is representative of a Babcock & Wilcox, or a Westinghouse type of reactor design. The core consists of a 5x5 array of pseudo-assemblies, each containing a 15x15 pin lattice. 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 "driver" zone. From one core to the next, the central pseudo-assembly was modified with gadolinium fuel pins, Ag-In-Cd, B4C control rods, or hollow tubes.

The geometry of Cores 18 through 20, is also illustrated in Fig. 4 in ¼ core symmetry. This geometry approximates a Combustion Engineering type of reactor design. The core consists of a 5x5 array of pseudo-assemblies, each containing a 16x16 pin lattice. All cores contain a high enrichment central area surrounded by a low enriched "driver" zone. The cores differ only in the number of gadolinium fuel pins present. Table 3 presents results for the new 586 group ENDF/B-VI CASMO library, with the 2D transport calculation performed in 8, 40, and 70 groups.

The MCNP-4C results reported in Table 3 (where available) were generated using the UTXS6 ENDF/B-VI library [15] with 50 million histories producing a 1σ standard deviation of 0.00010 for all cases. Overall, the CASMO-5 run with the 586 group library demonstrates excellent agreement with the experiments and show no obvious bias with the introduction of absorber perturbations.

**Table 3**: ENDF/B-VI CASMO-5 k-effective results for BAW Criticals (1810 Series).

| | MCNP-4C | 8 Grps | 40 Grps | 70 Grps |
|---|---|---|---|---|
| **15x15** | | | | |
| **Core 01** | 1.00078 | 1.00112 | 1.00000 | 0.99987 |
| **Core 02** | | 1.00033 | 0.99938 | 0.99926 |
| **Core 03** | | 1.00058 | 0.99951 | 0.99939 |
| **Core 04** | | 1.00102 | 1.00009 | 0.99997 |
| **Core 05** | 1.00021 | 1.00012 | 0.99909 | 0.99897 |
| **Core 06** | | 1.00020 | 0.99930 | 0.99918 |
| **Core 07** | | 1.00014 | 0.99911 | 0.99898 |
| **Core 08** | | 1.00017 | 0.99916 | 0.99904 |
| **Core 09** | | 0.99996 | 0.99906 | 0.99894 |
| **Core 10** | | 0.99999 | 0.99899 | 0.99886 |
| **Core 12** | 0.99957 | 1.00127 | 1.00006 | 0.99991 |
| **Core 13** | | 1.00114 | 1.00029 | 1.00018 |
| **Core 14** | 0.99985 | 1.00068 | 0.99948 | 0.99935 |
| **Core 15** | | 1.00092 | 0.99999 | 0.99987 |
| **Core 16** | | 1.00067 | 0.99945 | 0.99932 |
| **Core 17** | | 1.00057 | 0.99959 | 0.99946 |
| **Average** | **1.00010** | **1.00056** | **0.99953** | **0.99941** |
| **Std. Dev.** | **0.00052** | **0.00044** | **0.00043** | **0.00042** |
| **16x16** | | | | |
| **Core 18** | | 1.00228 | 1.00105 | 1.00091 |
| **Core 19** | | 1.00181 | 1.00058 | 1.00044 |
| **Core 20** | | 1.00163 | 1.00038 | 1.00018 |
| **Average** | | **1.00191** | **1.00067** | **1.00051** |
| **Std. Dev.** | | **0.00034** | **0.00034** | **0.00037** |

## 7. Conclusions

The new Studsvik Scandpower lattice physics code CASMO-5 incorporates both new numerical models, e.g., the quadratic gadolinium depletion model, characteristics based Dancoff factors, default azimuthal depletion of Gd pins and new neutron/gamma data libraries applicable for both PWR and BWR analysis. The CASMO-5M version of the code adds generalized multi-assembly capability and higher-order Pn-scattering capabilities. Using the new 586 group ENDF/B-VI library, CASMO-5 has demonstrated to provide very good results for simple criticals. This new neutron data library provides energy condensation capabilities and flexibility in CASMO-5 that has not previously been available in the CASMO code family. CASMO-5 provides the lattice physics data for the SIMULATE-4 advanced nodal code and is a crucial component of the next generation reactor physics tools at Studsvik Scandpower. Comprehensive benchmarking of CASMO-5 versus both actual reactor models and continuous energy Monte Carlo depletion calculations is currently underway.

## Acknowledgements

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## References

1. "HELIOS methods" in program manual Rev 3, Program HELIOS-1.5, Studsvik-Scandpower (1998).
2. M. Edenius, *et. al.*, "CASMO-3 User's Manual Rev. 3, "STUDSVIK/NFA-89/3, Studsvik of America (1993).
3. J. Rhodes, *et. al.*, "CASMO-4 User's Manual Rev. 4, "SSP-01/400 Rev 4, Studsvik Scandpower (2004).
4. T. Bahadir, S-O Lindahl and S. Palmtag, "SIMULATE-4 multigroup nodal code with microscopic depletion model," Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications, Avignon, France, (2005).
5. T. Bahadir, S-O Lindahl, "SIMULATE-4 pin power calculations," PHYSOR 2006, Vancouver, Canada, (2006).
6. K. Smith, *et. al.*, 'SIMULATE-3 Methodology", Studsvik/SOA-95/18, (1995).
7. M.J. Halsall, "CACTUS, A characteristics solution of the neutron transport equations in complicated geometries," AEEW-R-1291, U.K. Atomic Energy Authority, (1990).
8. S. Kosaka, and E. Saji, "The characteristics transport calculation for a multi-assembly system using neutron path linking technique," Proc. Int. Conf. Mathematical and Computation Reactor Physics and Environmental Analysis in Nuclear Applications, Madrid, Spain, (1999).
9. D. Knott, M. Edenius, "Validation of the CASMO-4 transport solution" Proc. Int. Mtg. Mathematical Methods and Supercomputing in Nuclear Applications. Karlsruhe, Germany, Vol 2, p 547, (1993).
10. K. Smith and J. Rhodes, "CASMO-4 characteristics methods for two-dimensional PWR and BWR core calculations," ANS/ENS International Winter Meeting and Embedded Topical Meetings, Washington D.C., Nov. (2000).
11. K. Smith and J. Rhodes "Full-Core, 2-D, LWR core calculations with CASMO-4E," PHYSOR 2002, Seoul, Korea, (2002).
12. M. Tohjoh, M. Watanabe, and A.Yamamoto, "Application of continuous-energy Monte Carlo code as a cross section generator of BWR core calculations," Annals of Nuclear Energy 32, p 857-875, (2005).
13. M.N. Baldwin and M.E. Stern, "Physics verification program, part III, task 4, summary report," Babcock and Wilcox Report BAW-3647-20 (1971).
14. L.W. Newman (Project Engineer), "Urania-gadolinia: nuclear model development and critical experiment benchmark," BAW-1810, Babcock & Wilcox, (1984).
15. M.S. Abdelrahman and N.M. Abdurrahman, "Cross section libraries for studies of plutonium disposition in light water reactors," ANRCP-1999-28, Amarillo National Resource Center for Plutonium, (1999).