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Development of an Automated Core Model for Nuclear Reactors

Russell D. Mosteller*

Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The objective of this project was to develop an automated package of computer codes that can model the steady-state behavior of nuclear-reactor cores of various designs. As an added benefit, data produced for steady-state analysis also can be used as input to the TRAC transient-analysis code for subsequent safety analysis of the reactor at any point in its operating lifetime. The basic capability to perform steady-state reactor-core analysis already existed in the combination of the HELIOS lattice-physics code and the NESTLE advanced nodal code. In this project, the automated package was completed by (1) obtaining cross-section libraries for HELIOS, (2) validating HELIOS by comparing its predictions to results from critical experiments and from the MCNP Monte Carlo code, (3) validating NESTLE by comparing its predictions to results from numerical benchmarks and to measured data from operating reactors, and (4) developing a linkage code to transform HELIOS output into NESTLE input.

Background and Research Objectives

The objective of this research project is to develop an automated package of computer codes that can model the steady-state behavior of nuclear-reactor cores of various designs. As an added benefit, the data produced for the steady-state analysis also can be used as input to the TRAC transient-analysis code (Reference 1) for subsequent safety analysis of the reactor at any point in its operating lifetime.

Reactor core analysis typically is performed with a "nodal" code that represents each fuel assembly as a stack of homogeneous blocks (nodes), each with its own unique isotopic composition and thermal-hydraulic conditions. The three-dimensional nodal model iterates between thermal-hydraulic and neutronic calculations to produce a consistent set of conditions in each of the nodes in the core.

In order to perform its neutronic calculations, the nodal code requires cross sections and other related data as input. These data are produced by two-dimensional lattice calculations with imposed thermal-hydraulic conditions. The lattice model typically

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contains a detailed representation of a single fuel type, and separate lattice calculations are performed for each fuel type. (A fuel type corresponds to a fuel assembly if the fuel isotopics initially are the same over its entire length; if the assembly contains different fuel enrichments or different absorber concentrations at different elevations, then a unique fuel type must be defined for each of those elevations.)

The lattice-physics code produces homogenized cross sections for a given fuel type, with the homogenized region corresponding to a node in the nodal code. However, additional lattice calculations have to be performed for each fuel type so that the entire range of anticipated thermal-hydraulic conditions is included. A linkage code then is needed to process the results from the sequence of lattice-physics calculations into cross-section input for the nodal code, so that the cross sections are represented as polynomial functions of the relevant thermal-hydraulic variables.

The basic capability to perform steady-state reactor-core analysis already existed in the HELIOS lattice-physics code (Reference 2) and the NESTLE advanced nodal code (Reference 3). This project has completed the automated package by (1) obtaining cross-section libraries for HELIOS, (2) validating HELIOS, (3) validating NESTLE, and (4) developing a linkage code that transforms HELIOS output into NESTLE input.

Importance to LANL's Science and Technology Base and National R&D Needs

LANL's ability to perform safety analyses and other evaluations for our customers, including the U. S. Department of Energy and the U. S. Nuclear Regulatory Commission, currently is limited by our ability to generate the input necessary for such calculations. In many transient or accident scenarios, the response of the reactor to upset conditions is determined by the isotopic inventory in different parts of the core. That inventory changes, both locally and globally, throughout the operating lifetime of the reactor. The availability of the automated core model developed in this project not only removes this limitation but also enables us to perform detailed analyses of reactors at normal operating conditions throughout their lifetimes.

This automated core model can be used for a number of different purposes. As noted previously, it can generate input to safety analyses at any point in the operating history of a reactor. In addition, given an operating history, it can provide reasonably detailed information about the actinide content of individual fuel assemblies upon their removal from the core. Finally, it can be used to determine steady-state safety margins, which are required for new or modified reactor designs. In particular, such determinations

must be made for fuel designs that would allow reactors to be used for the disposition of weapons-grade plutonium or the production of tritium.

Scientific Approach and Accomplishments

As noted above, this project has four complementary components: (1) cross-section libraries for HELIOS, (2) validation of HELIOS, (3) validation of NESTLE, and (4) development of a linkage code to couple HELIOS and NESTLE. Each of these four components will be discussed separately.

Cross Section Libraries

When LANL purchased HELIOS from Scandpower in 1992, no modern cross-section library was available for it. As part of this project, we purchased a set of three cross-section libraries that Scandpower had developed in the interim. These libraries differ only in the number of energy groups they employ (34, 89, or 190), and all of them are derived from version VI of the Evaluated Nuclear Data File (ENDF/B-VI), the most up-to-date nuclear data library available in the United States. The libraries that we purchased initially are based on Release 2 of ENDF/B-VI, and Scandpower subsequently gave us updated versions of those libraries that are based on Release 3. In fact, Scandpower gave us two versions of each library. The first version is derived directly from ENDF/B-VI Release 3, while the second version incorporates a reduction in the resonance integral of ^{238}U but is otherwise identical.

Validation of HELIOS

HELIOS was validated by comparisons with results from the MCNP Monte Carlo Code (Reference 4) for two sets of benchmarks. The first set was established by the Benchmark Committee of the Reactor Physics Division of the American Nuclear Society (Reference 5) and is based on critical experiments with lattices of UO_2 fuel pins. The second set is a modification (Publication 1) of benchmarks established by the Cross Section Evaluation Working Group (Reference 6) that are based on critical experiments with mixed-oxide (UO_2 and PuO_2) fuel pins. In addition, the fuel-temperature model in HELIOS has been verified by comparing results from it (Publication 2) with a previously-established benchmark for Doppler feedback (Reference 7).

The inner portion of the UO_2 benchmarks contains a 3 x 3 array of pressurized-water-reactor (PWR) fuel assemblies with the fuel rods arranged in a 15 x 15 lattice. The nine assemblies are surrounded by a buffer of 2,396 UO_2 fuel rods, and the entire arrangement is immersed in borated water. For core A, all of the locations in the central nine assemblies contain fuel rods, producing a uniform core. For core B, the fuel rods are removed from 17 of the locations in each assembly so that the geometry corresponds to a

typical PWR assembly. For core C, Pyrex burnable poison rods are placed in 16 of the 17 empty locations from core B. The results from MCNP and HELIOS for these three benchmarks are shown in Tables I, II, and III, respectively.

The HELIOS calculations with the unmodified 89-group library produces generally good agreement with MCNP, but the modified 89-group library produces values for k_{eff} that are closer to unity. In addition, it should be noted that the 34-group libraries consistently produce values for k_{eff} that are approximately 0.003 δk higher than those from their 89-group counterparts.

The six mixed-oxide benchmarks contain fuel pins arranged on a uniform pitch and are immersed in water. Three different pitches are used, and there are two benchmarks at each pitch, one of which contains (essentially) unborated water and the other of which contains borated water. A brief summary of the benchmarks and the results obtained from MCNP and HELIOS is presented in Table IV. The boron content in the water is given in parts per million (PPM), by weight.

The HELIOS results for the mixed-oxide benchmarks are not as consistent with those from MCNP as were the results for the UO_2 benchmarks. The HELIOS value for k_{eff} generally is lower than that from MCNP, but it is slightly higher in one case (PNL-30) and much lower in another (PNL-34). We were not able to resolve these discrepancies within the time frame for this project.

Validation of NESTLE

NESTLE has been validated by comparisons to numerical benchmarks and to measured data from PWRs. The numerical benchmarks include cases representative of PWRs, boiling water reactors (BWRs), CANDU heavy water reactors (HWRs), and high-temperature gas-cooled reactors (HTGRs). The measured PWR data include critical soluble boron concentrations and isothermal temperature coefficients of reactivity (ITCs).

NESTLE solves the few-group neutron-diffusion equations using the nodal expansion method (NEM) in conjunction with a nonlinear iteration strategy. At the user's option, however, the nonlinear iterations can be omitted from NESTLE's iteration strategy. In such cases, the solution degenerates to the standard finite-difference method (FDM). Although this feature is of no practical importance (it is well known that, in contrast to NEM, FDM requires a very fine spatial mesh to produce an accurate solution), it allows the validation of NESTLE to proceed along two complementary paths: (1) comparison of its FDM solution with other FDM solutions, and (2) comparison of its NEM solution with reference solutions.

NESTLE results were obtained for both two-dimensional (2D) and three-

dimensional (3D) versions of benchmarks for PWRs, BWRs, and HWRs and for a 2D version of a benchmark for an HTGR (the specification for the 3D version of the HTGR benchmark was incomplete). The HTGR benchmark has hexagonal geometry, while the geometry for the others is Cartesian. The benchmark specifications were taken from supplements 2 and 3 of the Argonne Benchmark Book (Reference 7). None of these benchmarks account for variations in thermal-hydraulic conditions, and therefore they are ideal tests of NESTLE's ability to solve the steady-state few-group diffusion equations correctly.

NESTLE results for the 3D benchmarks are compared against those from other codes in Tables V, VI, and VII, while NESTLE results for the 2D HTGR benchmark are compared to those from other codes in Table VIII. VENTURE (Reference 8) is based on FDM, as are CERKIN (Reference 9) and CERBERUS (Reference 10). ARROTTA (Reference 11) and QUANDRY (Reference 12) are based on the analytic nodal method (ANM). GRIMHX (Reference 13) can solve the few-group diffusion equations using either standard FDM or a higher-order coarse-mesh FDM (CMFDM). The extrapolated VENTURE solution ("Extrap." in the Tables) was obtained by extrapolating from a series of calculations with finer and finer spatial meshes. More information about the numerical benchmark calculations, as well as the power distributions obtained, can be found in the literature (Publication s 3 and 4).

Although it only identifies them by a letter rather than their actual names, Reference 14 provides detailed descriptions of the core design and loading pattern for the first cycle of four PWRs. Table IX briefly summarizes the first cycle of each of those plants, including differences in the type of lumped burnable poison rods (LBPRs). All of the measurements discussed herein were made at hot-zero-power conditions at beginning of plant life, prior to ascension to power.

The cross sections for NESTLE were not generated as part of this project. Instead, cross sections that had been generated previously (Reference 14) for ARROTTA simply were translated into NESTLE input format. Because NESTLE's cross-section representation is a superset of that employed by ARROTTA, no approximations were required for the translation.

NESTLE's predictions for critical soluble boron concentrations and ITCS for these plants are compared with the measured values and the predictions from ARROTTA in Tables X and XI, respectively. As the tables demonstrate, NESTLE produces excellent agreement with both the measured values and the values predicted by ARROTTA. Furthermore, the consistent agreement in critical soluble boron concentration with different control-rod banks inserted shows that NESTLE accurately predicts control-rod worth.

The results from the numerical benchmarks demonstrate that the NESTLE FDM calculations replicate the calculations from other FDM codes and that the NESTLE NEM calculations produce excellent agreement with reference solutions. In addition, the comparisons with measured data show that NESTLE predicts the behavior of a variety of PWRs very accurately at static conditions.

Development of a Linkage Code

The PHONICS linkage code was developed to process HELIOS output into NESTLE input for cross sections and related data. PHONICS is written entirely in Fortran 90, and it contains 31 subroutines, 23 common blocks, and nearly 5,000 lines of active coding. A manual describing its methodology, file and subroutine structures, and user input has been written and should be available as a LANL report in the near future.

Publications

1. Mosteller, R., "Two-Dimensional Benchmark Calculations for PNL%30 through PNL%35," *Trans. Am. Nucl. Soc.* (forthcoming).

2. Mosteller, R., "Comparison of Doppler Coefficients from ENDF/B%V and ENDF/B%VI," *Trans. Am. Nucl. Soc.*, **74**, 331 (June 1996).

3. Mosteller, R., "Static Benchmarking of the NESTLE Advanced Nodal Code," *Proceedings of the Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications*, Vol. 2, pp. 1596-1605 (October 1997).

4. Mosteller, R., "Validation of NESTLE Against Static Reactor Benchmark Problems," *Trans. Am. Nucl. Soc.*, **74**, 310 (June 1996).

5. Mosteller, R., "Benchmarking of NESTLE against Measured PWR Data at Beginning of Life," *Trans. Am. Nucl. Soc.*, **73**, 369 (October 1995).

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Table I. Results for Core A

Code	Energy Groups	k_{eff}
MCNP	C	0.9956±0.0003
HELIOS	89	0.9956
	89*	0.9992
	34	0.9988
	34*	1.0025

*Includes Scandpower modification to ^{238}U

Table II. Results for Core B

Code	Energy Groups	k_{eff}
MCNP	C	0.9957±0.0003
HELIOS	89	0.9971
	89*	1.0004
	34	1.0005
	34*	1.0038

*Includes Scandpower modification to ^{238}U

Table III. Results for Core C

Code	Energy Groups	k_{eff}
MCNP	C	0.9940±0.0003
HELIOS	89	0.9917
	89*	0.9951
	34	0.9942
	34*	0.9977

*Includes Scandpower modification to ^{238}U

Table IV. Results for Mixed-Oxide Benchmarks

Case	Fuel Pins	Soluble Boron (PPM)	Pitch (cm)	k_{eff}, MCNP	k_{eff}, HELIOS	
					89 Groups	34 Groups
PNL-30	469	2	1.7780	0.9941±0.0008	0.9966	1.0017
PNL-31	761	681	1.7780	0.9982±0.0008	0.9941	0.9993
PNL-32	195	1	2.2098	0.9975±0.0008	0.9948	0.9999
PNL-33	761	1090	2.2098	1.0083±0.0008	1.0022	1.0079
PNL-34	160	2	2.5146	1.0030±0.0007	0.9918	0.9970
PNL-35	689	767	2.5146	1.0078±0.0007	1.0042	1.0101

Table V. Results for 3D PWR Benchmark

Code	Method	Mesh Spacing (cm)		k_{eff}	Peak Relative Power
		Planar	Axial		
VENTURE	FDM	5	10	1.02864	2.504
		Extrap.	Extrap.	1.02903	2.354
ARROTTA	ANM	20	20	1.02899	NR[a]
NESTLE	FDM	5	10	1.02864	2.504
	NEM	5	10	1.02907	2.340
		20	20	1.02899	2.304

[a] Not reported

Table VI. Results for Static 3D BWR Benchmark

Code	Method	Mesh Spacing (cm)		k_{eff}	Peak Relative Power
		Planar	Axial		
QUANDRY	ANM	7.5	25[a]	0.99639	NR[b]
		15	25[a]	0.99644	NR[b]
NESTLE	NEM	7.5	7.5	0.99638	3.462
		15	15	0.99627	3.210

[a] 15 cm in axial reflector

[b] Not reported

Table VII. Results for 3D CANDU HWR Benchmark

Code	Method	Mesh Spacing (cm)		k_{eff}	Power Fraction		
		Planar	Axial		Outer Core, Front and Back	Outer Core, Sides	Inner Core
CERKIN	FDM	NR[a]	NR[a]	1.00355	0.2752	0.3106	0.4142
CERBERUS	FDM	30 / 60[b]	60	1.00356	0.2752	0.3106	0.4142
NESTLE	FDM	30	60	1.00315	0.2739	0.3099	0.4162
	NEM	30	60	1.00357	0.2743	0.3114	0.4143
		15	60	1.00351	0.2742	0.3111	0.4147

[a] Not reported

[b] 30 cm near fuel/reflector interface, 60 cm elsewhere

Table VIII. Results for 2D HTGR Benchmark

Code	Method	Mesh Spacing (cm)	k_{eff}	Relative Peak Power
VENTURE	FDM	36.2	1.12725	1.423
		Extrap.	1.11835	1.418
GRIMHX	FDM	36.2	1.12725	1.464
	CMFDM	12.1	1.11863	1.323
NESTLE	FDM	36.2	1.12722	1.465
	NEM	36.2	1.11852	1.327

Table IX. Plant Characteristics

Plant	Rated Power (MWt)	Number of Assemblies	Type of Assemblies	Type of LBPR	Fuel Enrichment (w/o)
B	3250	193	15 x 15	Full	2.248, 2.789, 3.292
C	2775	157	17 x 17	Part	1.6, 2.4, 3.1
D	3411	193	17 x 17	Full	1.6, 2.4, 3.1
F	2560	217	14 x 14	Part	1.9, 2.3, 2.8

Table X. Measured and Predicted Critical Soluble Boron Concentrations

Plant	Temperature (EF)	Control-Rod Banks Inserted	Critical Boron Concentration (PPM)		
			Measured	ARROTTA[a]	NESTLE
B	547	None	1350	1314	1312
		D[b]	1348	C	1310
		C[c], D	1203	C	1170
		B[b], C, D	1085	C	1063
		A[c], B, C, D	940	C	914
C	557	None	1189	1190	1187
D	557	None	975	997	996
		D	902	933	932
		C, D	816	841	837
F	532	None	952	951	953
		5, 6, 7	844	813	823
		2, 3, 4, 5, 6, 7	606	580	605

[a] Values taken from Reference 14
[b] 200 Steps Withdrawn (Fully Withdrawn at 220 Steps)
[c] 180 Steps Withdrawn (Fully Withdrawn at 220 Steps)

Table XI. Measured and Predicted ITCs

Plant	Temperature (EF)	Control-Rod Banks Inserted	Critical Boron Concentration (PPM)	ITC (pcm/EF)		
				Measured	ARROTTA[a]	NESTLE
B	547	D[b]	1348	-1.3±0.3	-1.6	-1.6
		C[c], D	1203	-5.2±0.3	-5.6	-5.3
		B[b], C, D	1085	-9.0±0.9	-9.1	-8.5
		A[c], B, C, D	940	-10.3±1.7	-10.7	-9.9
C	557	None	1189	3.5	1.3	2.1
D	557	None	975	-1.7	-3.2	-2.7
		D	902	-2.8	-4.3	-3.9
		C, D	816	-8.0	-8.9	-8.0
F	532	None	952	0.8	-0.8	-0.9
		5, 6, 7	844	-4.1	-5.4	-4.9
		2, 3, 4, 5, 6, 7	606	-10.4	-10.3	-8.1

[a] Values taken from Reference 14
[b] 200 Steps Withdrawn (Fully Withdrawn at 220 Steps)
[c] 180 Steps Withdrawn (Fully Withdrawn at 220 Steps)