

## SIMULATE-4 Pin Power Calculations

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### Abstract

A new pin power reconstruction module has been implemented in Studsvik Scandpower's next generation nodal code, SIMULATE-4. Heterogeneous pin powers are calculated by modulating multi-group pin powers from the submesh solver of SIMULATE-4 with pin form factors from single-assembly CASMO-5 lattice calculations. The multi-group pin power model captures instantaneous spectral effects, and actinide tracking on the assembly submesh describes exposure-induced pin power variations. Model details and verification tests against high order multi-assembly transport methods are presented. The accuracy of the new methods is also demonstrated by comparing SIMULATE-4 calculations with measured critical experiment pin powers.

**KEYWORDS:** *T. Bahadır; S.-O. Lindahl*

### 1. Introduction

SIMULATE-4 [1] is Studsvik Scandpower's next generation nodal code developed to address deficiencies of existing reactor physics tools for today's aggressive core designs. Multi-group cross sections and other data for SIMULATE-4 are generated from Studsvik's new lattice physics code, CASMO-5 [2] which supports latest data libraries and includes new numerical models. The major features of SIMULATE-4 can be summarized as:

- Arbitrary number of energy groups are employed
- Diffusion or simplified  $P_3$  equations are solved
- Microscopic depletion model including 50 heavy nuclides and fission products is used to describe cross sections
- Axial heterogeneities are treated explicitly
- Fuel assemblies are divided into heterogeneous radial submeshes, overcoming shortcomings of traditional assembly-averaged cross sections/discontinuity factors and the quadratic transverse leakage approximation

Details of the three-dimensional global neutronic solver of SIMULATE-4 can be found in Reference [1].

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As part of the new development, the pin power reconstruction of SIMULATE-3 [3, 4] has also been replaced. This paper describes the new pin power model of SIMULATE-4 and the results of numerical tests which demonstrate the accuracy of the new method.

## 2. Pin Power Model

The pin power calculation is based on a submesh model. The core is divided into a number of 2D slices where each assembly (or quarter-assembly) is divided into  $N \times N$  rectangular subnodes or “submeshes” (typically  $N=5$ ). The submesh boundaries are chosen to coincide with either the water/control-rod(CR) gaps of a BWR or with pin cell boundaries. Thus, a subnode consists of  $I \times J$  pin cells or of a section of a water/CR gap. In PWRs, the outer layer is chosen to be one pin-cell wide in order to accurately describe intra-assembly gradients. All reflector regions outside the active core are treated in an analogous manner, and PWR baffles are treated explicitly.

Submesh interfaces of adjacent assemblies need not match geometrically, which is common in BWR cores with mixed fuel assembly designs.

The submesh module of SIMULATE-4 solves the multi-group diffusion or the simplified P3 (SP3) equations by assuming the flux in each group and subnode to be given as [1]

$$\phi(x, y) = \sum_{i=1}^4 K_i v_i(x, y) + c_0 + \sum_{l=1}^2 (c_{xl} P_l(x) + c_{yl} P_l(y)) \quad (1)$$

where  $P_l$  is the Legendre polynomial and

$$v_1 = e^{-\kappa_x x} \quad , \quad v_2 = e^{+\kappa_x x} \quad , \quad v_3 = e^{-\kappa_y y} \quad , \quad v_4 = e^{+\kappa_y y} \quad . \quad (2)$$

The unknown expansion coefficients  $K_i$  are found from four boundary conditions (submesh average side fluxes). The  $c_i$  coefficients are determined by the fission and scattering source expansions.

Submesh cross sections,  $\Sigma_{\alpha g, s}$ , and discontinuity factors (as well as assembly-averaged cross sections and discontinuity factors) are computed by CASMO-5 as a function of control rod, burnup, moderator density, etc. Submesh cross sections are corrected for local submesh burnup, fuel temperature, xenon, moderator density, and concentration of  $U^{235}$ ,  $U^{238}$ ,  $Pu^{239}$ ,  $Pu^{240}$ , and  $Pu^{241}$ . The correction term is labeled  $\Delta \Sigma_{\alpha g, s}$ . Note that ~50 heavy nuclides and fission products are tracked for each node, and they are used to correct assembly-averaged cross sections. The five heavy nuclides are tracked for each submesh by solving the decay and conversion chains using submesh fluxes. Thus, SIMULATE-4 carefully describes the physics of control rods and assembly interfaces. The multi-group formulation captures instantaneous spectral effects, and the tracking of the important heavy nuclides describes local isotopic details.

The submesh calculations follow a three-step scheme.

*Step 1 – Full 2D calculation:* The 2D submesh diffusion (or SP3) equations are solved one axial slice at a time, with explicit reflectors.

*Step 2 – Single-Assembly (SA) calculation:* For each assembly, the diffusion (or SP3) submesh equations are solved with zero net-current boundary conditions.

*Step 3 – Renormalization:* The full 2D and single-assembly calculations are used to correct CASMO-5 single-assembly cross sections and discontinuity factors for local leakage effects (details given in Reference 1).

By integrating Eq. 1 over each pin cell of the submesh, “homogenous” pin powers are obtained. To account for the heterogeneity of the submesh, form functions from CASMO-5 are superimposed on the homogeneous powers:

$$P_i = \sum_{g=1}^{G_p} P_{gi}^{CAS} \frac{P_{gi}^{2D}}{P_{gi}^{SA}} \quad (3)$$

where  $P_{gi}^{CAS}$  is the CASMO-5 multi-group pin power form factor and

$$\left. \begin{aligned} P_{gi}^{2D} &= \sum_{g'=G_1}^{G_2} \frac{\kappa_{g's}}{\nu_{g's}} \left( \nu \Sigma_{fg's} + \Delta \nu \Sigma_{fg's} \right) \cdot \phi_{g'i}^{2D} \\ P_{gi}^{SA} &= \sum_{g'=G_1}^{G_2} \frac{\kappa_{g's}}{\nu_{g's}} \nu \Sigma_{fg's} \cdot \phi_{g'i}^{SA} \end{aligned} \right\} \quad (4)$$

Index  $i$  denotes pin cell and  $s$  denotes submesh. The calculation of Eq. 3 can be performed in either the same number of groups used in the submesh solution ( $G_p=G$ ) or in two groups ( $G_p=2$ ).

Axial smearing of different axial enrichment/burnable absorber zones or spacers is avoided by performing explicit pin power reconstruction for each unique axial zone of a node (see the axial homogenization technique in Reference 1). Pin burnups are obtained by explicitly integrating pin powers over time.

The neutron detector response is computed using the reconstructed flux at the detector position:

$$R_n = \sum_{g=1}^G \left[ \sigma_{fg,det}^{CAS} \phi_{g,det}^{CAS} \right] \frac{\phi_{g,det}^{2D}}{\phi_{g,det}^{SA}} \quad (5)$$

The gamma detector responses in BWRs are computed using pin powers of the four surrounding assemblies and pin-power based detector response functions:

$$R_\gamma = D_\gamma^{CAS} \sum_i w_i P_i \quad . \quad (6)$$

The weights  $w_i$  depend on detector-pin distance and angle of view.

### 3. Verification Tests

#### 3.1 B&W Critical Experiments

SIMULATE-4 pin power calculations have been verified using B&W critical cores [5] which provided high quality pin-by-pin fission rate (power) measurements. Relatively large cores (five fuel assemblies in diameter) were built with fresh fuel in two mechanical designs (15x15 fuel with small water rods and 16x16 fuel with large water rods). Fuel assemblies differed in enrichment and the number of gadolinium pins. For several core configurations, each pin in the central assembly was gamma scanned to infer power distributions, and the pin-power uncertainties were very small (~0.5%).

SIMULATE-4 pin power calculations were performed in two, four, and eight energy groups, with data generated from single-assembly CASMO-5 calculations. Results are compared against the six B&W core configurations having measured pin powers, as summarized in Table 1. CASMO-5M results generated with explicit full-core calculations in 16 energy groups are also displayed in Table 1. Detailed pin power distribution comparisons for two of these cores are presented in Fig. 1. Calculated and measured pin powers were normalized to unity in the central assembly. SIMULATE-4 results were generated with eight energy groups in the nodal solution and with pin power form factors described by two energy groups. The SIMULATE-4 calculations and measurements agreed very well, having nearly the same trends as seen between CASMO-5M and measurement.

**Table 1** Summary of B&W criticals: eigenvalue and pin power errors

Core #		1	5	12	14	18	20	Mean ± 1 sigma(pcm)
Fuel Assembly Design		2.46% 15x15 0 Gd	2.46% 15x15 12 Gd	4.02% 15x15 0 Gd	4.02% 15x15 12 Gd	4.02% 16x16 0 Gd	4.02% 16x16 16 Gd	
CASMO-5M	k <sub>eff</sub>	1.00180	1.00079	1.00212	1.00130	1.00336	1.00245	1.00197±90
	RMS(%)	0.51	0.55	0.72	0.73	0.83	0.92	
S4 2 group	k <sub>eff</sub>	1.00250	1.00147	1.00127	1.00137	1.00444	1.00249	1.00226±120
	RMS(%)	0.55	0.58	0.76	0.74	0.87	1.01	
S4 4 group	k <sub>eff</sub>	1.00224	1.00087	1.00040	1.00077	1.00368	1.00200	1.00166±123
	RMS(%)	0.55	0.62	0.76	0.72	0.87	0.98	
S4 8 group	k <sub>eff</sub>	1.00194	1.00049	1.00002	1.00043	1.00336	1.00171	1.00133±125
	RMS(%)	0.55	0.62	0.77	0.71	0.87	0.98	

**Figure 1:** Fission rate (pin power) comparisons for B&W cores 18 and 20

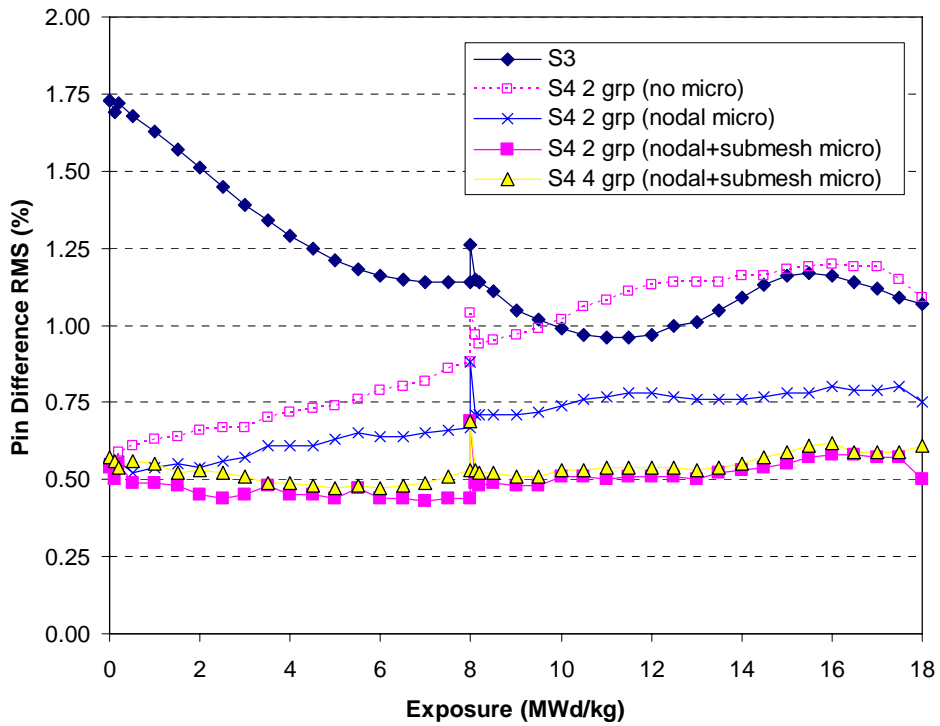
Water		Core 18						Water		Core 20																		
1.21	1.08	Measured (C5-Meas)*100 (S4-Meas)*100						1.28	1.11	Measured (C5-Meas)*100 (S4-Meas)*100																		
0.6	0.8							0.1	0.3																			
0.6	1.1	1.03	1.02	1.07	1.08	1.01	0.17	0.9	0.9	0.6	0.8	-0.4	Gd															
1.03	1.02	1.07	1.06	1.06	1.24	1.04	1.08	1.27																				
0.4	1.2	1.7	-0.5	0.3	-1.2	0.5	0.2	1.0	1.04	1.03	1.07	1.28	1.28	1.08														
0.4	1.3	1.6	-0.2	0.8	-0.7	0.7	0.5	1.1	-0.7	-0.4	-1.1	-2.4	-0.6	0.8														
1.00	1.01	1.23	1.04	1.18	1.17	1.00	1.04	1.03	1.07	1.28	1.28	1.08	-0.6	-0.3	-0.9	-2.4	-0.7	0.9										
0.3	1.8	-1.4	0.96	0.98	1.04	1.18	1.17	1.00	1.02	0.97	0.16	0.97	1.05	0.96	0.16	0.4	-0.4	-0.2	2.8	-0.4	-0.2	-0.2						
0.3	1.9	-1.7	0.4	-0.3	-0.1	-0.6	-0.4	1.3	0.5	-0.6	-0.3	3.0	-0.4	-0.3	-0.3	0.1	-0.1	-0.1	-0.4	-1.1	-0.2	-0.5						
0.98	1.01	1.20	0.4	-0.3	0.1	-0.8	-0.4	1.6	0.5	-0.6	-0.3	3.0	-0.4	-0.3	-0.3	0.1	0.1	0.0	-0.4	-1.2	-0.2	-0.4						
0.6	0.6	-0.1	0.94	0.95	0.96	0.97	0.97	0.92	0.89	1.01	0.98	0.95	1.00	1.00	0.98	0.90	0.93	0.5	0.6	-0.2	0.91	0.91	0.93	0.92	0.91	0.89	0.87	0.83
0.5	0.6	-0.2	0.1	-0.1	-0.1	-0.4	-1.1	-0.2	-0.5	0.9	1.6	0.1	-0.8	0.2	-1.1	1.1	-0.1	0.1	0.1	0.0	0.9	0.5	-1.3	-1.3	-0.9	-0.4	-0.5	0.5
0.96	0.98	1.04	1.18	1.17	1.00	1.3	1.6	1.2	1.4	-0.5	-0.8	0.3	-1.4	0.7	-0.3	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5		
0.4	-0.3	-0.1	-0.6	-0.4	1.3	1.6	0.91	0.98	0.95	1.00	1.00	0.98	0.90	0.93	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5			
0.4	-0.3	0.1	-0.8	-0.4	1.6	0.89	0.87	0.83	1.2	1.4	-0.5	-0.8	0.3	-1.4	0.7	-0.3	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5	
0.94	0.95	0.96	0.97	0.97	0.92	0.89	0.87	0.83	1.2	1.4	-0.5	-0.8	0.3	-1.4	0.7	-0.3	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5	
0.1	-0.1	-0.1	-0.4	-1.1	-0.2	-0.5	0.87	0.83	1.2	1.4	-0.5	-0.8	0.3	-1.4	0.7	-0.3	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5	
0.1	0.1	0.0	-0.4	-1.2	-0.2	-0.4	0.83	0.7	1.2	1.4	-0.5	-0.8	0.3	-1.4	0.7	-0.3	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5	
0.91	0.91	0.93	0.92	0.91	0.89	0.87	0.83	1.2	1.4	-0.5	-0.8	0.3	-1.4	0.7	-0.3	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5		
0.9	0.5	-1.3	-1.3	-0.9	-0.4	-0.5	0.5	1.2	1.4	-0.5	-0.8	0.3	-1.4	0.7	-0.3	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5		
1.0	0.6	-1.2	-1.1	-0.8	-0.3	-0.4	0.7	1.2	1.4	-0.5	-0.8	0.3	-1.4	0.7	-0.3	1.0	0.6	-1.2	1.0	0.9	-1.3	-1.3	-0.9	-0.4	-0.5	0.5		

### 3.2 Mini-Core BWR

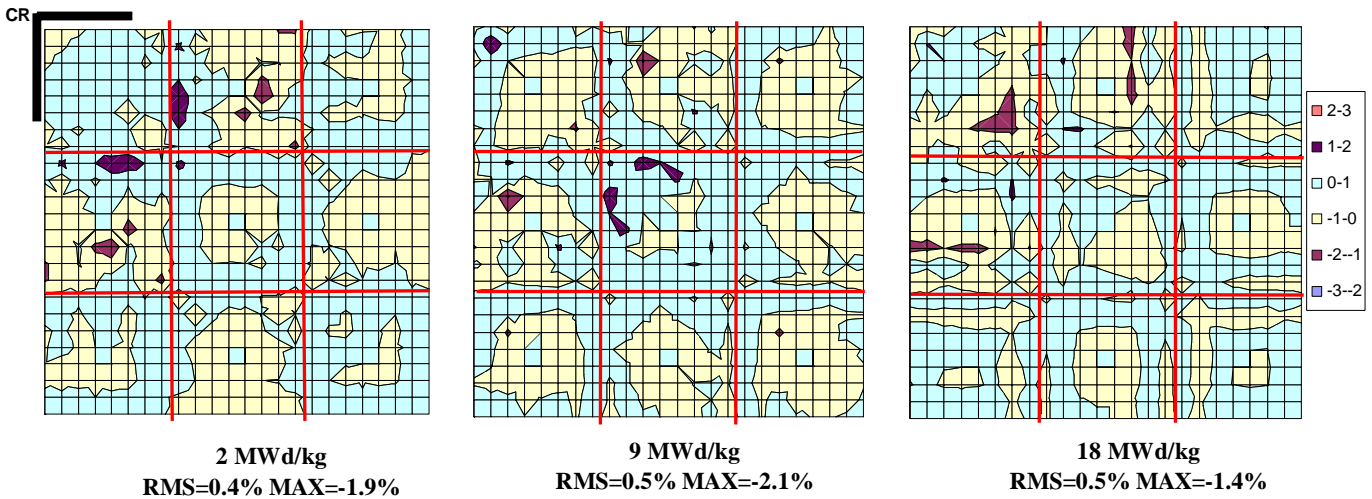
A 3x3 arrangement of BWR 8x8 assemblies was modeled with three fuel types having average enrichments of 1.3 wt%, 2.5 wt% and 3.8wt%, the latter two including Gd<sub>2</sub>O<sub>3</sub> bearing pins. The mini core was depleted with one control rod inserted until 8 MWd/kg and the control rod was then withdrawn for the remainder of the depletion. The reference solution was obtained from CASMO-5M with 16 energy groups. Pin powers were evaluated by SIMULATE-4 with various cross-section models and results were compared to SIMULATE-3 and to the reference CASMO-5M solution.

Results presented in Fig. 2 show that SIMULATE-4 models have reduced errors in BOL pin powers by a factor of three compared to SIMULATE-3. At zero exposure, the improvement in the SIMULATE-4 model clearly comes from more accurate representation of homogeneous pin powers obtained from the submesh flux solution. Fig. 2 also shows that without microscopic cross-section modeling, the accuracy of SIMULATE-4 pin powers degrade with burn-up. Microscopic cross-section modeling (which tracks the node-averaged number densities for approximately 50 isotopes) is necessary for accurately predicting assembly powers [1]. However, the nodal microscopic cross-section model is insufficient for capturing the effect of the control rod - which impacts the local decay/build-up rates of Pu isotopes. When submesh isotope tracking with five actinides was added to the node-averaged isotope tracking, the BOL accuracy is maintained throughout depletion. Addition of more energy groups had no impact on results. Detailed pin-by-pin comparisons at 2, 10 and 18 MWd/kg are presented in Fig. 3. The figures show that errors are fairly evenly distributed across the controlled assembly, i.e.; SIMULATE-4 described the rapidly changing conditions near the control rod.

**Figure 2:** Pin RMS difference  $[(C5-S4) \times 100]$  for a 3x3 BWR core



**Figure 3:** Pin-by-pin comparisons  $[(C5-S4) \times 100]$  for a 3x3 BWR problem

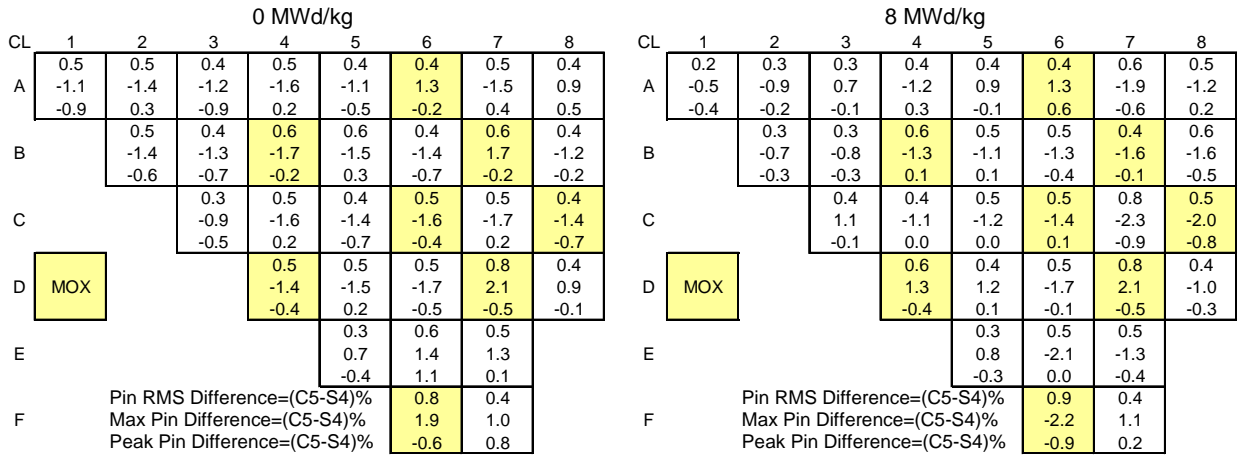


The pin exposures calculated by SIMULATE-4 were also compared against reference CASMO-5M results at 18 MWd/kg core exposure. The RMS difference in pin exposure was 0.12 MWd/kg with the maximum difference of 0.49 MWd/kg at one of the  $Gd_2O_3$  pin locations which was at 9.92 MWd/kg. The error at the peak pin exposure location was 0.15 MWd/kg for a  $UO_2$  pin at 24.38 MWd/kg.

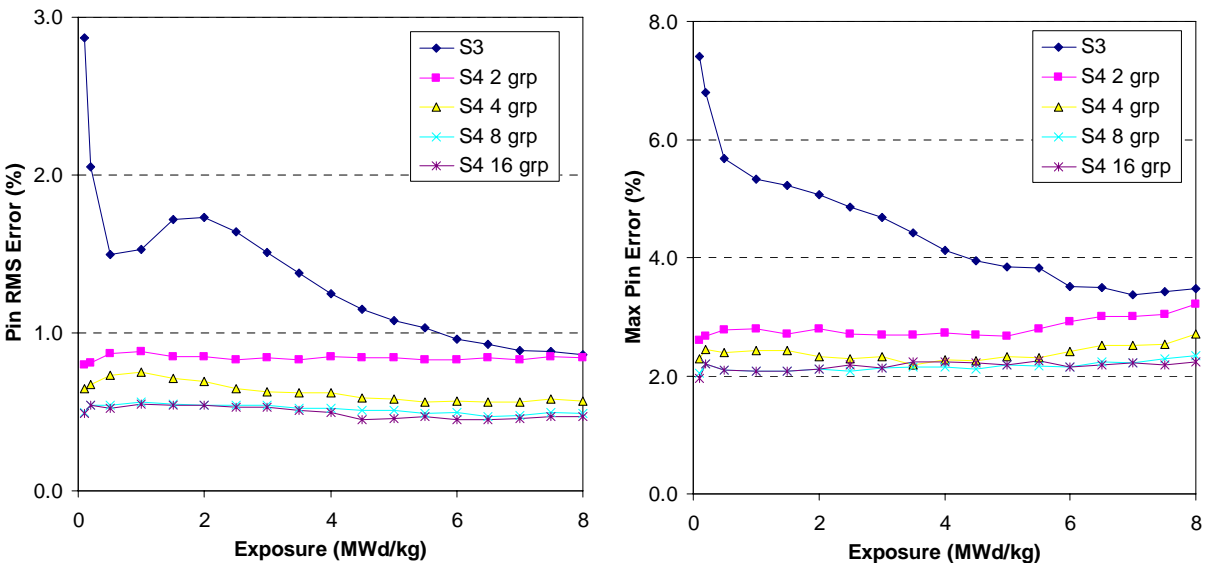
### 3.3 2D PWR MOX Core

A quarter-core PWR with MOX fuel was also analyzed [6], and the reference solution was obtained from quarter-core 2D CASMO-5M calculation performed in 16 groups. The core was depleted to 8 MWd/kg at fixed boron concentration. SIMULATE-4 calculations were performed in 2, 4, 8 and 16 energy groups with the SP3 model. Fig. 4 displays the core configuration and shows the errors (at 0 and 8 MWd/kg) in SIMULATE-4 pin powers for each assembly with the eight-group solution. Fig. 5 presents the core-wide RMS and absolute value of maximum error in SIMULATE-4 pin powers. SIMULATE-4 pin power predictions with four or more energy groups were in excellent agreement with the reference solution, and core-wide pin power RMS was 0.5% and the maximum difference in pin powers was approximately 2% over the entire depletion.

**Figure 4:** PWR 1/8 core assembly pin power distribution error at 0 and 8 MWd/kg (8 group)



**Figure 5:** PWR 1/8 core pin RMS difference and maximum error



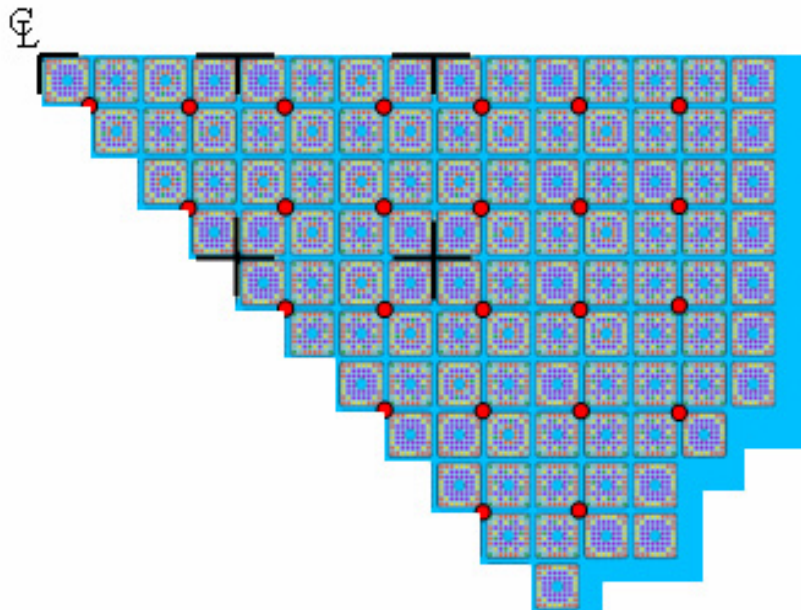
The effect of explicit baffle modeling was studied by treating the baffle/reflector nodes as homogenized (the SIMULATE-3 model). The maximum error in pin powers for peripheral assemblies (such as those at core locations D8 and E7) increased 1-2%, whereas the difference in assembly pin RMSs for the same assemblies was less than 0.2%. No significant impact on the core eigenvalue, relative assembly powers, or pin powers in non-peripheral assemblies was observed. Thus, the effects of explicit baffle modeling are very local.

Results presented in Fig. 4 and 5 were generated using the two-group pin form factors (i.e.,  $G_p=2$  in Eq. 3). A SIMULATE-4 calculation employing eight-group pin form factors produced differences in both maximum and RMS error of less than 0.1%, confirming that two-group form factors are sufficient for capturing the heterogeneity effects - even for this difficult MOX/ $UO_2$  problem.

### 3.4 2D BWR Detector Response Calculations

To verify the accuracy of neutron and gamma detector response calculations in SIMULATE-4, a quarter-core BWR core was considered. The fuel designs were the same as those of the previously mentioned 3x3 mini-core test problem. A reference solution for detector responses was obtained from a 16 energy group CASMO-5M calculation. Detectors were assumed to be located at each narrow-narrow gap, as depicted in Fig. 6. SIMULATE-4 calculations were performed with two, four and eight-energy groups. Core-averaged detector responses were normalized to unity, and a comparison of results are presented in Fig.7. Very good agreement was obtained for both neutron and gamma detectors. These results indicate that there is group sensitivity, as predictions improve when more than two energy groups are used.

**Figure 6:** Core configuration for 1/8 BWR problem





**Figure 7:** Neutron and gamma detector response comparisons for 1/8 core BWR problem

CL	1	2	3	4	5	6	7
A	2.7	2.4	2.2	0.9	0.9	-1.3	-1.0
	0.1	-0.2	0.2	-0.7	1.0	-0.2	-0.2
	0.0	-0.3	0.2	-0.7	1.1	-0.1	-0.4
B		2.1	1.6	0.5	0.2	-1.4	-1.7
		-0.3	-0.3	-0.8	0.5	-0.2	-0.3
		-0.3	-0.4	-0.7	0.4	-0.1	-0.1
C			1.7	0.2	0.7	-2.0	-1.5
			0.5	-0.2	1.5	-0.6	-0.6
			0.5	-0.2	1.5	-0.5	-0.9
D				0.3	-0.9	-1.9	-0.8
				0.9	0.2	-0.4	0.0
			RMS(%)	1.2	0.2	-0.3	-0.1
(C5-S4 2grp) %			1.4		-0.3	-0.6	
(C5-S4 4grp) %			0.6		1.0	0.2	
(C5-S4 8grp) %			0.6		1.2	0.1	

**Neutron Detectors**

CL	1	2	3	4	5	6	7
A	2.4	2.2	1.8	0.7	-0.4	-0.5	-0.9
	-0.2	-0.4	-0.3	-0.8	-0.4	0.6	0.2
	-0.2	-0.3	-0.3	-0.8	-0.3	0.7	0.0
B		2.1	1.2	0.6	-0.9	-0.4	-1.1
		-0.4	-0.8	-0.8	-0.8	0.8	0.4
		-0.3	-0.7	-0.6	-0.8	0.9	0.3
C			0.8	-0.4	-0.8	-0.8	-1.1
			-0.5	-0.9	-0.1	0.5	0.1
			-0.5	-0.8	0.0	0.6	-0.2
D				1.0	0.0	-0.8	-0.8
				1.4	1.0	0.7	-0.1
			RMS(%)	1.7	1.1	0.6	-0.3
(C5-S4 2grp) %			1.1		0.3	-0.8	
(C5-S4 4grp) %			0.7		1.6	0.1	
(C5-S4 8grp) %			0.7		1.5	-0.2	

**Gamma Detectors**

## 4. Conclusion

The new pin power reconstruction methodology based on a submesh model has been implemented in SIMULATE-4. The model has been verified against the B&W criticals and higher-order CASMO-5M transport solutions. The multi-group model captures instantaneous spectral effects, and the submesh actinide tracking model captures exposure-induced variations near node interfaces and control rods. Excellent agreement in pin powers are obtained for difficult problems - such as BWRs with control rods inserted and MOX/ $UO_2$  loaded PWRs. More accurate pin powers also translate into more accurate pin exposures and detector responses. Extensive core follow testing of CASMO-5/SIMULATE-4 is currently in progress.

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