

## SIMULATE-4 developments

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### Abstract

This paper details the new thermal-hydraulics and shutdown margin calculation modules of Studsvik Scandpower's next generation nodal code, SIMULATE-4.

SIMULATE-4's BWR thermal-hydraulics (TH) models an entire vessel loop: core, chimney (for natural circulation reactors), upper plenum, standpipes, steam separators, down comer, re-circulation pumps, and lower plenum. The PWR thermal-hydraulics models the region from lower to upper tie plate. The core portion of the TH models of PWR and BWRs are treated essentially identically, with each assembly having an active channel and a number of parallel water channels. In each axial node of a channel, the total mixture mass, steam mass, mixture enthalpy, and mixture momentum balance equations are solved. The 3-D fuel temperatures are evaluated in the TH module by solving the radial heat conduction equation for the average pin of each node. The BWR assembly may be divided into four radial sub-channels. Assembly or nodal cross flow is allowed for PWRs.

A new three-dimensional shutdown margin (SDM) method based on "mini-core" concept has been developed in SIMULATE-4. "Mini-core" geometry is used as a fast screening tool where full 3D calculations are performed for those rods identified with SDM smaller than the user's input criteria.

Various numerical test results are presented to illustrate improvements with each module.

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### 1. Introduction

SIMULATE-4 (Bahadir et al, 2005, Bahadir and Lindahl, 2006) is Studsvik Scandpower's next generation nodal code, which has been developed to address deficiencies of existing reactor physics tools for today's advanced core designs with increased heterogeneity and aggressive operating strategies.

The code is based largely on true physics and true geometry. The major features of the neutronics of SIMULATE-4 are:

- Arbitrary number of energy groups
- Diffusion or simplified  $P_3$  transport equations
- Cross sections evaluated with a microscopic depletion model with 50 heavy nuclides and fission products
- Axial heterogeneities treated explicitly

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- Fuel assemblies divided into heterogeneous radial sub-meshes, eliminating shortcomings of traditional assembly-averaged cross sections/discontinuity factors and quadratic transverse leakage approximations
- Pin powers, pin burnups, and detector signals based on superposition of lattice code pin powers and sub-mesh fluxes.

Multi-group cross sections and physics data for SIMULATE-4 are generated with the CASMO-5 lattice physics code (Rhodes et al, 2006), which uses an ENDF/B-VII library.

The details of the neutronics solver along with the pin power reconstruction can be found in Bahadir et al, 2005 and Bahadir and Lindahl, 2006.

This paper describes the latest SIMULATE-4 developments in thermal hydraulics and shutdown margin modules.

## 2. Thermal Hydraulics

The purpose of the thermal hydraulics module of SIMULATE-4 is two-fold:

1. To provide quantities essential for other modules of the core simulator like fuel temperature and coolant density distributions used in the cross section evaluation and coolant flow needed by thermal margin calculations.
2. To provide information about the static thermal hydraulic state of the reactor and components of interest to those studying the core and designing its fuel assemblies.

The thermal-hydraulic module can be executed as a stand-alone module, in which case the external power distribution is described via user input, or as part of a complete core analysis including neutronics.

### 2.1. BWR Thermal-Hydraulics

The SIMULATE-4 BWR thermal-hydraulics (TH) models the entire vessel loop: core, chimney (for natural circulation reactors), upper plenum, stand pipes, steam separators, steam dome, upper and lower down comer, re-circulation pumps, and lower plenum.

Each assembly of the core is analysed in detail. The assembly consists of a number of parallel flow

channels (active coolant, water rod(s)), which are treated individually.

The bypass gaps between the fuel assemblies are, at the user's discretion, lumped into zones. Thus, the two extremes of the lumping are a) all gaps constitute one bypass channel and b) each assembly is surrounded by its own bypass channel. The bypass flow is assumed to be one-dimensional, i.e. there is no radial cross flow.

In addition to the ordinary axial nodalisation, (typically 25 nodes per channel), the conventional nodes are axially divided into subnodes such that each is materially homogeneous. For each subnode, the average power is known from the 3-D global neutronic solution. This power constitutes the feedback from the neutronics to the thermal hydraulics.

SIMULATE-4 offers as an option a TH evaluation of each quarter-bundle of a BWR assembly. First, the full assembly is analysed in the "conventional" manner. Results from this analysis are used as boundary conditions (total assembly inlet flow, water rod flow conditions) to evaluate each quarter bundle (e.g., Q-bundle).

For each type of assembly, the user specifies one of three alternatives to handle cross flow:

1. Closed Q-assemblies (no cross flow): The Q-channel flow rates are adjusted until the total pressure drop of the sub-channels are identical. This option may be used for the SVEA fuel of Westinghouse.
2. Cross flow driven by the lateral pressure difference: Lateral momentum equation (Eq. 1 below) is employed to compute cross flow, with turbulent mixing and void drift effects assumed to be negligible. At the bundle inlet, all four Q-channel flow rates are equal. This ad hoc assumption is justified by the fact that whatever incorrect inlet distribution exists will quickly disappear a few nodes up the assembly.
3. Cross flow driven by the lateral pressure difference: The cross flow is adjusted such that the pressure is equalized at each of the four node outlets at every axial level.

The numerical difference between these three options with respect to internal density distribution is very minor. This is explained by the fact that the difference in void and density between the Q-assemblies is mainly power driven and not so much affected by the cross flow. Especially, options 2 and 3 are close. Option 3, which is less physical than

option 2, is offered since it has superior convergence properties.

For options 2 and 3, the dispersing effect of spacers is also included in the cross flow calculation.

The lateral flow rate  $w_{ij}$ , of option 2, between sub-channels  $i$  and  $j$  is governed by the transverse momentum equation

$$\frac{\ell}{s \Delta z} \frac{\partial(u_{ax} w_{ij})}{\partial z} + k \frac{1}{2 \rho_l} \frac{w_{ij} |w_{ij}|}{S_{ij}^2 \Delta z^2} \phi^2 = p_i - p_j \quad (1)$$

where

- $p_i$  - Pressure of channel  $i$
- $u_{ax}$  - Axial coolant speed of donor channel
- $\phi^2$  - Two-phase multiplier
- $\Delta z$  - Node height
- $s / \ell$  - Pin separation distance / Cross flow lateral reach
- $S_{ij} \Delta z$  - Cross flow area between channels  $i$  and  $j$
- $k$  - Lateral loss coefficient.

Substantial differences in coolant conditions between quarter-channels appear wherever there are strong radial power gradients within an assembly. This happens, for instance, in controlled bundles and at the core periphery.

## 2.2. PWR Thermal-Hydraulics

The PWR thermal-hydraulics models the core region only from lower to upper tie plate.

The BWR and PWR cores are treated essentially identically, with each assembly having an active channel and a number of parallel water channels.

SIMULATE-4 offers two ways of computing the PWR assembly flow distribution. The most accurate one is via the cross flow model described later. An approximate '1D' method is based on the assumptions

- No cross flow.
- Equal pressure drops for all assemblies.
- Zero power when computing pressure drops for the flow evaluation. This is done to avoid complications if voiding occurs.

With such a model, differences in flow rate between assemblies are mainly due to different spacer properties.

The optional PWR cross flow calculation of SIMULATE-4 follows the 'conventional' TH analysis with the 1D model.

The cross flow model is close to that of the COBRA IIIC code (Rowe, 1973) with balance equations for flow rate, energy, axial momentum, and lateral momentum.

The following assumptions are made:

1. Any cross flow is driven by lateral pressure imbalance. Turbulent mixing and void drift effects are negligible.
2. The channel inlet flow rate is given either by the 1D flow results or by a fixed flow distribution. The core inlet cross flow is zero.
3. All channels have the same outlet pressure. There is no attempt to equalize pressures at the bottom of the channels.
4. Water rod flow rates are not affected by the cross flow analysis.
5. The cross flow has the same liquid/steam composition as the coolant of the donor channel.

The cross flow option is typically not used for routine PWR calculations, but may be employed for special studies like fuel assembly entrance blockages (see Section 4.3).

Any deviation in PWR flow rates from a uniform distribution has minor impact on the neutronics (unless there is voiding at the top of the core). The importance of a correct flow rate lies in DNB calculations. SIMULATE-4 offers a DNB evaluation based on the Doroshuck correlation (Doroshuck 1975).

## 2.3. Equations

For each node of the reactor vessel, requirements have to be met regarding mass, energy, and momentum balance. Basically, SIMULATE-4 has a drift flux formulation with total flow rate, vapour flow rate, liquid/vapour mixture enthalpy, and local pressure as primary variables. Knowing mass flow, enthalpy, and pressure at the inlet of a node, the balance requirements determine the values of corresponding parameters at the node outlet.

In the most general case, the flow paths in and out of a node are illustrated in Figure 1. Because of the subnode concept, where each subnode has materially and geometrically unique characteristics, water rod inlets and outlets will occur at the node

lower and upper boundaries. Any cross flow is assumed to enter/leave at the node vertical side midpoints.

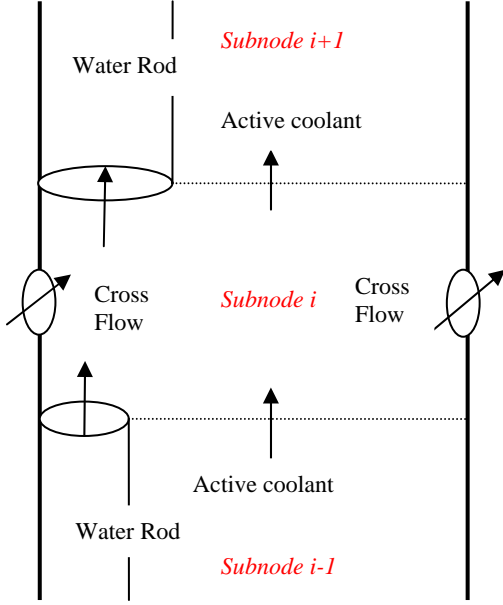


Fig. 1. Node flow paths.

Correlations are used to determine flow quality, void fraction, two-phase friction multipliers, and heat transfer coefficients. A library, easy to amend, exists for these functions. For each assembly type, the user may specify which correlations to use.

The power of a bypass or a water rod node is built up via two mechanisms; heat conduction through the box/water rod wall and through direct gamma/neutron heating. By solving the one-dimensional heat conduction equation, the power of the bypass (or water rod) node is found to be

$$Q_{bp} = \gamma_{bp} \cdot Q_{fis} + \gamma_{box} Q_{fis} h_{tot} \left( \frac{d_{box}}{2\lambda_{box}} + \frac{1}{h_{act}} \right) + h_{tot} (T_{act} - T_{bp}) A_{box} \quad (2)$$

$$\frac{1}{h_{tot}} = \frac{1}{h_{act}} + \frac{d_{box}}{\lambda_{box}} + \frac{1}{h_{bp}} \quad (3)$$

$$\gamma_x = a_x + b_x \rho_{act} \quad (4)$$

where

- $Q_{fis}$  - Fission power of node
- $\gamma_x$  - Fraction of fission power radiated to region  $x$
- $a_x, b_x$  - Assembly type dependent coeff.
- $\rho_{act}$  - Active coolant density
- $T_x$  - Coolant temperature of region  $x$
- $d_{box}, A_{box}$  - Box wall thickness and surface area
- $\lambda_{box}$  - Box wall conductivity
- $h_x$  - Dittus-Boelter heat transfer coeff.

The fuel bundle lift force is also calculated as part of the pressure calculations.

#### 2.4. Flow Distributions

The flow split between fuel assemblies and between active flow and water rods within an assembly is obtained by requiring that the pressure drop shall be equal for parallel channels. The simple observation that the total pressure drop along a channel has two components, one that is proportional to the square of the flow rate and one that is constant (the elevation pressure drop),

$$\Delta p_{tot} = coeff \cdot w^2 + \Delta p_{elev} \quad (5)$$

provides a mechanism for adjusting the flow rates.

#### 2.5. Fuel Temperature Model

The 3D fuel temperature distribution is evaluated in the TH module by solving the one-dimensional, annular heat conduction equation for the average fuel pin of each node.

The thermal hydraulics module provides the temperature of the coolant surrounding the pin. This serves as the boundary condition for the fuel temperature calculation.

The heat conduction equation for the fuel pellet is (Lahey, 1993)

$$\frac{1}{r} \frac{\partial}{\partial r} r k_f \frac{\partial T}{\partial r} + Q = 0 \quad (6)$$

$T$  is the radial temperature distribution array,  $k_f$  is the fuel thermal conductivity and  $Q$  represents the heat sources. A similar equation is solved for the heat conduction in the cladding.

The fuel and cladding thermal conductivities are temperature and burnup dependent. Temperature dependent conduction properties for  $\text{UO}_2$  are tabulated based on data sets from the Nuclear Fuel Industries as described in Lanning, et al, 2005. The gap conductance model is taken from the fuel performance code INTERPIN-4 (Hagrman, et al 2007) and it is functionalized versus exposure and temperature. The following physical effects for the gap are modelled: (a) fuel pellet cracking, (b) fuel pellet irradiation swelling, (c) fuel pellet and clad thermal expansion, (d) clad compression caused by irradiation at high temperature and (e) gas gap composition changes as a result of fission gas release.

The radial distribution of the volumetric heat source in the pellet is dependent on the fuel depletion. The intra-pellet radial power profiles, as a function of rod burnup, have been computed with CASMO-5 for typical  $\text{UO}_2$  pins with 4.5% enrichment and for reactor grade MOX pins. The data is evaluated based on the pellet average exposure by interpolating in pre-computed tables. The intra-pellet power distribution of the heat source peaks at the outer edge of the fuel pin, with exposure-dependent relative peaking values.

The convective heat transfer coefficient is determined from one of the different possible modes of heat transfer according to classical boiling formulation: (a) single phase liquid forced convection, (b) nucleate boiling, (c) transition boiling, (d) film boiling, and (e) single phase vapour forced convection.

### 3. Shutdown Margin Calculations

Since hundreds of shutdown margin (SDM) calculations need be performed for different core configurations, fast running and accurate methods are essential. Traditionally, two-dimensional methods have been used for SDM evaluations either as a main engine for such calculations or as a screening tool for determining the limiting rods for which the three-dimensional methods are to be employed. However, aggressive fuel designs with axially varying burnable absorbers, enrichment, and part-length fuel rods introduce significant error in two-dimensional shutdown margins models. Accordingly, a three-dimensional shutdown margin method based on “mini-core” concept has been developed in SIMULATE-4.

This method is based on the observation that the neutron flux near the withdrawn control rod decreases rapidly in the radial direction, causing the shutdown margin evaluation to be a local phenomenon. SIMULATE-4 employs the following shutdown margin computational strategy:

1. For the region around the evaluated control rod, a 3D mini-core is constructed. The SDM is computed by a fast scanning method which solves the two-group diffusion equation by assuming the buckling within each node to be isotropically distributed in the x, y, and z directions. Hence, the problem of evaluating a transverse leakage and its shape does not appear. The scanning method has an accuracy of a few hundred to one thousand pcm.
2. If the flux does not decrease as rapidly as expected, an enlarged mini core is defined and re-evaluated.
3. If the mini-core SDM exceeds a user-specified threshold, the SDM is accepted and the next control rod is evaluated.
4. Otherwise, the mini-core SDM is re-evaluated with the Analytic Nodal Method (ANM).
5. If the ANM based SDM is less than a second user-specified threshold, a full-core SIMULATE-4 SDM calculation is performed.

## 4. Numerical Testing

### 4.1. Void in Four BWR Sub-Channels

A test of BWR TH models is presented for an assembly with a 64% inserted control rod. In such a case, the power is highly peaked towards the detector corner of the assembly, and intra-bundle cross flow is computed. The resulting void distributions in the four sub-channels are shown in Figure 2. At the tip of the control rod, the void in the sub-channel adjacent to the rod is 14 %, while it is 54 % in the detector quadrant.

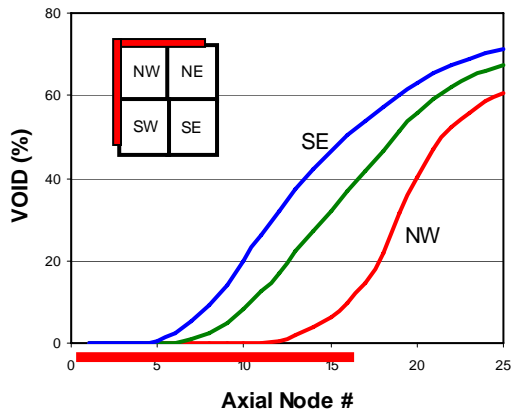


Fig. 2. Void profiles in a controlled BWR assembly.

When the same assembly is modelled assuming non-communicating channels, one obtains results fairly close to those of Figure 2. Thus, one concludes that the flow is essentially one-dimensional, and the quadrant voids are principally determined by the sub-assembly power distributions.

Modelling of a BWR assembly as four sub-channels has an important impact on the local pin power predictions. Figure 3 presents the % difference in pin powers for four different pins for the same assembly with and without the sub-channel modelling. The difference is significant, ~10%, for pin(1,1) which is located next to the control rod.

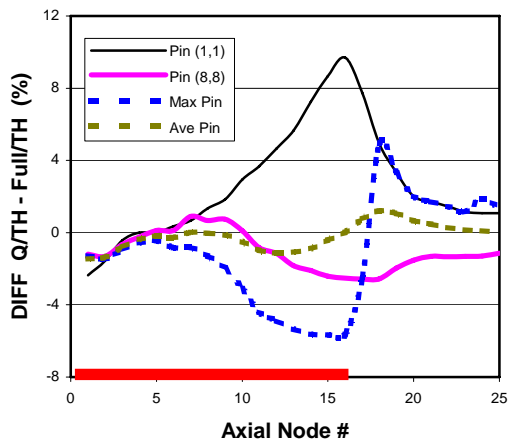


Fig.3. Difference in pin powers for a controlled BWR assembly with and without Q-channel TH modelling

#### 4.2. PWR cross flow and 1D flow models

Assembly average flow rates for a PWR core with fuel assemblies with mixed spacer types are calculated with

1. Channel cross flow (reference solution)
2. Uniform assembly flow distribution
3. The 1D flow model.

The resulting flow distribution and the deviations from the reference solution for the two approximate methods are shown in Figure 4. Obviously, the 1D method, with a maximum error of 1.6 kg/s, is superior to the uniform approach, which has a maximum error of 8.0 kg/s.

86.4	77.0	86.9	76.8	86.9	76.8	77.7	78.6
6.7	-2.8	7.2	-2.9	7.2	-2.9	-2.0	-1.1
-0.1	1.3	-0.6	1.5	-0.6	1.5	0.5	-0.4
76.9	76.9	77.1	77.9	77.9	78.5	77.8	79.0
-2.8	-2.8	-2.6	-1.8	-1.8	-1.2	-1.9	-0.7
1.3	1.3	1.1	0.3	0.3	-0.3	0.5	-0.8
86.8	77.1	77.1	87.5	77.4	78.5	79.0	
7.1	-2.6	-2.6	7.7	-2.3	-1.2	-0.7	
-0.5	1.2	1.1	-1.1	0.9	-0.3	-0.8	
76.8	77.9	87.3	77.3	87.6	77.8	79.6	
-3.0	-1.8	7.6	-2.4	7.9	-1.9	-0.1	
1.5	0.3	-1.0	0.9	-1.3	0.4	-1.4	
86.9	77.9	77.4	87.8	77.7	79.2		
7.2	-1.8	-2.3	8.0	-2.1	-0.5		
-0.6	0.4	0.9	-1.4	0.6	-1.0		
76.7	78.5	78.4	77.9	79.2			
-3.0	-1.3	-1.3	-1.8	-0.5			
1.6	-0.3	-0.2	0.4	-1.0			
77.6	77.6	79.0	79.5				
-2.1	-2.1	-0.8	-0.2				
0.6	0.6	-0.8	-1.4				
78.2	87.8						
-1.5	8.0						
0.0	-1.5						

Ref = Cross Flow (kg/s)  
Uniform - Ref.  
1D - Ref.

Fig. 4. Flow rates in PWR core with different spacers.

#### 4.3. Flow Blockage in a PWR

A test of PWR cross-flow is presented by simulating a flow blockage of an assembly in the core. Coolant flow rate for each axial node obtained from no-blockage case is compared to a case when inlet flow of an open channel assembly is restricted to 1% of its normal value. Coolant is quickly sucked into the channel from surrounding assemblies. One

meter up the channel the effect of the blockage has essentially disappeared, as illustrated in Figure 5.

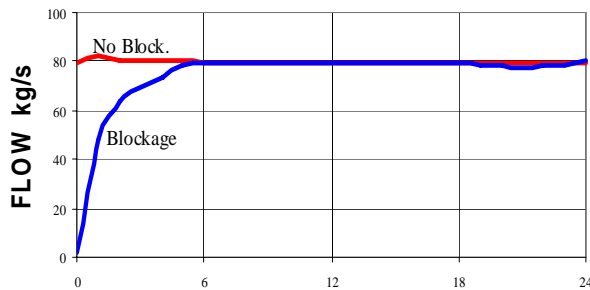


Fig. 5. Flow blockage in a PWR assembly.

#### 4.4. SDM calculations

Shutdown margins for a typical BWR core have been computed using mini-cores with 10×10 assemblies. A reference solution has been found by employing a full-core SIMULATE-4 model (32×32 assemblies). Table 1 compares the  $k_{\text{eff}}$  calculated for mini-cores with the Isotropic Buckling and the Analytical Nodal Models (ANM) against the reference full core ANM. Figure 6 compares the calculated SDMs for each control rod in the lower right quadrant of the core. The maximum error of the mini-core SDMs is 0.69%. This occurs at the core periphery, where the margin is anyhow large. The mini-core execution time is a factor of 50 smaller than that of the reference calculation.

## 5. Conclusions

SIMULATE-4 provides an accurate description of the thermal hydraulics behaviour of BWR and PWR cores by modelling fluid flows in various leakage paths, vertical channels, and horizontal cross flow channels. The radial void distribution within BWR assemblies is also calculated.

SIMULATE-4 accurately computes shutdown margins by using a fast-running model that closely reproduces direct full-core SDM evaluations. All axial bundle complexities are treated with a three-dimensional model.

With all the major neutronic and thermal-hydraulics modules of SIMULATE-4 now complete, extensive validation/benchmarking studies of operational core-follow analysis of both BWRs and PWRs are underway.

Table 1. Shutdown Margin Comparison: Full Core Analytical Nodal Model (ANM) versus Mini Core ANM and Isotropic Buckling Models

Rod		Mi	Full Core		Mini	Mini
I	J	Co	SDM	ANM	ANM	IsoBuck
		Siz	(%)	$k_{\text{ref}}$	$k_{\text{eff}}-k_{\text{ref}}$	$k_{\text{eff}}-k_{\text{ref}}$
					(pcm)	(pcm)
12	9	10	0.81	0.98122	27	-42
11	9	10	1.33	0.97611	21	-99
8	8	10	1.38	0.97566	11	-119
12	8	10	1.74	0.97222	29	-84
11	10	10	1.79	0.97177	12	-127
10	9	10	1.80	0.97166	25	14
11	8	10	2.30	0.96693	16	-142
13	10	10	2.32	0.96671	23	1
10	10	10	2.46	0.96539	4	-199
11	14	10	2.47	0.96529	7	-4
12	10	10	2.48	0.96522	29	-131
11	11	10	2.52	0.96482	20	-92
12	11	10	2.72	0.96296	40	-14
12	13	10	2.78	0.96234	4	1
9	8	10	2.98	0.96047	-31	-112
12	14	10	2.99	0.96044	-5	222
13	9	10	2.99	0.96038	4	-48
9	13	10	3.01	0.96023	4	-49
10	14	10	3.13	0.95916	12	-50
10	8	12	3.29	0.95765	23	47
13	11	10	3.40	0.95658	-7	-170
9	9	12	3.41	0.95655	45	35
12	12	12	3.69	0.95394	35	69
13	8	12	4.17	0.94956	-1	-66
14	9	12	4.18	0.94945	-9	-47
14	8	12	4.58	0.94582	-99	-132
13	13	12	4.65	0.94520	-106	59
15	8	26	4.74	0.94441	-63	283
15	9	26	4.75	0.94427	-51	216
15	10	26	4.80	0.94380	-96	104
15	11	26	4.86	0.94331	-179	-236
Average					-10	-10
Min Diff					-179	-236
Max					45	283

Fehler!							
1,38	2,99	3,30	2,31	1,76	4,19	4,59	4,78
1,37	3,02	3,27	2,29	1,73	4,19	4,71	5,17
-0,01	0,03	-0,03	-0,02	-0,03	0,00	0,12	0,39
2,98	3,41	1,80	1,36	0,88	3,01	4,19	4,76
3,02	3,36	1,78	1,34	0,85	3,00	4,20	5,07
0,04	-0,05	-0,02	-0,02	-0,03	-0,01	0,01	0,31
3,29	1,80	2,46	1,80	2,50	2,32	3,12	4,80
3,26	1,77	2,46	1,79	2,47	2,30	3,11	5,17
-0,03	-0,03	0,00	-0,01	-0,03	-0,02	-0,01	0,37
2,30	1,33	1,79	2,52	2,72	3,40	2,47	4,86
2,28	1,31	1,77	2,50	2,68	3,41	2,46	5,55
-0,02	-0,02	-0,02	-0,02	-0,04	0,01	-0,01	0,69
1,74	0,81	2,48	2,72	3,69	2,78	2,99	
1,71	0,78	2,45	2,67	3,65	2,78	2,99	
-0,03	-0,03	-0,03	-0,05	-0,04	0,00	0,00	
4,17	2,99	2,32	3,40	2,80	4,65		
4,17	2,99	2,29	3,41	2,80	4,77		
0,00	0,00	-0,03	0,01	0,00	0,12		
4,58	4,18	3,14	2,52	3,03			
4,69	4,19	3,13	2,51	3,03			
0,11	0,01	-0,01	-0,01	0,00			
4,74	4,75	4,80	4,86	Full Core ANM SDM (%)			
5,04	5,06	5,17	5,53	Mini Core ANM SDM (%)			
0,30	0,31	0,37	0,67	Diff (Mini-Full)			

Fig. 6. SDM Comparisons for a BWR quarter-core

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