

## Parameterization of nuclear cross-sections for coupled neutronic-thermalhydraulic codes

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### Abstract

The present work consists of developing an in-house methodology, called SIMTAB, to characterize, in a simplified way, the reactor core of LWR Nuclear Power Plants. Specifically, a cross-sections and kinetic parameters set are obtained as a function of the prompt and control variables. So that, the core can be modeled using a limited number of neutronic regions, in such a way that the reactor kinetic behavior is properly characterized. This simplification of the reactor core permits, from an operative point of view, the use of few cross sections data sets in coupled 3D neutronic-thermalhydraulic codes.

**KEYWORDS:** *Nuclear cross-sections homogeneization, Nuclear cross-sections functionalization, 3D coupled codes.*

### 1. Introduction

Neutronic and coupled neutronic-thermalhydraulic codes have limited computational capability, for instance, they have to use a reduced number of neutronic compositions data. In order to satisfy this necessity we developed a methodology to characterize the reactor core of light water reactors (LWR) in a simplified way using a small number of neutronic compositions. Specifically, we obtain a cross-sections set as a function of the prompt thermodynamic and control variables.

This methodology uses data provided by CASMO4/SIMULATE3 code [1][2]. Calculations are performed in core average conditions and the data obtained are used to tabulate the cross-sections in terms of the exposure. It is important to model the cross sections in terms of local properties of the fuel elements: water density (void fraction), fuel temperature, exposure, control rod fraction, etc.

Cross-sections dependences are determined by means of CASMO4 burnup code following, the structure shown in Tab. 1.

The real concentration of nuclides and therefore the cross-section in any node depend on the previous conditions of this node during the exposure historic of the core. So, it is necessary for nodal codes to consider the effects on the exposure and the dependences on the other parameters. This can be achieved solving the equations of the nuclides exposure in each node of the reactor model and tabulating the microscopic cross sections as a function of the state variables: fuel temperature, moderator density (void fraction), control rod fraction and boron concentration. The dependences of the macroscopic cross-sections with the historic of the variables are determined using CASMO4 code by means of exposure calculations in each fuel element for different historic allowing the functionalization of them.

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However, SIMULATE3 uses an indirect method for the treatment of the isotopes in the nodes, using a model of the historic that preserves the list of the state variables depending on the exposure. For example: historic of the moderator density, boron concentration, etc. The macroscopic cross sections for each node behave as function of the historic of the state variables.

**Table 1:** Stationary points calculation conditions depending on the exposure (Mwd/kg).

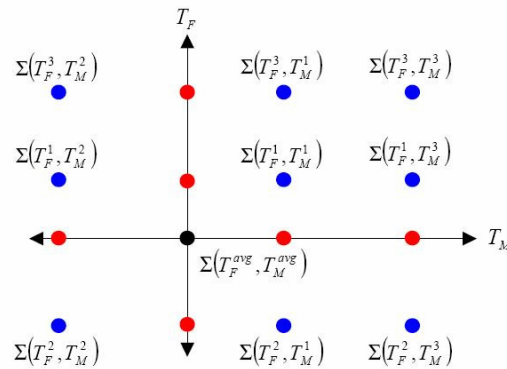
Condition	Branch or Depletion	Stationary calculus points							
		0.0	0.5	1.0	2.0	5.0	7.5	10.0	12.5
BOR High TMO Medium TFU Medium	Depletion	X	X	X	X	X	X	X	X
TMO High	Branch	X				X		X	.....
BOR High	Branch	X				X		X	.....
BOR Medium TMO Medium TFU Medium	Depletion	X	X	X	X	X	X	X	X
TMO Low	Branch	X				X		X	.....
BOR Low	Branch	X				X		X	.....
TFU Low	Branch	X				X		X	.....
CRD Inserted	Branch	X				X		X	.....
BOR Medium TMO Low TFU Medium	Depletion	X	X	X	X	X	X	X	X
	Exposure (Mwd/kg)	0.0	0.5	1.0	2.0	5.0	7.5	10.0	12.5
where	TMO is the water density TFU is the fuel temperature BOR is the boron concentration CRD is the control rod insertion HTMO is the moderator temperature historical HBOR is the boron historical								

## 2. Parameterization of the cross sections

The cross-sections generation has been calculated by means of the simultaneous variation of various thermalhydraulic parameters in SIMULATE3 following the methodology developed in PSU [3].

Fig. 1 shows the origin of the value of the cross sections obtained for averaged values of the local variables (exposure, control rod insertion (yes or not), historic, boron concentration, moderator temperature and fuel temperature) and around of this value it has been generated variations of the cross-sections by means of the perturbation of the moderator temperature and fuel temperature. This terms are named "Cross Term Cross-Sections" and they have a 2D dependence that can be generalized to a 4D dependence when also includes the perturbation of boron concentration and control rod insertion.

**Figure 1:** Origin of the cross section values from local variables.



### 3. Implementation of the methodology

The nuclear parameters code generator has been called SIMTAB [4]. This code uses the function AUDIT of SIMULATE3 to obtain the cross-sections.

Fig. 2 shows the process of generating the cross-sections set used by this computer code.

The unique input deck needed by this program is the file *DECISIO* that contains the exposure criterion that the user imposes in function of exposure differences to distinguish two fuel elements segments. Another data that the user has to introduce is the number of axial neutronic regions that consider different and the variation range of fuel temperature and moderator density in which the obtained tables are valid.

The output files are *nemtab* and *nemtabr* which contain the cross-sections for rodded and unrodded conditions respectively, as function of the moderator density and fuel temperature.

The methodology runs in UNIX (64 or 32 bits), LINUX and PC platforms. The calculation to obtain 4500 compositions takes approximately seven minutes of real time in a LINUX platform (64 bits) against a time of 30 minutes that takes in a PC platform. In both platforms the Intel<sup>®</sup> Fortran 90 compiler has been used.

## 4. Results and discussion

### 4.1 Steady state neutronic calculations

In the process of a transient simulation by 3D neutronic-thermalhydraulic codes it is essential to obtain an accurate steady state characterization of the reactor. For that purpose, it is necessary to obtain a simplified core with the thermalhydraulic codes RELAP/PARCS [10] and RELAP/VALKIN [6][7] coherent with the core of the stationary coupled neutronic-thermalhydraulic code SIMULATE3. The obtained core should be the most simplified core that can be obtained and adjusted at the specific point of analysis and it should characterize the behaviour and the neutronic state of the core in that starting point.

Therefore, we studied different LWR cores in order to test the SIMTAB methodology.

We compare the results from the neutronic modules PARCS and VALKIN with the ones from SIMULATE3.

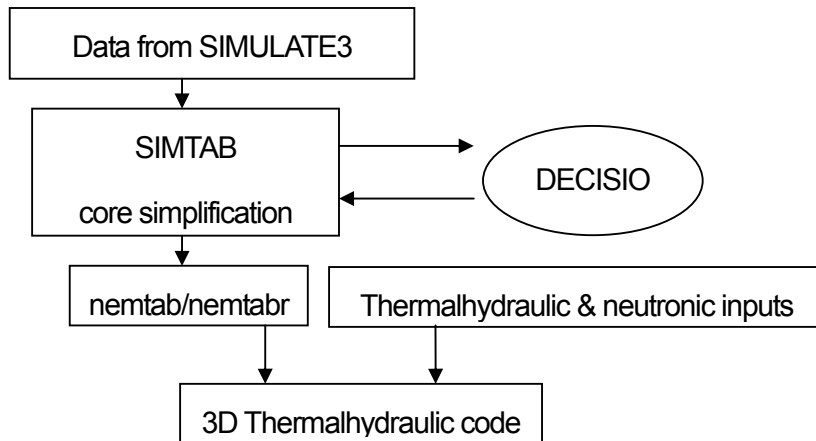
The first case studied corresponds to hot zero power (HZP) at BOC conditions for a very homogeneous case in a PWR: Almaraz NPP.

Tab. 2 shows the values of the effective  $k_{eff}$  for different simulations. The number of compositions depends on the exposure criterion that the user imposes. The different power

axial power profiles computed with VALKIN code for the HZP core for different neutronic compositions appears in Fig. 3.

The  $k_{eff}$  values have been obtained using the VALKIN code in a stand-alone run in conditions of HZP. As we can see the results are very similar, being the differences in  $k_{eff}$  and axial profile between SIMULATE (all compositions) and the VALKIN code (few compositions) very small.

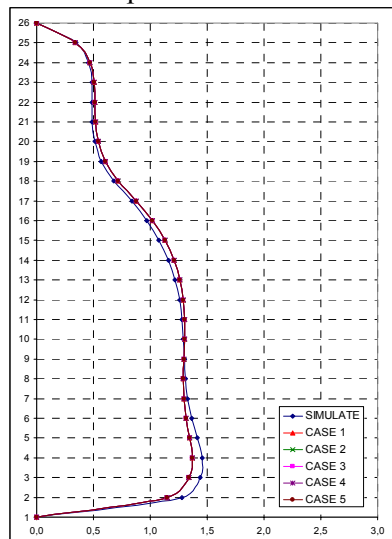
**Figure 2:** SIMTAB Methodology.



**Table 2:** Values of  $k_{eff}$  of different simulations of Almaraz NPP.

CASES	$k_{eff}$	Relative error with respect to SIMULATE value (%)
<b>SIMULATE3</b>	0.98229	0.000
<b>CASE I – 224 comp</b>	0.97908	-0.327
<b>CASE II – 263 comp</b>	0.98015	-0.218
<b>CASE III – 315 comp</b>	0.97993	-0.240
<b>CASE IV – 483 comp</b>	0.97993	-0.240
<b>CASE V – 579 comp</b>	0.97973	-0.261

**Figure 3:** Axial profile at HZP of Almaraz NPP.



The next analyzed case corresponds to Trillo NPP (PWR). For this reactor two operational points have been analyzed: BOC and EOC, both in HZP conditions.

The Trillo NPP core presents more different fuel types and non symmetric axial power profile than Almaraz nuclear core configuration. For this reason, it is necessary a bigger number of neutronic compositions to describe adequately the plant behaviour of a transient simulation.

The obtained results of  $k_{eff}$  of the BOC case are presented in Tab. 3. The absolute error with respect to SIMULATE3 is the same using 483 and 611 neutronic compositions. Comparing the axial power profile we obtain the same conclusion. In Fig. 4 we show the power axial profile in BOC conditions using PARCS and VALKIN neutronic codes with 483 neutronic compositions compared with SIMULATE3. Tab. 4 summarizes the statistical errors associated to the simplified core configurations.

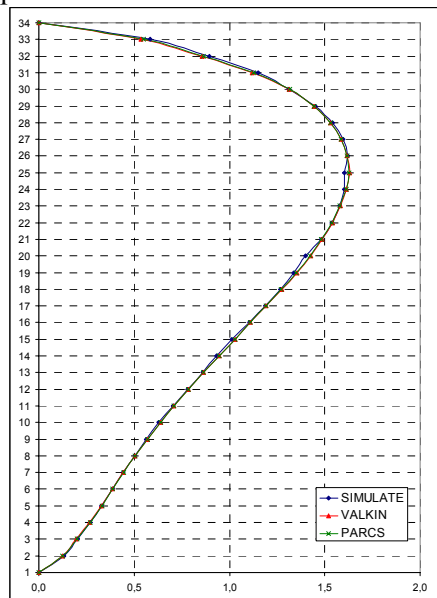
We can see that in the same way like the Almaraz NPP, the errors are very small.

Tab. 5 and Fig. 5 present the same parameters in EOC conditions. In this case the core is not very homogeneous, hence we need to increase the number of neutronic compositions to simplify the core without losing accuracy. Tab. 6 summarizes the statistical errors.

**Table 3:** Values of  $k_{eff}$  of BOC case of Trillo NPP.

CASES	$k_{eff}$	Absolut error respect to SIMULATE3 value (pcm)
<b>SIMULATE3</b>	1.00000	0.000
<b>VALKIN – 483 comp</b>	1.00025	25
<b>PARCS – 483 comp</b>	1.00045	45
<b>VALKIN – 611 comp</b>	1.00025	25
<b>PARCS – 611 comp</b>	1.00045	45

**Figure 4:** Power axial profile at BOC of Trillo NPP with 483 neutronic compositions.



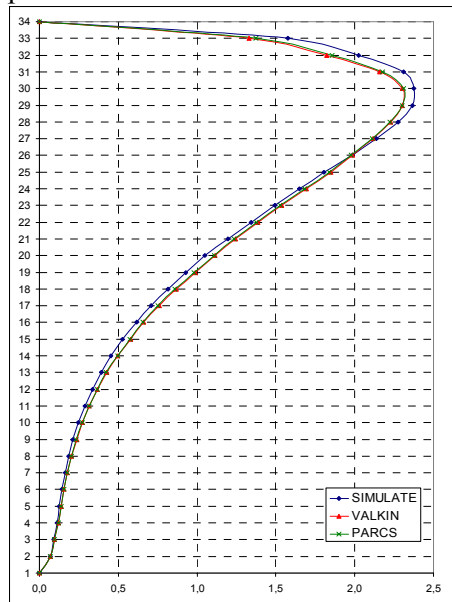
**Table 4:** Statistical errors of BOC case of Trillo NPP.

PARAMETERS	483 compositions		611 compositions	
	VALKIN	PARCS	VALKIN	PARCS
AXIAL RMS	0.015	0.012	0.015	0.012
AXIAL MIN. ABS. ERROR	-0.046	-0.035	-0.047	-0.035
AXIAL MAX. ABS. ERROR	0.026	0.024	0.026	0.024
RADIAL RMS	0.048	0.026	0.040	0.017
RADIAL MIN. ABS. ERROR	-0.091	-0.086	-0.094	-0.033
RADIAL MAX. ABS. ERROR	0.053	0.061	0.058	0.057

**Table 5:** Values of  $k_{eff}$  of EOC case of Trillo NPP.

CASES	$k_{eff}$	Absolute error respect to SIMULATE3 value (pcm)
SIMULATE3	1.00000	0
VALKIN – 483 comp	1.00102	102
PARCS – 483 comp	1.00141	141
VALKIN – 611 comp	1.00115	115
PARCS – 611 comp	1.00154	154
VALKIN – 771 comp	1.00128	128
PARCS – 771 comp	1.00168	168
VALKIN – 963 comp	1.00128	128
PARCS – 963 comp	1.00168	169

**Figure 5:** Power axial profile at EOC of Trillo NPP with 963 neutronic compositions.



**Table 4:** Statistical errors of EOC case of Trillo NPP.

PARAMETERS	483 compositions		611 compositions	
	VALKIN	PARCS	VALKIN	PARCS
AXIAL RMS	0.074	0.064	0.072	0.062
AXIAL MIN. ABS. ERROR	-0.250	-0.208	-0.247	-0.205
AXIAL MAX. ABS. ERROR	0.067	0.064	0.067	0.061
RADIAL RMS	0.024	0.028	0.028	0.037
RADIAL MIN. ABS. ERROR	-0.055	-0.044	-0.093	-0.073
RADIAL MAX. ABS. ERROR	0.051	0.052	0.043	0.065
PARAMETERS	771 compositions		963 compositions	
	VALKIN	PARCS	VALKIN	PARCS
AXIAL RMS	0.071	0.061	0.071	0.061
AXIAL MIN. ABS. ERROR	-0.246	-0.203	-0.246	-0.203
AXIAL MAX. ABS. ERROR	0.067	0.060	0.066	0.060
RADIAL RMS	0.030	0.039	0.031	0.039
RADIAL MIN. ABS. ERROR	-0.091	-0.072	-0.094	-0.075
RADIAL MAX. ABS. ERROR	0.050	0.065	0.046	0.068

#### 4.2 Steady state coupled thermalhydraulic-neutronic calculations

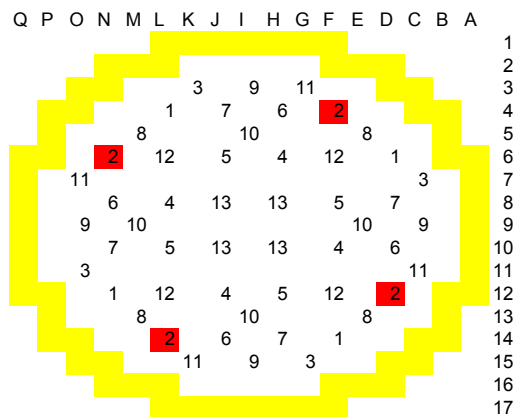
RELAP/PARCS and RELAP/VALKIN are the coupled codes used to perform these calculations. The analyzed cases correspond to EOC and HZP conditions in Trillo NPP, control rod bank 2 is partially and completely inserted (Fig. 6). In Tab. 7 and in Fig. 7 we show the obtained  $k_{eff}$  and the axial power profiles. Tab. 8 and 9 summarizes the statistical errors these cases.

The results confirm that with few neutronic compositions it is possible to have an adequate neutron core simplification.

Finally, Fig. 8 presents the three codes comparison of  $k_{eff}$  values depending on the insertion level of all control rod banks.

The results are very satisfactory, confirming the adequacy of the SIMTAB methodology to simplify adequately the nuclear core using few neutronic compositions. This simplification makes possible transient calculations with a reduction of the CPU time.

**Figure 6:** Power axial profiles at EOC of Trillo NPP.

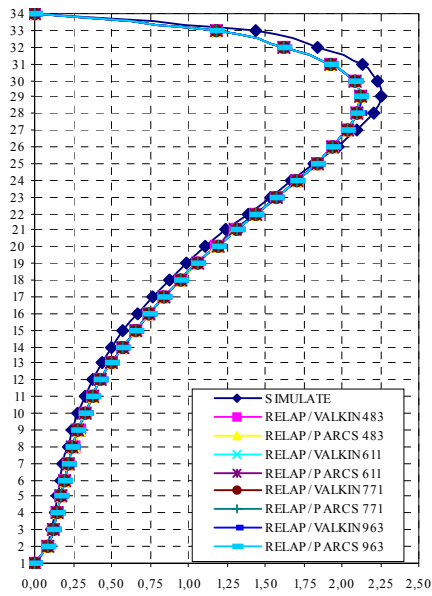


**Table 7:** Values of  $k_{eff}$  of Trillo NPP at EOC (control rod bank 2 partially and totally inserted).

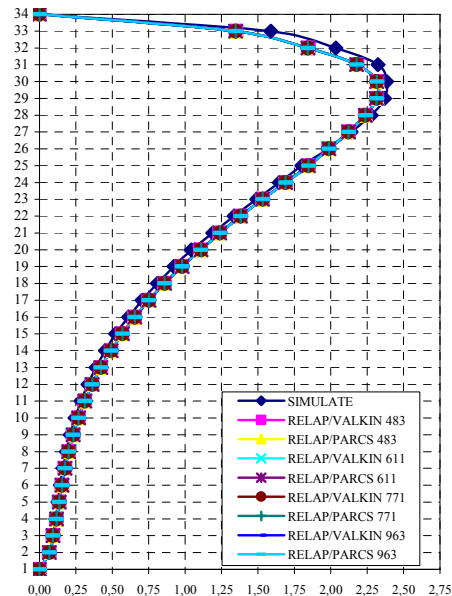
CASE	$k_{eff}$ SIMULATE3	$k_{eff}$ RELAP/VALKIN	$k_{eff}$ RELAP/PARCS	error RELAP/VALKIN	error RELAP/PARCS
BOC-483	0.998850	0.999718	0.999914	86.8	106.4
BOC-611	0.998850	0.999716	0.999912	86.6	106.2
EOC-483	0.998850	0.999491	0.999858	64.1	100.8
EOC-611	0.998850	0.999595	0.999967	74.5	111.7
EOC-771	0.998850	0.999706	1.000078	85.6	122.8
EOC-963	0.998850	0.999721	1.000092	87.1	124.2
EOC-1155	0.998850	0.999726	1.000098	87.6	124.8
EOC-1923	0.998850	0.999726	1.000098	87.6	124.8

CASE	$k_{eff}$ SIMULATE3	$k_{eff}$ RELAP/VALKIN	$k_{eff}$ RELAP/PARCS	error RELAP/VALKIN	error RELAP/PARCS
BOC-483	0.995840	0.995948	0.996159	10.8	31.9
BOC-611	0.995840	0.995994	0.996157	15.4	31.7
EOC-483	0.995840	0.996645	0.996980	80.5	114
EOC-611	0.995840	0.996739	0.997082	89.9	124.2
EOC-771	0.995840	0.996802	0.997162	96.2	132.2
EOC-963	0.995840	0.996827	0.997169	98.7	132.9
EOC-1155	0.995840	0.996827	0.997170	98.7	133
EOC-1923	0.995840	0.996825	0.997169	98.5	132.9

**Figure 7:** Power axial profiles at EOC of Trillo NPP.



Partially inserted control bank 2



Totally inserted control bank 2



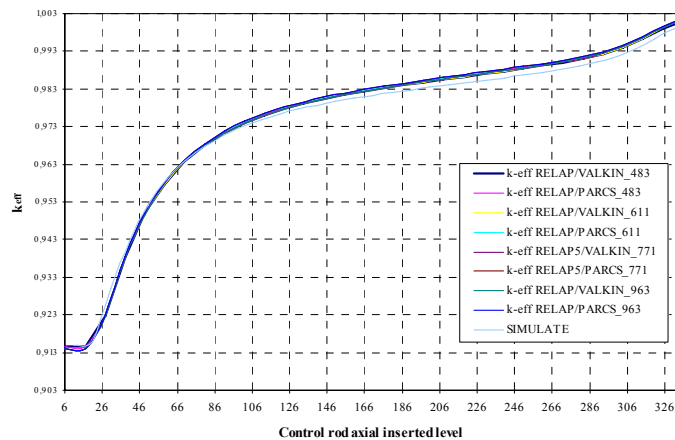
**Table 8:** Statistical errors of EOC-partially inserted control bank 2 case of Trillo NPP.

PARAMETERS	483 compositions		611 compositions	
	VALKIN	PARCS	VALKIN	PARCS
AXIAL RMS	0.040	0.040	0.040	0.040
AXIAL MIN. ABS. ERROR	-0.084	-0.084	-0.085	-0.085
AXIAL MAX. ABS. ERROR	0.256	0.256	0.255	0.255
RADIAL RMS	0.018	0.023	0.026	0.033
RADIAL MIN. ABS. ERROR	-0.043	-0.035	-0.083	-0.064
RADIAL MAX. ABS. ERROR	0.037	0.046	0.042	0.066
PARAMETERS	771 compositions		963 compositions	
	VALKIN	PARCS	VALKIN	PARCS
AXIAL RMS	0.040	0.040	0.040	0.040
AXIAL MIN. ABS. ERROR	-0.086	-0.086	-0.086	-0.086
AXIAL MAX. ABS. ERROR	0.256	0.256	0.256	0.256
RADIAL RMS	0.026	0.033	0.027	0.034
RADIAL MIN. ABS. ERROR	-0.079	-0.063	-0.083	-0.065
RADIAL MAX. ABS. ERROR	0.043	0.067	0.045	0.065

**Table 9:** Statistical errors of EOC-totally inserted rod bank 2 case of Trillo NPP.

PARAMETERS	483 compositions		611 compositions	
	VALKIN	PARCS	VALKIN	PARCS
AXIAL RMS	0.029	0.029	0.030	0.030
AXIAL MIN. ABS. ERROR	-0.062	-0.062	-0.064	-0.064
AXIAL MAX. ABS. ERROR	0.238	0.238	0.241	0.241
RADIAL RMS	0.022	0.024	0.028	0.037
RADIAL MIN. ABS. ERROR	-0.050	-0.040	-0.103	-0.079
RADIAL MAX. ABS. ERROR	0.038	0.049	0.043	0.073
PARAMETERS	771 compositions		963 compositions	
	VALKIN	PARCS	VALKIN	PARCS
AXIAL RMS	0.030	0.030	0.030	0.030
AXIAL MIN. ABS. ERROR	-0.065	-0.065	-0.064	-0.064
AXIAL MAX. ABS. ERROR	0.242	0.242	0.241	0.241
RADIAL RMS	0.028	0.037	0.029	0.038
RADIAL MIN. ABS. ERROR	-0.096	-0.075	-0.1010	-0.079
RADIAL MAX. ABS. ERROR	0.046	0.074	0.047	0.073

**Figure 8:**  $k_{eff}$  as a function of all control rod banks insertion at EOC of Trillo NPP.



## 5. Conclusions

The methodology SIMTAB characterizes, in a simplified way, the reactor core of LWR NPP. Cross-sections are obtained as a function of the control rod and thermalhydraulic variables (fuel temperature and moderator density) for a specific point of operation (History and Exposure).

With the SIMTAB methodology the reactor core can be modelled using few neutronic regions, in such a way that the nuclear kinetic behaviour is adequately characterized. This simplification permits the use of few cross-sections data set in coupled 3D neutronic-thermalhydraulic codes, saving memory and CPU times in simulation of real transients in LWR NPP.

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