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NEW PROCEDURE FOR CRITICALITY SEARCH USING COARSE MESH NODAL METHODS

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ABSTRACT

The coarse mesh nodal methods have as their primary goal to calculate the neutron flux inside the reactor core. Many computer systems use a specific form of calculation, which is called nodal method. In classical computing systems that use the criticality search is made after the complete convergence of the iterative process of calculating the neutron flux. In this paper, we proposed a new method for the calculation of criticality, condition which will be over very iterative process of calculating the neutron flux. Thus, the processing time for calculating the neutron flux was reduced by half compared with the procedure developed by the Nuclear Engineering Program of COPPE / UFRJ (PEN/COPPE/UFRJ).

1. INTRODUCTION

Either calculations of optimization models in of nuclear reactor reload or in calculation of monitoring operation of nuclear reactors, the reactor core must be critical. Therefore, it is necessary to a search procedure criticality, where the concentration of soluble boron is changed until the multiplication factor reaches the value equal to one. In the program developed in PEN/COPPE/UFRJ, calculate of the boron concentration takes place after the complete convergence of the iterative process of calculating the neutron flux and the factor multiplication, and so continued until the multiplication factor reaches the value equal to one. This procedure can spend a lot of computational time, because for each new value of boron concentration the iterative process of calculating the neutron flux is repeated until convergence is reached again [1].

This paper proposed adopt a new procedure in which the criticality is made concurrently with the iterative process of calculating the neutron flux. In other words, obtain the boron concentration, which makes the system critical along the iterative process of calculating the neutron flux and the multiplication factor, where is expected that one iterative process be necessary to calculation new boron concentration and multiplication factor equal to one.

In sections 2 and 3 are presented, respectively, the formulations of the nodal expansion method and critical search. In section 4 is a brief explanation of the method adopted in the algorithm made by the PEN/COPPE/UFRJ. In section 5 will be presented the new method developed and in subsequent sections will present the results and conclusions.
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2. NODAL EXPANSION METHOD

Modern coarse mesh nodal methods provide, quickly and very accurately, average fluxes in the nodes, the net current and average fluxes in the faces of these nodes. Nodal Expansion Method (NEM)[2], which will be used in this paper, is today one of the most common nodal methods.

The main equations of the NEM, taking part in the iterative process of calculating both the neutron flux (ϕ_g^n) and the multiplication factor (k_{eff}) are as follows:

2.1. Nodal Balance Equation

$$(\sum_{u=x,y,z} 2A_{0gu}^n / a_u^n + \Sigma_{Rg}^n)\phi_g^n = \frac{1}{k_{eff}} \chi_g \sum_{g'=1}^{2} \nu\Sigma_{fg'}^n \phi_{g'}^n + \sum_{\substack{g'=1 \\ g' \neq g}}^{2} \Sigma_{gg'}^n \phi_{g'}^n + \sum_{u=x,y,z} 2A_{0gu}^n (2(J_{gur}^{-n} + J_{gul}^{+n}) - c_{4gu}^n) / a_u^n \quad (1)$$

2.2. Partial Currents

$$J_{gul}^{-n} = A_{0gu}^n (\phi_g^n + c_{4gu}^n) + A_{1gu}^n J_{gul}^{+n} + A_{2gu}^n J_{gur}^{-n} - A_{3gu}^n c_{3gu}^n \quad (2)$$

and

$$J_{gur}^{+n} = A_{0gu}^n (\phi_g^n + c_{4gu}^n) + A_{2gu}^n J_{gul}^{+n} + A_{1gu}^n J_{gur}^{-n} + A_{3gu}^n c_{3gu}^n \quad (3)$$

Where:

$$A_{0gu}^n \equiv \frac{6(D_g^n / a_u^n)}{(1+12(D_g^n / a_u^n))} \quad (4)$$

$$A_{1gu}^n = \frac{(1-48(D_g^n / a_u^n)^2)}{((1+12(D_g^n / a_u^n))(1+4(D_g^n / a_u^n)))} \quad (5)$$

$$A_{2gu}^n = \frac{-8(D_g^n / a_u^n)}{((1+12(D_g^n / a_u^n))(1+4(D_g^n / a_u^n)))} \quad (6)$$

and

$$A_{3gu}^n = \frac{6(D_g^n / a_u^n)}{(1+4(D_g^n / a_u^n))} \quad (7)$$

2.3. Primary Coefficients

$$c_{1gu}^{n} = (J_{gur}^{+n} + J_{gur}^{-n}) - (J_{gul}^{+n} + J_{gul}^{-n}) \tag{8}$$

and

$$c_{2gu}^{n} = \phi_{g}^{n} - ((J_{gur}^{+n} + J_{gur}^{-n}) + (J_{gul}^{+n} + J_{gul}^{-n})) \tag{9}$$

2.4. Secondary Coefficients

These coefficients (c_{3gu}^{n} and c_{4gu}^{n}) are obtained through the technique of weighted residuals applied to the following one-dimensional diffusion equation:

$$-D_{g}^{n}\frac{d^{2}}{du^{2}}\psi_{gu}^{n}(u) + \Sigma_{Rg}^{n}\psi_{gu}^{n}(u) = \frac{1}{k_{eff}}\chi_{g}\sum_{g'=1}^{2}\nu\Sigma_{fg'}^{n}\psi_{g'u}^{n}(u) + \sum_{g'=1}^{2}\Sigma_{gg'}^{n}\psi_{g'u}^{n}(u) - L_{gu}^{n}(u) \tag{10}$$

2.5. Transverse Leakage

The term cross leakage ($L_{gu}^{n}(u)$) is approximated by a polynomial as follows:

$$L_{gu}^{n}(u) = \sum_{i=0}^{2}\alpha_{igu}^{n}h_{i}(u/a_{u}^{n}) \tag{11}$$

whose coefficients are thus calculated:

$$\alpha_{0gu}^{n} \equiv \overline{L}_{gu}^{n} = \sum_{\xi=v,w}((J_{g\xi r}^{+n} - J_{g\xi r}^{-n}) - (J_{g\xi l}^{+n} - J_{g\xi l}^{-n}))/a_{\xi}^{n} \tag{12}$$

$$\alpha_{1gu}^{n} = \frac{1}{2}(L_{gur}^{n} - L_{gul}^{n}) \tag{13}$$

and

$$\alpha_{2gu}^{n} = \overline{L}_{gu}^{n} - \frac{1}{2}(L_{gur}^{n} + L_{gul}^{n}) \tag{14}$$

with,

$$L_{gul}^{n} = (a_{u}^{n-1}\overline{L}_{gu}^{n} + a_{u}^{n}\overline{L}_{gu}^{n-1})/(a_{u}^{n-1} + a_{u}^{n}) \tag{15}$$

and

$$L_{gur}^{n} = L_{gul}^{n-1} \tag{16}$$

and the L^n_{gus} are obtained imposing the continuity of the function $L^n_{gu}(u)$ and its first derivative at the interface between nodes.

3. CRITICALITY SEARCH

The nuclear reactor needs to operate in critical condition at all times of the operation cycle. That is to say, that the effective multiplication factor of the reactor core always be the value equal to one.

In reactor physics codes there is a module that specific to the calculation of the value concentration of soluble boron to the reactor becomes critical. This hypothesis is to relate the variation of boron concentration with the variation of the effective multiplication factor is linear.

When it relates directly to the effective multiplication factor with the boron concentration is detected a problem with the angular coefficient. As the iterations of the search are going the angular coefficient has the freedom to change signal, it can cause an uncertainty in the value boron concentration. This problem occurs when there are great variations of the effective multiplication factor. So, some methods were developed to avoid this problem, which are explained in the following subsections.

3.1. Fixed Angular Coefficient Method

The new boron concentration used in the calculation of new macroscopic cross sections is calculated as follows:

$$C_B = C_B^{(anterior)} + \Delta C_B \tag{17}$$

Where C_B is the new boron concentration, $C_B^{(anterior)}$ is the concentration of boron above and ΔC_B is the amount of boron that must be added so that the multiplication factor reaches the value 1. This ΔC_B is given by:

$$\Delta C_B = \frac{k_{eff}^{(alvo)} - k_{eff}}{\alpha} \tag{18}$$

It is observed that when k_{eff} is larger $k_{eff}^{(alvo)}$, more boron will be needed in the reactor core, then ΔC_B will be positive, on the other hand, when k_{eff} is less than $k_{eff}^{(alvo)}$ has to remove boron in the core, so ΔC_B will be negative. For this reason α, which is the angular coefficient of the line, assume a negative value. The value of α was set at -10^{-4}.

3.2. Deviation Method

To not use the fixed slope, there is another way to perform the calculation of the new boron concentration, which is well done:

$$\Delta C_B = \frac{k_{eff}^{(alvo)} - k_{eff}}{\alpha} \tag{19}$$

where C_B is the boron concentration, α is an unknown factor that multiplies the initial boron concentration of $C_B^{(0)}$, which is known a priori. It also defined the deviation (E) between the effective current multiplication factor, i.e. the value found in the last iteration, and the value of the effective multiplication factor that we want to achieve ($k_{eff}^{(alvo)}$) using the following equation.

$$E = k_{eff}^{(alvo)} - k_{eff} \tag{20}$$

Finally, the relationship between E and the multiplicative factor is made by a linear function as explained below.

$$E = a\alpha + b \tag{21}$$

So, looking at equation (20), to that k_{eff} scope $k_{eff}^{(alvo)}$ the deviation (E) must be zero and this implies that:

$$\alpha = -\frac{b}{a} \tag{22}$$

The parameters *a* and *b* are calculated from two consecutive values of C_B and k_{eff}, i.e. values corresponding to two successive iterations. Thus, the equation (21) follows that:

$$E^{(i-1)} = k_{eff}^{(alvo)} - k_{eff}^{(i-1)} = a\alpha^{(i-1)} + b \tag{23}$$

$$E^{(i)} = k_{eff}^{(alvo)} - k_{eff}^{(i)} = a\alpha^{(i)} + b \tag{24}$$

Subtracting the equation (24) the equation (23) we have that

$$a = \frac{E^{(i-1)} - E^{(i)}}{\alpha^{(i-1)} - \alpha^{(i)}} \tag{25}$$

And replacing the equation (25) in equation (23) comes

$$b = \frac{\alpha^{(i-1)} E^{(i)} - \alpha^{(i)} E^{(i-1)}}{\alpha^{(i-1)} - \alpha^{(i)}} \tag{26}$$

It may be noted that for each iteration of the search term and the slope of the line are updated independently. However, the first two values of C_B and k_{eff} are obtained for $\alpha^{(0)}$ and $\alpha^{(1)}$ predetermined.

3.3. Controlled Variations Method

Another way is impose control over the variations of the angular coefficient and the variation of boron concentration. The new boron concentration used in the calculation of new macroscopic cross sections is calculated as shown in equation (17). But with ΔC_B as follows:

$$\Delta C_B = \frac{k_{eff}^{(alvo)} - k_{eff}^{(atual)}}{\frac{dk_{eff}}{dC_B}} \tag{27}$$

where $k_{eff}^{(alvo)}$ is the multiplication factor that we want to achieve in the case of criticality search takes the value one, $k_{eff}^{(atual)}$ is the current value of the multiplication factor and $\frac{dk_{eff}}{dC_B}$ is the coefficient of the line that relates k_{eff} to C_B, which in this case is type:

$$\Delta k_{eff} = \alpha.\Delta C_B \tag{28}$$

It is observed that the first iteration of the search values of $C_B^{(anterior)}$ and $\frac{dk_{eff}}{dC_B}$ are given. The new value of the derivative is obtained as follows:

$$\frac{dk_{eff}}{dC_B}^{(atual)} = \frac{k_{eff}^{(atual)} - k_{eff}^{(anterior)}}{C_B^{(atual)} - C_B^{(anterior)}} \tag{29}$$

The control condition on the variation of the derivative is made so it does not exceed a maximum permissible variation with respect to the previous derivative. The relative variation is calculated thus:

$$\delta_{relativo} = \frac{\frac{dk_{eff}}{dC_B}^{(atual)} - \frac{dk_{eff}}{dC_B}^{(anterior)}}{\frac{dk_{eff}}{dC_B}^{(anterior)}} \tag{30}$$

It is a comparison between the absolute value of $\delta_{relativo}$, found by equation (30), and maximum possible variation, the value that will be used will is lowest value found. And the new value of the derivative is calculated as follows:

$$\frac{dk_{eff}}{dC_B} = \frac{dk_{eff}}{dC_B}^{(anterior)} \quad x\ \{1+(\pm)\,x\,\delta_{relativo}\} \tag{31}$$

where $(\pm)$ is the signal $\delta_{relativo}$ calculated.

The control over the variation of boron concentration (ΔC_B) is given also using the lower of (ΔC_B), calculated by equation (27), and a tenth of the difference between $C_B^{máximo}$ and $C_B^{mínimo}$, which are input data of the problem. Finally, the new boron concentration calculated from the equation (17) must be between $C_B^{máximo}$ and $C_B^{mínimo}$, because if it is outside those boundaries will be used the value of the limit values.

3.4. Macroscopic cross section

All cross sections, the macroscopic cross section of absorption, scattering and fission - vary according to the boron concentration, fuel temperature, moderator temperature and density of the moderator. Using Taylor series expansion [3] truncated at first order, we can write:

$$\Sigma_{xg}^{n} = \Sigma_{xg}^{n,0} + \frac{\partial \Sigma_{xg}^{n}}{\partial c_B}(c_B - c_B^0) + \frac{\partial \Sigma_{xg}^{n}}{\partial \sqrt{T_F}}(\sqrt{T_F^n} - \sqrt{T_F^0}) + \frac{\partial \Sigma_{xg}^{n}}{\partial T_M}(T_M^n - T_M^o) + \frac{\partial \Sigma_{xg}^{n}}{\partial \rho_M}(\rho_M^n - \rho_M^0) \tag{32}$$

where Σ_{xg}^{n} and $\Sigma_{xg}^{n,0}$ are defined as follows:

$$\Sigma_{xg}^{n} \equiv \Sigma_{xg}^{n}(c_B, T_F^n, T_M^n, \rho_M^n) \tag{33}$$

and

$$\Sigma_{xg}^{n,0} \equiv \Sigma_{xg}^{n,0}(c_B^0, T_F^{n,0}, T_M^{n,0}, \rho_M^{n,0}) \tag{34}$$

where c_B is the boron concentration, T_F^n is the fuel temperature, T_M^n is the moderator temperature of and ρ_M^n is the moderator density for a node n. The values of $\Sigma_{xg}^{n,0}$ are the initial data problem, as the initial values of the variables mentioned above.

As this paper does not perform calculations thermohydraulic, only the concentration of boron is considered, thus, equation (35) becomes:

$$\Sigma_{xg}^{n} = \Sigma_{xg}^{n,0} + \frac{\partial \Sigma_{xg}^{n}}{\partial c_B}(c_B - c_B^0) \tag{35}$$

and the macroscopic cross sections are just redefined:

$$\Sigma_{xg}^{n} \equiv \Sigma_{xg}^{n}(c_B) \tag{36}$$

$$\Sigma_{xg}^{n,0} \equiv \Sigma_{xg}^{n,0}(c_B^0) \tag{37}$$

4. CONVENTIONAL ALGORITHM

Some computer models, as developed by the PEN/COPPE/UFRJ, of neutronic calculations for a nuclear reactor, are based on the scheme displayed in Figure 1.

The initialization module is responsible for entering geometric data of the reactor core, nuclear data and it also fixed the values of tolerance (ε_k and ε_ϕ).

After initialization, goes into action the module that specifically handles the solution of neutron diffusion equation, where all the calculations of coefficients of the NEM method. The verification of convergence, as shown in Figure 1, is done using the following tests.

$$\left| \frac{k_{eff}^{atual} - k_{eff}^{anterior}}{k_{eff}^{atual}} \right| \leq \varepsilon_k \tag{38}$$

and

$$\max_{n,g} \left| \frac{\phi_{n,g}^{atual} - \phi_{n,g}^{anterior}}{\phi_{n,g}^{atual}} \right| \leq \varepsilon_\phi \tag{39}$$

The algorithm does not come out of the flux calculation module while the values of the flux and the effective multiplication factor do not meet the criteria of convergence, equations (38) and (39). Therefore, the computational time is directly proportional to the time it takes for these conditions are met. Normally, the values set for the tolerances are 10^{-5} for the effective multiplication factor (ε_k) and 10^{-3} for average nodal flux (ε_ϕ), as are values that provide reasonable accuracy with a low computational time.

After the convergence of the average flux and the effective multiplication factor, the program checks whether the reactor is critical regarding the boron concentration present, if not the module to adjust the concentration of soluble boron is driven to be calculated the new boron concentration, and so returns to the beginning to redo all the procedures again. This process is repeated until the value of the effective multiplication factor becomes one.

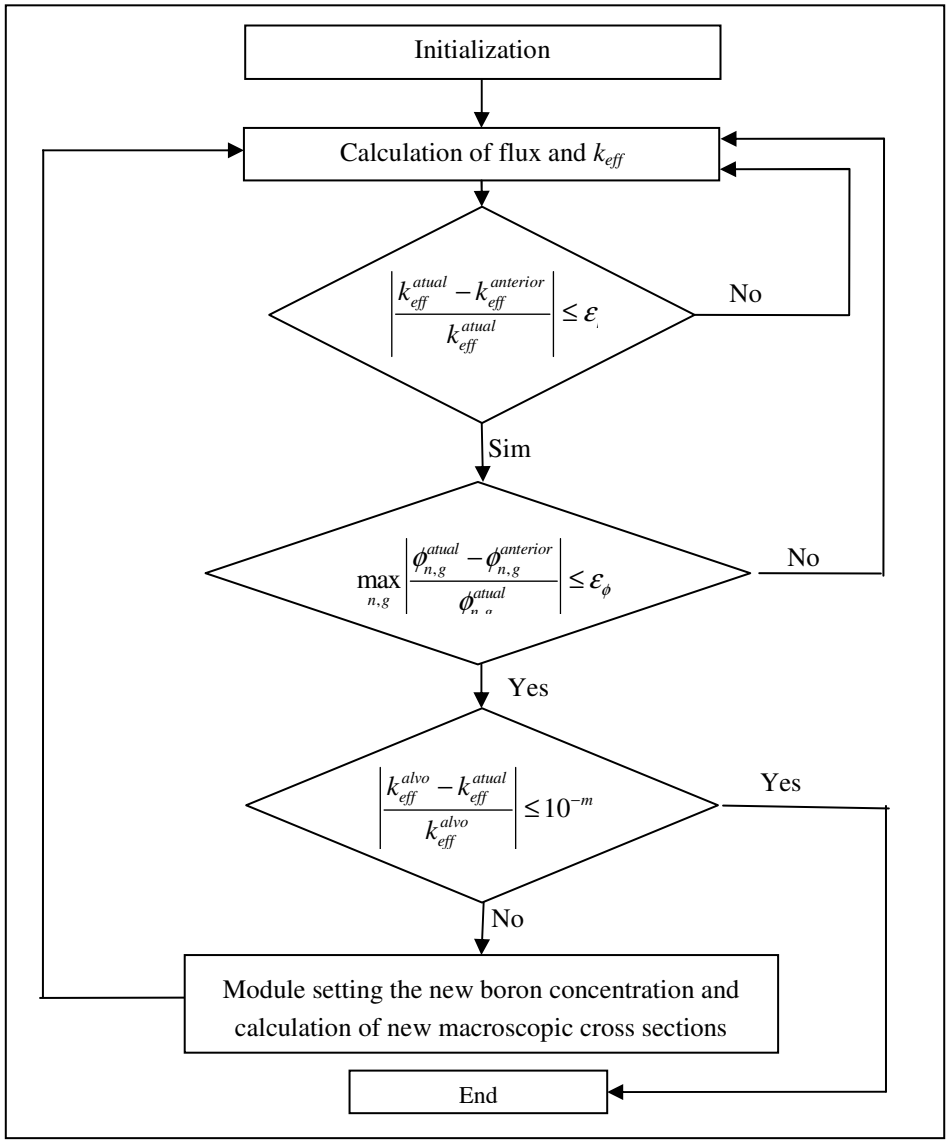

Figure 1: Computational model simplified to the classic process

After adjusting the boron concentration, the program recalculates the absorption macroscopic cross section to repeat the process for calculating the average flux and the effective multiplication factor.

5. DYNAMIC PROCESS FOR CRITICALITY SEARCH

This procedure, the program performs criticality search along the iterative process of calculating the neutron flux according to some predetermined parameter

To make the necessary changes in the program developed by the PEN/COPPE/UFRJ, that realizes the criticality search along the iterative process of calculation, was necessary a study on the behavior of the effective multiplication factor along of the iterations without the adjusting the boron concentration.

The behavior of the multiplication factor along of the iterations, as can be seen in Figure 2, it quickly reaches a real value. The convergence of the multiplication factor takes values around 10^{-3} around the fifteenth iteration. As the values of effective multiplication factors of the four reactors studied: NEACRP [3], ZION [4], PWR [5] and LMW [7]. A normalization was performed at the highest value, of the values for each iteration of the K_{eff}. It can be observed that the behavior of convergence is not an attribute of the reactor. The convergence of the effective multiplication factor is a property of the method used in this case was NEM.

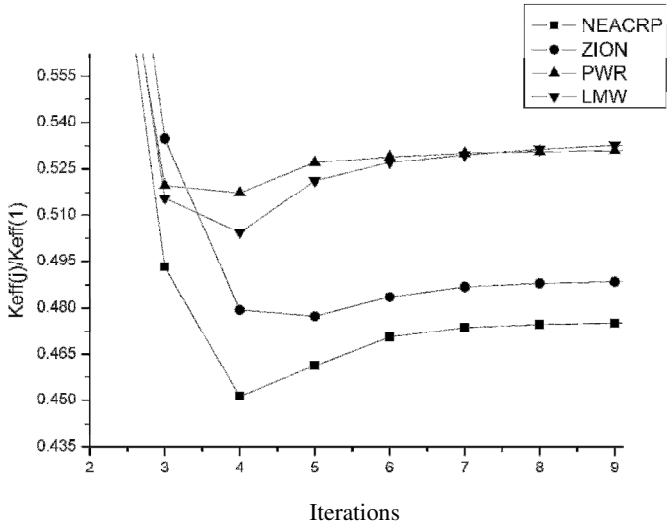

Figure 2: Graph of the behavior of K_{eff} versus the number of iterations.

The programming logic was changed so as to shorten the time criticality of the module enter action, that is, the program does not wait for the end of the iterative process to verify the criticality of the reactor studied. With this, a parameter was introduced to stop the iterative process, first, this parameter was set in order to pause the iterative process in a predetermined value of iteration, where the values are n = 3, 5 and 10. Another method is determining a preliminary value for the convergence of the effective multiplication factor parameter called pre-convergence, the value was always set at 0.05.

Equation (38) was used to check the pre-convergence of the effective multiplication factor, in this case by the parameter ε_k equals the pre-convergence. If the equality is not met the program continues the iterative process for calculating the flux and the effective multiplication factor, otherwise the program stop all the calculations and checks if the reactor is critical, it will seek a new boron concentration and from the point of the pause will continue to do the calculations to find the neutron flux. Figure 3 illustrates the changes.

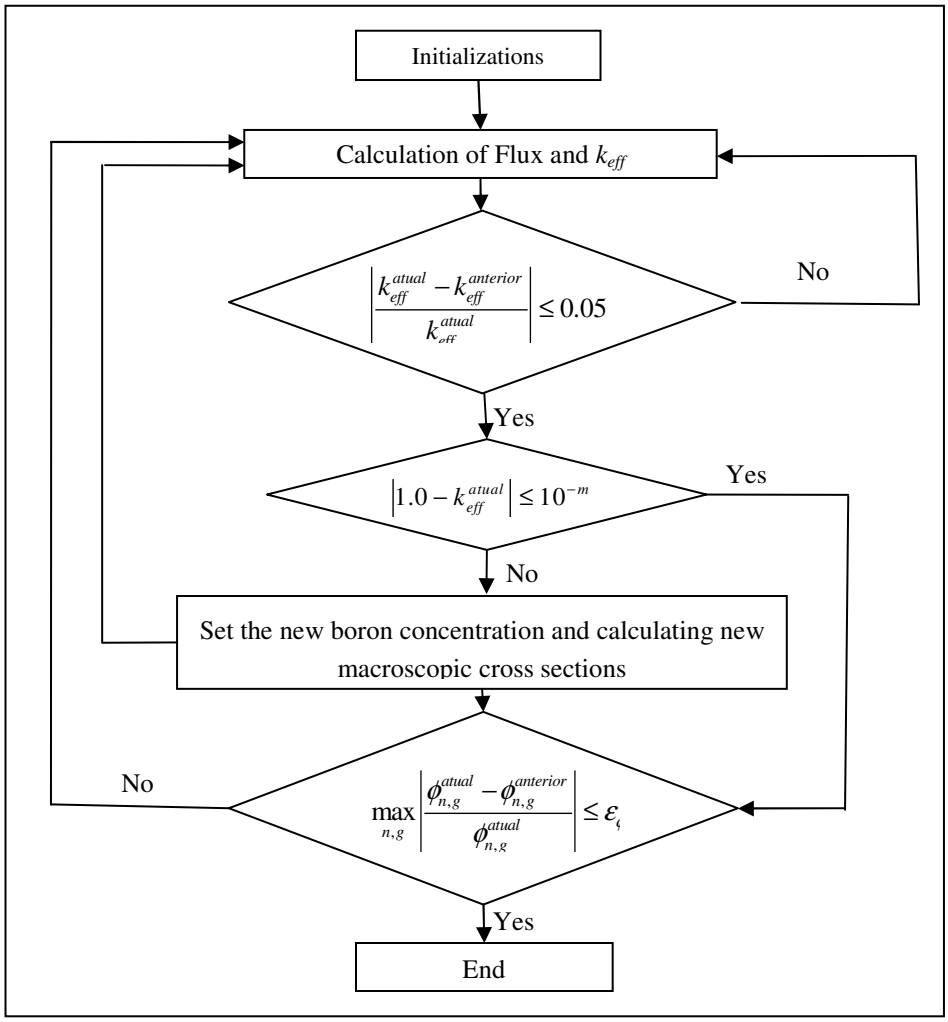

Figure 3: New procedure for activating the module to adjust the concentration of soluble boron using the pre-convergence factor.

6. RESULTS AND DISCUSSION

To test different criticality search methods, taking into account the different types of mathematical relationships presented in Section 3, the reactor NEACRP PWR-335-L [3] was used. This reactor was used because their data sets are complete found in the literature, i.e., the data has all the core values for the macroscopic cross sections and their derivatives with respect to fuel temperature, moderator temperature and density and concentration of soluble boron.
All results shown in this section were obtained using equation (35) for upgrading the macroscopic cross sections due to the change in boron concentration.

The NEACRP PWR-335-L has a symmetry of the eighth core and a total height of 427.3 cm and 30 cm for top and bottom reflectors, therefore, an active height of 367.3 cm. The fuel

elements have dimensions of 21.606 x 21.606 cm^2, thus the nodes have 21.606 x 21.606 x 20.4056 cm^3, a total of 1280 nodes.

Table 1 are shown the results for both the Fixed Angular Coefficient Method and the classic method. In the same table are the results obtained with the dynamic process, using the default parameters for n = 3, 5 and 10.

Table 1: Method of Fixed Slope

		Computational Time (seconds)	k_{eff}	C_B (ppm)
	Classic Process	3,58	1,00000000	1895
Dynamic Process	n = 3	3,62	0,99999995	1895
	n = 5	3,45	1,00000000	1895
	n = 10	3,42	0,99999993	1895

One can see, the results shown in Table 1, there is not much difference between the values obtained in the various procedures used, noting that there is no significant reduction in computational time.

Table 2 shows the results obtained by having the angular coefficient that relates the effective multiplication factor to the boron concentration, varied each time the module criticality would take action.

Table 2: Deviation Method

		Computational Time (seconds)	k_{eff}	C_B (ppm)
	Classic Process	4,7	1,00000000	1895
Dynamic Process	3	3,12	0,99999999	1895
	5	3,75	0,99999997	1895
	10	4,64	0,99999996	1895

Analyzing the results presented in Table 2, has values for the effective multiplication factor, using the angular coefficient variable, is more dispersed than employing a Fixed Angular Coefficient Method, however is not large differences between the values. Note that there is a significant improvement in computational time using n equal to 3 and 5 in the new dynamic. The computational time, using n = 3, is reduced to 66.38% and using n = 5 is 79.78% of the time spent by the classic process.

Table 3 shows the results for cases that use the control on the variation of the angular coeffiecient and the variation of boron concentration

Table 3: Method of Controlled Variations

		Computational Time (seconds)	k_{eff}	*CB* (ppm)
	Classic Process	3,25	0,99999995	1895
Dynamic Process	$n = 3$	4,58	1,00000000	1895
	$n = 5$	4,14	1,00000008	1895
	$n = 10$	3,36	1,00000006	1895

It appears that using the dynamic process to control the number of iterations, combining with the method of control over the variations of boron concentration and the angular coeffiecient, Controlled Method of Variations, the computational time increases in relation to the classic process.

In Table 4 the results are found when using the pre-factor for the convergence k_{eff} in 0.05, a procedure described in section 5, for the three methods of calculating the boron concentration.

Table 4: Comparison of computational time using the Pre-Convergence Factor

	Computational Time (seconds)	k_{eff}	*CB* (ppm)
Method of Fixed Slope	3,68	1,00000000	1895
Deviation Method	2,93	0,99999991	1895
Method of Controlled Variations	1,81	0,99999999	1894

It may be noted that using the procedure using the Method of Controlled Variations computational time is reduced to about 55.69% of the time of the classical process using the same method. It method using the dynamic process wear out 38.51% of the time that the Deviation of the Method with the classic process, spend to make the criticality search and, finally, it still spends about 50.56% of the time that the Fixed Angular Coefficient Method, using the classical process.

Table 5 shows the comparison of computational times for all methods used in this study to relate the effective multiplication factor to the boron concentration and the different types of processes.

Table 5: Comparison of times for all methods and processes

	Classic process Time (seconds)	Dynamic Process Time (seconds)			
		With Pre-Convergence Factor	$n = 10$	$n = 5$	$n = 3$
Method of Fixed Slope	4,7	2,93	4,64	3,75	3,12
Deviation Method	3,58	3,68	3,42	3,45	3,62
Method of Controlled Variations	3,25	1,81	3,36	4,14	4,58

Comparing the results above can be seen that the dynamic process used to pre-convergence factor and the Method of Controlled Variations is the fastest of all used. It spends half the time that the classical process using the Deviation of the Method, which is considered the standard method, to perform criticality search.

7. CONCLUSIONS

All results of this paper were obtained by comparing the classical method, which is await the full convergence of the effective multiplication factor of the neutron flux to see if the reactor is critical or not, change the boron concentration and perform another iterative process. These results, obtained by the program developed by the PEN/COPPE/UFRJ, as nodal average neutron flux and multiplication factor, were considered as references to evaluate possible deviations caused by dynamic processes. As we can see the deviations obtained are not relevant. The largest deviation found in the boron concentration to the reactor NEACRP was about 0.05%.

Clearly the new procedure for the detection of criticality using the Method of Controlled Variations, with the factor of pre-convergence is faster than the classical method. The new procedure takes only 38.5% of the time it takes for the classic process perform the same calculation.

Whereas the calculations of a power reactor only consider five decimal significative values for the K_{eff} value and none to the value of boron concentration, the new procedure is reliable with regard to the figures at the end of the flux calculation.

The values for the average nodal fluxes present a largest deviation of 0.5%. Therefore, the new procedure is reliable for the values of the neutron fluxes and boron concentration that causes the reactor to operate critical.

Studying the behavior of the new process using a pre-convergence parameter in the neutron flux is a suggestion of future work, since the flux takes longer to converge. Evaluate the

behavior of neutron flux along the iterations of criticality research is of vital importance for the development of new processes.

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