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SOLUTION OF THE NEUTRON POINT KINETICS EQUATIONS BY APPLYING THE ROSENBROCK METHOD

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Abstract. *In this work, the solution of the Neutron Point Kinetics equations is presented by applying the fourth-order and four-stage Rosenbrock method. The objective of this paper is to validate this methodology already used in Yang and Jevremovic (2009) to apply it, in future works, to the Neutron Point Kinetics equations including the effects of temperature and poisons in the final analysis of neutron density behavior. In the resolution, one and six groups of delayed neutron precursors are considered for reactivities of the type: constant, ramp, quadratic, sinusoidal, zig-zag, and pulsed source with constant time step. The Numerical results are compared with those found in the literature. The numerical results obtained have achieved good precision as the time step is reduced, ensuring that the system stiffness is overcome. Thus, this study contributed to guarantee the safe operation of nuclear reactors by analyzing the neutron density behavior for different reactivity insertions.*

Keywords: *Neutron Point kinetics equations, Rosenbrock Method, Nuclear Engineering.*

1. INTRODUCTION

Nuclear energy is an important alternative available in the world. The advantages of its use are: it does not release greenhouse gases, obeying the objectives of the Kyoto Protocol (1997) and, more recently, the Paris Agreement (2015); little space is required for its construction; fuel availability; it is the most efficient source for energy generation; independent of climatic factors, in addition to others.

In studies of reactor physics, the main focus is the distribution of neutrons that determines the rate at which various nuclear reactions occur within the reactor. Besides, by studying the behavior of the neutron population, measures can be taken to control the chain reaction, allowing stability and safety in the nuclear reactor.

For that, mathematical models serve as great allies in the simulation of neutron density. The Neutron Point Kinetics equations are models that describe the temporal behavior of the neutron population and also the decay of delayed neutron precursors, important for the reactor's operational control.

Many works have been published on the Neutron Point Kinetics equations (NPKE), among them the Nahla (2011) which presents the New Analytic Method (NAM) based on the roots of the Inhour Equation using the Elimination Gaussian method to solve the NPKE with constant type reactivities, ramp and temperature feedback; Ganapol (2013) performs a numerical procedure that uses the Implicit Euler method and the Finite Difference scheme (BEFD); Mohideen Abdul Razak and Rathinasamy (2018) present a new way to solve the inverse Point Kinetics equations, using Haar's wavelet transform, transforming the inverse Point Kinetics equations into a set of linear equations. In (Picca *et al*., 2013) develop Kinard and Allen's (2004) improved enhanced piecewise approach (EPCA). In (Aboanber *et al*., 2012) use the Analytical Perturbation method for a group of delayed neutron precursors with temperature feedback, based on approximations with small parameters for neutron density. Recently, in (Paganim *et al*.,2020) solved the Neutron Point Kinetics equations considering not only the effects of the main neutron poisons as well as the effects of some transuraniums through a decomposition method that expands nonlinear terms in an infinite series obtaining a recursive system, dealing with non-linearity by the Adomian polynomials.

Due to the stiffness of this model, caused by the great lifetimes difference between the prompt and delayed neutrons, there is a need to look for methods to circumvent this characteristic. Curtiss and Hirschfelder (1952) were the first authors to verify that rigid problems require implicit methods due to their region of unlimited stability.

Therefore, the Rosenbrock method has been shown in the literature to be satisfactory in solving stiff problems. Schippmann and Burchard (2011) focused their attention on investigating Rosembrock's computational efficiency compared to the methods of Runge-Kutta and Patankar. In Galina (2016), numerical solutions are presented for rigid problems of radioactive decay chains involving natural and artificial chains using the Rosembrock method, producing consistent

results.Recently, in chemical kinetics, Sehnem (2018) uses the method to solve a stiff system of ODE in order to moderate the degree of stiffness and decrease the number of species involved in the combustion of the methane element. In conclusion, the Rosenbrock method showed high precision, high efficiency and stable solution.Yang and Jevremovic (2009) solve the Neutron Point Kinetics equations by the Rosenbrock method in which the results were satisfactory.

The objective of this work is to solve the Neutron Point Kinetics equations by the Rosenbrock method in order to validate the methodology. After validation of the methodology, it is intended to apply it to more complex models such as the inclusion of equations describing the effects of temperature and poisons.

Many works have already been done taking into account the effects of temperature, as in Silva (2011) which uses the decomposition method present in Petersen (2011) to obtain an analytical solution to the problem, where nonlinearity is treated using the Adomian polynomials. Tumelero (2015) presents a solution for the Neutron Point Kinetics equations applying the method of polynomial approximation, also considering the effects of temperature.

In the literature some works that take into account the effects of the poisons on the Point Kinetics model, as in Espinosa (2016) that works with the Neutron Point Kinetics equations taking into account the effects of the Xenon-135 and Samarium-149 poisons on the reactor, in which the new system of equations is solved through a method of decomposition that expands the non-linear terms into an infinite series obtaining a recursive system, treating nonlinearity by the Adomian polynomials. Recently, Paganim, Bodmann, Vilhena (2020) solve the Point Kinetics of Neutrons equations considering not only the effects of the main neutron poisons as well as the effects of some transuranics by the same method of Espinosa (2016) obtaining results consistent with the expected.

In our knowledge, the exclusivity before the literature in the second part of this work, after independent validation of the models with temperature effects and also with the poisons, is to include and analyze these two effects together with the model of Neutron Point Kinetics.

2. MODEL

The Neutron Point Kinetics equations form a system containing seven time-dependent coupled differential equations that describe the behavior of the neutron population and the decay of delayed neutron precursors, described in Eq. (1):

$$\begin{aligned} \frac{d}{dt}n(t) &= \frac{\rho(t)-\beta}{\Lambda}n(t) + \sum_{i=1}^{6}\lambda_i C_i(t), \\ \frac{d}{dt}C_i(t) &= \frac{\beta_i}{\Lambda}n(t) - \lambda_i C_i(t), \end{aligned} \tag{1}$$

for $i = 1 : 6$. With the following initial conditions:

$$\begin{aligned} n(0) &= n_0, \\ C_i(0) &= \frac{\beta_i}{\lambda_i \Lambda}n_0, \end{aligned} \tag{2}$$

for $i = 1 : 6$.

2.1 Rosenbrock Method

The Rosenbrock methods belong to one of the classes of the Runge-Kutta methods. They consist of linearizing the implicit Runge-Kutta methods, thus facilitating the implementation of the code since instead of solving non-linear systems, a sequence of linear systems is solved. The structure of the Rosenbrock method used in this work found in Yang and Jevremovic (2009) is defined as follows:

$$\begin{aligned} k_1 &= Bf(y_0, t_0) + Bhc_1\frac{\partial f}{\partial t}, \\ k_2 &= Bf(y_0 + a_{21}k_1, t_0 + h) + B\left[hc_2\frac{\partial f}{\partial t} + \frac{c_{21}k_1}{h}\right], \\ k_3 &= Bf(y_0 + a_{31}k_1 + a_{32}k_2, t_0 + h) + B\left[hc_3\frac{\partial f}{\partial t} + \frac{c_{31}k_1 + c_{32}k_2}{h}\right], \\ k_4 &= Bf(y_0 + a_{31}k_1 + a_{32}k_2, t_0 + h) + B\left[hc_4\frac{\partial f}{\partial t} + \frac{c_{41}k_1 + c_{42}k_2 + c_{43}k_3}{h}\right], \\ y(t_0 + h) &= y(t_0) + b_1k_1 + b_2k_2 + b_3k_3 + b_4k_4. \end{aligned} \tag{3}$$

in which $B = [\frac{1}{\gamma h}I - \frac{\partial f}{\partial y}]^{-1}$, where I is the identity matrix $m \times m$, h is the size of the integration step, γ is one of the roots of the Laguerre polynomial, $\frac{\partial f}{\partial y}$ is the Jacobian matrix in relation to y and $\frac{\partial f}{\partial t}$ is the Jacobian matrix in relation to t.

The parameters for the fourth order, fourth stage Rosenbrock method defined in Yang and Jevremovic (2009) used in this work are: $\alpha_{21} = 2,\ \alpha_{31} = 1.92,\ \alpha_{32} = 0.24, c_{21} = -8,\ c_{31} = 14.88,\ c_{32} = 2.4,\ c_{41} = -0.896,\ c_{42} = -0.432,\ c_{43} = -0.4,\ b_1 = 19/9,\ b_2 = 0.5,\ b_3 = 25/108,\ b_4 = 125/108,\ c_1 = 0.5,\ c_2 = -1.5,\ c_3 = 2.42,\ c_4 = 0.116,\ e_1 = 17/54,\ e_2 = 7/36,\ e_3 = 0$ and $e_4 = 125/108$.

3. RESULTS

The results are obtained for one and six groups of delayed neutron precursors, considering reactivities of the type: Constant, Ramp, Quadratic, Sinusoidal, Zig-zag, and Pulsed Source and with a constant time step of $0.0001s$ and $0.00001s$. The results presented in this section are compared with the Polynomial Approximation Method (PAM) present in Tumelero (2015), with the Enhanced Piecewise Constant Approximation (EPCA) of Picca, Furfaro, and Ganapol (2013), and with the work of Ganapol (2013) which performs a numerical procedure using the Implicit Euler method and the Finite Differences scheme. The software used was SciLab 6.0.2 (http://www.scilab.org/) in a computer with the following configurations: Intel® Core™ i74930k CPU 3.40GHz, 16 GB RAM, 64-bit operating system, x64-based processor.

3.1 Insertion of Constant Reactivity

The Neutron Point Kinetics equations are solved by the Rosenbrock method for constant reactivity using the kinetics parameters presented in Tumelero (2015). Four constant reactivity values are considered, two of them subcritical ($\rho = -1\beta$ e $\rho = -0.5\beta$) and two other supercriticals (prompt subcritical: $\rho = 0.5\beta$ and prompt critical: $\rho = 1\beta$). The results for the neutron density in cm^{-3} are presented in Tab. 1, together with the respective relative deviations. Figure 1 shows the graph of neutron density behavior for cases of constant reactivity $\rho = -1\beta$, $\rho = -0.5\beta$, $\rho = 0.5\beta$ and finally, $\rho = 1\beta$.

Analyzing the table and graphs, one notices an excellent performance of the Rosenbrock method when compared to the BEFD method when reaching an accuracy of up to 9 decimal places. Analyzing Tab. 1, it can be seen that the largest relative error happens for the prompt critical case, $\rho = 1\beta$, at time $t = 100s$ with a error of $3.8513620727 \times 10^{-7}$ and an accuracy of 8 decimal places. The graphics for constant reactivity insertion behave, for all reactivity values, in a satisfactory way when coinciding with the reference points of the literature.

Table 1: Neutron density in cm^{-3} for constant reactivity insertion

Reactivity	t(s)	**ROS** $\Delta t = 0.0001s$	BEFD	Relative Errors
$\rho = -1\beta$	0.1	0.5205642859	0.5205642866	$1.34469462853 \times 10^{-9}$
	1	0.4333334453	0.4333334453	0
	10	0.2361106508	0.2361106508	0
	100	0.0286676425	0.02866764245	$3.4882533565 \times 10^{-9}$
$\rho = -0.5\beta$	0.1	0.6989252253	0.6989252256	$4.2923046559 \times 10^{-10}$
	1	0.6070535656	0.6070535656	0
	10	0.3960776907	0.3960776907	0
	100	0.0715828544	0.07158285444	0
$\rho = 0.5\beta$	0.1	1.533112646	1.533112646	0
	1	2.5114942915	2.511494291	$1.990846651 \times 10^{-10}$
	10	14.215025242	14.21502524	$1.406961975 \times 10^{-10}$
	100	80061435.624	80061435.62	$4.996163220 \times 10^{-11}$
$\rho = 1\beta$	0.1	2.5157661414	2.515766141	$1.589972905 \times 10^{-10}$
	1	32.183540946	32.18354095	$1.2428713192 \times 10^{-10}$
	10	3246978898	3246978898	0
	100	2.596485E+89	2.596484E+89	$3.8513620727 \times 10^{-7}$

3.2 Insertion of time-dependent reactivity

3.2.1 Insertion of Ramp Reactivity

For the second case of reactivity to be analyzed, the kinetics parameters presented in Tumelero (2015) are used, considering insertion of linear reactivity $\rho(t) = at$, where $a = 0.1\$$. The values for neutron density in cm^{-3} are shown in the Tab. 2 along with the relative errors. The graph is shown in Fig. 2 generated in the range of $0s$ to $8s$.

Analyzing the table and graph of the ramp reactivity, it is noticed that there is an agreement with the results of the BEFD method. In Tab. 2, it can be seen that as the time step is reduced, convergence is achieved, obtaining more accurate results

when compared to the benchmark data in the literature. Analyzing the relative errors for this case, with $\Delta t = 0.00001s$, it can be seen that the largest relative error is $t = 11s$, with a value of $2.04993979 \times 10^{-4}$. The neutron density behavior for inserting this reactivity presented in Fig. 2 is satisfactory when coinciding with the BEFD method points.

Table 2: Neutron density in cm^{-3} for ramp reactivity insertion

Reactivity	t(s)	**ROS** $\Delta t = 0.0001s$	**ROS** $\Delta t = 0.00001s$	BEFD	Relative Errors **ROS** $\Delta t = 0.00001s$
$\rho = 0.1\beta t$	2	1.3382136087	1.3382014099	1.338200050	$1.0162157743 \times 10^{-6}$
	4	2.2284808046	2.2284457943	2.228441897	$1.2037244514 \times 10^{-6}$
	6	5.582286602	5.5820357692	5.582052449	$2.98811237486 \times 10^{-6}$
	8	42.790022391	42.786668501	42.78629573	$8.7123924527 \times 10^{-6}$
	10	451457.69528	451193.02182	451163.6239	$6.5120217807 \times 10^{-5}$
	11	1.795892E+16	1.792581D+16	1.792213607E+16	$2.04993979 \times 10^{-4}$

3.2.2 Insertion of Quadratic Reactivity

For the case of quadratic reactivity, it uses the kinetic parameters of Tumelero (2015) with $\lambda = 1 \times 10^{-4}$ and reactivity defined as:

$$\rho(t) = at + bt^2, \tag{4}$$

where a and b are arbitrary constants.

For this analysis, parameter b is fixed and only the a varies, considering three values for a: $-b/10$, 0 and $b/10$ as in Petersen (2011). The behavior of neutron density in cm^{-3} until $1.2s$ for these three cases is shown in Fig. 2.

For this case of reactivity, no numerical data were found in the literature to compare, therefore, only the graph is presented. The neutron density graph for this case, presented in Fig. 2, behaved as expected when comparing with the literature.

3.2.3 Insertion of Sinusoidal Reactivity

For periodic insertion of reactivity, $\rho(t) = \rho_0 sen(t)$, with $\rho_0 = 0.00073$, the Neutron Point Kinetics equations are solved using the kinetic parameters found in Tumelero (2015). In the Tab 3, neutron density is shown in cm^{-3}, where the relative errors are also found. Its respective graph is shown in Fig. 2, generated until $10s$.

Analyzing the table and graph, one can see that the Rosenbrock method produces satisfactory results when compared to the Polynomial Approximation (PAM) method. As can be seen in Tab. 3, the largest relative error is $6.44960321971 \times 10^{-7}$ in $t = 3s$. Note also the approximation of the results of the Rosenbrock method with those of the literature (PAM), since the relative error also decreases when the time step is reduced. The graph again behaves satisfactorily by coinciding with the points of the Polynomial Approximation method of Tumelero (2015).

Table 3: Neutron density in cm^{-3} for insertion of sinusoidal reactivity with six groups of delayed neutron precursors

Reactivity	t(s)	**ROS** $\Delta t = 0.0001s$	**ROS** $\Delta t = 0.00001s$	PAM $\Delta t = 0.0001s$	Relative Errors (**ROS** $\Delta t = 0.00001s$ and PAM)
$\rho = 0.00073 sen(t)$	1	1.1239352929	1.123941089	1.123940509	$5.1604154788 \times 10^{-7}$
	2	1.1688911711	1.168889413	1.168888959	$3.8840301852 \times 10^{-7}$
	3	1.0744909323	1.074484010	1.074484703	$6.44960321971 \times 10^{-7}$
	4	0.9538336925	0.953829729	0.953829290	$4.6025007263 \times 10^{-7}$
	5	0.9073533104	0.907353473	0.907353490	$1.87358071439 \times 10^{-8}$
	6	0.961534792	0.961539100	0.961539576	$4.95039426229 \times 10^{-7}$
	7	1.0874527064	1.087458291	1.087458911	$5.71056058963 \times 10^{-7}$
	8	1.171670565	1.171671201	1.171671274	$6.23041646747 \times 10^{-8}$
	9	1.1113100446	1.111304995	1.111304437	$5.0211263576 \times 10^{-7}$
	10	0.9846856831	0.984680857	0.984680323	$5.4230798313 \times 10^{-7}$

3.2.4 Insertion of Zig-zag Reactivity

For this case, the NPKEs are solved considering the reactivity of the zig-zag type defined as:

$$\rho(t) = \begin{cases} 0.0075t, & 0 \leq t \leq 0.5, \\ -0.0075(t-0.5) + 0.00375, & 0.5 \leq t \leq 1, \\ 0.0075(t-1), & 1 \leq t \leq 1.5, \\ 0.00375, & t \geq 1.5. \end{cases} \tag{5}$$

The parameters found in Tumelero (2015) are used. The numerical results for the neutron density in cm^{-3} until $10s$ are found in Tab. 4 and the graph generated until $2s$, in Fig. 2. To calculate the relative errors, found in the same table, the numerical data of the EPCA method was used.

When looking at the table and graph of this case, one notices that the numerical results found are close to those of the PAM and EPCA methods as the integration step are reduced, obtaining the largest relative error of $7.69677438301 \times 10^{-6}$ in $t = 0.5s$. The graph of neutron density behavior for zig-zag reactivity insertion behaves satisfactorily by coinciding with the data in the literature, in this case with the EPCA method.

Table 4: Neutron density in cm^{-3} for insertion of zig-zag reactivity

t(s)	**ROS** $\Delta t = 0.0001s$	**ROS** $\Delta t = 0.00001s$	PAM $\Delta t = 0.0001s$	EPCA	Relative Errors (**ROS** $\Delta t = 0.00001s$ and EPCA)
0.5	1.7212899131	1.7214091726	1.721422393	1.721422422	$7.69677438301 \times 10^{-6}$
1	1.211194194	1.2111340908	1.211127399	1.211127415	$5.5120542374 \times 10^{-6}$
1.5	1.8920831062	1.8922118385	1.892226104	1.892226140	$7.55802897850 \times 10^{-6}$
2	2.5215662131	2.5216043656	2.521600526	2.521600530	$1.5210973960 \times 10^{-6}$
10	12.047004216	12.047116659	12.04710533	12.04710535	$9.3873172612 \times 10^{-7}$

3.2.5 Insertion of Pulsed Source Reactivity

For the case of pulsed source reactivity, one group of neutron precursors delayed in a thermal reactor is considered, with $\beta = 0.006502$, $\lambda = 0.077/s$, $\Lambda = 5 \cdot 10^{-4}s$ and the reactivity defined by:

$$\rho(t) = \begin{cases} 4\beta exp(-2t^2), & t < 1s, \\ 0, & t > 1s. \end{cases} \tag{6}$$

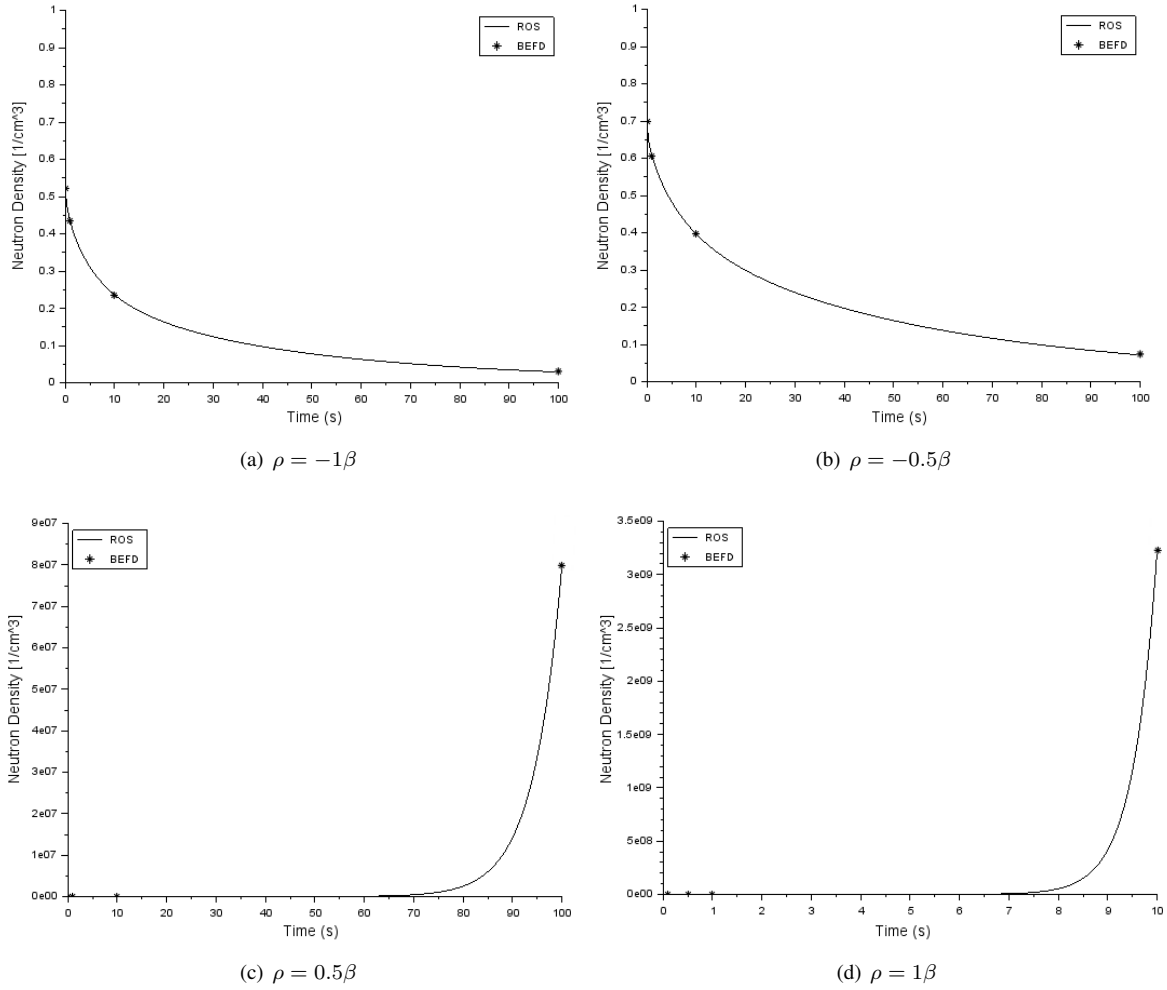
Table 5 shows the results for neutron density, with relative errors and Fig. 2 shows the graph for this case. According to the graph and the table, it can be seen that the Rosenbrock method is very close to the compared results. However, it can be seen that both the method proposed in this paper and the PAM method achieve greater discrepancies in this case of reactivity when compared to the BEFD method, considered benchmark (standard results) in the literature. Table 4 shows that the largest relative error is $2.030486431 \times 10^{-4}$ in $t = 0.8s$ and all other values of relative deviations are in this approximation order. Again, the graph of neutron density behavior for the insertion of pulsed source type reactivity is satisfactory when coinciding with the reference data, in this case, the BEFD method.

Table 5: Neutron density in cm^{-3} for insertion of pulsed source reactivity

t(s)	**ROS** $\Delta t = 0.0001s$	**ROS** $\Delta t = 0.00001s$	PAM $\Delta = 0.0001s$	BEFD	Relative Errors (**ROS** $\Delta t = 0.00001s$ e BEFD)
0.5	9369944.7406	9379086.787	9380592.423	9380044.272	$1.020768103 \times 10^{-4}$
0.8	169116284.16	169443203.99	169487791.0	169477616.1	$2.030486431 \times 10^{-4}$
1	107261206.3	107495133.74	107519618.5	107513170.4	$1.677627023 \times 10^{-4}$
2	4824400.113	4833134.9073	4834396.081	4834106.369	$2.009599967 \times 10^{-4}$
3	4824186.5874	4832920.8993	4834182.039	4833892.339	$2.009642813 \times 10^{-4}$

4. CONCLUSION

In this work, we report a solution of the Neutron Point Kinetics equations applying the fourth-order and four-stage Rosenbrock method, considering inserts of constant and time-dependent reactivities (ramp, quadratic, sinusoidal, zig-zag



(a) $\rho = -1\beta$ (b) $\rho = -0.5\beta$

(c) $\rho = 0.5\beta$ (d) $\rho = 1\beta$

Figure 1: Neutron density for cases with constant reactivity, for (a) $\rho = -1\beta$, (b) $\rho = -0.5\beta$, (c) $\rho = 0.5\beta$ e (d) $\rho = 1\beta$.

and pulsed source). Therefore, because of results, it was possible to verify that the Rosenbrock method produced consistent results as expected, overcoming the stiffness characteristic of the models. As shown in the tables, it can be noticed that by decreasing the time step, the solution tends to converge to the results presented in the literature. Besides, the graphs behave expectedly way when passing over the neutron density points presented by the cited literature references. It is worth mentioning here that this work is the first step of the general aim of this research, seeking to validate at this moment the methodology for the set of equations. In future works, we intend to apply the presented methodology to the Neutron Point Kinetics model including the temperature feedback and poisons effects. Through these equations, we also intend to simulate the accident in the 4th Unit of the nuclear power station at Chernobyl to show the importance of the effects of temperature and poisons in the safe operation of a nuclear reactor.

5. ACKNOWLEDGEMENTS

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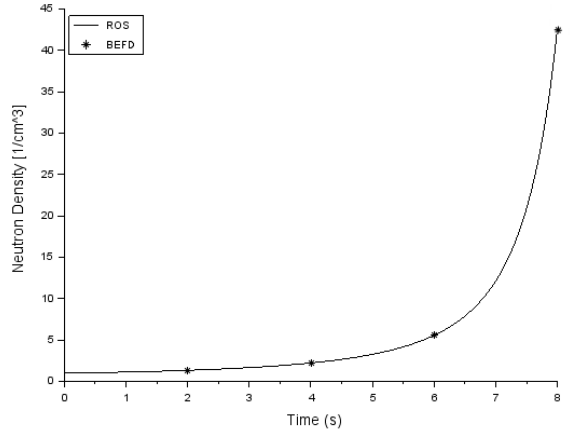
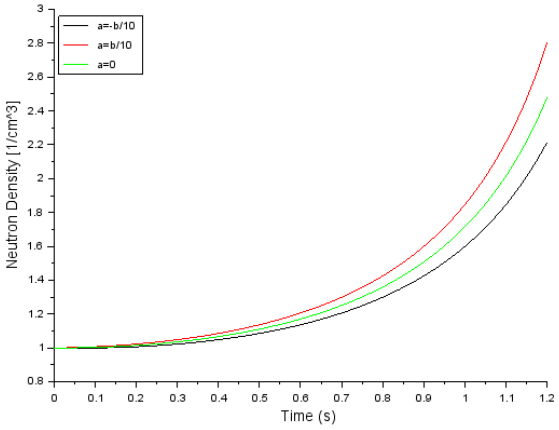
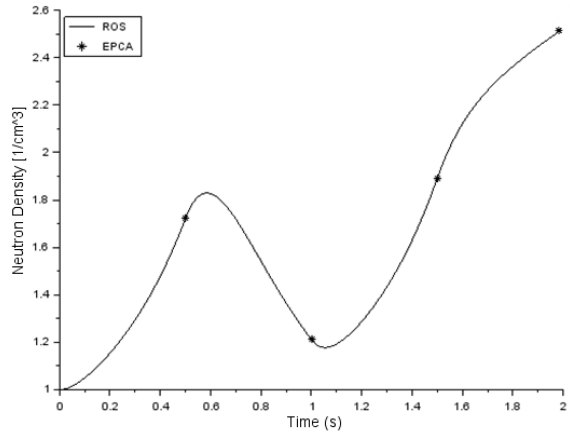


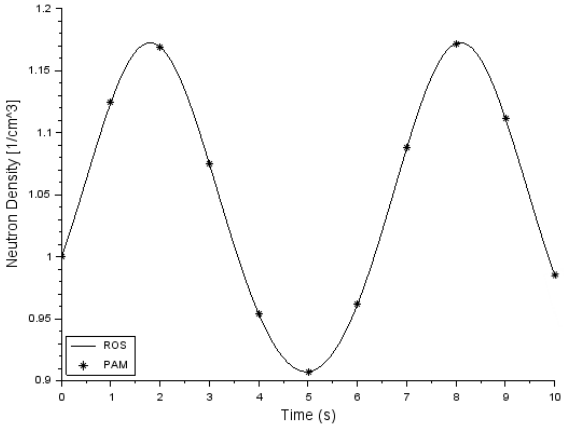
(a) Ramp reactivity



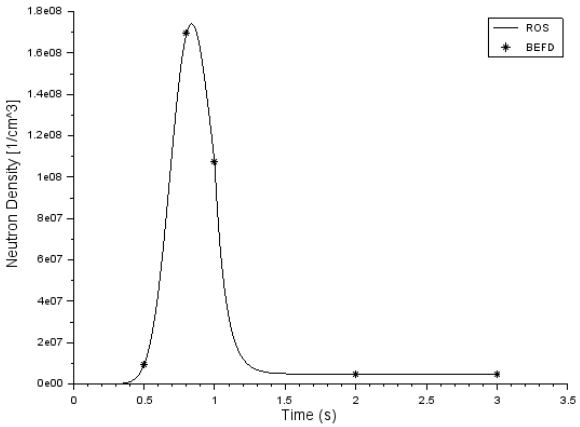
(b) Quadratic reactivity



(c) Zig-zag reactivity



(d) Sinusoidal reactivity



(e) Pulsed source reactivity

Figure 2: Neutron density for cases with reactivity dependent on t.

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