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ON THE NUMERICAL SOLUTION OF STOCHASTIC POINT KINETICS EQUATIONS WITH FEEDBACK EFFECTS USING THE IMPLICIT MILSTEIN METHOD WITH STEP EXTERNAL REACTIVITY

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ABSTRACT

In this work, the iterative schemes Taylor order-two (TO2) and Implicit Milstein with Diagonal Brownian (IMDB) are employed to provide a numerical solution to both the deterministic and stochastic point kinetics equations with feedback effects. The different numerical experiments are performed with 500 Brownian motions, their results are compared with the values reported in the literature, these comparisons showed how the proposed schemes produce good approximations in the calculation of the expected values for neutron density and reactivity, determining the time to the peak where the maximum in neutron density occurs with different step external reactivities for a reactor with feedback effects.

Keywords: stochastic point kinetic equation, temperature feedback effects, taylor order-two, neutron density, reactivity.

1. INTRODUCTION

The point kinetic equations (PKE) [1] model the time evolution of the core of a nuclear reactor, in terms of the different events that modify the population of neutrons and the combustible material in the reactor core, some of these events are: neutron capture by the combustible material, the decay of fission products emitting neutrons, the same fission processes that give rise to new neutrons, among other events. However, this theoretical model does not explain why at low power levels the neutron density and the concentration of precursor groups exhibit fluctuations.

The Stochastic point kinetic equations (SPKE) [2] are a more general model of the temporal evolution of the reactor core, since this includes the random and probabilistic aspects of neutrons, fission processes and decay processes, as well as the variation of the parameters involved in the reactor core such as the small variations in pressure, of the control rods, among others. The *SPKE* consists of a system of $m + 1$ strongly coupled non-linear stochastic differential equations, with $m + 2$ random variables, the m variables are the number of precursor groups to be considered, generally $m = 6$ provides information accurate enough. The other two random variables are the neutron density and the reactivity. The latter accounts for the rate of neutron production in the reactor core. The production of neutrons in the core releases large amounts of energy thereby raising the core's temperature, in turn, this increase in energy causes a lower rate of fission processes with a consequent decrease in the production of neutrons. That is why the reactivity presents feedback effects, the consideration of this effect provides a better understanding of the dynamics of nuclear reactors. The *SPKE* model does not have an analytical solution, therefore it is necessary to use iterative numerical schemes that provide precise approximate solutions.

In this work, the Taylor order-two (TO2) scheme is used to give approximate numerical solutions to the PKE and the Implicit Milstein with Diagonal Brownian (IMDB) for SPKE, this scheme has already been shown to be efficient in the numerical solution of the SPKE model [3]. The results obtained by TO2 and IMDB are compared with the Split-Step Forward Euler-Maruyama Method (EMM), the Derivative-Free Miltein Method (DFMM), the Analytical Exponential Technique (AET) [4], the RK2-2st Method [5], the ITS2 Method [6] and the ABM8 Method [1]. In the next section the theoretical aspects of the SPKE model with feedback effects are analysed.

2. THEORETICAL CONSIDERATIONS

STOCHASTIC POINT KINETIC EQUATIONS

The SPKE model was first introduced in [2], the matrix expression deduced by those authors is:

$$\frac{d}{dt}|P(t)\rangle = \hat{A}|P(t)\rangle + |Q(t)\rangle + \hat{B}^{1/2}\frac{d}{dt}|\omega(t)\rangle \quad (1)$$

where $|P(t)\rangle$ is the vector of random variables defined by equation (2), which accounts for the temporal evolution of the neutron and precursor populations, $\hat{A}$ is the matrix of expected values defined in equation (3), $|Q(t)\rangle$ is the vector of external sources defined in equation (4), $\hat{B}^{1/2}$ is the square root of the variance matrix defined in equation (5), $|\omega(t)\rangle$ is the Wiener process vector defined in equation (6) or by $\sqrt{\Delta t}|\eta\rangle$, where $|\eta\rangle$ is a vector of random numbers with mean zero and standard deviation unity, and Δt is the time step.

$$|P(t)\rangle = \begin{bmatrix} n(t) \\ C_1(t) \\ C_2(t) \\ \vdots \\ C_m(t) \end{bmatrix} \quad (2)$$

$$\hat{A}=\begin{bmatrix} \frac{\rho(t)-\beta}{\Lambda} & \lambda_1 & \lambda_2 & \cdots & \lambda_m \\ \frac{\beta_1}{\Lambda} & -\lambda_1 & 0 & \cdots & 0 \\ \frac{\beta_2}{\Lambda} & 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\beta_m}{\Lambda} & 0 & 0 & \cdots & -\lambda_m \end{bmatrix} \quad (3)$$

$$|Q(t)\rangle=\begin{bmatrix} q(t) \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad (4)$$

$$\hat{B}^{1/2}=\begin{bmatrix} B_{1,1} & B_{1,2} & B_{1,3} & \cdots & B_{1,m+1} \\ B_{2,1} & B_{2,2} & B_{2,3} & \cdots & B_{2,m+1} \\ B_{3,1} & B_{3,2} & B_{3,3} & \cdots & B_{3,m+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_{m+1,1} & B_{m+1,2} & B_{m+1,3} & \cdots & B_{m+1,m+1} \end{bmatrix} \quad (5)$$

$$|\omega(t)\rangle=\begin{bmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \\ \vdots \\ \omega_{m+1} \end{bmatrix} \quad (6)$$

$$\rho(t)=\rho_{ext}-\alpha\left[T(t)-T_0\right] \quad (7)$$

$$\frac{d}{dt}T(t)=K_c n(t) \quad (8)$$

where, n is the neutron density, C_m is the concentration of precursors of the *m-th* group, $\rho(t)$ is the reactivity which accounts for neutron production, β is the total fraction of delayed neutron precursors, Λ is the mean neutron generation time, λ_m is the decay constant of class m of delayed neutron precursors, q is the magnitude of the external source of neutrons, ω_m are Wiener processes which are continuous-time and independent stationary increment stochastic processes, ρ_{ext} is the external reactivity, α is the reactivity temperature coefficient, K_c is the reciprocal of the reactor´s thermal capacity coefficient, $T(t)$ is the reactor temperature and T_0 is the initial temperature of the reactor. The elements of the matrix $\hat{B}^{1/2}$ are described as follows:

$$\begin{aligned} B_{1,1}&=\sqrt{\xi} \\ B_{i,i}&=\sqrt{r_{i-1}-\frac{a_{i-1}^2}{\xi}}\ ;\ i=1,2,3,...,m+1 \\ B_{1,i}&=B_{i,1}=\frac{a_{i-1}}{\sqrt{\xi}}\ ;\ i=1,2,3,...,m+1 \\ B_{i,j}&=\frac{b_{i,j}\frac{a_{i-1}a_{j-1}}{\xi}}{\left(B_{i,i}B_{j,j}\right)^{1/2}+B_{i,i}}\ ;\ i>j \quad \begin{matrix} i=2,3,...,m+1 \\ j=3,4,...,m+1 \end{matrix} \end{aligned} \quad (9)$$

where the parameters ξ, a_i, r_i y $b_{i,j}$ are:

$$\xi=\gamma n(t)+\sum_{i=1}^{m}\lambda_i C_i(t)+q(t) \quad (10)$$

$$\gamma=\frac{-1-\rho+\upsilon(1-\beta)^2+2\beta}{\Lambda} \quad (11)$$

$$a_i=\frac{\beta_i\left[\upsilon(1-\beta)-1\right]}{\Lambda}n(t)-\lambda_i C_i(t) \quad (12)$$

$$r_i=\frac{\upsilon\beta_i^2}{\Lambda}n(t)+\lambda_i C_i(t) \quad (13)$$

$$b_{i,j}=\frac{\upsilon\beta_{i-1}\beta_{j-1}}{\Lambda}n(t) \quad (14)$$

where υ is the average number of neutrons generated per fission event. Equations (7) and (8) include the thermal feedback effects, these are not considered in [2]. Note as if in equation (1) $\hat{B}^{1/2}=0$, the *PKE* model is obtained. A non-matrix way is:

$$\begin{aligned} \frac{d}{dt}n(t)&=\frac{\rho(t)-\beta}{\Lambda}n(t)+\sum_{i=1}^{m}\lambda_i C_i(t)+q(t) \\ \frac{d}{dt}C_i(t)&=\frac{\beta_i}{\Lambda}n(t)-\lambda_i C_i(t)\quad ;\quad i=1,2,3,...,m \end{aligned} \quad (15)$$

In the next section the order-two Taylor scheme for PKE is shown. The Implicit Milstein Scheme applied to SPKE with the Diagonal Brownian variance reduction.

3. ORDER-TWO TAYLOR SCHEME

The order-two Taylor iterative scheme for the neutron density variables and for the m groups of precursors is:

$$n_{k+1} = n_k + h\frac{d}{dt_k}n_k + \frac{h^2}{2!}\frac{d^2}{dt_k^2}n_k$$
$$C_{i,k+1} = C_{i,k} h\frac{d}{dt_k}C_{i,k} + \frac{h^2}{2!}\frac{d^2}{dt_k^2}C_{i,k}\ ;\ i = 1,2,3,...,m \quad (16)$$

Note that the first-time derivatives correspond to the system (15), and the second-time derivatives stem from deriving the system (15), these derivatives have been calculated analytically, and replaced into equation (16). The resulting system of equations can be rewritten in matrix form in the following way:

$$P_{k+1} = P_k + h\left(A_k P_k + Q_k\right) + \frac{h^2}{2}A_k' P_k \quad (17)$$

where the matrix A_k' has the following form:

$$A_k' = \begin{bmatrix} a_{1,1}' & a_{1,2}' & a_{1,3}' & \cdots & a_{1,m+1}' \\ a_{2,1}' & a_{2,2}' & 0 & \cdots & 0 \\ a_{3,1}' & 0 & a_{3,3}' & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m+1,1}' & 0 & 0 & \cdots & a_{m+1,m+1}' \end{bmatrix} \quad (18)$$

being

$$a_{1,1}' = \frac{1}{\Lambda}\left(\frac{d}{dt_k}\rho_k + \frac{\left(\rho_k - \beta\right)^2}{\Lambda} + \sum_{i=1}^{m}\lambda_i\beta_i\right)$$
$$a_{1,i}' = \lambda_{i-1}\left(\frac{\left(\rho_k - \beta\right)}{\Lambda} - \lambda_{i-1}\right);\ i = 2,3,4,...,m \quad (19)$$
$$a_{i,1}' = \frac{\beta_{i-1}}{\lambda_{i-1}\Lambda}a_{1,i}'\ ;\ i = 2,3,4,...,m$$
$$a_{i,i}' = \lambda_{i-1}\left(\frac{\beta_{i-1}}{\Lambda} - \lambda_{i-1}\right);\ i = 2,3,4,...,m$$

In short, the scheme called *TO2* used to give an approximate numerical solution to the PKE in this work is:

$$P_{k+1} = P_k + h\left(A_k + \frac{h}{2}A_k'\right)P_k + hQ_k \quad (20)$$

4. IMPLICIT MILSTEIN SCHEME

Milstein´s iterative scheme is the result of truncating the Itô-Taylor expansion at the fourth term [3,7], this expansion is the stochastic version of the popular Taylor series. Equation (21) describes the discrete Milstein's scheme. This scheme has a convergence order of 1.0.

$$x_{n+1} = x_n + a_n + b_n\Delta\omega + \frac{1}{2}b_n\frac{\partial}{\partial x_n}b_n\left[\left(\Delta\omega\right)^2 - \Delta\right] \quad (21)$$

where

$$\Delta = t_{n+1} - t_n \quad (22)$$

$$\Delta\omega = \omega_{n+1} - \omega_n \quad (23)$$

Equation (23) introduces a Wiener process. This is characterised by being a continuous-time stochastic process with independent stationary increments, $\omega_{t=0} = 0$ with probability unity and $\omega_t - \omega_s \sim \aleph(0, t-s)$ for $0 \le s \le t$, where $\aleph(\mu, \sigma^2)$ denotes the normal distribution with expected value μ and variance σ^2 [9]. With the property introduced in equation (24), which is useful for the simulations.

$$\Delta\omega = \sqrt{\Delta}\aleph(0,1) \quad (24)$$

However, the use of Milstein´s implicit version for a better approximation is considered, given the strong coupling and the nonlinearity that point kinetics exhibits in both its deterministic and stochastic formulation, this scheme is:

$$x_{n+1} = x_n + a_{n+1}h + b_n\Delta\omega + \frac{1}{2}b_n\frac{\partial}{\partial x_n}b_n\left[\left(\Delta\omega\right)^2 - h\right] \quad (25)$$

Applying equation (25) to the S*PKE* we get

$$P_{k+1} = P_k + \left[A_{k+1}P_{k+1} + Q_{k+1}\right]h + B_k^{1/2}\Delta\omega_k + \frac{1}{2}B_k^{1/2}\frac{d}{dP_k}B_k^{1/2}\left[\left(\Delta\omega_k\right)^2 - h\right] \quad (26)$$

Solving for P_{k+1} we get

$$P_{k+1} = \left(I - hA_{k+1}\right)^{-1}\left[\begin{matrix} P_k + Q_{k+1}h + B_k^{1/2}\Delta\omega_k \\ + \frac{1}{2}B_k^{1/2}\frac{d}{dP_k}B_k^{1/2}\left[\left(\Delta\omega\right)^2 - h\right]\end{matrix}\right] \quad (27)$$

where I is the identity matrix. The calculation of the inverse of $I - h\,A_{k+1}$ has already been presented analytically [3] and its result will be used in this work. Thus, Milstein's implicit scheme applied to SPKE turns out to be:

$$P_{k+1} = S_{k+1}\left[\begin{matrix} P_k + Q_{k+1}h + B_k^{1/2}\Delta\omega_k \\ + \frac{1}{2}B_k^{1/2}\frac{d}{dP_k}B_k^{1/2}\left[\left(\Delta\omega_k\right)^2 - h\right]\end{matrix}\right] \quad (28)$$

where

$$\hat{S} = \begin{bmatrix} S_{1,1} & S_{1,2} & S_{1,3} & \cdots & S_{1,m+1} \\ S_{2,1} & S_{2,2} & S_{2,3} & \cdots & S_{2,m+1} \\ S_{3,1} & S_{3,2} & S_{3,3} & \cdots & S_{3,m+1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ S_{m+1,1} & S_{m+1,2} & S_{m+1,3} & \cdots & S_{m+1,m+1} \end{bmatrix} \quad (29)$$

with

$$S_{1,j} = \frac{1}{\zeta_{k+1}}\left[1+\left(\frac{\lambda_{j-1}\Delta}{1+\lambda_{j-1}\Delta}-1\right)\left(1-\delta_{1,j}\right)\right];\ j=1,2,3,...,m+1$$
$$\zeta_{k+1} = 1-\frac{\rho_{k+1}-\beta}{\Lambda}\Delta-\frac{\Delta^2}{\Lambda}\sum_{i=1}^{m}\frac{\lambda_i\beta_i}{1+\lambda_i\Delta} \quad (30)$$
$$S_{i,j} = \frac{1}{1+\lambda_i\Delta}\left[1\frac{\beta_{i-1}\Delta}{\Lambda}S_{1,j}+\delta_{1,j}\right];\ \begin{matrix} i=2,3,4,...,m+1 \\ j=1,2,3,...,m+1 \end{matrix}$$

In addition, the following product is approximated as:

$$B_k^{1/2}\frac{d}{dP_k}B_k^{1/2} = \begin{bmatrix} B_{1,1}\frac{d}{dn_k}B_{1,1} & B_{1,2}\frac{d}{dn_k}B_{1,2} & \cdots & B_{1,m+1}\frac{d}{dn_k}B_{1,m+1} \\ B_{2,1}\frac{d}{dC_{1k}}B_{2,1} & B_{2,2}\frac{d}{dC_{1k}}B_{2,2} & \cdots & B_{2,m+1}\frac{d}{dC_{1k}}B_{2,m+1} \\ \vdots & \vdots & \ddots & \vdots \\ B_{m+1,1}\frac{d}{dC_{mk}}B_{m+1,1} & B_{m+1,2}\frac{d}{dC_{mk}}B_{m+1,2} & \cdots & B_{m+1,m+1}\frac{d}{dC_{mk}}B_{m+1,m+1} \end{bmatrix} \quad (31)$$

5. DIAGONAL BROWNIAN

The implicit Milstein scheme with Brownian diagonal considers a new independent Brownian motion which multiplies the terms of the main diagonal of the square root of the variance matrix in the following way:

$$B_{1,1} = \Delta\omega_t\sqrt{\xi}$$
$$B_{i,i} = \Delta\omega_t\sqrt{r_{i-1}-\frac{a_{i-1}^2}{\xi}} \quad ;\quad i=1,2,3,...,m+1 \quad (32)$$

6. RESULTS

Taylor's method of order-two (*TO2*) and implicit Milstein with diagonal Brownian (IMDB) have been applied to the PKE and SPKE models with feedback effects, respectively, for a graphite reactor $^{235}_{92}U$, the physical parameters of this type of reactor are: thermal coefficient of reactivity $\alpha = 5x10^{-5}\ (K^{-1})$, reciprocal coefficient of thermal capacity of the reactor $K_c = 0{,}05\ \left(\frac{K}{MW}\right)$, average number of neutrons generated per fission event $\upsilon = 2{,}5$, neutron generation time $\Lambda = 5x10^{-5}\ (s)$, partial fractions of precursor groups $\beta_i = [0{,}00021\ 0{,}00141\ 0{,}00127\ 0{,}00074\ 0{,}00027]$, total fraction of precursors $\beta = \sum\beta_i$ and decay constants $\lambda_i = [0{,}0124\ 0{,}0305\ 0{,}111\ 0{,}301\ 1{,}13\ 3{,}0]\ (s^{-1})$.

The different numerical experiments are carried out for external reactivities of 0.50 ($), 0.75 ($), 1.00 ($), 1.50 ($) and 2.00 ($), where the sign ($) refers to dollars. These experiments are carried out with a magnitude of the external source of neutrons $q(t) = 0$ and initial conditions $n(0) = 1\ \left(\frac{g}{cm^3}\right), C(0) = \frac{\beta}{\lambda_1\Lambda}n(0)\ \left(\frac{g}{cm^3}\right)$. The deterministic method *TO2* uses a time step of 10^{-5}, the stochastic method proposed, *IMDB*, uses a time step of 10^{-3} with 500 Brownian motions as in the different stochastic methods reported in the literature.

Table-1 shows results of the proposed method and some of the methods reported in the literature. The maximum values of neutron density and the time-to-peak in which this is reached for the different external reactivities are reported 0.50 ($), 0.75 ($) and 1.00 ($). Since the results using the deterministic methods *ITS2* and *ABM8* were not reported in the literature, the *TO2* method is implemented in order to compare the precision of the stochastic methods. The results produce good numerical approximations of the proposed *IMDB* method since the time-to-peak in which the maximums of the neutron density occur are very similar to the other stochastic methods and the *TO2* reference method.

Table-1. Maximum peak of neutron density and its corresponding time for external reactivity.

Method	$\rho_{ext} = 0{,}50$ ($)		$\rho_{ext} = 0{,}75$ ($)		$\rho_{ext} = 1{,}00$ ($)	
	peak	*time*	*peak*	*time*	*peak*	*time*
DFMM [4]	46,260	27,840	164,220	8,950	769,238	1,057
RK2-2ST [5]	45,820	27,800	163,492	8,900	805,446	1,000
EMM [4]	46,4939	28,3400	163,707	8,795	760,589	1,065
IMDB	46,065	28,183	164,434	8,522	811,926	0,991
ITS2 [6]	-	-	-	-	807,868	0,953
ABM8 [1]	-	-	-	-	807,868	0,954
TO2	45,703	28,301	163,283	8,811	807,860	0,953

Increased the value of the external reactivity, the results of the different experiments considering the greater reactivities 1.50 ($) and 2.00 ($) are presented in Table-2. For these values of reactivity there are reference values using the deterministic methods ITS2 and ABM8, thus the two reference methods would be of better precision than

the *TO2* method, however, the values are not very different and for our purpose of comparing with the stochastic methods, it turns out to be appropriate. The times to peak are very similar among the different stochastic methods, although IMDB seems to calculate by excess the maximum values of the neutron density, the time in which these maximums occur is according to the reference values.

Table-2. Maximum peak of neutron density and its corresponding time for external reactivity.

Method	$\rho_{ext} = 1,50$ (\$)		$\rho_{ext} = 2,00$ (\$)	
	peak	***time***	***peak***	***time***
RK2-2ST [5]	39472,347	0,169	148565,750	0,100
IMDB	44990,492	0,164	188180,805	0,093
AET [4]	33119,580	0,174	128083,100	0,101
ITS2 [6]	43024,605	0,168	167845,682	0,098
ABM8 [1]	43024,600	0,168	167845,600	0,098
TO2	43043,262	0,168	167990,418	0,098

Figures 1a-1e show the different numerical experiments previously carried out to obtain the neutron density depending on the external reactivity. The stochastic behaviour is clearly seen for external reactivities 0.50 (\$), 0.75 (\$) and 1.00 (\$), being more noticeable for small reactivities. It is observed how the average value calculated by the proposed IMDB method using the 500 Brownian motions approximates the deterministic value calculated with the *TO2* method. For high reactivities 1.50 (\$) and 2.00 (\$), the stochastic effects seem to decrease.

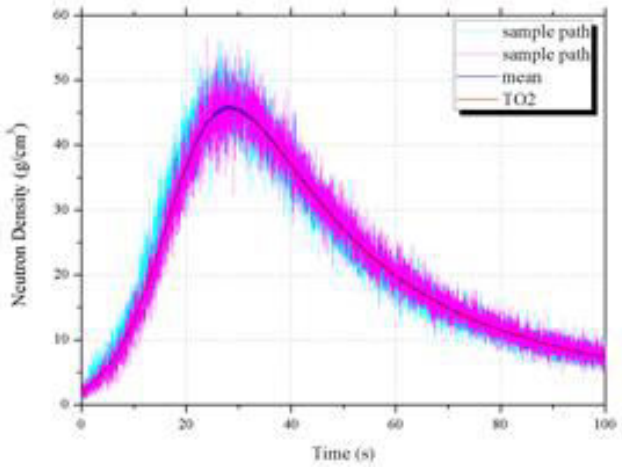

Figure-1a $\rho_{ext} = 0,50$ (\$).

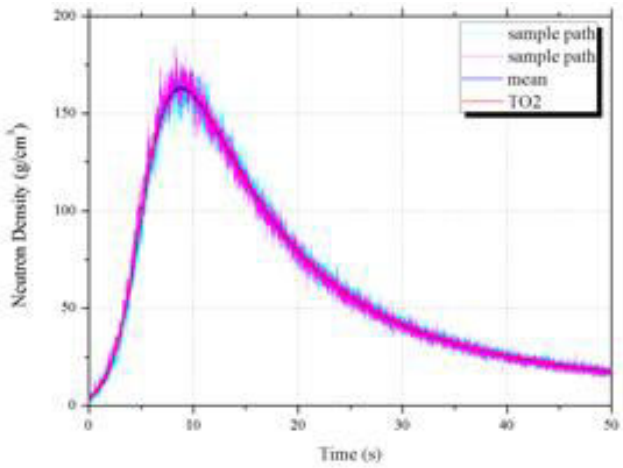

Figure-1b. $\rho_{ext} = 0,75$ (\$).

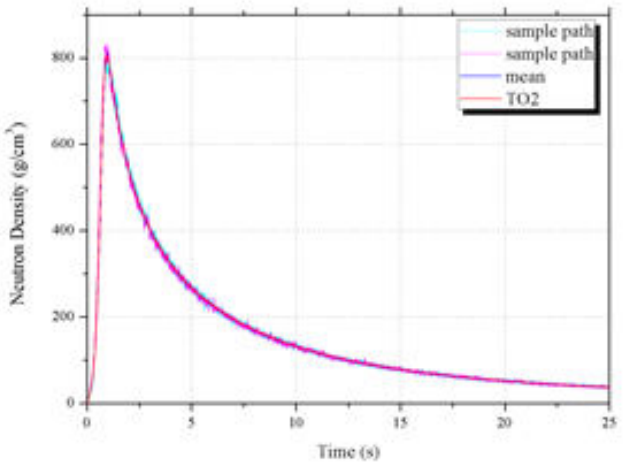

Figure-1c. $\rho_{ext} = 1,00$ (\$).

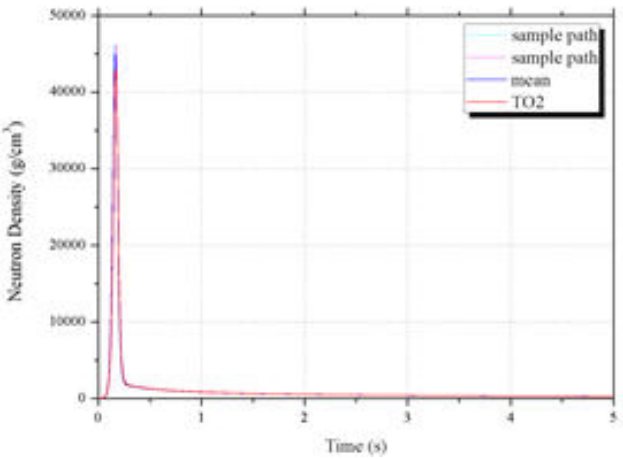

Figure-1d. $\rho_{ext} = 1{,}50$ (\$).

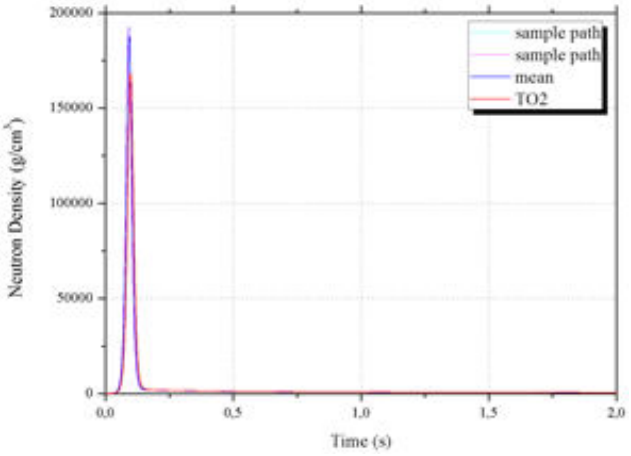

Figure-1e. $\rho_{ext} = 2{,}00$ (\$).

Table-3 shows the expected values for the density of the neutron population and the reactivity for different values of external reactivity and simulation times considered in this work, and those reported in the literature. Figure-2 shows the behaviour of reactivity over time for the different values of external reactivity. It is observed that the reference method and the proposed method have an increasing difference when the value of external reactivity increases.

Table-3. Values of the neutron density and reactivity by the proposed method.

$\boldsymbol{\rho_{ext}}$ (\$)	$\boldsymbol{time}$ $(\boldsymbol{s})$	*Method*			
		IMDB		***TO2***	
		$E[n(t)]$	$E[\rho(t)]$ (\$)	$n(t)$	$\rho(t)$ (\$)
0,50	100	7,365	-0,35395	7,302	-0,35271
0,75	50	17,180	-0,48698	17,168	-0,48620
1,00	25	37,016	-0,59147	37,062	-0,59039
1,50	5	231,429	-0,54481	233,794	-0,52372
2,00	2	487,162	-0,79767	505,142	-0,67752

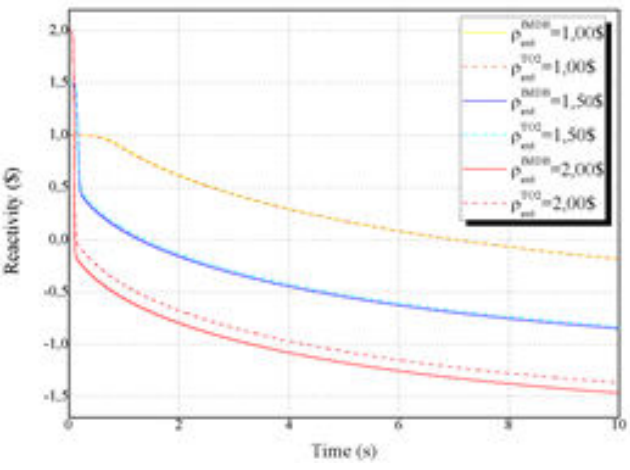

Figure-2. Reactivity for each step external reactivity.

7. CONCLUSIONS

In this work, the proposed implicit Milstein with diagonal Brownian (IMDB) method to solve stochastic equations of point kinetics with feedback effects considering different step external reactivity values was presented. Comparison of the obtained results with those in the literature shows that the proposed method has good precision and its results were validated with some very high-precision deterministic methods such as the *ITS2* and *ABM8* methods. When the values reported in the literature were not available, our results were compared with the deterministic method using the order-two Taylor series (*TO2*). Our method of calculation has some important advantages such as a low computational cost, since it does not require the calculation of inverse matrices nor derivatives since they can be calculated analytically and are easy to implement.

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