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A NEW NUMERICAL APPROXIMATION FOR REACTIVITY CALCULATION

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ABSTRACT

In this work, a new numerical approximation to solve the inverse point kinetics equation is presented. The integral of the historic of the neutron population density is discretized, based on the approximation of Euler-Maclaurin formula, considering an extra term in this procedure to obtain a better approximation using two Bernoulli numbers. Reactivity is calculated for different numerical experiments, with different neutron population density forms and different time steps. In order to validate the accuracy of the proposed method, we compare the results obtained with different numerical experiments reported in the literature. The results suggest that the method shown can be used in a real time reactivity digital meter.

Keywords: inverse point kinetics equation, reactivity, neutron population density, simulation.

INTRODUCTION

The nuclear reactions that occur inside nuclear reactors are product of the fission of uranium (U^{235}) located in the reactor core. When bombarded with a beam of thermal neutrons, a chain reaction is produced. This chain reaction frees a great amount of energy and several neutrons that can be either instantaneous or delayed. It is necessary to control this chain reaction that depends of the interaction of the fission neutrons with different materials. To control the chain reaction, it is important to know the parameter that allows to operate safely the nuclear reactor which is known as reactivity. Furthermore, it is possible to determine the time dependent behavior of the neutron distribution and the change in time of the fissionable material composition due to the neutron interactions (Stacey, 2018).

A great variety of scientific work has been done over the years around the calculation of reactivity to find a method that shows a better accuracy while reduces the computational cost. For reactivity calculation, several of these methods have been reported in the literature based on the discretization of the neutron population density history (Shimazu *et al*., 1987, Ansari, 1991, Binney *et al*., 1989, Hoogenboom *et al*., 1988, Malmir *et al*., 2013, Suescún *et al*., 2007, Kitano *et al*., 2000). Another method was published using the discrete version of the Laplace transform (Suescún *et al*., 2008), where the linear part is characterized by a filter called Finite Impulse Response (FIR) (Haykin S, 2002). This was done to discretize the integral of the neutron population density as a convolution sum. Although this method showed good results, it has high computational cost.

In this work, it is proposed the discretization of the integral of the historic of the neutron population density, using the Euler-Maclaurin formula (Suescún *et al*., 2013), considering up to second Bernoulli number.

THEORETICAL ASPECTS

The point kinetic equations can be obtained from the neutron diffusion equations. Their representation is given by (Duderstadt, 1976),

$$\frac{dP(t)}{dt}=\left[\frac{\rho(t)-\beta}{\Lambda}\right]P(t)+\sum_{i=1}^{6}\lambda_i C_i(t) \tag{1}$$

$$\frac{dC_i(t)}{dt}+\lambda_i C_i(t)=\frac{\beta_i}{\Lambda}P(t) \quad ; \quad i=1,2,\ldots,6 \tag{2}$$

Constrained by the following initial conditions:

$$P(t=0)=P_0 \tag{3}$$

$$C_i(t=0)=\frac{\beta_i}{\Lambda\lambda_i}P_0 \tag{4}$$

Where C_i is the concentration of the *i-th* group of delayed neutron precursors, $P(t)$ is the neutron population density, $\rho(t)$ is the reactivity, Λ is the neutron generation time, β is the total effective fraction of delayed neutrons, λ_i is the decay constant of the *i-th* group of delayed neutron precursors and β_i is the *i-th* fraction of delayed neutrons.

Isolating $\rho(t)$ on equation (1) we obtain an expression for the reactivity:

$$\rho(t)=\beta+\frac{\Lambda}{P(t)}\frac{dP(t)}{dt}-\frac{\Lambda}{P(t)}\sum_{i=1}^{6}\lambda_i C_i(t) \tag{5}$$

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When solving equation (2), and applying the initial conditions shown on equations (3) and (4), an expression for the precursor concentration can be obtained:

$$C_i(t) = \frac{\beta_i}{\Lambda}\left[\frac{e^{-\lambda_i t}}{\lambda_i}P_0 + \int_0^t e^{-\lambda_i (t-t')}P(t')dt'\right] \tag{6}$$

Replacing equation (6) on equation (5) we get:

$$\rho(t) = \beta + \frac{\Lambda}{P(t)}\frac{dP(t)}{dt} - \frac{\langle P_0\rangle}{P(t)}\sum_{i=1}^{6}\beta_i e^{-\lambda_i t} - \frac{1}{P(t)}\sum_{i=1}^{6}\int_0^t \lambda_i\beta_i e^{-\lambda_i (t-t')}P(t')dt' \tag{7}$$

Equation (7) represents the inverse point kinetics equation; this equation cannot be used directly to calculate the reactivity, due to the dependence it has on the neutron density history, which implies a very high computational cost.

PROPOSED METHOD

The method proposed in this section, to obtain a better approximation and reduce the computational cost for the reactivity calculation, is based on the discretization of the integral of the neutron population density history given on equation (7), using the Euler-Maclaurin formula (Arfken, 2013), using two Bernoulli numbers in the following equation:

$$\int_0^n F(k)dk = \sum_{s=1}^{n-1}F[s] + \frac{1}{2}\left[F[0]+F[n]\right] - \sum_{m=1}^{\infty}\frac{B_m}{(2m)!}\left[F^{(2m-1)}[n] - F^{(2m-1)}[0]\right] \tag{8}$$

These first two Bernoulli numbers represented on equation (8) by the term B_m are $B_1 = \frac{1}{6}$ and $B_2 = \frac{1}{30}$

We define the response of the system to a unitary impulse (Suescún et al., 2008) as:

$$h_i(t-t') = \lambda_i\beta_i e^{-\lambda_i (t-t')} \tag{9}$$

Replacing expression (9) in the neutron population density history on equation (5) we get:

$$F(t') = h_i(t-t')P(t') \tag{10}$$

It is also possible to get a discrete version of equation (10) of the form:

$$F[s] = h_i[n-s]P[s] \tag{11}$$

The reactivity for the first Bernoulli number (Suescún *et al*., 2013), using equation (8) is defined as:

$$\begin{aligned}\rho[n] &= \beta + \frac{\Lambda}{P[n]}P^{(1)}[n] - \frac{\langle P_0\rangle}{P[n]}\sum_{i=1}^{6}\beta_i e^{-\lambda_i nT} \\ &- \frac{T}{P[n]}\sum_{i=1}^{6}\left[\sum_{s=1}^{n}h_i[n-s]P[s] - \frac{1}{2}[h_i[n]P[0] + h_i[0]P[n]]\right] \\ &+ \frac{T^2}{12P[n]}\sum_{i=1}^{6}[h_i^{(1)}[0]P[n] + h_i[0]P^{(1)}[n] - h_i^{(1)}[n]P[0] - h_i[n]P^{(1)}[0]]\end{aligned} \tag{12}$$

Where T is the step size in the calculation of reactivity, n indicates the discrete time, and its relation with the continuous time is given by $t = nT$.
Deriving three time the equation (11), we express:

$$\begin{aligned}F^{(3)}[s] &= h_i^{(3)}[n-s]P[s] + 3(h_i^{(2)}[n-s]P^{(1)}[s]) \\ &+ 3(h_i^{(1)}[n-s]P^{(2)}[s]) + h_i[n-s]P^{(3)}[s]\end{aligned} \tag{13}$$

Now, we evaluate equation (11) at $s = n$ and $s = 0$, we have:

$$F[n] = h_i[0]P[n] \tag{14}$$

$$F[0] = h_i[n]P[0] \tag{15}$$

By replacing equations (14) and (15) on equation (13), we get:

$$\begin{aligned}F^{(3)}[n] &= h_i^{(3)}[0]P[n] + 3(h_i^{(2)}[0]P^{(1)}[n]) \\ &+ 3(h_i^{(1)}[0]P^{(2)}[n]) + h_i[0]P^{(3)}[n]\end{aligned} \tag{16}$$

$$\begin{aligned}F^{(3)}[0] &= h_i^{(3)}[n]P[0] + 3(h_i^{(2)}[n]P^{(1)}[0]) \\ &+ 3(h_i^{(1)}[n]P^{(2)}[0]) + h_i[n]P^{(3)}[0]\end{aligned} \tag{17}$$

It is possible to find an equation to calculate the reactivity with the second Bernoulli number, making *m=2* on equation (8) and then replacing on equation (10) and equation (11), is possible to verify the following expression:

$$\int_0^n h_i(t-t')P(t')dt' = \sum_{s=0}^{n-1} h_i[n-s]P[s] + \frac{1}{2}\left[F[0]+F[n]\right] - \frac{1}{12}\left[F^{(1)}[n]-F^{(1)}[0]\right] + \frac{1}{720}\left[F^{(3)}[n]-F^{(3)}[0]\right] \quad (18)$$

Replacing equations (14) through (17) on equation (18) it is possible to obtain:

$$\begin{aligned}\int_0^t F(k)dk = \int_0^t h_i(t-t')P(t')dt' = T\left[\sum_{s=0}^{n} h_i[n-s]P[s] - \frac{1}{2}[h_i[n]P[0]+h_i[0]P[n]]\right]\\ -\frac{T^2}{12}[h_i^{(1)}[0]P[n]+h_i[0]P^{(1)}[n]-h_i^{(1)}[n]P[0]+h_i[n]P^{(1)}[0]]\\ +\frac{T^4}{720}[h_i^{(3)}[0]P[n]+3(h_i^{(2)}[0]P^{(1)}[n])+3(h_i^{(1)}[0]P^{(2)}[n])+h_i[0]P^{(3)}[n]\\ -h_i^{(3)}[n]P[0]-3(h_i^{(2)}[n]P^{(1)}[0])-3(h_i^{(1)}[n]P^{(2)}[0])-h_i[n]P^{(3)}[0]]\end{aligned} \quad (19)$$

Replacing equation (19) on equation (7), we can write the following expression:

$$\rho[n] = \rho_{FIR} + C_{EM} - C_{B_2} \quad (20)$$

Where,

$$\begin{aligned}\rho_{FIR}[n] = \beta + \frac{\Lambda}{P[n]}P^{(1)}[n] - \frac{\langle P_0\rangle}{P[n]}\sum_{i=1}^{6}\beta_i e^{-\lambda_i nT}\\ -\frac{T}{P[n]}\sum_{i=1}^{6}\left[\sum_{s=1}^{n} h_i[n-s]P[s] - \frac{1}{2}\left[h_i[n]P[0]+h_i[0]P[n]\right]\right]\end{aligned} \quad (21)$$

$$C_{EM} = \frac{T^2}{12P[n]}\sum_{i=1}^{6}[h_i^{(1)}[0]P[n]+h_i[0]P^{(1)}[n]-h_i^{(1)}[n]P[0]-h_i[n]P^{(1)}[0]] \quad (22)$$

$$C_{B_2} = -\frac{T^4}{720P[n]}\sum_{i=1}^{6}\left[\begin{aligned}h_i^{(3)}[0]P[n]+3(h_i^{(2)}[0]P^{(1)}[n])+3(h_i^{(1)}[0]P^{(2)}[n])+h_i[0]P^{(3)}[n]\\ -h_i^{(3)}[n]P[0]-3(h_i^{(2)}[n]P^{(1)}[0])-3(h_i^{(1)}[n]P^{(2)}[0])-h_i[n]P^{(3)}[0]\end{aligned}\right] \quad (23)$$

Equation (20) represents the proposed method to calculate the reactivity making use of two Bernoulli numbers.

In the following section we present the results for different numerical experiments, for different forms of the neutron population density, with different time step to calculate reactivity.

RESULTS AND DISCUSSIONS

In this section, the results of the reactivity calculation using two Bernoulli numbers are presented; the reactivity was calculated for different forms of the neutron population density and different time steps. The values for the physical constants are presented on Table-1 and the reference method is given by the analytical solution of equation (7), which is the point of comparison to understand the accuracy of the method. As an abbreviation for the name of the proposed method, we will use $B_{m=2}$.

Table-1. Typical constants for ^{235}U.

Group	1	2	3	4	5	6
$\lambda_i[s^{-1}]$	0.0127	0.0317	0.115	0.311	1.4	3.87
β_i	0.000266	0.001491	0.001316	0.002849	0.000896	0.000182
$\Lambda = 2\times10^{-5}\ [s]$						
$\beta = 7\times10^{-3}$						

First, we consider a neutron nuclear density of the form $P(t)=e^{\omega t}$ with $\omega = 0.00243$ for different time step in the reactivity calculation up to a final time of $t = 1000\ s$. On Table-2 it is possible to observe that the reactivity method with two Bernoulli numbers has a better approximation compared with the Euler-Maclaurin method (Suescún *et al.*, 2013). For time step $T \le 0.5\ s$, it is evident that the proposed method, using two Bernoulli numbers, has a better approximation than the Euler-Maclaurin method (Suescún *et al.,* 2013) and Adams-Bashforth-Moulton (Suescún *et al*., 2016). Figure-1 show the curve of the reactivity for a neutron population density of the form $P(t)=e^{\omega t}$ with $\omega = 0.00243$.

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Table-2. Difference in the reactivity for $P(t)=e^{\omega t}$ with $\omega = 0.00243$, $t = 1000\ s$.

T [s]	Euler-Maclaurin	Hamming	ABM V	$B_{m=2}$
0.01	6.20×10^{-08}	2.08×10^{-11}	2.48×10^{-11}	4.50×10^{-11}
0.05	3.84×10^{-05}	2.88×10^{-08}	5.66×10^{-08}	3.20×10^{-08}
0.1	6.14×10^{-04}	9.01×10^{-07}	1.25×10^{-06}	2.04×10^{-06}
0.2	9.73×10^{-03}	3.25×10^{-05}	5.40×10^{-05}	1.29×10^{-04}
0.5	3.6×10^{-01}	8.47×10^{290}	2.48×10^{307}	2.93×10^{-02}
1	4.66×10^{0}	Infinite	Not Reported	1.49×10^{0}

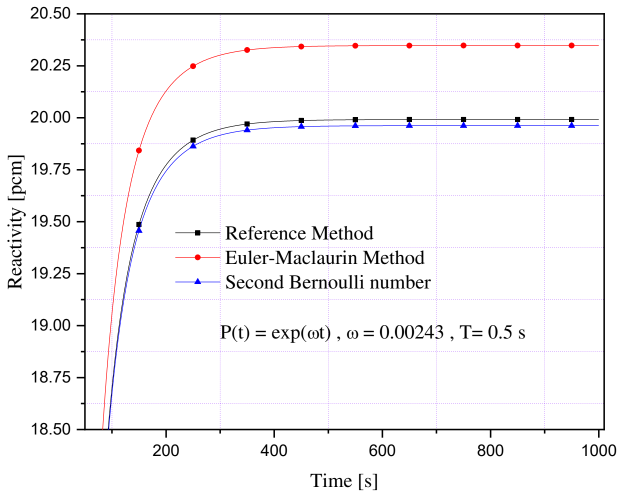

Figure-1. Reactivity curve in pcm for a neutron population density described by $P(t)=e^{\omega t}$ with a value of $\omega = 0.00243$.

Next, we take the same exponential form, but this time we change the value of ω from $\omega = 0.01046$ *to* $\omega = 0.12353$. On Tables 3 through 5 we see the accuracy of the method, using two Bernoulli numbers, for all different time step and time intervals when compared with the Hamming () [15] and Adams-Bashforth-Moulton (Suescún *et al*., 2016) methods; when comparing the reactivity with two Bernoulli numbers and the five-points Lagrange method (Malmir *et al*., 2013), we observe that when $T = 0.1\ s$, which is a value commonly used when calculating reactivity in real time, the numerical results show that the proposed method has a better approximation. Figure-2 shows the curve of the reactivity for a neutron population density of the form $P(t) = e^{\omega t}$ with $\omega = 0.12353$, we can see the accuracy of the proposed method, it is compared with the Euler-Maclaurin method.

Table-3. Difference in the reactivity for $P(t)=e^{\omega t}$ with $\omega = 0.01046, t = 800\ s$.

T [s]	Euler-Maclaurin	Hamming	ABM V	$B_{m=2}$
0.01	6.20×10^{-08}	1.062×10^{-10}	2.37×10^{-05}	3.87×10^{-12}
0.05	3.87×10^{-05}	2.43×10^{-07}	3.98×10^{-04}	3.23×10^{-08}
0.1	6.18×10^{-04}	5.29×10^{-06}	1.14×10^{-03}	2.06×10^{-06}
0.2	9.8×10^{-03}	1.37×10^{-04}	Not Reported	1.30×10^{-04}
0.5	3.58×10^{-01}	7.86×10^{228}	1.04×10^{-02}	2.76×10^{-03}
1	4.69×10^{0}	Infinite	1.83×10^{-02}	5.60×10^{-01}

Table-4. Difference in the reactivity for $P(t)=e^{\omega t}$ with $\omega=0.02817, t=600\ s$.

T [s]	Euler-Maclaurin	Hamming	ABM V	$B_{m=2}$
0.01	6.30×10^{-08}	2.88×10^{-10}	6.38×10^{-05}	3.39×10^{-12}
0.05	3.93×10^{-05}	6.56×10^{-07}	1.06×10^{-03}	3.31×10^{-08}
0.1	6.28×10^{-04}	1.42×10^{-05}	3.05×10^{-03}	2.11×10^{-06}
0.2	9.96×10^{-03}	3.85×10^{-04}	Not Reported	1.33×10^{-04}
0.5	3.64×10^{-03}	4.44×10^{182}	2.65×10^{-02}	3.03×10^{-02}
1	4.76×10^{0}	Infinite	4.36×10^{-02}	1.54×10^{0}

Table-5. Difference in the reactivity for $P(t)=e^{\omega t}$ with $\omega=0.12353, t=300\ s$.

T [s]	Euler-Maclaurin	Hamming	ABM V	$B_{m=2}$
0.01	6.85×10^{-08}	1.27×10^{-09}	2.78×10^{-04}	3.06×10^{-12}
0.05	4.28×10^{-05}	2.88×10^{-06}	4.50×10^{-03}	3.75×10^{-08}
0.1	6.83×10^{-04}	6.24×10^{-05}	1.24×10^{-02}	2.39×10^{-06}
0.2	1.08×10^{-02}	1.46×10^{-03}	Not Reported	1.51×10^{-04}
0.5	3.9×10^{-01}	3.30×10^{78}	8.29×10^{-02}	3.41×10^{-02}
1	5.13×10^{0}	1.25×10^{254}	9.46×10^{-02}	1.72×10^{0}

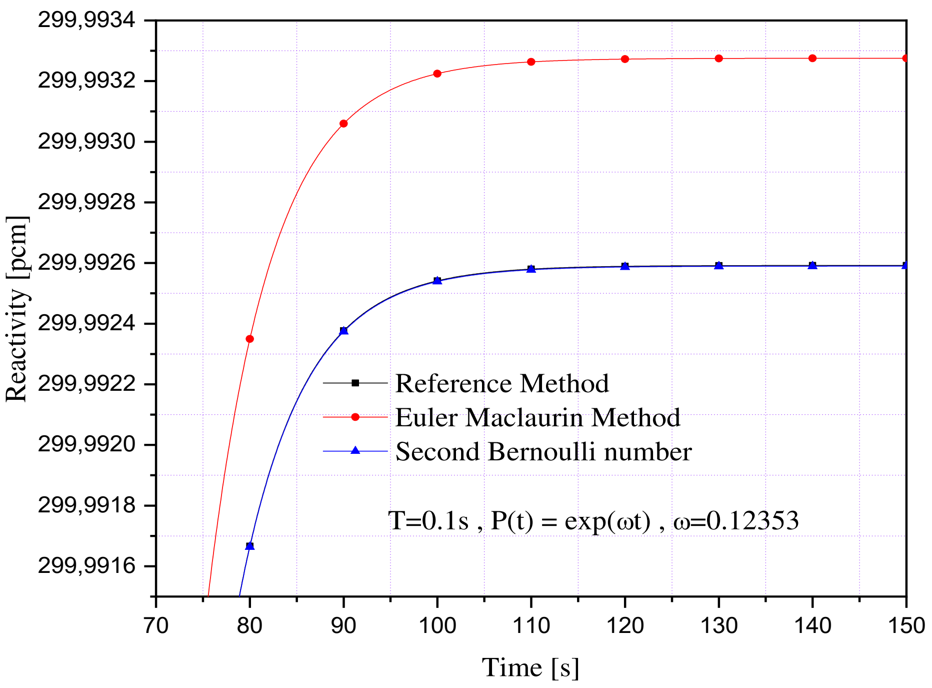

Figure-2. Reactivity curve in pcm for a neutron population density described by $P(t)=e^{\omega t}$ with a value of $\omega=0.12353$.

Finally, we consider the neutron population density of the form $P(t)=a+bt^3$. The results are shown on Table-6 with different time step for the calculation of the reactivity. We observe that the proposed method using the second Bernoulli number for this neutron density form has a constant behavior and of less difference compared to the highest precision methods reported on the literature, such as the derivative method (Suescún *et al*., 2007) and the most recently reported method in the literature, which is matrix formulation method (Suescún *et al*., 2018). With this experiment we show the advantage of the proposed method when the neutron density form has low values of the reactivity.

Table-6.

T [s]	a	B	Derivatives Method	Matrix Formulation Method	$B_{m=2}$
0.1	1	$(0.0127)^5/9$	3.89×10^{-03}	1.42×10^{-05}	2.04×10^{-06}
0.1	1	$(0.0127)^4/40$	6.20×10^{-02}	9.57×10^{-05}	2.04×10^{-06}
0.1	1	$(0.0127)^4/4$	6.21×10^{-01}	4.38×10^{-04}	2.04×10^{-06}

CONCLUSIONS

In this work we presented a new approximation for the calculation of the reactivity, making use of a correction of two Bernoulli numbers and considering the Euler-Maclaurin series. The numerical experiments show very good approximation for the different forms of the neutron population density when compared with several values reported on the literature. The proposed method, due to the high precision it has, can be implemented on real time digital reactivity meter.

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