A toy model for determining the critical size condition in fission chain reaction

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Received 26 November 2023; accepted 27 May 2024

The geometric Buckling in the analytical solutions of the steady-state one group neutron diffusion equation are used to compare with numerical results of the Monte Carlo Method in the determination of the size condition yielding the minimum critical mass in three basic geometries. The survival fraction value, f_s (which is also called as the multiplication factor, k) is calculated for the criticality condition in these geometries and the results are tabulated for each one. Our numerical results by Monte Carlo Method show that the minimum critical mass is obtained in the case of spherical shape of fuel element, and they are in agreement with those of analytical solutions.

Keywords: Applications of Monte Carlo methods; neutron transport: diffusion and moderation; nuclear fission power.

DOI: https://doi.org/10.31349/RevMexFisE.22.010213

Introduction

The fuel material's critical size and mass in a fission chain reaction have extreme importance in nuclear power plants and nuclear weapons [1–3]. There is a certain analogy between the analytical solutions of the steady-state one-group diffusion equation with size and type of material in the sustainable fission process. It is well known that the nuclear fission reaction is a random process and its simulation can also be studied by the Monte Carlo Method (MCM) [4]. In random processes of such a reaction, the critical size and the corresponding mass of the fuel material can be determined by using a simple computer program via MCM. One can simulate the one-group steady state neutron diffusion equation by MCM method in rectangular, cylindrical and spherical geometries.

The purpose of this paper is first to review briefly in three basic geometries the solution of steady-state one-group diffusion equation for bare systems, and then to figure out the critical size condition of the hypothetical fuel material in these geometries by a modified Monte Carlo Method (MCM) which is well formulated and disseminated in PHYSNET [5].

As far as our knowledge, there is no such a simple presentation for the application of the MCM for determining the critical size condition in three different basic geometries. For example, in their paper Brandon *et al*. [6] calculate the critical mass by MCM due to the purity, shape, mean-free path and energy ranges of neutrons and find out that the lowest critical mass is the spherical one. Ibrahim *et al*. [7, 8] investigate the best description of multiplication factor by MCM, and show that there are direct connections among the critical mass and all other parameters such as the dimension of the system, energy range and generation of random points for neutrons. There are many other studies in literature such as Gray [9] and Hiroshi *et al.* [10] for the determination of critical mass for different types of mixtures without and with a reflector by applying some advanced versions of MCM packaged programs using the data libraries such as JEF-2.2, JENDL-3.2 and ENDF/B-VI. All these valuable studies are focused on the calculation of critical mass but in very advanced level for undergraduate and also for graduate students in science and engineering branches: They need advanced calculations and/or ready-packaged programs and naturally require also some extra data-library. On the other hand, the method in this study for undergraduate and also for graduate level students in any branches of science and engineering is very easy, simple and directly applicable for the application of MCM to steady-state one-group diffusion equation. It builds up connection between the results of analytical solutions of neutron diffusion equation for the critical size condition and the MCM method. As far as it is known, there is no such a simple calculation of critical size condition of a reactor system by a MCM [11].

In Sec. 2, we briefly present a review of the solution of the continuity equation and obtain the Buckling parameters. In Sec. 3, we give basics of our modified MCM approach and its applications in three basic different geometries. We present our results in Tables and it is clearly seen that the results are exactly in agreement with those of Neutron Diffusion Theory. In the last section, a short conclusion is presented.

Diffusion equation

If V is the volume of multiplicative medium, three options exist as followings: First, neutrons are produced within the volume. Second, neutrons are absorbed in the volume, and the third one is neutrons escaping (leakage) from the volume.

It is clear that all these reactions take place in volume per unit time and they continue randomly. Thus, the rate of change of neutrons in such a volume is given by a simple equation called as the steady-state diffusion equation [1, 12, 13]:

$$D\,\nabla^2\Phi - \Sigma_a\Phi + S = 0, \tag{1}$$

where Φ is the neutron flux function, Σ_a is the total absorption cross section for the homogeneous mixture of fuel and moderator, D is the diffusion coefficient, and S is the neutron source in the given medium. It should also be noted here that other materials such as coolant and various structural components of the core can be included in the determination of the total absorption cross section. However, we only consider a reactor with homogeneous mixture of fuel and moderator for the simplicity of the solution. Therefore the source term can be defined by the following procedure: $\Sigma_{\rm aF}$ is the fuel element's absorption cross section and f is the fraction for total number of neutrons absorbed by the fuel element to the total number of neutrons absorbed by the mixture of fuel and moderator in the reactor volume, and given as $f = \Sigma_{\rm aF}/\Sigma_{\rm a}$. If η is the average number of fission neutrons emitted per neutron absorbed by the fuel, then the source term is given by

$$S = \eta f \Sigma_a \Phi, \tag{2}$$

where *f* is called as the *fuel utilization coefficient*. If we write the multiplication factor, *k*, for an infinite reactor where no neutrons are escaped (but fully absorbed) in the reactor volume, all neutrons are absorbed either in the fuel or by the moderator eventually. Thus, the absorption rate of $\Sigma_{\rm a}\ \Phi$ neutrons in one generation will lead to the absorption rate of $\eta {\rm f}\Sigma_{\rm a}\ \Phi$ neutrons. Since the multiplication factor, *k*, is defined as the division of total number of fissions in one generation by that of in the preceding generation, one can give the multiplication factor for an infinite reactor as

$$k_\infty = \frac{\eta f \Sigma_a \Phi}{\Sigma_a \Phi} = \eta f. \tag{3}$$

This result is applicable for only an infinite reactor volume. The source term in Eq. (2) can now be written as

$$S = k_\infty \Sigma_a \Phi. \tag{4}$$

Replacing Eq. (4) into Eq. (1) one gets

$$D\,\nabla^2\Phi - \Sigma_a\Phi + k_\infty\Sigma_a\Phi = 0, \tag{5}$$

for a critical reactor. If one defines L^2 which is called as *diffusion area*, by

$$L^2 = \frac{D}{\Sigma_a}, \tag{6}$$

then Eq. (5) is now called as the one-group reactor equation and written as

$$\nabla^2\Phi + B_m^2\Phi = 0, \tag{7}$$

where $B_m^2 = (k_\infty - 1)/L^2$ called as the material Buckling parameter. Since the Laplacian operator in Eq. (7) depends on the geometry of the system under investigation, an expression is obtained that is proportional to the curvature of the neutron flux in the reactor, which gives a measure of the way in which the flux "buckles" and that it depends on the geometry of the reactor. Thus the Buckling parameters for a critical reactor is now written as

$$B_m^2 = \frac{k_\infty - 1}{L^2} = B_g^2, \tag{8}$$

where B_g is called as the geometric Buckling depending on the solution of Eq. (7) and B_m is the material Buckling, respectively. Using Eq. (7) one can find geometric Bucklings for sphere, rectangular parallelepiped and finite cylinder shapes (without the extrapolation distance) as followings: $B_g^2 = (\pi/R)^2$ for spherical shape; $B_g^2 = (\pi/a)^2 + (\pi/b)^2 + (\pi/c)^2$ for rectangular parallelepiped; and $B_g^2 = (\pi/H)^2 + (2.405/R)^2$ for cylinder shapes. Here a, b, c are side lengths of rectangular parallelepiped; R is radius of sphere and cylinder; and H is height of cylinder [1]. (We also need here to note that solutions of Eq. (7) can be found in detail in many Reactor Physics texbooks such as [1–3].

If B_g is known then B_m can be calculated, or vice versa: A greater material Buckling -meaning of a larger fission cross section, a smaller absorption cross section, and/or smaller D- means a more favorable condition for criticality. Conversely, a small geometric Buckling is favored with respect to criticality (shape notwithstanding) as this infers a larger size and thus a larger core. However, the material composition of the core and its shape and size are obviously dependent factors; the criticality is not possible without the combination of these two parameters being satisfied. This condition is satisfied when the Buckling equality is given as $B_g^2 = B_m^2$ corresponding to a state where the survival fraction value $f_s = 1$. Thus, one can conclude $B_m^2 \geq B_g^2$ for the supercriticality $f_s \geq 1$, and conversely $B_g^2 \geq B_m^2$ stands for the subcritical condition $f_s < 1$ [14].

Applications of the MCM

Critical size for a bare rectangular reactor

It assumed that the piece of fissile is a rectangular block of dimensions $a \times a \times b$ and random points for the coordinates x_0, y_0 and z_0 are subject to the following conditions:

$$\left(-\frac{a}{2}\right) \leq x_0 \leq \left(\frac{a}{2}\right), \qquad \left(-\frac{a}{2}\right) \leq y_0 \leq \left(\frac{a}{2}\right),$$
$$\left(-\frac{b}{2}\right) \leq z_0 \leq \left(\frac{b}{2}\right). \tag{9}$$

It is fact that for all fissile nuclei the distributions of fission prompt neutrons are well known and it would be more logical (in the framework of the Monte-Carlo Method) to draw this number (from 2 to 3 or 4) from the frequency distribution function for a sustainable fission chain reaction. However, we assume in this study that only two neutrons are emitted during the fission process and may travel in any directions,

in order to keep our approach as much as simple. In three dimensional space, a direction can be defined by two angles: θ the polar angle, and ϕ, the azimuth angle. If the emitted neutrons have an "isotropic" distribution (depending on the assumptions of Fick's Law), *i.e.*, all directions are equally likely probable, then the probability of a neutron emitted from the point $(x_0,\ y_0,\ z_0)$ hitting any area on a surrounding unit sphere depends only on the size of the area. We shall assume that a neutron emitted during a fission reaction can hit another nucleus after it moves *freely* any distance of d which is random, and whose distribution should depend significantly on the composition of the breeding medium between (unrealistically) 0 and 1, with equal probability for the meaning of mean-free path of neutron in such systems. Since any neutron emerges from the point (x_0, y_0, z_0) and moves along a direction (θ, ϕ), we can determine the coordinates of the point (x_1, y_1, z_1) where it would hit another fissile nucleus using the geometrical relations:

$$x_1 = x_0 + d\sin\theta\cos\phi,$$
$$y_1 = y_0 + d\sin\theta\sin\phi, \qquad z_1 = z_0 + d\cos\theta. \tag{10}$$

For the survival fraction, we only need to generate as much as large number of random points (as fission reactions) and to keep a count of the number of neutrons, N_{in}, which lie inside the block (as sustainable fission reaction). To generate random fission points, we need nine random numbers $r_1, r_2, \ldots, r_9$, which lie between 0 and 1. These nine quantities are generated according to the following set: Three random numbers for initial coordinates; four random numbers are for angular positions of two emitted neutrons; two random numbers are for distance travelled by two emitted neutrons, respectively. This insures that each of the nine parameters will lie in the proper range. For each neutron from a random fission we need to determine the neutron endpoint from Eq. (10), and then test if the point is inside or outside of the block. The survival fraction f_s is then given by $f_s = N_{in}/N$. In the usage of MCM [5] to find the survival fraction f_s, one is actually integrating a function F with nine variables $F\,(x_0, y_0, z_0, \theta, \phi, d, \theta', \phi', d')$ which represents the number of fissions induced by two emitted neutrons for particular values of the variables $x_0, y_0, \ldots, d'$. In our case, we search the critical size of rectangular blocks for $a \times a \times b$ for its simplicity. For the shape in hand, we first define the parameter S, where $S = a/b$, and keep it fixed, and then vary the mass of the block, *M*, until the survival fraction satisfies the condition $f_s \geq 1$. Then, we vary S to find out the critical mass for each shape. Assuming a direct relation between mass and density which is a hidden parameter here, one can write a relation among a, b, S and M as followings:

$$a = (M \times S)^{1/3}, \qquad b = \left(M/S^2\right)^{1/3} \tag{11}$$

The inputs in our program are: *N*=number of randomly generated neutrons; *M*=mass of the rectangular block, and *S*=ratio of length to thickness (shape of block). Since the accuracy of the calculation is increased by using higher values of *N*, we first search a relation, if existing, among parameters *N*, *M*, and *S* used as indicative parameters of the statistical fluctuations presented in our Monte Carlo calculation, as shown in Table I. We run all calculations for *10* number of experiments throughout the text, and $\overline{f}_s$ is the average value of 10 experiments: $\bar{f}_s = (\sum_{i=1}^{10} f_{s,i})/10$.

In Table I, it is seen that *N* has no direct effect in the calculation of $\bar{f}_s$ value. Therefore, we search for effects of other parameters. We try to get the relation among the parameters M, S and N as following: Since $\bar{f}_s$ is converging a certain value after $N = 10^6$, one can set $N = 10^6$ and $S = 1$ for all runs, and then search for the critical mass value for which the survival fractions becomes/reaches 1.0. We present our results in Table II. Because a certain amount of fissile material

TABLE I. The relation between N and f_s, for the rectangular block.

1^{st} set ($S = 1$ and $M = 1$ are constants)						
N	10^2	10^3	10^4	10^5	10^6	10^7
	0.98	0.876	0.8887	0.89652	0.895712	0.895665
	0.80	0.867	0.8835	0.89657	0.895789	0.895789
	1.02	0.899	0.8933	0.89416	0.895131	0.895478
	0.95	0.916	0.8894	0.89689	0.897115	0.895496
	0.92	0.915	0.8941	0.89231	0.895246	0.895299
f_s	0.78	0.907	0.9030	0.89351	0.896667	0.895235
	0.93	0.897	0.8888	0.89557	0.894426	0.895358
	0.75	0.880	0.8887	0.89472	0.895771	0.895251
	0.98	0.921	0.8837	0.89323	0.896237	0.895426
	0.86	0.929	0.9025	0.89337	0.894728	0.895507
$\bar{f}_s$	0.89	0.901	0.89157	0.894685	0.895682	0.89545

TABLE II. The relation between *M* and f_s, for the rectangular block.

2^{nd} set ($N = 10^6$ and $S = 1$ are constants)							
M	0.1	0.5	1.0	1.5	2	8	16
	0.41712	0.70826	0.895712	0.98202	1.05220	1.34947	1.46378
	0.41496	0.70816	0.895789	0.98380	1.05554	1.34802	1.47017
	0.41499	0.71201	0.895131	0.98618	1.05647	1.34572	1.46916
	0.41532	0.71282	0.897115	0.98274	1.05786	1.34940	1.46560
	0.41329	0.70627	0.895246	0.98403	1.05748	1.34998	1.46658
f_s	0.41268	0.70915	0.896667	0.98401	1.05866	1.34868	1.46628
	0.41559	0.70811	0.894426	0.98344	1.06063	1.35077	1.46519
	0.41393	0.70884	0.895771	0.98472	1.04900	1.34813	1.46278
	0.41596	0.70762	0.896237	0.98418	1.05645	1.34764	1.46507
	0.41559	0.70922	0.894728	0.98679	1.05656	1.34851	1.47142
$\bar{f}_s$	0.41494	0.70905	0.89568	0.98419	1.05608	1.34863	1.46661

TABLE III. The relation between S and f_s, for the rectangular block.

3^{rd} set ($N = 10^6$ and $M = 1$ are constants)							
S	0.1	0.5	1.0	1.5	2	8	16
	0.59333	0.83839	0.895712	0.86717	0.84029	0.59258	0.45720
	0.60203	0.83717	0.895789	0.86393	0.83499	0.59015	0.45949
	0.59678	0.83897	0.895131	0.86696	0.83323	0.59511	0.45592
	0.59575	0.83666	0.897115	0.86606	0.83097	0.59166	0.45710
	0.59409	0.83948	0.895246	0.86712	0.83959	0.59240	0.45666
f_s	0.59892	0.83483	0.896667	0.86542	0.83666	0.59062	0.45738
	0.59544	0.83753	0.894426	0.86762	0.83707	0.58934	0.45629
	0.59372	0.83747	0.895771	0.86465	0.83567	0.59073	0.45842
	0.59349	0.84017	0.896237	0.86315	0.83951	0.58791	0.45771
	0.59588	0.84036	0.894728	0.86577	0.83795	0.59321	0.45602
$\bar{f}_s$	0.59594	0.83810	0.89568	0.86578	0.83659	0.59137	0.45722

is required for reaching the criticality, a point at which the number of neutrons generated through fission reaction balances out the number of neutrons absorbed in the volume and lost through the surface of shape by leakage. It is clear that the minimum mass required to reach at criticality depends on the geometry of system. Therefore, the optimal shape for the minimum amount of fissile material to make the reactor system be critical should be determined.

From Table II, one can say that the critical mass exists between $M = 1.5$ and $M = 2.0$ because the survival fraction is about 1.0 there. Although we can estimate the critical mass between $M = 1.5$ and $M = 2.0$, one also needs to calculate that one for non-cubic rectangular blocks and needs to repeat the procedure via using certain values of S for the certainty. We set $S = 0.1$, 0.5, 1.0, 1.5, 2.0., 8.0 and 16 and repeat the calculation.

We present our results in Table III. It is clearly seen that the highest value of $\bar{f}_s = 0.89568$ is around $S = 1$, and it implies that one cannot reach to the criticality via changing the shape of block S for $M = 1$. Therefore one must search for the corresponding mass value M by changing S, for example, from 0.1 to 5.0 and ask if the survival fraction f_s is equal to or greater than one in this process.

We present the corresponding minimum critical mass for each value of $S = 0.1$, 0.2, 0.3.... etc, for $N = 10^6$ random points as shown in the Table IV. When $S = 1$, the smallest critical mass is obtained as $M = 1.61$ for $\bar{f}_s \geq$ condition. So, the minimum mass is in the cubic shape. As shown in Table IV, the mass value changes from higher to lower for $S = 0.1$ to $S = 1.0$ and then it increases gradually. Theoretically, one needs to support our results: The volume of the rectangular parallelepiped (for the simplicity of sides lengths $a \times a \times b$) shape is $V = a^2\, b$ and the length to thickness ratio

TABLE IV. The relation among the parameters S, M and $\bar{f}_s$, for the block of $a \times a \times b$.

$N = 10^6$					
S	*M*	$\bar{f}_s$	*S*	*M*	$\bar{f}_s$
0.1	6.28	1.00253	2.6	2.38	1.00144
0.2	3.46	1.00211	2.7	2.47	1.00286
0.3	2.55	1.00147	2.8	2.52	1.00146
0.4	2.18	1.00600	2.9	2.6	1.00211
0.5	1.93	1.00301	3.0	2.70	1.00069
0.6	1.75	1.00137	3.1	2.73	1.00000
0.7	1.69	1.00300	3.2	2.84	1.00255
0.8	1.62	1.00026	3.3	2.95	1.00086
0.9	1.62	1.00055	3.4	3.07	1.00299
1.0	**1.61**	**1.00069**	3.5	3.13	1.00003
1.1	1.62	1.00338	3.6	3.23	1.00103
1.2	1.63	1.00058	3.7	3.28	1.00043
1.3	1.66	1.00605	3.8	3.39	1.00251
1.4	1.68	1.00099	3.9	3.48	1.00123
1.5	1.70	1.00083	4.0	3.58	1.00022
1.6	1.79	1.00601	4.1	3.66	1.00239
1.7	1.81	1.00049	4.2	3.77	1.00136
1.8	1.86	1.00177	4.3	3.90	1.00181
1.9	1.95	1.00404	4.4	4.02	1.00151
2.0	1.98	1.00075	4.5	4.08	1.00053
2.1	2.05	1.00067	4.6	4.22	1.00307
2.2	2.12	1.00125	4.7	4.31	1.00316
2.3	2.16	1.00163	4.8	4.43	1.00251
2.4	2.25	1.00332	4.9	4.56	1.00207
2.5	2.32	1.00144	5.0	4.61	1.00270

TABLE V. The relation between *N* and f_s, for the finite cylinder.

1^{st} set ($S = 1$ and $M = 1$ are constants)						
N	10^2	10^3	10^4	10^5	10^6	10^7
	1.00	0.926	0.9533	0.94424	0.945162	0.945761
	1.01	0.895	0.9335	0.94829	0.944673	0.945918
	0.99	0.969	0.9398	0.95008	0.94639	0.945648
	0.82	0.968	0.9378	0.94717	0.945653	0.945252
	0.95	0.953	0.9545	0.94569	0.945749	0.945371
f_s	0.97	0.952	0.9384	0.94269	0.945933	0.945952
	1.03	0.951	0.944	0.94507	0.945596	0.945776
	0.83	0.919	0.9564	0.94571	0.946023	0.945521
	0.95	0.924	0.9404	0.94889	0.94638	0.945372
	0.89	0.935	0.9437	0.94774	0.947706	0.945649
$\bar{f}_s$	0.944	0.9392	0.94418	0.946557	0.9459265	0.945622

TABLE VI. The relation between *M* and f_s, for the finite cylinder.

2^{nd} set ($N = 10^6$ and $S = 1$ are constants)							
M	0.1	0.5	1.0	1.5	2	8	16
	0.44454	0.76004	0.94516	1.06297	1.14433	1.47582	1.59049
	0.44302	0.75984	0.94467	1.06186	1.14513	1.47445	1.59219
	0.44418	0.75939	0.94632	1.06259	1.14441	1.47454	1.5921
	0.44379	0.75951	0.94565	1.06253	1.14512	1.47428	1.59215
	0.44341	0.75861	0.94574	1.0623	1.14577	1.47464	1.59171
f_s	0.44396	0.75881	0.94593	1.0616	1.1436	1.47465	1.59233
	0.44384	0.75954	0.94559	1.06142	1.14482	1.47513	1.59187
	0.44442	0.76083	0.94602	1.06188	1.1433	1.47452	1.59185
	0.44425	0.75988	0.9463	1.06191	1.14538	1.47395	1.59272
	0.44532	0.75862	0.94771	1.0613	1.14409	1.475689	1.59201
$\bar{f}_s$	0.44407	0.75951	0.94592	1.06204	1.14459	1.47477	1.59194

is assumed to be $S = a/b \implies a = S\,b$. For the geometric Buckling; $B^2 = (\pi/\,a\,)^2 + (\pi/\,b\,)^2 + (\pi/\,a)^2$. Substituting $a = S\,b$ and for the minimum Buckling with constant V, one has to consider the case: $dB^2/dS = 0$. After some algebra one finds $S = 1$ that satisfies the condition for critically. It implies $a = b = c$, so the minimum critical volume gives us a cubic shape for which we have found the same result as shown in Table IV by using the MCM.

Critical size for a bare cylindrical reactor

Running our modified program for a finite cylinder of radius r with height h, we first define $S = h/r$. Following the previous steps, we present our results from Table V to Table VIII for cylinder system. In Table V, we present the effect of "N" for constant values of S and M. If M and S are kept constant, the effect of N is not obvious in the calculation of "f" parameter. Therefore, we set $S = 1$ and $N = 10^6$ (as in previous case) to observe the effect of M. In Table VI it is clearly seen that $\bar{f}_s$ increases as M increases.

It is an expected result because most of neutrons in greater volume (higher mass value) are highly absorbed and they have less chance for leakage throughout the surface of the shape. The effect of S in the calculation of f is shown in Table VII. It is obvious that the value of $\bar{f}_s$ increases in the range between $S = 0.1$ and $S = 1.5$, and then it decreases from $S = 2$ to $S = 16$. So, there should be a value between $S = 1.5$ and $S = 2.0$ approaching the critically condition for $M = 1$.

In Table VII, the mass M is equal to 1 and it is seen that the mass must be increased to make the survival fractions f_s be equal or greater than 1 for constant value of *S*. To find out what the minimum critical mass for each value of the height-

TABLE VII. The relation between *S* and f_s, for the finite cylinder.

3^{rd} set ($N = 10^6$ and $M = 1$ are constants)							
S	0.1	0.5	1.0	1.5	2	8	16
	0.473204	0.833021	0.945162	0.974038	0.973057	0.789682	0.667238
	0.473037	0.833278	0.944673	0.973834	0.972689	0.791315	0.666464
	0.473429	0.831187	0.94639	0.975304	0.972443	0.789842	0.666526
	0.474000	0.834288	0.945653	0.974584	0.971732	0.790225	0.667443
	0.474007	0.833894	0.945749	0.974453	0.971965	0.790856	0.66776
f_s	0.471869	0.833012	0.945933	0.974003	0.973622	0.789742	0.668019
	0.472911	0.833061	0.945596	0.973749	0.972911	0.790628	0.666612
	0.473482	0.832978	0.946023	0.974984	0.972269	0.789082	0.667165
	0.473736	0.833592	0.94638	0.973228	0.972172	0.791213	0.666558
	0.473801	0.83354	0.947706	0.974169	0.970597	0.790452	0.667485
$\bar{f}_s$	0.473347	0.833185	0.945926	0.974234	0.972345	0.790304	0.667127

TABLE VIII. The relation among the parameters S, M and $\bar{f}_s$, for the finite cylinder.

$N = 10^6$					
S	M	$\bar{f}_s$	S	M	$\bar{f}_s$
0.1	27.991	1.001	2.6	1.200	1.001
0.2	8.200	1.000	2.7	1.220	1.003
0.3	4.260	1.000	2.8	1.240	1.001
0.4	2.790	1.001	2.9	1.260	1.001
0.5	2.100	1.000	3.0	1.270	1.001
0.6	1.750	1.001	3.1	1.290	1.001
0.7	1.550	1.001	3.2	1.310	1.002
0.8	1.400	1.001	3.3	1.320	1.001
0.9	1.310	1.001	3.4	1.340	1.001
1.0	1.250	1.002	3.5	1.360	1.001
1.1	1.210	1.002	3.6	1.380	1.002
1.2	1.180	1.001	3.7	1.400	1.002
1.3	1.160	1.003	3.8	1.410	1.000
1.4	1.140	1.001	3.9	1.430	1.000
1.5	1.140	1.002	4.0	1.460	1.002
1.6	1.130	1.002	4.1	1.480	1.002
1.7	1.130	1.002	4.2	1.490	1.001
1.8	**1.120**	**1.000**	4.3	1.510	1.001
1.9	1.130	1.003	4.4	1.530	1.001
2.0	1.140	1.002	4.5	1.550	1.002
2.1	1.150	1.002	4.6	1.570	1.000
2.2	1.150	1.001	4.7	1.590	1.001
2.3	1.160	1.001	4.8	1.610	1.000
2.4	1.170	1.002	4.9	1.630	1.001
2.5	1.180	1.001	5.0	1.640	1.000

TABLE IX. The relation between N and f_s, for the spherical reactor where $M = 1$ ($R = 0.62035$).

1^{st} set ($M = 1$ and $R = 0.62035$)						
N	10^2	10^3	10^4	10^5	10^6	10^7
	1.11	1.081	1.0765	1.08025	1.079055	1.0795062
	1.05	1.094	1.0829	1.07873	1.078407	1.0795276
	1.08	1.075	1.0975	1.08197	1.080221	1.0798335
	0.98	1.072	1.0697	1.07738	1.079912	1.0796746
	1.01	1.074	1.0773	1.07759	1.080022	1.0797197
f_s	1.23	1.088	1.0906	1.07516	1.078738	1.0797584
	1.02	1.098	1.0706	1.07756	1.079784	1.0798805
	0.99	1.113	1.0888	1.08207	1.079915	1.0799033
	1.12	1.097	1.0835	1.07789	1.079364	1.0797344
	0.89	1.071	1.083	1.08052	1.079512	1.0799324
$\bar{f}_s$	1.048	1.0863	1.08204	1.078912	1.079493	1.07974706

TABLE X. The relation between M and f_s, for the spherical reactor.

2^{nd} set ($N = 10^6$ and r proportional to M)							
M	0.1	0.5	1.0	1.5	2	8	16
	0.50245	0.85972	1.07906	1.22369	1.32693	1.71484	1.81662
	0.50230	0.85856	1.07841	1.22491	1.32702	1.71549	1.81686
	0.50137	0.85993	1.08022	1.22434	1.32843	1.7141	1.81761
	0.50203	0.85905	1.07991	1.22486	1.32756	1.71526	1.81713
	0.50247	0.85819	1.08002	1.22377	1.32732	1.71596	1.81684
f_s	0.50295	0.85932	1.07874	1.22291	1.32857	1.71641	1.8178
	0.50268	0.85888	1.07978	1.22511	1.32756	1.71544	1.81753
	0.50112	0.85902	1.07992	1.22361	1.32772	1.71567	1.81654
	0.50261	0.85883	1.07936	1.22317	1.32825	1.71583	1.81748
	0.50232	0.86017	1.07953	1.22423	1.32706	1.71533	1.81679
$\overline{f}_s$	0.50223	0.85918	1.07949	1.22406	1.32764	1.71543	1.81712

TABLE XI. The relation among parameters S, M and $\bar{f}_s$, for the spherical reactor.

$N = 10^6$					
S	M	$\bar{f}_s$	S	M	$\bar{f}_s$
0.01	0.133650	0.232794	2.51	0.843066	1.40785
0.11	0.297235	0.518616	2.61	0.854117	1.42043
0.21	0.368731	0.641612	2.71	0.864888	1.43242
0.31	0.419846	0.731956	2.81	0.875399	1.44579
0.41	0.460855	0.802502	2.91	0.885662	1.4569
0.51	0.495633	0.865500	3.01	0.895693	1.46772
0.61	0.526114	0.917306	3.11	0.905504	1.47775
0.71	0.553422	0.963154	3.21	0.915107	1.48938
0.81	**0.578272**	**1.00713**	3.31	0.924513	1.49851
0.91	0.601152	1.046452	3.41	0.933731	1.50809
1.01	0.622411	1.082393	3.51	0.942771	1.5174
1.11	0.642310	1.115561	3.61	0.951640	1.52693
1.21	0.661047	1.146565	3.71	0.960347	1.53269
1.31	0.678777	1.176063	3.81	0.968899	1.54129
1.41	0.695627	1.200577	3.91	0.977303	1.54837
1.51	0.711698	1.226552	4.01	0.985564	1.55774
1.61	0.727074	1.249039	4.11	0.993692	1.56304
1.71	0.741826	1.27203 3	4.21	1.001685	1.57081
1.81	0.756014	1.292766	4.31	1.009554	1.57512
1.91	0.769688	1.309722	4.41	1.017302	1.58301
2.01	0.782893	1.330617	4.51	1.024934	1.58908

to-radius ratio is and to know what the exact critical dimensions of cylinder are, we modify our code for cylinder system and present our results in Table VIII for a range of S from 0.1 to 5.0 with corresponding critical mass M satisfying the condition $f \geq 1.0$. It is seen in Table VIII that the minimum critical mass is obtained when $S = h/r = 1.8$.

As we show for parallelepiped, the volume of the cylinder shape is $V = \pi\, r^2 \times h$ and the height to radius ratio is $S = h/r$. Substituting $h = S \times r$ in B_g^2 of cylinder shape, and then defining $r = \sqrt{V/\pi H}$ and considering the case $dB^2/dS = 0$ one finds $S = 1.82$ that satisfies the mini-

mum critical mass. The modified MCM program developed in Mathematica^{TM}for the case of the bare cylinder is presented in Appendix as an example of the work carried out for the interested readers.

Critical size for a bare spherical reactor

In the determination of the critical size of a spherical reactor, there is a direct connection between the mass and the radius of sphere. Therefore, the change in the mass changes the radius (or vice versa) until it satisfies $f \geq 1.0$. Following the same procedures in the previous sections, we present our results in Tables IX and X. As seen in Table IX, N has no direct effect on values of f. Since we set $M = 1$, the results show that the system is almost critic. Therefore we can search for which mass (or radius) value is the most appropriate one. The system will become critical via changing the mass M (or radius). We set $N = 10^6$ and show our results in Table X. The effect of increase in the mass can be observed clearly on the value of $\bar{f}_s$: It is seen that the minimum critical mass is between $M = 0.5$ and $M = 1$. In summary, the increase in the volume of core will subsequently leads to the increase in the value of survival fraction because of decrease in number of leakage neutrons. To find out the minimum critical mass for the spherical system, we run our code for different values of S from 0.01 to 4.51 through the survival fractions when f to be equal or greater than one. We present results in Table XI.

Conclusion

In this paper, we show a simple application of MCM to calculate the minimum critical size condition satisfied for a hypothetical fissile material in three different geometries: For the bare rectangular-parallelepiped shape, we find that the minimum critical size condition exists when $S = a/b = 1.0$ which is in the shape of a cube. For the bare finite-cylinder, the minimum critical mass requires the condition $S = H/R \simeq 1.8$. For the bare spherical system, the minimum critical size is obtained when the radius of the sphere is equal to 0.57. These results are in agreement with those of neutron diffusion equation for Zero Boundary Flux in the determination of the minimum critical mass calculations for $dB^2/dS = 0$.

One can also conclude throughout these results that the most optimum shape for the minimum critical size condition is the spherical one.

As a future study, one can repeat these calculations for the Extrapolated Boundary Flux in other geometries. Our approach can also be modified by considering the energy of neutrons, corresponding cross-section values of target element and other parameters such as mean-free path etc. The calculation of the critical mass in such simple reactor geometries with reflectors can also be studied for future studies. Thus, it would be very good opportunity to compare the results of systems without/with reflectors, which are good materials at reducing the amount of fuel element required for the core to become critical. Finally, there is also possibility to modify our approach to determine the critical mass in other particular geometries and to compare results among them.

Appendix

A. Example program for bare-cylinder reactor

```
(*PROGRAM BARECYLINDER
This program determines the critical mass of a bare cylinder.
The check point is to control if f_s=>1.0 for criticality.*)
  Unprotect["`*"];
  ClearAll["`*"];
  ClearAll["Global`*"];
  (*number of incident neutrons input here*)
  numn = 10000;
  (*if required, the number of repetation input here(it is 10 in paper)*)
  numexp = 1;
  (*The range for S from "ilk" to "son"*)
  ilk = 13;
  son = 23;
  Do[
   (*S value changes here: from 1.3 to 2.3*)
   S = KM*0.1;
   Svalue[KM] = S;
   (*M changes from initial value to final value by step number of dM=0.01*)
   M = 0.1;
   dM = 0.01;
   Label[mbegin];
   M = M + dM;
   Mass[KM] = M;
   (* Determine the Radius and Height of cylinder in terms of M and S *)
 R = (M / (S*Pi))^(1/3);
 H = (M*S*S / Pi)^(1/3);
 Do[(*Number of experiments from 1-to-numexp starts here*)
   nin = 0.; (*initial number of generated neutrons as result of fission in volume*)
   Do[(*incident neutrons makes target fission here*)
    (*initial fission coordinates generation in volume*)
    theta = RandomReal[{0, 360}];
    D1 = RandomReal[];
    x0 = R*Cos[theta Degree]*D1;
    y0 = R*Sin[theta Degree]*D1;
    z0 = H*(RandomReal[] - 0.5);
    Do[
     (*two random neutrons coordinates generated here: from fissions n=1,2*)
     theta1 = RandomReal[{0, 360}];
     cosphi1 = 2*(RandomReal[] - 0.5);
     sinphi1 = Sqrt[1. - cosphi1^2];
     d = RandomReal[{0, 1}];
     xnew = x0 + d*Cos[theta1 Degree]*sinphi1;
     ynew = y0 + d*Sin[theta1 Degree]*sinphi1;
     znew = z0 + d*cosphi1;
     cnew = Sqrt[xnew^2 + ynew^2];
     (*check if generated neutrons' coordinates are "in" the volume or "not"*)
     If[cnew <= R && Abs[znew] <= H / 2., nin = nin + 1., zz = 99],
     {n, 1, 2}],
    {nn, 1, numn}];
   SF[IJ] = nin / numn,
   {IJ, 1, numexp}];
 AvgF = 0.;
 (* Calculate the Average value of survival factor for all experiments *)
 Do[AvgF = AvgF + SF[IJ], {IJ, 1, numexp}];
 AvgF = AvgF / numexp;
 SS = H / R;
 HtoR[KM] = SS;
 FFraction[KM] = AvgF;
 (* compare if f_s >= 1.0, then Print results *)
 If[AvgF >= 1.0,
  Print["Loop= ", KM, "  ", "S= ", SetAccuracy[S, 4], "  ",
                        "Mass= ", SetAccuracy[M, 4], "  ",
                        "AvgF= ", SetAccuracy[AvgF, 4], "  ",
    "Height/Radius= ", SetAccuracy[SS, 4]],
   Goto[mbegin]],
  {KM, ilk, son}]
 (*If necessary, save the Results in a "dat" file*)
 SwwS = Table[{KM, SetAccuracy[Svalue[KM], 4], SetAccuracy[Mass[KM],
 4], SetAccuracy[FFraction[KM],
 4], SetAccuracy[HtoR[KM], 4]}, {KM, ilk, son}];
 Export["D:\\Cylinder.dat", SwwS]
```

Acknowledgment

One of the authors (O. Ozer) would like to thank the Rosatom Technical Academy for its hospitality in Obninsk and St. Petersburg, Russian Federation. The authors are also very much indebted to the referee(s) for useful comments and suggestions.

Conflict of interest

The authors declare that they have no conflict of interest.

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