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Optimization of a microreactor core's dimensions using metaheuristic methods

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ABSTRACT

This article proposes the use of the multi-group diffusion equations with four groups to determine the dimensions of the microreactor of the TERRA project. With this intent, the values of the radius and height of the cylinder that represents the core, as well as its enrichment were optimized through a framework called LOF. This tool has several metaheuristics methods already implemented, which provides a considerable time gain. So any particular method implemented, or a combination of some of them, could be utilized without any concerns regarding implementation time. In addition to the application of the metaheuristic methods for the proposed optimization, there was also a concern about altering the search parameters used in each of the metaheuristics, which eventually caused an improvement in the results. With this method, the radius and height dimensions achieved were quite reasonable for a microreactor. As for the enrichment, the value of 19.75% was achieved, limited by the Non-Proliferation Treaty.

Keywords: **Multigroup diffusion, core optimization, microreactor, LOF, metaheuristics.**

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1. INTRODUCTION

In the past years, the Institute for Advanced Studies of the Brazilian Air Force (IEAv) has been working on the concept of a nuclear microreactor. In this context, the Advanced Fast Reactors Technology (TERRA) project has been conceived to provide a reactor that would work as a source of electrical and thermal energy capable of providing the means to ensure human survival, as well as the operation of essential equipment. This technology can be useful not only in outer space, but also in very remote areas, such as in deep sea. The core of this reactor is designed to provide 1,200 kW_{th} of power over a period of 8 years.

One of the desired characteristics pursued, similarly to several other projects currently being developed around the world, is the low level of enrichment (percentage of Uranium-235 in relation to the total uranium in the fuel), in order not to violate the Non-Proliferation of Nuclear Weapons Treaty. One solution would be to employ HALEU (High Assay Low Enriched Uranium) as fuel, with a maximum enrichment of 19.75%. Another challenge lies is the development of a reactor that relies exclusively on the use of national materials and technologies.

Considering the high complexity of the neutron transport equation, which cannot be solved analytically, this work proposes the optimization of the core's dimensions and enrichment by using the LOF software (LEV Optimization Framework, LEV – Laboratório de Engenharia Virtual), which has several metaheuristic methods implemented in its database. Some research will show that metaheuristic methods have already been used in several other works for core design and optimization, such as seen in [1] and [2].

2. MATERIALS AND METHODS

The first step was to briefly demonstrate the Multigroup Diffusion equation model used in this work. Then, the necessary constants for the proposed method were presented and calculated. After that, the C/C++ code was implemented and operated with the LOF software, which makes use of several metaheuristic calculation tools. At the end, the results were presented and it was possible to determine which of the solutions found was more suitable for solving this particular problem and, consequently, which were the optimal dimensions and enrichment calculated for the core of the TERRA project.

2.1. The Multigroup Diffusion method

The method chosen and used to model the behavior of the neutron population in the nucleus was the Multigroup Diffusion. This method is derived from the neutron transport equation, which despite being exact, cannot be solved for practical and realistic situations. Taking this into account, the diffusion approximation, which considers that the angular flux is weakly dependent on the angle (linearly anisotropic), is commonly used [3]. Therefore, in order to obtain a first approximation for the quantities involved in this problem, the use of the Multigroup Diffusion equation (Eq. 1) is adequate.

$$\frac{1}{v_g}\frac{\partial \varphi_g}{\varphi_t} - \nabla . D_g \nabla \varphi + \Sigma_{tg}\varphi_g(r,t) = \sum_{g=1}^{G} \Sigma_{sg'g}\varphi_{g'} + X_g \sum_{g=1}^{G} v_g \Sigma_{fg'}\varphi_{g'} + S_g \quad (1)$$

where ν_g represents the average number of neutrons emitted by fission, φ the neutron flux in $cm^{-2}s^{-1}$, t the time in s, D the neutron diffusion coefficient in cm, Σ_t, Σ_f and $\Sigma_{sg'g}$, respectively, the macroscopic total, fission and scattering cross section with energy change from group g' to group g in cm^{-1}, X the fission spectrum, S_g external sources of neutrons and the g index refers to each energy group.

Another common simplification is to assume that the neutrons of a given energy group, when scattered, can only lose energy so as to fall to the next lower group. This makes multigroup equations directly coupled. Considering that when $E_{g-1} / E_g > 150$ the probability of this happening is greater than 99% [3], such approximation is coherent in this work.

In order to solve this model, one last manipulation must be done. Firstly it must be noted that, as it will be later explained, the core is considered homogeneous, despite being made up of several different elements. Then, assuming that scattered neutrons can only lose enough energy to move to thenext lower group, making the equations directly coupled, and that the fluxes are all characterized bythe same spatial form [3], the model for four energy groups can then be represented by the matrix form described in Eq. 2:

$$M\phi = \frac{1}{k} F\phi \qquad (2)$$

where the matrices *M* and *F* and the vector ϕ are given by Eqs. 3, 4 and 5, the term Σ_{Rg} represents the removal cross section of each energy group and *k* stands for the multiplicity factor.

$$M = \begin{bmatrix} D_1 B^2 + \Sigma_{R1} & 0 & 0 & 0 \\ -\Sigma_{S12} & D_2 B^2 + \Sigma_{R2} & 0 & 0 \\ 0 & -\Sigma_{S23} & D_3 B^2 + \Sigma_{R3} & 0 \\ 0 & 0 & -\Sigma_{S34} & D_4 B^2 + \Sigma_{R4} \end{bmatrix} \qquad (3)$$

$$F = \begin{bmatrix} v_1 X_1 \Sigma_{f1} & v_2 X_1 \Sigma_{f2} & v_3 X_1 \Sigma_{f3} & v_4 X_1 \Sigma_{f4} \\ v_1 X_2 \Sigma_{f1} & v_2 X_2 \Sigma_{f2} & v_3 X_2 \Sigma_{f3} & v_4 X_2 \Sigma_{f4} \\ v_1 X_3 \Sigma_{f1} & v_2 X_3 \Sigma_{f2} & v_3 X_3 \Sigma_{f3} & v_4 X_3 \Sigma_{f4} \\ v_1 X_4 \Sigma_{f1} & v_2 X_4 \Sigma_{f2} & v_3 X_4 \Sigma_{f3} & v_4 X_4 \Sigma_{f4} \end{bmatrix} \qquad (4)$$

$$\phi = \begin{bmatrix} \phi 1 \\ \phi 2 \\ \phi 3 \\ \phi 4 \end{bmatrix} \qquad (5)$$

This system has five unknown variables (the flux ϕ for each energy group and the multiplicity factor *k*) and four equations, so it is indeterminate. For it to be possible, the determinant must be equal to zero. This was accomplished with the cofactor method, in order to calculate *k* that satisfies this condition.

2.2. The core model

The core of the TERRA project considered in this article is based on [4] and consists of a homogeneous cylinder of radius R and height H. This, in turn, is composed of a mixture of 90% uranium nitride (UN) and 10% lead (Pb). Both N and Pb are used in their natural forms, that is, the composition of their isotopes is identical to that found in nature, which simplifies the manufacturing process.

As for the uranium, it presents an enrichment of α% in ^{235}U, that is, α% of the uranium is in the form of ^{235}U, which is fissile, and the rest (100 - α%) in the form of ^{238}U.

Such mentioned values of R, H and α are precisely the design variables that will be calculated in this work in order to optimize the core.

2.3. Obtaining the required parameters

The microscopic cross-section values of transport σ_{tr}, fission σ_f, radiative capture σ_γ, scattering to another group $\sigma_{sg'g}$ and ν for ^{235}U and ^{238}U, for each of the 4 energy groups, were extracted directly from Argonne National Laboratory publications [5].

However, as the Pb and N data are presented in tables with 16 energy groups, the values selected were the ones closest to the four energy groups given in Table 1 for the U. In the absence of data, the ^{14}N parameters were defined as the arithmetic mean of the oxygen and carbon values, which was considered acceptable for a first approximation, since nitrogen has a similar nuclear arrangement and mass equivalent to the mean value. And the ^{15}N data was defined as the mean value between the calculated ^{14}N and O data. As for the Pb, the absence of lower energy data values motivated the definition of the data for the third and fourth energy groups as equal to the values of the lowest energy group given in the mentioned tables.

Afterwards, additional calculations were performed to obtain the parameters needed to solve Eqs. 2 to 5. The absorption (Eq. 6) and removal (Eq. 7) microscopic cross sections were calculated as follows:

$$\sigma_a = \sigma_f + \sigma_\gamma \tag{6}$$

$$\sigma_R = \sigma_a + \sigma_{sg'g} \tag{7}$$

Then, the number densities and all macroscopic cross sections were obtained, as given by Eqs. 8 and 9, where N_a represents Avogadro's number, M the molar mass and ρ the specific mass for each material.

$$N = N_a \frac{M}{\rho} \tag{8}$$

$$\Sigma = N\sigma \tag{9}$$

The last necessary values are the constants D and B_g (geometric Buckling number for the cylinder), given by Eqs. 10 and 11, which is only valid for a homogeneous core:

$$D = \frac{1}{3\Sigma_{tr}} \tag{10}$$

$$B_g = \left(\frac{v_0}{\tilde{R}}\right)^2 + \left(\frac{\pi}{\tilde{H}}\right)^2 \tag{11}$$

The constant v_0 refers to the smallest zero of the Bessel function and the values of $\tilde{R}$ and $\tilde{H}$ are obtained through Eqs. 12, 13 and 14, where z_0 refers to the extrapolation distance.

$$\tilde{R} = R + z_0 \tag{12}$$

$$\tilde{H} = H + z_0 \tag{13}$$

$$z_0 = \frac{0.7104}{\Sigma_{tr}} \tag{14}$$

The values of all necessary parameters to solve the model, whether they were extracted from the cited references or calculated through Eqs. 6 to 14, are presented in Tables 1 and 2.

Table 1: Required parameters used for the model calculations.

Parameter		**Energy groups**			
		1 (1,353 Mev)	**2 (9,12 keV)**	**3 (0,4 ev)**	**4 (0 ev)**
^{235}U	σ_f	$1,3.10^{-28}$ m²	$1,4.10^{-28}$ m²	$23,0.10^{-28}$ m²	490.10^{-28} m²
	ν	2,65	2,55	2,5	2,5
	σ_{tr}	$4,7.10^{-28}$ m²	$7,0.10^{-28}$ m²	$51,0.10^{-28}$ m²	$597,0.10^{-28}$ m²
	$\sigma_{sg'g}$	$1,4.10^{-28}$ m²	0	$0,01.10^{-28}$ m²	0
	σ_r	$2,8.10^{-28}$ m²	$1,7.10^{-28}$ m²	$41,01.10^{-28}$ m²	587.10^{-28} m²
^{238}U	σ_f	$0,53.10^{-28}$ m²	0	0	0
	ν	2,65	0	0	0
	σ_{tr}	$4,7.10^{-28}$ m²	$7,0.10^{-28}$ m²	$11,0.10^{-28}$ m²	$13,0.10^{-28}$ m²
	$\sigma_{sg'g}$	$2,1.10^{-28}$ m²	0	$0,01.10^{-28}$ m²	0
	σ_r	$2,67.10^{-28}$ m²	$0,18.10^{-28}$ m²	$0,81.10^{-28}$ m²	$2,4.10^{-28}$ m²
^{14}N	σ_{tr}	$1,30.10^{-28}$ m²	$3,65.10^{-28}$ m²	$4,04.10^{-28}$ m²	$4,04.10^{-28}$ m²
	$\sigma_{sg'g}$	$0,253.10^{-28}$ m²	$0,385.10^{-28}$ m²	$0,546.10^{-28}$ m²	0
	σ_r	$0,753.10^{-28}$ m²	$0,535.10^{-28}$ m²	$0,756.10^{-28}$ m²	$0,211.10^{-28}$ m²
^{15}N	σ_{tr}	$1,24.10^{-28}$ m²	$3,68.10^{-28}$ m²	$3,84.10^{-28}$ m²	$3,841.10^{-28}$ m²
	$\sigma_{sg'g}$	$0,222.10^{-28}$ m²	$0,361.10^{-28}$ m²	$0,480.10^{-28}$ m²	0
	σ_r	$0,732.10^{-28}$ m²	$0,481.10^{-28}$ m²	$0,665.10^{-28}$ m²	$0,185.10^{-28}$ m²
Pb	σ_{tr}	$4,44.10^{-28}$ m²	$4,92.10^{-28}$ m²	$11,0.10^{-28}$ m²	$11,0.10^{-28}$ m²
	$\sigma_{sg'g}$	$1,1.10^{-28}$ m²	0	0	0
	σ_r	$1,161.10^{-28}$ m²	$0,087.10^{-28}$ m²	$0,005.10^{-28}$ m²	$0,005.10^{-28}$ m²

Table 2: Other necessary parameters obtained.

M ^{235}U (g/mol)	235,0439	**ρ Pb (kg/m³)**	11.340
M ^{238}U (g/mol)	238,0508	**ρ UN (kg/m³)**	14.080
M ^{14}N (g/mol)	14,0031	X_1 **(%)**	57,5
M ^{15}N (g/mol)	15,0001	X_2 **(%)**	42,5
M (g/mol)	207,2169	X_3 **(%)**	0
^{14}N (%)	99,63	X_4 **(%)**	0

2.4. The solving method

After building the model and taking into account all the considerations made in the previous sections regarding optimization, the implementation in C/C++ language was made, as it can be seen in Annex C, and the code was operated with the LOF framework.

To be considered optimal, the core should meet the following three criteria:

1. Have a multiplicity factor (k) as close as possible to 1.25, as in [2];
2. Minimize the enrichment (α);
3. Minimize the volume (V).

The last two criteria are intended to lower the core's costs, while the first one has the goal turning it as safe and controllable as possible. Thus, the following objective function was created (Eq. 15):

$$minimize f(R,H,\alpha) = P_1 \left| \frac{(k-1{,}25)}{\Delta k_0} \right| + P_2 \frac{V}{V_0} + P_3 \frac{\alpha}{\alpha_0} \quad (15)$$

Considering the differences in the quantities involved, a normalization of the parameters in the objective function is performed, through the terms Δk_0, V_0 and α_0. The values of P_1 = 0.6, P_2 = 0.2 and P_3 = 0.2 are the weights assigned to each part of the objective function. In addition to the greater importance given to the multiplicity factor (higher P_1), the following penalties to the objective function were defined:

1. If $k > 2$ or $k < 1$, the function f is penalized by having 10^6 added to its value; and
2. If $k > 1.5$ or $k < 1.1$, the penalty is 10^3.

After implementing it in C/C++ and interacting it with the LOF framework, the constants previously calculated, in addition to the range in which the variables R, H and α should be searched, were inserted as inputs. In order to obtain realistic dimensions and enrichment, R and H were searched in between 0.05 m and 10 m, and α in between 0 and 19.75%.

The outputs selected were α, k and V. Additionally, four s-metaheuristics and five p-metaheuristics were chosen, in order to find the best solution using a wide variety of techniques. Finally, three sets of search parameters for each method were tested, the default values in LOF, one with slightly higher and another with slightly lower parameter values. Each of them was run 15 times, and the number of objective functions computed was 10,000 for each of them. The other parameters initially used for each metaheuristic were the ones defined as standard in the LOF software.

3. RESULTS AND DISCUSSION

Table 3 summarizes the best results achieved by each metaheuristic method. The *Tabu Search* was the best in all criteria except for the time spent, which put the *Evolutionary Algorithm* method as the best overall. The minimum value of the objective function found is not in any of the results shown in Table I, but in one of the *Evolutionary Algorithm* variations that had a worse overall result than the one presented in this table.

The *Sea Turtle* also presented very good results and *Sine Cosine*, despite presenting high mean and standard deviation due to its poor ability to escape local minima, usually had excellent results as well. These first four methods would probably deserve more attention in future studies for this problem. The others were not very impressive, at least considering the three sets of parameters tried.

Table 3: Comparison of the best versions of each metaheuristic.

Metaheuristic	Time spent (s)	Minimum	Average	Median	Standard

					deviation
Evolutionary Algorithm	4.202,21	1,12247	1,12310	1,12278	$6{,}601.10^{-4}$
Tabu Search	5.247,74	1,12245	1,12252	1,12251	$4{,}911.10^{-5}$
Sea Turtle	5.015,26	1,12260	1,12459	1,12345	$2{,}578.10^{-3}$
Sine Cosine	5.216,87	1,12247	1,17625	1,12303	$1{,}658.10^{-1}$
Vortex Search	5.396,31	1,12374	1,12922	1,12801	$4{,}376.10^{-3}$
Gravitational Search	4.209,96	1,12385	1,15133	1,14909	$2{,}640.10^{-2}$
Simulated Annealing	4.305,50* (6,951 O. F. computed)	1,15141	1,19577	1,19133	$2{,}693.10^{-2}$
Black Hole	5.748,38	1,14074	1,17756	1,18230	$2{,}028.10^{-2}$
Modified Vortex Search	5.752,15	1,14686	1,20250	1,18977	$4{,}610.10^{-2}$

Finally, Table 4 summarizes some of the best results obtained after applying all three set of parameters variations for each of the nine different metaheuristics used in the LOF framework. A number of different metaheuristics showed very similar results. Taking into account that each of them has its own search method, the results achieved have greater credibility than if they were achieved using a single search method, especially when considering that there was also a study of the search parameters, which increased the confidence on the results. Thus, it can be said that the core must have 19.75% enrichment as expected, radius of 0.921 meters and height of 1,742 meters.

Table 4: Best results compiled at the end of all calculations.

Metaheuristic	**Objective function**	**Radius (m)**	**Height (m)**	**Enrichment (%)**	**Volume (m^3)**	**Multiplicity factor**

Evolutionary Algorithm	1,12242	0,921	1,742	19,75	4,637	1,198
Tabu Search	1,12245	0,922	1,749	19,75	4,673	1,198
Evolutionary Algorithm	1,12247	0,931	1,729	19,75	4,704	1,198
Sine Cosine	1,12247	0,930	1,729	19,75	4,694	1,198
Sine Cosine	1,12252	0,917	1,727	19,75	4,559	1,197
Sea Turtle	1,12260	0,924	1,763	19,75	4,734	1,198
Sea Turtle	1,12289	0,907	1,729	19,75	4,471	1,197
Gravitational Search	1,12298	0,913	1,803	19,75	4,719	1,198

4. CONCLUSION

This work began with a presentation of the multigroup diffusion equations, showing its validity, especially for these preliminary calculations in order to define the optimal dimensions of the core for the TERRA project. Future works could improve the model applied considering 16 or more energy groups, instead of 4. Another upgrade, which would increase the complexity, but would be extremely relevant, would be the consideration of two regions in the core, where the second one would represent the reflectors around the core. Such modifications, in addition to bringing the results closer to reality, would allow the sizing of the reflectors in order to reduce the core or even the enrichment.

Then the necessary constants used in the calculations were presented. For the purpose of time saving, some approximations were made. In future works, such constants could be obtained more accurately from nuclear data libraries, such as JEF, ENDF/B and others.

Afterwards, the results obtained by the optimization calculations using the LOF framework were given. This tool proved to be valuable as it already has several metaheuristic methods implemented, which saves considerable time and eliminates the ease of implementation advantage some methods have, such as *Simulated Annealing*. This way, the user can implement any one, or a combination of several techniques, without worrying about the implementation time.

Another concern was the alteration of the search parameters used in each of the metaheuristics, which allowed some methods with initially poor performances to present excellent results, such as the *Tabu Search,* and increase the reliability of the results achieved.

In the end, the values calculated of the radius (0.921 meters) and height (1.742 meters) were quite reasonable for a microreactor's core. The enrichment for this optimized case ended up being 19.75%, which was already expected.

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