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Optimization of a microreactor core's dimensions using metaheuristic methods

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1. Introduction

In the past years, the Institute for Advanced Studies (IEAv) has been developing the concept of a nuclear microreactor, known as the Advanced Fast Reactors Technology project (TERRA), that could work as a source of electrical and thermal energy and would be useful not only in outer space, but also in very remote areas, such as in deep sea. The core is designed to provide 1,200 kW_{th} of power over a period of 8 years.
One of the desired characteristics pursued is the low level of enrichment in order not to violate the Non-Proliferation 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 in 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 framework, which has several metaheuristic methods implemented in its database.

2. Methodology

The model used to calculate the behavior of the neutron population in the nucleus was the Multigroup Diffusion, as given by Eq. 1 [1].

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

where v_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 the total macroscopic cross section in cm^{-1}, $\Sigma_{sg'g}$ the macroscopic scattering cross section in cm^{-1} with energy change from group g' to group g, X the fission spectrum, Σ_f the macroscopic fission cross section in cm^{-1}, S_g external sources of neutrons and the g index refers to each energy group.
Assuming that scattered neutrons can only lose enough energy to move to the next lower group, making the equations directly coupled, and that the fluxes are all characterized by the same spatial form [1], the model for four energy groups can then be represented by the matrix form described in Eq. 2:

$$M\phi = \frac{1}{k}F\phi \tag{2}$$

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.

$$M = \begin{bmatrix} D_1B^2+\Sigma_{R1} & 0 & 0 & 0 \\ -\Sigma_{S12} & D_2B^2+\Sigma_{R2} & 0 & 0 \\ 0 & -\Sigma_{S23} & D_3B^2+\Sigma_{R3} & 0 \\ 0 & 0 & -\Sigma_{S34} & D_4B^2+\Sigma_{R4} \end{bmatrix} \tag{3}$$

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

$$\phi=\begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix} \quad (5)$$

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.

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 four energy groups, were directly extracted or interpolated from the data in [3]. The absorption and removal microscopic cross sections were calculated through Eqs. 6 and 7:

$$\sigma_a=\sigma_f+\sigma_\gamma \quad (6)$$

$$\sigma_R=\sigma_a+\sigma_{sg'g} \quad (7)$$

The number densities and macroscopic cross sections for each isotope were obtained through Eqs. 8 and 9, where Na represents Avogadro's number, M the molar mass and ρ the specific mass.

$$N=N_a\frac{M}{\rho} \quad (8)$$

$$\Sigma=N\sigma \quad (9)$$

The last needed values are D and geometric Buckling number B_g, given by Eqs. 10 and 11:

$$D=\frac{1}{3\Sigma_{tr}} \quad (10)$$

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

v_0 refers to the smallest zero of the Bessel function and the values of the extrapolated radius, $\widetilde{R}$, and height, $\widetilde{H}$, are obtained through Eqs. 12, 13 and 14, in which z_0 refers to the extrapolation distance.

$$\widetilde{R}=R+z_0 \quad (12)$$

$$\widetilde{H}=H+z_0 \quad (13)$$

$$z_0=\frac{0.7104}{\Sigma_{tr}} \quad (14)$$

The core consists of a homogeneous cylinder composed of 90% UN and 10% Pb. Both N and Pb are used in their natural isotopic forms, which simplifies the manufacturing process. [2] 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, that is, minimize the difference to 1.25;
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):

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

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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 the implemention 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. Then the following restrictions were imposed to obtain realistic dimensions and enrichment:

1. $0.05 \text{ m} < R < 10 \text{ m}$;
2. $0.05 \text{ m} < H < 10 \text{ m}$;
3. $0 < \alpha < 19.75\%$.

The outputs selected were *α*, *k* and *V.* Additionally, four s-metaheuristics and five p-metaheuristics were the chosen methods, 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 of 10,000 for each of them.

3. Results and Discussion

Table I 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 I: 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 II 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

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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 II: 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

4. Conclusions

This work began presenting the multigroup diffusion equations. Future works could improve such model by considering more than 4 energy groups. Another upgrade would be the consideration of two regions in the core, where the second would represent the reflectors. This would bring the results closer to reality and allow the sizing of the reflectors in order to reduce the core or even the enrichment.

Then the necessary constants for the model 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 or 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 more methods without worrying about 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) achieved were quite reasonable for a microreactor. The enrichment for this optimized case ended up being 19.75%, which was already expected.

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