

Generating optimal configurations for neutron source distribution in subcritical systems. A linear-programming approach

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ABSTRACT

This paper presents an approach to generate optimal configurations for the neutron source distribution in subcritical systems. These optimal configurations are modeled as linear programming optimization problems (LPOP), whose goal is to minimize the intensity of the neutron source distribution under constraints that define prescribed power density distribution in the subcritical system. The neutron source distribution simulates the neutrons released in spallation events in accelerator-driven subcritical reactors. Numerical results are given to illustrate that this approach can be used as an initial step of a computational tool to be used in the design of subcritical nuclear reactors. The supplementary computational tool aims at finding subcritical core configurations that can reduce the complexity of the high-energy particle accelerator.

1. Introduction

An accelerator driven subcritical (ADS) reactor is a nuclear reactor design formed by coupling a fission nuclear reactor core with a high-energy particle accelerator (Nifenecker et al., 2003; Hossain et al., 2015). The reactor core in an ADS system operates in a subcritical state, meaning that the fission events do not generate sufficient neutrons to sustain an ongoing chain reaction. However, the subcritical reactor core can achieve a steady neutron population, commonly referred to as neutronic stability, by increasing neutron production through spallation nuclear reactions (Nema, 2011; Faw and Shultis, 2012). This is accomplished by inserting heavy metal targets into the reactor core and bombarding them with high-energy protons from the charged particle accelerator. This process releases tens of neutrons in the target area, which can then move to the surrounding fuel areas, inducing new fission events and thus sustaining the fission chain reaction within the reactor core.

The ADS reactor possesses distinct features that prioritize safety and prevent criticality incidents. Turning off the accelerator is all it takes to shut down the reactor since the core is subcritical. Additionally, the ADS reactor's core subcriticality provides opportunities for transmutation and the disposal of heavy actinides, especially the fission fuel generated by conventional nuclear reactors (Nifenecker et al., 2003; Kapoor, 2002). However, these positive features contrast with the expense of requiring a particle accelerator, which significantly increases the overall complexity of ADS systems compared to commercial critical nuclear reactors. Relying on an external neutron

source adds complexity, for example, in terms of accelerator operation, maintenance, and integration with the reactor system. The accelerator must be reliable, generating a consistent proton flux and delivering sufficient power to operate the reactor.

In this work, we describe a linear programming-based methodology to determine the minimal source distribution needed to drive a subcritical system to a prescribed power density distribution. This preliminary study is a first step for the development of a supplementary computational tool for use in subcritical nuclear reactor analysis and design. This tool aims at finding subcritical core configurations that shall reduce the dependence on the particle accelerator. As the development of affordable and reliable particle accelerators that can achieve high values for the beam power is still a challenging ongoing research topic, offering potential subcritical core configurations that can reduce the complexity of the needed particle accelerator is of great interest in our point of view.

A basic schematic configuration of the supplementary computational tool operation is given in Fig. 1. The process presented in Fig. 1 stops when a configuration that meets the design requirements is found. Nonetheless, it can be extended to find and compare multiple possible configurations that meet the design requirements. Analyzing the scheme in Fig. 1, we can notice that the viability of the computational tool depends on the design requirements and efficiencies of the methods used in steps I–III. At this point, we remark that as this work is an initial step toward the supplementary tool's construction, we do not offer

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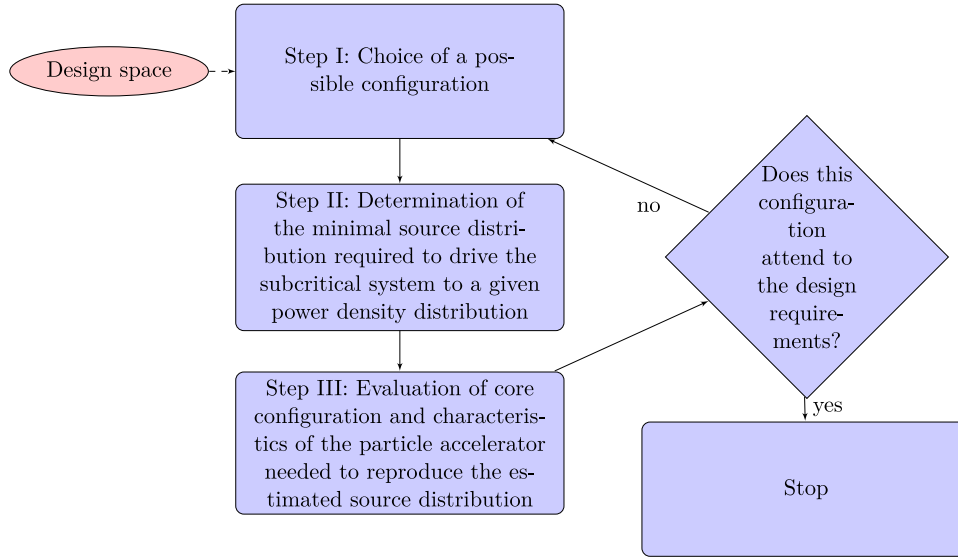


Fig. 1. Basic schematic configuration of a supplementary computational tool to subcritical nuclear reactor design.

any efficiency analysis. Instead, we focus on offering a methodology to represent step II in Fig. 1.

A summary of the remainder of this paper is given next. In Section 2, we present a linear programming-based methodology to determine the minimum neutron source distribution that drives a subcritical core to a prescribed power density level. The prescribed power density distribution and the neutron source distribution are correlated through the adjoint technique (Gandini, 1987, 1967). The neutron sources considered in this methodology intend to simulate the neutrons generated by spallation events in the reactor core. Therefore, the generated neutron source distribution gives an overall idea of the required intensity that the particle accelerator needs to produce to drive the reactor to a prescribed power density distribution. In Section 3, we present numerical results for two model problems, and we close this paper with a brief discussion in Section 4.

At this point, we emphasize that, to our knowledge, this is the first time that the adjoint technique is applied in the context of the optimization of neutron source distributions to drive subcritical systems to steady power level. Moreover, it is important to mention that an earlier version of this paper was presented at the 2023 International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering and was published in the Proceedings (Moraes et al., 2023).

2. Methodology

We begin by considering a two-dimensional rectangular domain composed of contiguous non-overlapping rectangular regions, i.e., $D = \mathcal{R}_1 \cup \mathcal{R}_2 \cup \dots \cup \mathcal{R}_k \cup \dots \cup \mathcal{R}_{T-1} \cup \mathcal{R}_T$, where T represents the total number of regions, viz. Fig. 2. The material parameters are considered spatially uniform inside each region $\mathcal{R}_k$ of the heterogeneous rectangular domain.

Now, let us introduce the functional

$$F = \sum_{k=1}^T \int_{h_{\mathcal{R}_k}} \int_{w_{\mathcal{R}_k}} \sum_{g=1}^G \sum_{m=1}^M Q_{k,g}^{\dagger} \Psi_{m,g}(x, y) \omega_m dx dy \equiv \langle Q^{\dagger}, \Psi \rangle, \quad (2.1)$$

which is linear with respect to both functions $Q^{\dagger}$ and Ψ . In Eq. (2.1), $m = 1, 2, \dots, M$ where $M = N(N+2)/2$ is the number of discrete directions with N being the order of the discrete ordinates (S_N) formulation, and $g = 1, 2, \dots, G$ with G being the number of energy groups in the multigroup formulation (Prinja and Larsen, 2010). Moreover, $\Psi_{m,g}(x, y)$ is the neutron angular flux in a point of the domain D , migrating in the discrete direction of motion (μ_m, η_m) with kinetic energy

within the energy group g . $Q_{k,g}^{\dagger}$ is a function termed adjoint source, whose meaning is tied to the definition of the functional F . Once we set a specific meaning to the functional F , we subsequently define the adjoint source term accordingly. In addition, $h_{\mathcal{R}_k}$ and $w_{\mathcal{R}_k}$ are, respectively, the height and width of region $\mathcal{R}_k$, and ω_m are the weights of the Level Symmetric angular quadrature (Lewis and Miller, 1993). The group neutron angular flux satisfies the multigroup S_N transport equation (Lewis and Miller, 1993) within region $\mathcal{R}_k$, i.e.,

$$\left(\mu_m \frac{\partial}{\partial x} + \eta_m \frac{\partial}{\partial y} + \Sigma_{t_{k,g}} \right) \Psi_{m,g}(x, y) = \frac{1}{4} \sum_{g'=1}^G \left(\Sigma_{s_{k,g' \rightarrow g}} + \chi_{k,g} \nu \Sigma_{f_{k,g'}} \right) \times \sum_{n=1}^M \Psi_{n,g'}(x, y) \omega_n + Q_{k,g}, \quad (2.2)$$

where $\Sigma_{t_{k,g}}$, $\Sigma_{s_{k,g' \rightarrow g}}$ and $\Sigma_{f_{k,g'}}$ are the total, scattering, and fission macroscopic cross sections, and ν and $\chi_{k,g}$ are respectively the average number of neutrons released in a fission event and the fission spectrum. The neutron source $Q_{k,g}$ is considered spatially uniform. Details about the mathematical model given in Eq. (2.2) can be found in Morató et al. (2020).

Based on the concept of neutron importance (Gandini, 1987, 1967; Moraes et al., 2022), we can rewrite the functional F , considering appropriate boundary conditions as (Moraes and Barros, 2022)

$$F = \sum_{k=1}^T \int_{h_{\mathcal{R}_k}} \int_{w_{\mathcal{R}_k}} \sum_{g=1}^G \sum_{m=1}^M Q_{k,g} \Psi_{m,g}^{\dagger}(x, y) \omega_m dx dy \equiv \langle Q, \Psi^{\dagger} \rangle, \quad (2.3)$$

where $\Psi_{m,g}^{\dagger}(x, y)$ represents the importance that one neutron inserted in the system traveling in a discrete direction of motion (μ_m, η_m) within the energy group g has to the quantity defined by F . The function $\Psi_{m,g}^{\dagger}(x, y)$ is also referred to as adjoint angular flux since it is the solution of the equation that is adjoint to Eq. (2.2) (Prinja and Larsen, 2010). That is,

$$\left(-\mu_m \frac{\partial}{\partial x} - \eta_m \frac{\partial}{\partial y} + \Sigma_{t_{k,g}} \right) \Psi_{m,g}^{\dagger}(x, y) = \frac{1}{4} \sum_{g'=1}^G \left(\Sigma_{s_{k,g \rightarrow g'}} + \chi_{k,g} \nu \Sigma_{f_{k,g'}} \right) \times \sum_{n=1}^M \Psi_{n,g'}^{\dagger}(x, y) \omega_n + Q_{k,g}^{\dagger}. \quad (2.4)$$

At this point, we remark that we shall use interchangeably the terms importance function and adjoint angular flux as references to $\Psi_{m,g}^{\dagger}(x, y)$.

Making use of Eqs. (2.1) and (2.3) we can write

$$\langle Q^{\dagger}, \Psi \rangle = \langle Q, \Psi^{\dagger} \rangle, \quad (2.5)$$

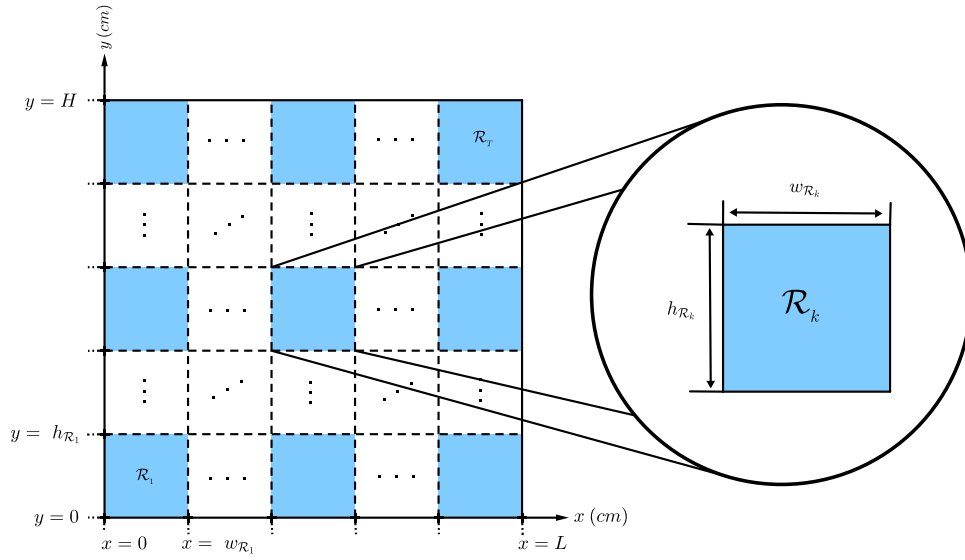


Fig. 2. Two-dimensional spatial domain (D) with T contiguous non-overlapping regions $\mathcal{R}_i$ of width $w_{\mathcal{R}_i}$ and height $h_{\mathcal{R}_i}$.

which is the well-known reciprocity relation (Moraes and Barros, 2022).

2.1. Linear Programming Optimization Problem (LPOP)

In the second step of Fig. 1, given a possible configuration of the subcritical system, we need to determine the minimum intensity of the neutron source distribution that will drive the subcritical core to a prescribed power distribution. We mathematically model this problem through the following linear programming optimization problem

$$\begin{aligned} & \text{Minimize} \quad \sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \\ & \text{Subjected to:} \\ & c_1^{\min} \leq P_1 \leq c_1^{\max}; \\ & c_2^{\min} \leq P_2 \leq c_2^{\max}; \\ & \vdots \\ & c_T^{\min} \leq P_T \leq c_T^{\max}; \\ & Q_{k,g} \geq 0, \end{aligned} \quad (2.6)$$

where $c_k^{\min}$ and $c_k^{\max}$ define the minimum and maximum possible values for the power density generated in region $\mathcal{R}_k$, i.e., P_k . At this point, we remark that not all regions $\mathcal{R}_k$ that compose the domain are necessarily composed of multiplying material (i.e., $\Sigma_{f,k,g} \neq 0$ for at least one energy group). In this case, we can proceed in two different paths, considering the constraints of the LPOP: (i) we consider one constraint for each multiplying region. Thus, the number of restrictions presented in Eq. (2.6) will be equal to the total number of fuel regions in the system; or (ii) we consider one constraint for every region $\mathcal{R}_k$ in the system and set both $c_k^{\min}$ and $c_k^{\max}$ as zero for non-multiplying regions. To make life simpler, we shall proceed in the second path, i.e., we consider one constraint for each region that composes the domain, setting $c_k^{\min}$ and $c_k^{\max}$ accordingly.

As we can notice from Eq. (2.6), some constraints are not, at a first glance, directly correlated with the neutron source distribution. We use the adjoint formulation to generate explicit relations between the neutron source distribution and the power density in region $\mathcal{R}_k$. As stated previously in this section, the definition of $Q^\dagger$ is tied to the meaning of the functional F . Therefore, as we want to correlate the neutron source distribution with the power density in the system, we consider the functional F as the power generated in region $\mathcal{R}_{k'}$ by unit of height. That is,

$$F = P_{k'} = \sum_{k=1}^T \int_{h_{\mathcal{R}_k}} \int_{w_{\mathcal{R}_k}} \sum_{g=1}^G \sum_{m=1}^M \epsilon \Sigma_{f,k,g} \delta_{k,k'} \Psi_{m,g}^\dagger(x, y) \omega_m dx dy \equiv \langle Q^\dagger, \Psi \rangle. \quad (2.7)$$

Analyzing Eq. (2.7), we can see that the adjoint source term $Q^\dagger$ is

$$Q_{k,g}^\dagger = \epsilon \Sigma_{f,k,g} \delta_{k,k'}, \quad (2.8)$$

where ϵ is the average energy released in a fission event, and $\delta_{k,k'}$ is a Kronecker delta function that is 1 if $\mathcal{R}_{k'} = \mathcal{R}_k$ and 0 otherwise. Substituting Eqs. (2.3) and (2.7) into Eq. (2.5), we obtain

$$P_{k'} = \sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{\dagger k'}, \quad (2.9a)$$

where we have defined

$$\Phi_{k,g}^{\dagger k'} = \int_{h_{\mathcal{R}_k}} \int_{w_{\mathcal{R}_k}} \sum_{m=1}^M \Psi_{m,g}^{\dagger k'}(x, y) \omega_m dx dy. \quad (2.9b)$$

The neutron importance in Eqs. (2.9) is obtained through the solution of Eq. (2.4) with adjoint source given in Eq. (2.8). Making use of Eqs. (2.9), we can rewrite the LPOP as

$$\begin{aligned} & \text{Minimize} \quad \sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \\ & \text{Subjected to:} \\ & c_1^{\min} \leq \sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{\dagger 1} \leq c_1^{\max}; \\ & c_2^{\min} \leq \sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{\dagger 2} \leq c_2^{\max}; \\ & \vdots \\ & c_T^{\min} \leq \sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{\dagger T} \leq c_T^{\max}; \\ & Q_{k,g} \geq 0. \end{aligned} \quad (2.10)$$

As we can see in Eq. (2.10), the objective function and constraints of the LPOP are now defined by linear expressions involving the neutron source distribution. This makes the LPOP suitable for well-established numerical methods such as the Interior Point (Potra and Wright, 2000; Nemirovski and Todd, 2008) method and the Simplex method (Nelder and Mead, 1965; Nash, 2000).

To solve Eq. (2.10), we adopt the Simplex method due to its simplicity and numerical stability (Nelder and Mead, 1965). This method, however, requires extra steps to deal with the inequality constraints. The definition of these steps can be tricky, especially for those unfamiliar with the method. Therefore, we present an explanation of

a solution process for Eq. (2.10) based on the Simplex method. We remark that some details of the method shall be intentionally omitted. Nonetheless, one can find detailed information about the Simplex method elsewhere (Nelder and Mead, 1965; Nash, 2000; Taha, 2019).

2.2. A solution process for the LPOP

Although it possesses underlying geometric concepts, operationally, the Simplex method can be viewed as an algebraic method since it is based on solving a system of equations (Taha, 2019). Therefore, the first step in the solution of Eq. (2.10) is to convert the inequality constraints into equality constraints.

The majority of constraints of Eq. (2.10) define intervals for power density in the regions that compose the domain. Considering, for example, region R_1 , we can split the constraint associated with this region into two different constraints. That is,

$$\sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{+1} \leq c_1^{max} \quad (2.11a)$$

and

$$\sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{+1} \geq c_1^{min}. \quad (2.11b)$$

To convert these inequalities into equality constraints, we use slack variables. We add a slack variable (V_1^+) to Eq. (2.11a) and subtract another one (V_1^-) from Eq. (2.11b), thus obtaining

$$\sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{+1} + V_1^+ = c_1^{max} \quad (2.12a)$$

and

$$\sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{+1} - V_1^- = c_1^{min}. \quad (2.12b)$$

By using slack variables, we can rewrite Eq. (2.10) in an equivalent augmented form as

$$\begin{aligned} &\text{Minimize} \quad \sum_{k=1}^T \sum_{g=1}^G Q_{k,g} + 0 \times \sum_{k=1}^T [V_k^+ + V_k^-] \\ &\text{Subjected to:} \\ &\sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{+1} + V_1^+ = c_1^{max}, \\ &\sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{+1} - V_1^- = c_1^{min}, \\ &\vdots \\ &\sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{+T} + V_T^+ = c_T^{max}, \\ &\sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \Phi_{k,g}^{+T} - V_T^- = c_T^{min} \\ &Q_{k,g} \geq 0; V_k^+ \geq 0; V_k^- \geq 0. \end{aligned} \quad (2.13)$$

Both forms of the LPOP, as presented in Eqs. (2.10) and (2.13), represent exactly the same problem. However, the form presented in Eq. (2.13) is much more convenient for algebraic manipulation and identifying feasible solutions. We have included the slack variables in the constitution of the objective function to clarify that the solution of the augmented problem also includes the slack variables. Nonetheless, as we multiply the slack variables by zero in the objective function, the solution of Eq. (2.13) is the same as Eq. (2.10).

Eq. (2.13) in a matrix form appears as

$$\begin{aligned} &\text{Minimize} \quad cQ \\ &\text{Subjected to:} \\ &AQ = b; \\ &Q_{k,g} \geq 0; V_k^+ \geq 0; V_k^- \geq 0, \end{aligned} \quad (2.14a)$$

where Q and c are $T(2+G)$ -dimensional column vectors defined as

$$Q = [Q_{1,1}, Q_{1,2}, \dots, Q_{T,G}, V_1^+, V_1^-, \dots, V_T^+, V_T^-]^t \quad (2.14b)$$

and

$$c = [1, 1, \dots, 1, 0, 0, \dots, 0], \quad (2.14c)$$

b is a $2T$ -dimensional column vector having the form

$$b = [c_1^{max}, c_1^{min}, \dots, c_T^{max}, c_T^{min}]^t, \quad (2.14d)$$

and A is a $2T \times T(2+G)$ matrix defined as

$$A = \begin{bmatrix} \Phi_{1,1}^{+1} & \Phi_{1,2}^{+1} & \dots & \Phi_{T,G}^{+1} & 1 & 0 & \dots & 0 & 0 \\ \Phi_{1,1}^{+1} & \Phi_{1,2}^{+1} & \dots & \Phi_{T,G}^{+1} & 0 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \Phi_{1,1}^{+T} & \Phi_{1,2}^{+T} & \dots & \Phi_{T,G}^{+T} & 0 & 0 & \dots & 1 & 0 \\ \Phi_{1,1}^{+T} & \Phi_{1,2}^{+T} & \dots & \Phi_{T,G}^{+T} & 0 & 0 & \dots & 0 & -1 \end{bmatrix}. \quad (2.14e)$$

In Eqs. (2.14) the superscript t represents transpose. Now, let us consider two column vectors Q_B and Q_N of order $2T$ and TG respectively. These vectors are sub-vectors of vector Q , so their concatenation represents the same vector Q , although in a possibly different organization. We chose $2T$ different terms of vector Q to define vector Q_B , and arranged the remaining terms of vector Q in vector Q_N , such that $Q \equiv [Q_B, Q_N]$. In this case, Eq. (2.14a) can be rewritten as

$$\begin{aligned} &\text{Minimize} \quad c_B Q_B + c_N Q_N \\ &\text{Subjected to:} \\ &BQ_B + NQ_N = b; \\ &Q_{k,g} \geq 0; V_k^+ \geq 0; V_k^- \geq 0. \end{aligned} \quad (2.15)$$

In Eq. (2.15), c_B and c_N are sub-vectors of vector c with order $2T$ and TG , respectively, and matrices B and N are sub-matrices of matrix A with order $2T \times 2T$ and $2T \times TG$ respectively. The constitution of c_B , c_N , B and N follows the organization adopted for Q_B and Q_N . From the linear system presented in Eq. (2.15), we have

$$Q_B = B^{-1} \{b - NQ_N\}, \quad (2.16)$$

provided B is invertible. If we consider Q_N as the null vector, Eq. (2.16) becomes

$$\hat{Q}_B = B^{-1} b. \quad (2.17)$$

Vector $\hat{Q}_B$ presented in Eq. (2.17) is called basic solution. By restriction, in order to the basic solution to be feasible, all terms of $\hat{Q}_B$ need to be greater than or equal to zero.

Substituting Eq. (2.16) into the objective function of Eq. (2.15) we obtain

$$\text{Minimize} \quad \hat{f} + rQ_N, \quad (2.18a)$$

where $\hat{f} = c_B \hat{Q}_B$ is the value of the objective function for the case Q_N is the null-vector, and

$$r = (c_N - c_B B^{-1} N) \quad (2.18b)$$

is a vector called relative cost. Analyzing Eqs. (2.18), we can note that if all terms of r are positive ($r \geq 0$), the solution that minimizes the objective function is $\hat{Q}_B$, and the minimum value of the objective function is $\hat{f}$. This condition is called optimality condition and, once satisfied, it guarantees that the best solution of the LPOP is $\hat{Q}_B$. Since by restriction Q_N can only assume values greater than or equal to zero, to assume any component of Q_N different from zero would increase the value of the objective function. However, if at least one component of r is less than zero, the optimal condition is not satisfied. We can decrease the value of the objective function by increasing the component of vector Q_N that multiplies the negative component of the vector r .

Since we seek the solution that minimizes the objective function, we need to change the initial configurations adopted for vectors $\mathbf{Q}_B$ and $\mathbf{Q}_N$ so that the optimality condition is satisfied.

We change the configuration of vectors $\mathbf{Q}_B$ and $\mathbf{Q}_N$ by switching selected components between these vectors. To select the component of vector $\mathbf{Q}_N$ that will enter the vector $\mathbf{Q}_B$, we analyze the components of $\mathbf{r}$, and select the negative component with the largest absolute value. Being negative and possessing a large absolute value, this component will have a heavy impact on decreasing the value of the objective function. Once we have selected the component that will leave $\mathbf{Q}_N$, we consider vector $\mathbf{Q}_N$ as composed of entries $\mathbf{Q}_{N_i}$, defined as

$$\mathbf{Q}_{N_i} = \begin{cases} \xi, & \text{if } n = i \\ 0, & \text{otherwise} \end{cases}, \quad (2.19)$$

where ξ is a positive constant, and n is the position of the negative component of vector $\mathbf{r}$ with the largest absolute value.

Now, to select the component of vector $\mathbf{Q}_B$ that will enter vector $\mathbf{Q}_N$, we substitute Eq. (2.19) into Eq. (2.16), thus obtaining

$$\mathbf{Q}_B = \hat{\mathbf{Q}}_B - \mathbf{z}\xi, \quad (2.20)$$

where $\mathbf{z} = \mathbf{B}^{-1} \mathbf{N}_n$ with $\mathbf{N}_n$ being the n th-column of matrix $\mathbf{N}$. By restriction, all components of vector $\mathbf{Q}_B$ must be greater than or equal to zero. With this in mind, let us suppose that all components of vector $\mathbf{z}$ are negative. In that case, the LPOP does not possess an optimal solution since we can continuously increase ξ (hence decreasing the objective function) and yet generate possible solutions. However, if at least one component of $\mathbf{z}$ is positive, we cannot increase ξ indefinitely since this would eventually contradict the restriction $\mathbf{Q}_B \geq 0$. The maximum value that ξ can have is

$$\xi = \frac{\hat{\mathbf{Q}}_{B_\ell}}{\mathbf{z}_\ell} = \text{minimum} \left\{ \frac{\hat{\mathbf{Q}}_{B_i}}{\mathbf{z}_i}, \quad \mathbf{z}_i > 0 \right\}. \quad (2.21)$$

Note that satisfying Eq. (2.21), at least one component of vector $\mathbf{Q}_B$ (Eq. (2.20)) will be zero. On the other hand, vector $\mathbf{Q}_N$ possesses one component that is different from zero (Eq. (2.19)). The optimal solution necessarily satisfies the optimality condition, which requires the vector $\mathbf{Q}_N$ to be the null vector. Therefore, we chose the component of vector $\mathbf{Q}_B$ that satisfies Eq. (2.21) to enter the vector $\mathbf{Q}_N$.

By switching these components, we change the initial configuration of vectors $\mathbf{Q}_B$ and $\mathbf{Q}_N$. Vectors $\mathbf{c}_B$ and $\mathbf{c}_N$, and matrices $\mathbf{B}$ and $\mathbf{N}$ follow this change, and need to be rearranged. Once we rearrange all vectors and matrices associated with the new organization for vectors $\mathbf{Q}_B$ and $\mathbf{Q}_N$, we repeat all steps starting from Eq. (2.15) until the optimality condition is satisfied.

2.2.1. Choice of the initial configuration for vector $\mathbf{Q}_B$

In order to use the Simplex method, we need to choose an initial configuration for vector $\mathbf{Q}_B$ such that the associated matrix $\mathbf{B}$ is invertible and $\hat{\mathbf{Q}}_B$ is a basic feasible solution, i.e., $\hat{\mathbf{Q}}_B \geq 0$. This task can be challenging since the constraints of the LPOP change with the problem's constitution.

To define an initial configuration for vector $\hat{\mathbf{Q}}_B$ that works regardless the problem's constitution, we add auxiliary variables (V_k^A) in the equality constraints of Eq. (2.13) associated with the minimum possible values for the power density in the system, and change the objective function to reflect this procedure. That is,

$$\begin{aligned} &\text{Minimize} \quad \sum_{k=1}^T \sum_{g=1}^G \mathbf{Q}_{k,g} + 0 \times \sum_{k=1}^T \left[V_k^+ + V_k^- \right] + \mathcal{M} \times \sum_{k=1}^T V_k^A \\ &\text{Subjected to:} \\ &\sum_{k=1}^T \sum_{g=1}^G \mathbf{Q}_{k,g} \Phi_{k,g}^{\dagger 1} + V_1^+ = c_1^{\max}, \\ &\vdots \\ &\sum_{k=1}^T \sum_{g=1}^G \mathbf{Q}_{k,g} \Phi_{k,g}^{\dagger T} + V_T^+ = c_T^{\max}, \\ &\sum_{k=1}^T \sum_{g=1}^G \mathbf{Q}_{k,g} \Phi_{k,g}^{\dagger T} - V_T^- + V_T^A = c_T^{\min} \\ &\mathbf{Q}_{k,g} \geq 0; V_k^+ \geq 0; V_k^- \geq 0; V_k^A \geq 0, \end{aligned}$$

$$\begin{aligned} &\sum_{k=1}^T \sum_{g=1}^G \mathbf{Q}_{k,g} \Phi_{k,g}^{\dagger 1} - V_1^- + V_1^A = c_1^{\min}; \\ &\vdots \\ &\sum_{k=1}^T \sum_{g=1}^G \mathbf{Q}_{k,g} \Phi_{k,g}^{\dagger T} + V_T^+ = c_T^{\max}; \\ &\sum_{k=1}^T \sum_{g=1}^G \mathbf{Q}_{k,g} \Phi_{k,g}^{\dagger T} - V_T^- + V_T^A = c_T^{\min} \\ &\mathbf{Q}_{k,g} \geq 0; V_k^+ \geq 0; V_k^- \geq 0; V_k^A \geq 0, \end{aligned} \quad (2.22)$$

where $\mathcal{M}$ is a large positive constant compared to $\mathbf{Q}$. As we are introducing new variables in constraints already defined by equality expressions (required by the Simplex method), the value of the auxiliary variables should be zero for these relations to remain the same. In order to force this situation (auxiliary variables as zero), we add the term $\mathcal{M} \times \sum_{k=1}^T V_k^A$ to the objective function. As the objective function should be minimized, and $\mathcal{M}$ is a large positive value, the Simplex method tends to allocate the auxiliary variables in the vector $\mathbf{Q}_N$ which is the null vector in the optimal solution. In this case, the solution of Eq. (2.22) will be the same as Eq. (2.13).

The introduction of these auxiliary variables guarantees that we can have an initial configuration for $\hat{\mathbf{Q}}_B$ that leads to an invertible matrix $\mathbf{B}$ and a basic feasible solution $\hat{\mathbf{Q}}_B \geq 0$. By selecting $\mathbf{Q}_B$ as

$$\mathbf{Q}_B = \left[V_1^+, V_1^A, V_2^+, V_2^A, \dots, V_T^+, V_T^A \right]^t, \quad (2.23)$$

matrix $\mathbf{B}$ can be written as the identity matrix. Since vector $\mathbf{b}$ is composed of entries which are greater than or equal to zero, the components of the basic solution associated with this organization are also greater than or equal to zero. Since $\mathbf{B}$ is the identity matrix, the basic feasible solution for the first configuration of vector $\mathbf{Q}_B$ is $\hat{\mathbf{Q}}_B = \mathbf{b}$.

2.2.2. Different interpretations of the solution of the LPOP

Mathematically, the solution of the LPOP presented in Eq. (2.10) determines the neutron source distribution that drives the subcritical system at a distribution of power density defined by the constraints of Eq. (2.10), and whose sum is minimal. However, different interpretations can be drawn through the solution of Eq. (2.10). We may consider $\mathbf{Q}_{k,g}$ as the number of neutrons within energy group g that are released in spallation events in region $\mathcal{R}_k$. In this case, the neutron source distribution represents the distribution of neutrons released in the spallation target areas. If we assume that interpretation for the neutron source distribution, we need to ensure that $\mathbf{Q}_{k,g}$ is zero in the regions that do not contain spallation material. This can be done by considering

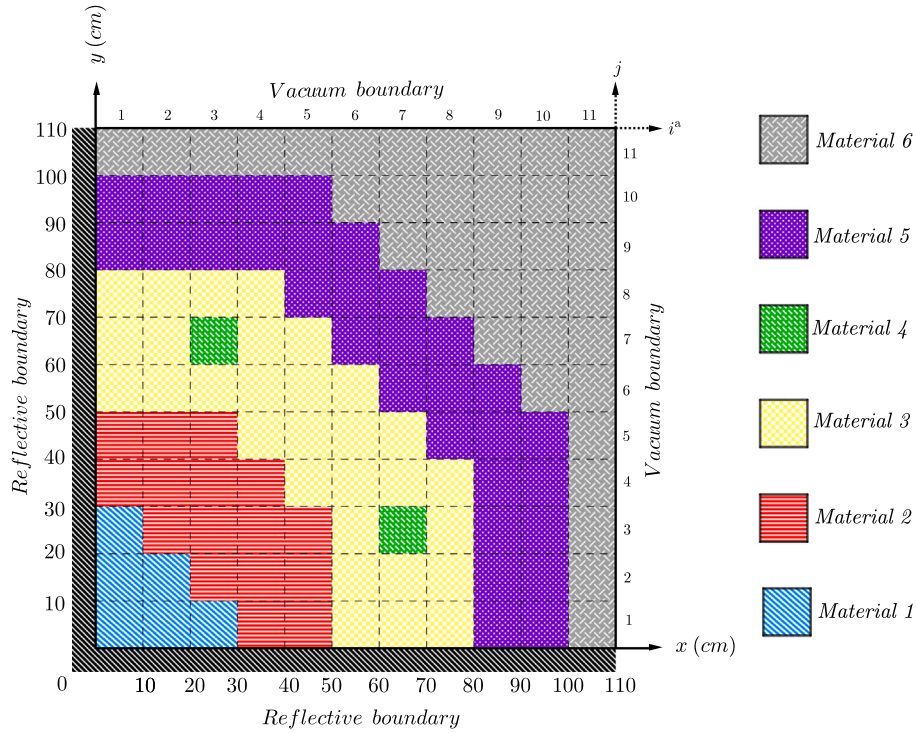
$$\mathbf{Q}_{k,g} = 0, \quad (2.24)$$

in the LPOP for each k different from the zones with spallation material, and g are the energy groups different from the energy groups of the neutrons released in spallation events.

Another possible interpretation for the solution of Eq. (2.10) is to consider $\mathbf{Q}_{k,g}$ as the number of neutrons within energy group g that arrive at region $\mathcal{R}_k$ from spallation events produced in a region different from $\mathcal{R}_k$. Look that this interpretation is entirely different from the previous one, but it can also be useful since the only assumption made is about the influence of the spallation events in zones other than the target zones. To represent this problem, we need to make sure that Eq. (2.24) is valid for regions $\mathcal{R}_k$ that contain the spallation material.

2.2.3. Prescribed power density distribution composed of given sets of fuel regions

As stated in Section 2.1, we consider one constraint for every region $\mathcal{R}_k$ in the system and set both $c_k^{\min}$ and $c_k^{\max}$ accordingly. The values of $c_k^{\min}$ and $c_k^{\max}$ for the multiplying regions ($c_k^{\min} = c_k^{\max} = 0$ for non-multiplying regions) should be provided through the prescribed power density distribution. However, depending on the way the prescribed



^a The values of i and j define the region $\mathcal{R}_k$. That is, $k = i + (j - 1) \times 11$.

Fig. 3. Geometry and material distribution of Model Problem I.

power density distribution is provided, we may not be able to define $c_k^{\min}$ and $c_k^{\max}$ for all multiplying regions in the domain.

To visualize this situation, let us consider a spatial domain composed of regions of two different multiplying materials. In addition, we assume that

$$c_{mat\ 1}^{\min} \leq \mathcal{P}_{mat\ 1} \leq c_{mat\ 1}^{\max} \quad (2.25a)$$

and

$$c_{mat\ 2}^{\min} \leq \mathcal{P}_{mat\ 2} \leq c_{mat\ 2}^{\max}, \quad (2.25b)$$

where $c_{mat\ u}^{\min}$ and $c_{mat\ u}^{\max}$ are the minimum and maximum values of the power density of all regions of material u , and $\mathcal{P}_{mat\ u}$ represents the power density of all regions of material u , such that $u = \{1 \text{ or } 2\}$. From Eqs. (2.25), we notice that we cannot obtain the values of $c_k^{\min}$ and $c_k^{\max}$ separately for all multiplying regions. Eqs. (2.25) instead state that the sum of the power density generated by all regions of material 1 and 2 should be in the intervals $[c_{mat\ 1}^{\min}, c_{mat\ 1}^{\max}]$ and $[c_{mat\ 2}^{\min}, c_{mat\ 2}^{\max}]$, respectively.

Since Eqs. (2.25) present the prescribed power density distribution as composed of values of power that are generated by the sum of the power generated by given sets of fuel regions, we sum the correspondent constraints of the LPOP presented in Eq. (2.6), so that Eqs. (2.25) are satisfied. In this case, Eq. (2.6) becomes

$$\begin{aligned} & \text{Minimize} \quad \sum_{k=1}^T \sum_{g=1}^G Q_{k,g} \\ & \text{Subjected to:} \\ & c_{mat\ 1}^{\min} \leq \mathcal{P}_{mat\ 1} \leq c_{mat\ 1}^{\max}, \\ & c_{mat\ 2}^{\min} \leq \mathcal{P}_{mat\ 2} \leq c_{mat\ 2}^{\max}, \\ & Q_{k,g} \geq 0. \end{aligned} \quad (2.26)$$

Analyzing Eq. (2.26), we observe that we do not need to solve the adjoint equations associated with the power density of each fuel region as in Eq. (2.6). Instead, to associate the constraints of Eq. (2.26) with

the neutron source distribution, we need to solve two distinct adjoint problems considering

$$Q_{k,g}^{\dagger} = \epsilon \sum_{f_{k,g}} \delta_{k,mat\ 1} \quad (2.27a)$$

and

$$Q_{k,g}^{\dagger} = \epsilon \sum_{f_{k,g}} \delta_{k,mat\ 2}. \quad (2.27b)$$

separately. In Eqs. (2.27), $\delta_{k,mat\ 1}$ and $\delta_{k,mat\ 2}$ are Kronecker delta functions that are equal to 1 if region $\mathcal{R}_k$ is composed of material 1 or 2, and zero otherwise. Substituting Eqs. (2.27) into Eq. (2.1), the functional F becomes the power density of all regions of material 1 and 2, respectively.

3. Numerical results

In this section, we present numerical results for two different model problems. In Model Problem I, we focus our attention on to provide insights into the LPOP's solution through the analysis of the importance function associated with the constraints of the LPOP (i.e., solution of Eq. (2.4)) and the potential presence of slack and auxiliary variables in the optimal solution. In Model Problem II, we slightly modify Model Problem I to illustrate the use of the offered methodology to select the configuration that decreases the intensity of the needed neutron source distribution.

For the numerical results presented in this section, we adopt that the average number of neutrons released in fission events is $\nu = 2.4$, and the average energy released in fission events is $\epsilon = 200$ MeV. Moreover, we used to model the adjoint problems (constraints of the LPOP) the S_4 formulation and the multigroup formulation with $G = 2$ energy groups. We remark that the geometry and material parameters considered in Model Problems I and II are fictitious. The idea is to demonstrate the application of the methodology described in the previous section and to show that this methodology can be used in step II of the supplementary tool whose schematic is illustrated in Fig. 1.

Table 1
Material parameters of Model Problem I.

Material parameters		Σ_{t_g} (cm ⁻¹)	Σ_{f_g} (cm ⁻¹)	$\Sigma_{s_{g \rightarrow g'}}$ (cm ⁻¹)		χ_g
				$g' = 1$	$g' = 2$	
Material 1	$g = 1$	2.31800E-01 ^a	0.00000E+00	1.82450E-01	1.56300E-02	1
	$g = 2$	8.38000E-01	0.00000E+00	0.00000E+00	7.33100E-01	
Material 2	$g = 1$	2.31800E-01	2.99700E-03	1.82400E-01	1.63800E-02	0
	$g = 2$	8.71460E-01	6.53510E-02	0.00000E+00	7.42840E-01	
Material 3	$g = 1$	2.36570E-01	3.68710E-03	2.09560E-01	1.45300E-02	1
	$g = 2$	8.22800E-01	8.37530E-02	0.00000E+00	7.06500E-01	
Material 4	$g = 1$	2.71520E-02	0.00000E+00	2.64812E-02	1.63800E-04	0
	$g = 2$	5.22800E-02	0.00000E+00	0.00000E+00	5.10840E-02	
Material 5	$g = 1$	3.37600E-01	0.00000E+00	3.03126E-01	1.01200E-03	0
	$g = 2$	9.99500E-01	0.00000E+00	0.00000E+00	3.13126E-01	
Material 6	$g = 1$	1.78120E-01	0.00000E+00	8.00710E-02	3.43400E-03	0
	$g = 2$	1.17616E+00	0.00000E+00	0.00000E+00	1.14458E-01	

^a Read as 2.31800×10^{-01} .

3.1. Model Problem I

For the first problem, we consider a square domain composed of 121 regions, 46 of which are composed of fuel materials. Fig. 3 displays the geometry and material distribution of Model Problem I, and Table 1 shows the material parameters of this problem. In Fig. 3, the term “Vacuum boundary” means that vacuum boundary conditions apply for the forward transport problem and zero adjoint angular flux in the outgoing directions apply for the adjoint problem, and “Reflective boundary” means that reflective boundary conditions apply for both the forward and adjoint problems.

3.1.1. First numerical experiment

To construct the LPOP given in Eq. (2.22), we need first to provide the prescribed power density distribution. In this case, we assume that the power density of all regions of material 2 and 3 should be in the interval $[4 \text{ MW cm}^{-1}, 5 \text{ MW cm}^{-1}]$ each. That is,

$$4 \text{ MW cm}^{-1} \leq P_{mat\ 2} \leq 5 \text{ MW cm}^{-1} \quad (3.28a)$$

and

$$4 \text{ MW cm}^{-1} \leq P_{mat\ 3} \leq 5 \text{ MW cm}^{-1}, \quad (3.28b)$$

where $P_{mat\ 2}$ and $P_{mat\ 3}$ represent the power generated by all regions composed of material 2 and 3 per unit length of core height, respectively.

Eqs. (3.28) are the initial constraints of the LPOP. To associate these constraints to the neutron source distribution, we solve two adjoint problems (Eq. (2.4)), varying the adjoint source term accordingly. The adjoint source terms associated with Eqs. (3.28) must be chosen such that the functional presented in Eq. (2.1) becomes the power density of all zones 2 and 3, respectively. To solve Eq. (2.4), we chose to use the coarse-mesh Response Matrix-Constant Nodal (RM-CN) method (da Silva et al., 2020; Moraes et al., 2021, 2020). Using the RM-CN method to generate accurate results for the importance function, we discretized the two-dimensional spatial domain in square cells of side 0.2 cm. The stopping criterion for the iteration scheme used in the RM-CN method requires that the maximum relative deviation between two consecutive estimates of the adjoint node-edge average scalar fluxes be no greater than 1×10^{-6} . Fig. 4 displays the group node-average adjoint scalar fluxes as a function of the node midpoints.

As briefly discussed in the previous section, the solution of the LPOP may have multiple interpretations. Thus, we consider $Q_{k,g}$ as the number of neutrons that are released in spallation events inside regions R_k , which are composed of spallation material. Assuming that the regions composed of material 1 are the regions where spallation events can occur, we need to add the constraint

$$Q_{k,g} = 0, \quad (3.29)$$

to the LPOP. Eq. (3.29) is valid for all regions composed of a material that is different from material 1. The LPOP associated with this numerical experiment is

$$\begin{aligned} \text{Minimize } & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} + 0 \times \sum_{u=1}^2 \left[V_u^+ + V_u^- \right] + \mathcal{M} \times \sum_{u=1}^2 V_u^A \\ \text{Subjected to: } & \\ & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{+mat\ 2} + V_1^+ = 5; \\ & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{+mat\ 2} - V_1^- + V_1^A = 4; \\ & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{+mat\ 3} + V_2^+ = 5; \\ & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{+mat\ 3} - V_2^- + V_2^A = 4; \\ & Q_{k,g} \geq 0 \text{ (regions of material 1);} \\ & Q_{k,g} = 0 \text{ (regions with material different than 1);} \\ & V_1^+ \geq 0; V_2^+ \geq 0; V_1^- \geq 0; V_2^- \geq 0; V_1^A \geq 0; V_2^A \geq 0, \end{aligned} \quad (3.30)$$

where $\mathcal{M} = 1 \times 10^{80}$. In the LPOP stated in Eq. (3.30) $\Phi_{k,g}^{+mat\ 2}$ and $\Phi_{k,g}^{+mat\ 3}$ are calculated through Eq. (2.9b) making use of the solutions of the adjoint problems associated with (3.28). The values of $\Phi_{k,g}^{+mat\ 2}$ and $\Phi_{k,g}^{+mat\ 3}$ for regions of material 1 are displayed in Table 2. We remark that we present the results of $\Phi_{k,g}^{+mat\ 2}$ and $\Phi_{k,g}^{+mat\ 3}$ only for regions composed of material 1 due to the extra constraint added in the LPOP, i.e., Eq. (3.29). As we assume that neutrons can be inserted into the system only in regions of material 1, the terms of $\Phi_{k,g}^{+mat\ 2}$ and $\Phi_{k,g}^{+mat\ 3}$ associated with regions composed of materials different from 1 will be multiplied by zero $Q_{k,g} = 0$ (regions with material different from zone 1), thus not contributing to the objective function nor with the constitution of the constraints.

Once we have the LPOP settled, we apply the Simplex method on Eq. (3.30), as discussed in the previous section, obtaining: $Q_{23,1} = 1.29743 \times 10^{15}$ neutrons/cm³s, $Q_{23,2} = 5.31066 \times 10^{14}$ neutrons/cm³s ($k = 23 \rightarrow i = 1$ and $j = 3$, according to Fig. 3), $V_1^+ = 1 \text{ MW cm}^{-1}$, and $V_2^- = 1 \text{ MW cm}^{-1}$. Moreover, $Q_{k,g} = 0$ for the remaining regions and energy groups, and $V_1^- = V_2^+ = V_1^A = V_2^A = 0$.

The solution of the LPOP can be explained by using the results displayed in Fig. 4 in conjunction with the values of the material parameters presented in Table 1. In Fig. 3a and b, we have results for the importance function associated with the power density of all regions composed of material 2, and in Fig. 3c and d, we have results for the importance function associated with the power density of all

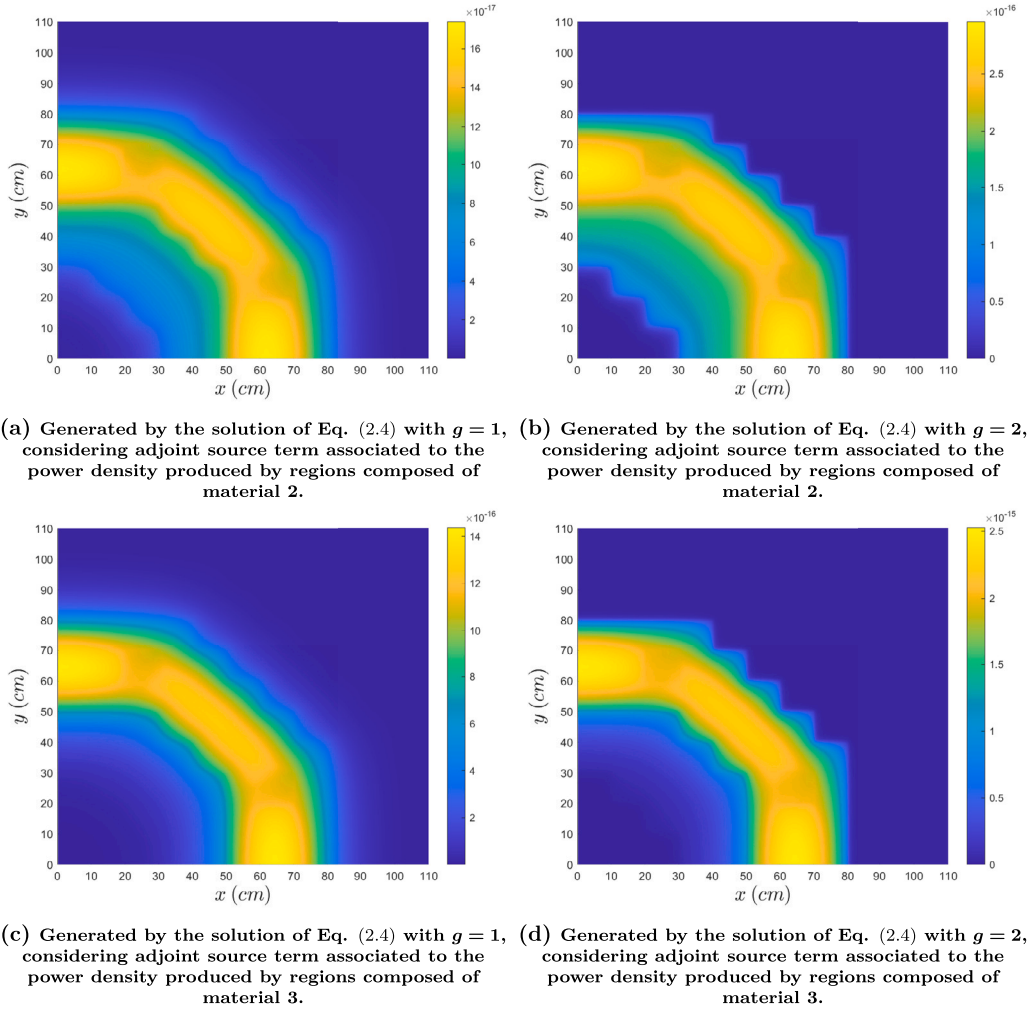


Fig. 4. Node-average adjoint scalar fluxes for the LPOP of the first numerical experiment.

Table 2

Values of $\Phi_{k,g}^{mat 2}$ and $\Phi_{k,g}^{mat 3}$ for regions of material 1 in Model Problem I.

Region	$\mathcal{R}_1$ ($i = 1$ and $j = 1$) ^a		$\mathcal{R}_2$ ($i = 2$ and $j = 1$)		$\mathcal{R}_3$ ($i = 3$ and $j = 1$)	
Energy group	$g = 1$	$g = 2$	$g = 1$	$g = 2$	$g = 1$	$g = 2$
$P_{mat 2}$	2.62143E-16 ^b	3.37746E-18	7.01933E-16	1.53210E-16	2.22868E-15	2.02699E-15
$P_{mat 3}$	2.59102E-16 ^c	1.27630E-18	7.30197E-16	5.64497E-17	2.90578E-15	1.26599E-15
Region	$\mathcal{R}_{12}$ ($i = 1$ and $j = 2$)		$\mathcal{R}_{13}$ ($i = 2$ and $j = 2$)		$\mathcal{R}_{23}$ ($i = 1$ and $j = 3$)	
Energy group	$g = 1$	$g = 2$	$g = 1$	$g = 2$	$g = 1$	$g = 2$
$P_{mat 2}$	7.01932E-16	1.53210E-16	1.74716E-15	1.76100E-15	2.22867E-15	2.02699E-15
$P_{mat 3}$	7.30190E-16	5.64491E-17	1.64634E-15	7.05129E-16	2.90573E-15	1.26597E-15

^a Values of i and j that define region $\mathcal{R}_k$ according to Fig. 3.^b Generated through the solution of Eq. (2.4) considering adjoint source such that function F becomes the power density of all regions of material 2. Read as 2.62143×10^{-16} .^c Generated through the solution of Eq. (2.4) considering adjoint source such that function F becomes the power density of all regions of material 3. Read as 2.59102×10^{-16} .

regions consisting of material 3. In both cases, the neutrons that migrate in the regions of material 3 are more important to the overall generation of power. If we analyze the macroscopic cross sections of materials 2 and 3, we notice that the fission cross sections of material 3 are higher than the fission cross sections of material 2. This means that neutrons migrating in regions composed of material 3 will induce more fission events than neutrons migrating in regions composed of material 2. Therefore, more neutrons will be released through fission

events in the regions composed of material 3 compared to regions of material 2. Some neutrons released in fission events in regions of material 3 will eventually migrate to regions composed of material 2, thus inducing new fission events. For that reason, neutrons migrating in regions composed of material 3 are also important to the generation of power in regions composed of material 2.

Based on this idea, a large number of neutrons in the first energy group (smaller cross sections) should be released in a region

Table 3

Power density generated through the solution of Eq. (2) with neutron source distribution obtained by solving the LPOP of the first numerical experiment.

Power density (MW cm ⁻¹)										Region $\mathcal{R}_k^a$
$i = 1$	$i = 2$	$i = 3$	$i = 4$	$i = 5$	$i = 6$	$i = 7$	$i = 8$	$i = 9$	$i = 10$	$i = 11$
										$j = 11$
										$j = 10$
										$j = 9$
										$j = 8$
0.24110	0.21394	0.17985	0.12062							$j = 7$
0.38998	0.33196		0.22077	0.12151						$j = 6$
0.39973	0.33581	0.26788	0.24067	0.18561	0.09808					$j = 5$
0.31948	0.22604	0.15108	0.19151	0.18304	0.13981	0.07210				$j = 4$
1.20309	0.46239	0.15007	0.09121	0.13126	0.13065	0.09850	0.04857			$j = 3$
	0.92170	0.14945	0.05823	0.05627	0.0993961		0.06380			$j = 2$
		0.08532	0.03653	0.03748	0.08627	0.09849	0.06582			$j = 1$
			0.02106	0.03107	0.08239	0.09892	0.06606			

^a The values of i and j define region $\mathcal{R}_k$. That is, $k = i + (j - 1) \times 11$.

composed of material 1, so that a considerable part of it can reach regions composed of material 3. Furthermore, in the path to reach the regions composed of material 3, some neutrons induce fission events in regions composed of material 2, which generates a value of power that is smaller than the prescribed for the regions of material 2. Thus, additional neutrons in the second energy group (higher cross sections) should also be released in spallation target areas, so that the total power generated by the regions composed of material 2 can achieve the prescribed value of power. Finally, the neutron source is located in region $\mathcal{R}_{23}$ ($i = 1$ and $j = 3$) because neutrons released in this region have to travel a shorter path to reach regions of material 3. This increases the probability of a neutron reaching regions composed of material 3. Thus, compared to other regions composed of material 1, a smaller number of neutrons need to be released in region $\mathcal{R}_{23}$ to generate the prescribed power considered for the regions of material 3.

In addition to the neutrons being inserted in region $\mathcal{R}_{23}$, the slack variables $V^+ = V^- = 1 \text{ MW cm}^{-1}$ are also part of the optimal solution. They are different from zero to ensure all constraints of the LPOP defined in Eq. (3.30) are equality constraints. To visualize this situation, we consider $Q_{k,g} = 0$ (except for region $\mathcal{R}_{23}$) in the constraints of the LPOP associated with the power generated in the system. That is,

$$\begin{aligned}
 \Phi_{23,1}^{mat 2} Q_{23,1} + \Phi_{23,2}^{mat 2} Q_{23,2} + V_1^+ &= 5; \\
 \Phi_{23,1}^{mat 2} Q_{23,1} + \Phi_{23,2}^{mat 2} Q_{23,2} - V_1^- + V_1^A &= 4; \\
 \Phi_{23,1}^{mat 3} Q_{23,1} + \Phi_{23,2}^{mat 3} Q_{23,2} + V_2^+ &= 5; \\
 \Phi_{23,1}^{mat 3} Q_{23,1} + \Phi_{23,2}^{mat 3} Q_{23,2} - V_2^- + V_2^A &= 4.
 \end{aligned} \tag{3.31}$$

Substituting $Q_{23,1}$ and $Q_{23,2}$ into Eq. (3.31), and considering the values displayed in Table 2, we have

$$\begin{aligned}
 4 + V_1^+ &= 5; \\
 4 - V_1^- + V_1^A &= 4; \\
 5 + V_2^+ &= 5; \\
 5 - V_2^- + V_2^A &= 4.
 \end{aligned} \tag{3.32}$$

As the goal is to minimize the objective function and the value considered for $\mathcal{M}$ is very large, the auxiliary variables V_1^A and V_2^A are going to be zero. Considering this, we solve the linear system presented in Eq. (3.32) obtaining $V_1^+ = V_2^- = 1 \text{ MW cm}^{-1}$ and $V_1^A = V_2^A = V_1^- = V_2^+ = 0$.

Now, to visualize if this source distribution drives the subcritical core to the prescribed power density distribution, we solve Eq. (2.2) with the same parameters of Model Problem I using the neutron source distribution generated by the solution of the LPOP. We remark that we also have used the RM-CN method to solve Eq. (2.2). The results are shown in Table 3.

If we sum the power generated in the regions composed of materials 2 and 3 we obtain, respectively, $P_{mat 2} = 4.00050 \text{ MW cm}^{-1}$ and $P_{mat 3} =$

$5.00410 \text{ MW cm}^{-1}$, which ensures that the methodology presented in Section 2 can potentially be used as the main part of step II shown in Fig. 1.

3.1.2. Second numerical experiment

In the second numerical experiment, we change one of the constraints considered in the first numerical experiment. Now, we consider the power density generated by regions of material 2 as

$$1 \text{ MW cm}^{-1} \leq P_{mat 2} \leq 2 \text{ MW cm}^{-1}. \tag{3.33}$$

Note that by changing this constraint, we do not need to solve the adjoint equation again since neither the material parameters nor the boundary conditions have changed.

With this different constraint, we solve the resulting LPOP generating the solution: $Q_{3,1} = 8.84878E + 14 \text{ neutrons/cm}^3 \text{ s}$ ($k = 3 \rightarrow i = 3$ and $j = 1$, according to Fig. 3), $V_1^- = 1 \text{ MW cm}^{-1}$, $V_2^+ = 2.09330 \text{ MW cm}^{-1}$, and $V_2^A = 1.09330 \text{ MW cm}^{-1}$. Moreover, $Q_{k,g} = 0$ for the remaining regions and energy groups, and $V_1^+ = V_2^- = V_1^A = 0$. Differently from the results generated for the first numerical experiment, an auxiliary variable V_2^A is part of the optimal solution. This indicates that the problem considered is not feasible, i.e., it is not possible to release neutrons in regions composed of material 1 and generate

$$1 \text{ MW cm}^{-1} \leq P_{mat 2} \leq 2 \text{ MW cm}^{-1} \tag{3.34a}$$

and

$$4 \text{ MW cm}^{-1} \leq P_{mat 3} \leq 5 \text{ MW cm}^{-1}. \tag{3.34b}$$

Following the first numerical experiment, the constraints associated with Eq. (3.34b) appear as

$$\sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{mat 3} + V_2^+ = 5 \tag{3.35a}$$

and

$$\sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{mat 3} - V_2^- + V_2^A = 4. \tag{3.35b}$$

By definition, we want to release the minimal quantity of neutrons in regions composed of material 1 so that Eqs. (3.34) hold. For the power density of regions composed of material 3 to be between 4 MW cm^{-1} and 5 MW cm^{-1} , a considerable number of neutrons must be released in regions of material 1 since part of these neutrons will eventually be absorbed while migrating in regions composed of material 2. However, part of the neutrons absorbed will induce fission events in regions composed of material 2, being the power density generated in this case greater than the maximum specified, i.e., $P_{mat 2} \leq 2 \text{ MW cm}^{-1}$. Therefore, the constraints of the LPOP do not represent a possible physical situation. To adequate the constraints to a possible situation: (i) either the maximum possible value for $P_{mat 2}$ should be increased,

Table 4

Power density generated through the solution of Eq. (2) with neutron source distribution obtained by solving the LPOP of the second numerical experiment.

Power density (MW cm ⁻¹)										Region $\mathcal{R}_k^a$
$i = 1$	$i = 2$	$i = 3$	$i = 4$	$i = 5$	$i = 6$	$i = 7$	$i = 8$	$i = 9$	$i = 10$	$i = 11$
										$j = 11$
										$j = 10$
										$j = 9$
										$j = 8$
0.03853	0.03838	0.03719	0.02830							$j = 7$
0.05772	0.05744		0.05738	0.04197						$j = 6$
0.04811	0.05034	0.05793	0.07607	0.08134	0.05703					$j = 5$
0.01822	0.02193	0.03283	0.07641	0.10645	0.10788	0.07059				$j = 4$
0.01257	0.02162	0.03406	0.05312	0.11129	0.13981	0.12823	0.07006			$j = 3$
	0.05108	0.08691	0.08715	0.08763	0.15555		0.10445			$j = 2$
		0.39482	0.24671	0.13095	0.19503	0.19277	0.12424			$j = 1$
			0.53594	0.18472	0.23207	0.22644	0.14000			

^a The values of i and j define the region $\mathcal{R}_k$. That is, $k = i + (j - 1) \times 11$.

maintaining the power density of regions composed of material 3 between 4 MW cm⁻¹ and 5 MW cm⁻¹; or (ii) the minimum value for $P_{mat 3}$ should be decreased, so that a smaller quantity of neutrons need to be released in regions of material 1 to reach regions of material 3, hence decreasing the power generated in regions of material 2. The LPOP aims to minimize the sum of the neutron source distribution. Thus the second option is the one inherently adopted in the solution process, and this is the reason V_2^A is part of the optimal solution. Rewriting Eq. (3.35b) as

$$\sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{mat 3} - V_2^- = 4 - V_2^A, \quad (3.36)$$

we can see that the auxiliary variable V_2^A is the one capable of decreasing the minimum value of the power density in regions of material 3, i.e., $c_{mat 3}^{min} = 4 - V_2^A$. Therefore, it must be moved to the optimal solution, even though it considerably increases the objective function.

To confirm our assertive, we solve Eq. (2.2) using the neutron source calculated, i.e., $Q_{3,1} = 8.84878E + 14$ neutrons/cm³ s and $Q_{k,g} = 0$ otherwise. Then, we calculate the power density in each fuel region, as illustrated in Table 4. By summing the power density of all regions 2 and 3, we have $P_{mat 2} = 2.00026$ MW cm⁻¹ and $P_{mat 3} = 2.90899$ MW cm⁻¹. As we can see, the solution of the LPOP satisfies the first constraint (Eq. (3.34a)) and decreases the power density in regions of material 3.

3.2. Model Problem II

In the second model problem, we consider a slight modification of Model Problem I. Now, regions that are adjacent to regions of material 1 are considered to be composed of material 3 instead of material 2, as in Model Problem I. Fig. 5 illustrates the geometry and material distribution of Model Problem II. The material parameters are the same as the ones displayed in Table 1.

3.2.1. Third numerical experiment

To construct the LPOP associated with this problem, we need to define the constraints of the LPOP. In this case, we assume that

$$4 \text{ MW cm}^{-1} \leq P_{mat 2^*} \leq 5 \text{ MW cm}^{-1} \quad (3.37a)$$

and

$$4 \text{ MW cm}^{-1} \leq P_{mat 3^*} \leq 5 \text{ MW cm}^{-1}, \quad (3.37b)$$

where $P_{mat 2^*}$ represents the power density generated by all regions composed of material 2 and regions of material 3 that are adjacent to regions of material 1, and $P_{mat 3^*}$ represents the power density of all remaining regions of material 3. We execute an analogous procedure to the one used in Model Problem I to associate the constraints displayed

in Eqs. (3.37) with the neutron source distribution. Fig. 6 shows the group node-average adjoint scalar fluxes as a function of the midpoints.

The LPOP associated with the third numerical experiment is

$$\begin{aligned} & \text{Minimize} \quad \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} + 0 \times \sum_{u=1}^2 \left[V_u^+ + V_u^- \right] + \mathcal{M} \times \sum_{u=1}^2 V_u^A \\ & \text{Subjected to:} \\ & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{mat 2^*} + V_1^+ = 5; \\ & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{mat 2^*} - V_1^- + V_1^A = 4; \\ & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{mat 3^*} + V_2^+ = 5; \\ & \sum_{k=1}^{121} \sum_{g=1}^2 Q_{k,g} \Phi_{k,g}^{mat 3^*} - V_2^- + V_2^A = 4; \\ & Q_{k,g} \geq 0 \text{ (regions of material 1);} \\ & Q_{k,g} = 0 \text{ (regions with material different than 1);} \\ & V_1^+ \geq 0; V_2^+ \geq 0; V_1^- \geq 0; V_2^- \geq 0; V_1^A \geq 0; V_2^A \geq 0; \end{aligned} \quad (3.38)$$

where we have also considered Eq. (2.24) as a constraint of the LPOP. In the LPOP stated in Eq. (3.38) $\Phi_{k,g}^{mat 2^*}$ and $\Phi_{k,g}^{mat 3^*}$ are calculated through the solution of the adjoint equation considering adjoint sources such that the functional F presented in Eq. (2.1) becomes the power density generated by all regions composed of material 2 and material 3 that are adjacent to regions of material 1, and the power density of all remaining regions of material 3 respectively. The values of $\Phi_{k,g}^{mat 2^*}$ and $\Phi_{k,g}^{mat 3^*}$ for regions of material 1 are displayed in Table 5.

Once we have the LPOP settled, we apply the Simplex method, following the procedure described in the previous section, obtaining: $Q_{23,1} = 5.27254E + 14$ neutrons/cm³ s, $Q_{23,2} = 3.57713E + 14$ neutrons/cm³ s ($k = 23 \rightarrow i = 1$ and $j = 3$, according to Fig. 3), $V_1^+ = 1$ MW cm⁻¹, and $V_2^- = 1$ MW cm⁻¹. Moreover, $Q_{k,g} = 0$ for the remaining regions and energy groups, and $V_2^+ = V_1^A = V_2^A = 0$. Comparing the results generated by the solution of Eqs. (3.30) and (3.38), we can see that the intensities of the neutron sources in the third numerical experiment are smaller than those generated in the first numerical experiment.

This can be explained by making use of the results displayed in Figs. 4 and 6. By analyzing these figures, we see that the change in the material parameters of the regions that are adjacent to regions of material 1 increases the importance of neutrons migrating in these regions and regions of material 2. Since the fission cross-sections of material 3 are higher than those of material 2, a larger number of fission events will take place in the regions adjacent to regions of material 1 (composed of material 3). Part of these neutrons will eventually migrate to the remaining regions of material 3, inducing new fission events.

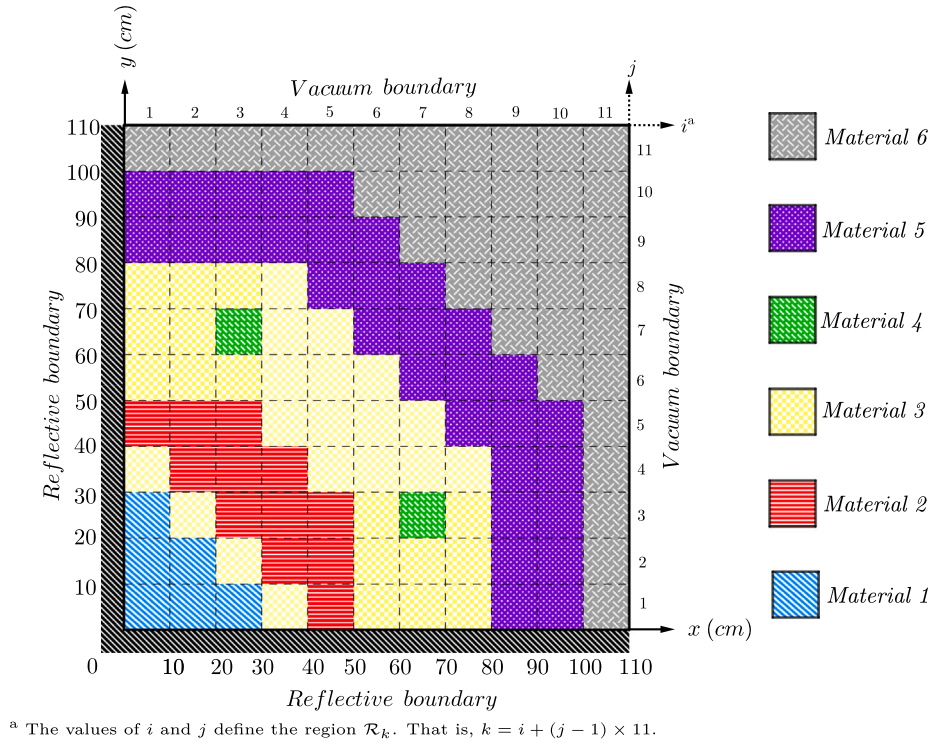


Fig. 5. Geometry and material distribution of Model Problem II.

Table 5

Values of $\Phi_{k,g}^{mat 2*}$ and $\Phi_{k,g}^{mat 3*}$ for regions of material 1 in Model Problem II.

Region	$\mathcal{R}_1$ ($i = 1$ and $j = 1$) ^a		$\mathcal{R}_2$ ($i = 2$ and $j = 1$)		$\mathcal{R}_3$ ($i = 3$ and $j = 1$)	
Energy group	$g = 1$	$g = 2$	$g = 1$	$g = 2$	$g = 1$	$g = 2$
$\mathcal{P}_{mat 2*}$	5.31431E-16 ^b	6.82166E-18	1.44126E-15	2.77338E-16	4.78052E-15	4.13588E-15
$\mathcal{P}_{mat 3*}$	6.39788E-16 ^c	4.31671E-18	1.76032E-15	1.77098E-16	6.82987E-15	3.91098E-15
Region	$\mathcal{R}_{12}$ ($i = 1$ and $j = 2$)		$\mathcal{R}_{13}$ ($i = 2$ and $j = 2$)		$\mathcal{R}_{23}$ ($i = 1$ and $j = 3$)	
Energy group	$g = 1$	$g = 2$	$g = 1$	$g = 2$	$g = 1$	$g = 2$
$\mathcal{P}_{mat 2*}$	1.44126E-15	2.77338E-16	3.57972E-15	3.36733E-15	4.78050E-15	4.13587E-15
$\mathcal{P}_{mat 3*}$	1.76030E-15	1.77096E-16	3.85724E-15	2.15154E-15	6.82975E-15	3.91091E-15

^a Values of i and j that defines region $\mathcal{R}_k$ according to Fig. 5.^b Generated through the solution of Eq. (2.4) considering adjoint source such that the function F becomes the power density of all regions of material 2 and regions of material 3 adjacent to regions of material 1. Read as 5.31431×10^{-16} .^c Generated through the solution of Eq. (2.4) considering adjoint source such that the function F becomes the power density of all remaining regions of material 3. Read as 6.39788×10^{-16} .

However, as the number of neutrons migrating from regions of material 2 to 3 will increase, the number of neutrons that need to be inserted in regions of material 1 should decrease. This increase of the neutron importance is illustrated in Table 6.

As the limits for the power density generated in the system are the same for the first and third numerical experiments, by increasing the values of $\Phi_{k,g}^{mat 2*}$ and $\Phi_{k,g}^{mat 3*}$ we need to decrease the values of $Q_{k,g}$, so that the constraints of the LPOP are satisfied.

Again, we follow the same procedure as in Model Problem I to verify the solution of the LPOP, i.e., we solve Eq. (2.2) with the parameters of Model Problem II using the neutron source distribution obtained by the solution of the LPOP given in Eq. (3.38) (see Table 7).

If we sum the power density of all regions composed of materials 2 and 3 (adjacent to regions of material 1), and sum the power density of all remaining regions of material 3, we obtain, respectively, $\mathcal{P}_{mat 2*} = 4.00060 \text{ MW cm}^{-1}$ and $\mathcal{P}_{mat 3*} = 5.00420 \text{ MW cm}^{-1}$.

By assessing Model Problem II, one can see that the offered methodology can be used to choose the core configuration that will reduce the

complexity of the particle accelerator. Thus increasing the efficiency of the system. In this case, the core configuration presented in Model Problem II shows a clear advantage when compared to the core configuration shown in Model Problem I. In fact the intensity that the neutron source distribution must have to drive the subcritical system at the prescribed power density distribution in the third numerical experiment is smaller than the one generated in the first numerical experiment.

4. Concluding remarks

Presented here is a methodology to generate optimal configurations for the neutron source distribution in subcritical systems. The optimization problem is mathematically modeled as an LPOP, where the goal is to minimize the intensity of the neutron source distribution under constraints that define the power density distribution in the subcritical system. In other words, the initial step of a supplementary computational tool that can be used in the design process of subcritical nuclear reactors. Numerical results were given in the previous section to: (i) illustrate the methodology's application; (ii) verify that the present

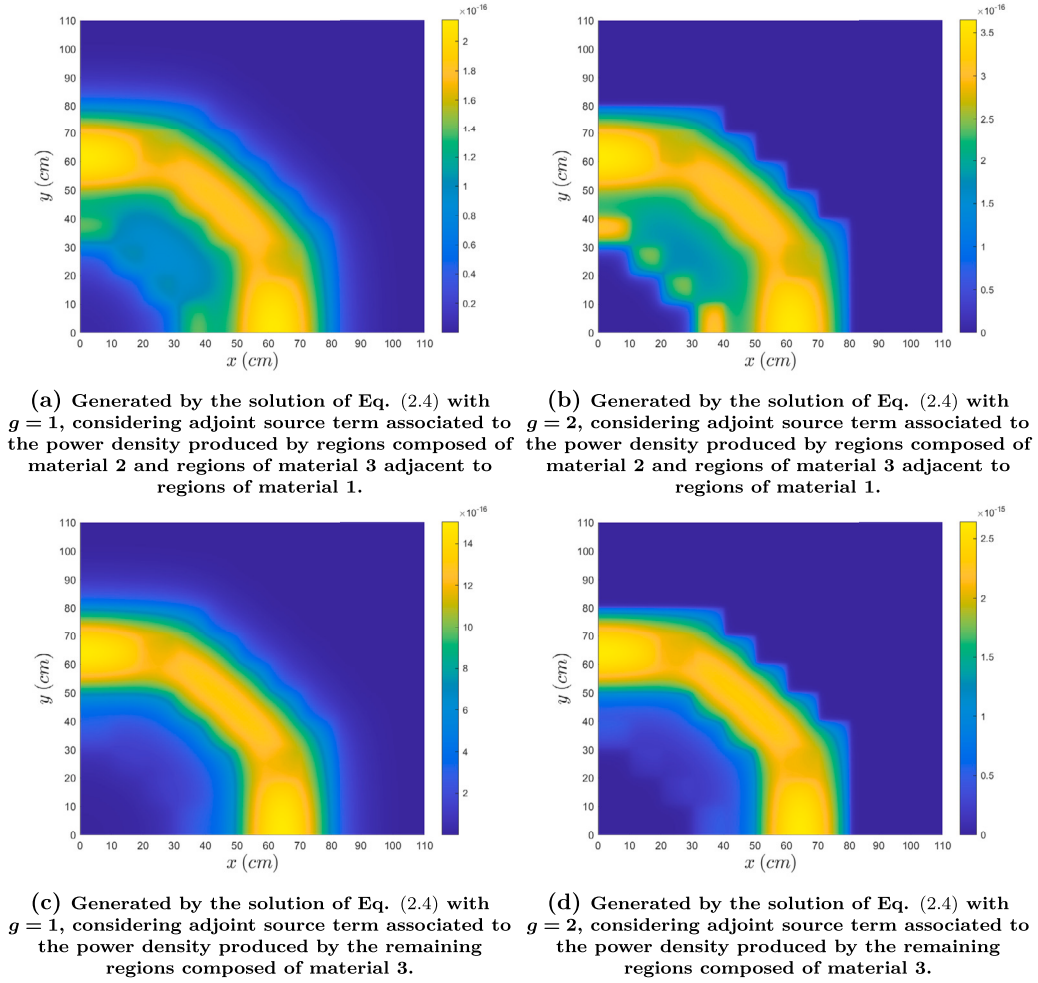


Fig. 6. Node-average adjoint scalar fluxes for the LPOP of the third numerical experiment.

Table 6

Increase of the neutron importance from Model Problem I to II.

Region	$\mathcal{R}_1$ ($i = 1$ and $j = 1$) ^a		$\mathcal{R}_2$ ($i = 2$ and $j = 1$)		$\mathcal{R}_3$ ($i = 3$ and $j = 1$)	
Energy group	$g = 1$	$g = 2$	$g = 1$	$g = 2$	$g = 1$	$g = 2$
$\frac{\phi_{i,g}^{mat 2*}}{\phi_{i,g}^{mat 2}}$	2.02725	2.01976	2.05327	1.81018	2.14501	2.04041
$\frac{\phi_{i,g}^{mat 3*}}{\phi_{i,g}^{mat 3}}$	2.46925	3.38221	2.41074	3.13727	2.35045	3.08927
Region	$\mathcal{R}_{12}$ ($i = 1$ and $j = 2$)		$\mathcal{R}_{13}$ ($i = 2$ and $j = 2$)		$\mathcal{R}_{23}$ ($i = 1$ and $j = 3$)	
Energy group	$g = 1$	$g = 2$	$g = 1$	$g = 2$	$g = 1$	$g = 2$
$\frac{\phi_{i,g}^{mat 2*}}{\phi_{i,g}^{mat 2}}$	2.05327	1.81018	2.04888	1.91217	2.14500	2.04040
$\frac{\phi_{i,g}^{mat 3*}}{\phi_{i,g}^{mat 3}}$	2.41074	3.13726	2.34293	3.05127	2.35044	3.08926

^a Values of i and j that define region $\mathcal{R}_k$ according to Figs. 3 and 5.

methodology can potentially represent step II of Fig. 1; and (iii) show the capability of this methodology in selecting a core configuration that reduces the intensity of the required neutron source distribution, hence the particle accelerator's complexity.

As an initial study, no efficiency analysis was conducted. However, the computational tool's viability will depend on the viability of the methods chosen to represent steps I to III. Therefore, an efficiency analysis of the methodology is of importance and should await future work. Nonetheless, even though an efficiency analysis needs to be performed, one can argue that the most costly part of the LPOP presented in

Eq. (2.10) resides in the constitution of the constraints associated with the power generated in the system. As currently stated, to generate the constraints of the LPOP, we need to solve one adjoint problem for each value of power that defines the prescribed power density distribution.

Different aspects may impact the efficiency concerning the generation of the constraints of the LPOP. Some examples are the characteristics of the power density distribution, the use of parallelization techniques, and the adequacy of the mathematical model used to represent the adjoint problems. The impact that the prescribed power density distribution has on the efficiency of the LPOP resides in the number of

Table 7

Power density generated through the solution of Eq. (2) with neutron source distribution obtained by solving the LPOP of the third numerical experiment.

Power generated (MW cm ⁻¹)										Region $\mathcal{R}_k^a$
$i = 1$	$i = 2$	$i = 3$	$i = 4$	$i = 5$	$i = 6$	$i = 7$	$i = 8$	$i = 9$	$i = 10$	$i = 11$
										$j = 11$
										$j = 10$
										$j = 9$
0.23939	0.21185	0.17749	0.11893							$j = 8$
0.38789	0.32870		0.21752	0.11973						$j = 7$
0.39987	0.33172	0.26288	0.23641	0.18289	0.09711					$j = 6$
0.33016	0.21921	0.14544	0.18678	0.18061	0.13931	0.07255				$j = 5$
1.25083	0.39039	0.13783	0.08840	0.13068	0.13184	0.10055	0.04991			$j = 4$
	0.88032	0.14652	0.05994	0.05799	0.10264		0.06615			$j = 3$
		0.12057	0.04540	0.04217	0.09203	0.10366	0.06905			$j = 2$
			0.04624	0.03916	0.09026	0.10575	0.070061			$j = 1$

^a The values of i and j define the region $\mathcal{R}_k$. That is, $k = i + (j - 1) \times 11$.

adjoint problems that need to be solved. The more restrictions on the power generated by the system are made, the more adjoint problems need to be solved to create the necessary constraints. One idea that can be explored in the future to approach this situation is the generation of auxiliary equations to be used in conjunction with the importance function associated with the total power density generated by the system. If we consider the adjoint source term such that the functional given in Eq. (2.1) is the power density generated by the whole system, the solution of Eq. (2.4) becomes the importance function associated with the total power density generated by the system. The adjoint source term is, in this case, composed of the sum of the adjoint source terms associated with the power density generated by each prescribed value of power. Therefore, as Eq. (2.4) is linear and the boundary conditions applied to Eq. (2.4) are homogeneous, the importance function associated with the total power density is equal to the sum of the importance functions associated with the prescribed value of power. Thus, instead of solving Eq. (2.4) for each prescribed value of power, one could potentially solve Eq. (2.4) only one time, for the total power density generated by the system and explore auxiliary equations that would allow separating from this importance function the contribution of the importance functions associated with each prescribed value of power.

In conjunction with the decrease in the number of constraints of the LPOP, the use of parallelization techniques is of particular interest. To generate the constraints of the LPOP, one has to solve one adjoint problem for each value of power defined in the prescribed power density distribution. Nonetheless, these adjoint problems are not coupled, and the only difference between them resides in the constitution of the adjoint source. Since they are not coupled, the solution process adopted to solve one specific adjoint problem is not dependent on the solution of another adjoint problem. Therefore, the solution process for all constraints of the LPOP can be executed in parallel. Thus, the use of parallelization techniques has the potential to improve the methodology's efficiency considerably.

Another way that may potentially increase the efficiency concerning the constraints of the LPOP is the exploration of low-order models to represent the adjoint problems. Analyzing Eq. (2.10), we notice that to define the constraints of the LPOP, we need to calculate Eq. (2.9b) for all regions and energy groups associated with each prescribed value of power density. That indicates that we do not necessarily need to know $\Psi^\dagger$ (adjoint angular flux) accurately, but instead, we need to calculate $\Phi^\dagger$ (adjoint scalar flux) accurately. Since the accurate calculation of $\Psi^\dagger$ is not directly needed, the exploration of low order models that can accurately calculate $\Phi^\dagger$ is of interest.

In conjunction with the topics of future work as discussed in this section, we intend to continue this work by developing/applying methods to represent steps I and III of Fig. 1. Regarding step I, the use of search tools/methods that can quickly move toward configurations meeting

the desired requirements is particularly appealing, as it can significantly alleviate the computational burden of the simulation. Moreover, concerning step III, as depicted in Fig. 1, a thorough evaluation of core configuration and the characteristics of the particle accelerator required to reproduce the estimated source distribution must be conducted. At this juncture, we highlight that opting to model the source distribution problem as a linear programming optimization problem also enables the consideration of characteristics beyond just power distribution. Essential constraints such as material temperature can be incorporated into the linear programming optimization problem, shaping the source distribution accordingly.

CRediT authorship contribution statement

Leonardo R.C. Moraes: Writing – original draft, Software, Project administration, Methodology, Investigation, Formal analysis, Conceptualization. **Ricardo C. Barros:** Writing – original draft, Supervision, Methodology, Conceptualization. **Richard Vasques:** Writing – original draft, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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