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Multi-material topology optimization of nuclear devices – principle and application

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Abstract. In this paper, we present a multi-material topology optimization procedure, capable of generating the best possible structure of a nuclear device from a list of design objectives and constraints. We propose an example of applying this new tool to calculate the structure of a neutron moderator, which will be used to generate an epithermal field for metrological applications at a facility of the Institute for Radiation Protection and Nuclear Safety (IRSN, France).

1 Introduction

Suppose a team wishes to design a nuclear device, e.g. a radiative shield minimizing the photon and neutron doses likely to be received by an operator, while being as light as possible, or a moderator that generates a neutron field whose intensity must be as high as possible, while having at the same time an energy spectrum as close as possible to a reference spectrum.

To design such devices, common in our fields, the team in charge of their development must first formulate with clarity the objective it wishes to achieve, which will be noted $O\varphi$. In our fields, O is a functional of the fluxes φ of particles which propagate in the device to be optimized, solutions of the Boltzmann equation, e.g. the value of a flux or a dose in this or that cell, to be min-maxed. The team must also identify the design constraints to be respected, which will be noted as $\mathbf{C}$. These constraints can for example be weight or maximum size constraints, spectral constraints to be respected, etc.

Once correctly identified, the design problem to be solved is then formulated as follows:

$$\begin{aligned} &\min_{\mathbf{x}}\max O\varphi \\ &\text{subject to} \quad C_1 \leq 0, \ldots, C_n \leq 0 \end{aligned} \qquad (1)$$

where $\mathbf{x}$ are the parameters that describe the structure of the device to be designed, e.g. the dimensions (radii, thicknesses, etc.) and materials of its components, which we wish to optimize.

Although it is simple to write, such a constrained optimization problem is nevertheless very complicated to solve in our fields. Indeed, the fluxes of particles that propagate in the

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device, and on which the objective O (and certain constraints **C**) depend, are non-linear, complex, non-analytical functions of the structural parameters **x**. For realistic applications, these fluxes can only be calculated numerically, using intensive calculation codes, mainly Monte-Carlo (MC) [1]. The classic techniques for solving problem (1), e.g. using gradient methods, are inapplicable here.

As there is no analytical link between the parameters **x** and O, one must proceed tentatively. The team in charge of development will have to (1) choose parameters **x** likely to impact the performance of the device, (2) vary each of these parameters in small steps, and in this way generate a large number of candidate structures; (3) for each structure thus generated, carry out a MC simulation of the performance of the device, to finally (4) determine among all the simulated configurations the best structure of the device.

This solution method is called parametric optimization, and it is universal in our fields – for lack of a better mean. This method, however, has two major limitations: (1) Suppose that the team in charge of the design has identified 5 parameters of interest to describe a candidate device [†], and varies these 5 parameters by taking 10 values each. The number of configurations to simulate is therefore 5^{10} or $\sim 10^7$. However, for a classic nuclear device, even a small one, the MC calculation time of particle fluxes can reach several hours per configuration on a modern server. Assuming that the team has access to a powerful computing farm, which allows this calculation time to be reduced to, say, 5 minutes, and to run 100 simulations in parallel, it will still take ~1 year to find the solution to this (tiny) parametric optimization problem. Therefore, a humanly compatible calculation time limits the number of usable parameters to half a dozen in practice, which only allows elementary geometries to be described, cf. section 3.2, even simplistic. (ii) The very choice of these parameters **x** is an unreliable prior. This choice is guided by intuition, literature, and feedback, which does not necessarily give a precise idea of the solution to the problem (1), or can even be counterproductive. If we do not know the solution to problem (1), we cannot in fact know in advance what the optimal structure is, therefore what are the parameters **x** to use. For these multiple reasons, (i) and (ii), a parametric optimization only allows exploring a tiny portion of the space of possible structures, and not necessarily in the right place. Except in cases specifically designed for, a parametric optimization has no chance of reaching the true optimum $\mathbf{x}_{opt}$ of problem (1).

To be able to solve the problem (1), and find the best possible structure of a nuclear device, we must find a better way to explore, exhaustively and without prejudice, the infinite space of possible structures, by increasing by several orders of quantities the number of parameters **x**, and making them not dependent on a choice. The description and application of this means is the subject of this paper.

In a series of articles, [2-4], we reported the development of a technique, called topological optimization (TopOpt), capable of solving a problem of type (1), in the particular case where $M \leq 2$ (number of materials) and $n = 1$ (number of constraints). This procedure, coupled with the Monte-Carlo MCNP transport code, allowed us to calculate, for example, the structure of a weight-constrained neutron concentrator [2], a distribution of low enriched uranium making it possible to reach criticality at minimum weight [3], the structure of a moderator taking 14 MeV neutrons as input and producing at output a typical spectrum of a fast reactor [3], or more recently the shape of heavy water moderators used in a neutron radiotherapy for maximizing the contrast between the dose deposited in a target tumor and those deposited in healthy tissues [4]. These topologically optimized devices presented elaborate shapes, inaccessible in their details to human intuition and parametric design techniques, and performance levels 30-40% higher than the best parametric devices. To solve

[†] 5 parameters to describe a structure is very few. Assuming that each component can only be defined by its radius, thickness and material, 5 parameters are barely enough to describe two components.

problem (1) in the general case, we still had to find a way to extend the capabilities of this TopOpt procedure to an arbitrarily large number of materials and constraints. This has now been done since 2023.

In this article, we will describe in section 2 the principle of such a multi-material multi-constraint topology optimization procedure. We will then propose in section 3 an example of practical application, the design of an epithermal moderator for a facility of the Institute for Radiation Protection and Nuclear Safety (IRSN, France).

2 Principle of a multi-material multi-constraint topology optimization algorithm

To solve a problem of type (1), let's start by discretizing it. Let us subdivide the volume of the device into a large number, $N >> 1$, of small volumes, $V_{i=1..N}$, called voxels, each of which can contain M different materials, in variable proportions but in fixed number. The first advantage of such discretization is to systematize the parameters $\mathbf{x}$, which are now the volume fractions $\chi_{i=1..N,j=1..M}$ of the materials in the voxels V_i, and no longer arbitrary and simplistic macroscopic parameters like radii or thicknesses.

The second advantage of this reformulation is that it becomes possible to solve problem (1) using the Karush-Kuhn-Tucker (KKT) conditions [5, 6]. These conditions imply that the optimal structure, $\boldsymbol{\chi}_{opt}$, of the nuclear device sought is the solution of a system of equations, which is written:

$$\frac{\partial L}{\partial \chi_{ij}} = 0, \forall i, j, \quad L = O\varphi + \sum_{k=1}^{n} \lambda_k C_k \quad (2)$$
$$\min\left(\lambda_k, \left|C_k\right|\right) = 0, \forall k$$

In (2), L is the Lagrangian of problem (1), and λ_k is the Lagrange multiplier associated with the constraint C_k.

As there is no analytical link between L and the fractions χ_{ij}, system (2) must be solved with an iterative procedure. At iteration 0, we start from an arbitrary distribution of materials, $\boldsymbol{\chi}_0$, in the voxels of the structure. This initial structure is often taken uniform. We compute the $N\times M$ derivatives of the Lagrangian, $\partial L/\partial \chi_{ij}$, with the MCNP6 code, using its sensitivity calculation module [1-3], then modify accordingly the volume fractions χ_{ij} in small steps, 1% max. e.g., simultaneously in the N voxels of the structure, in the right direction [‡]. We iterate until convergence towards the $\boldsymbol{\chi}_{opt}$ solution of problem (1)-(2).

Other mathematical or computer tricks are necessary to further reduce the calculation time and make it humanly compatible with practical applications, e.g. the use of adaptive steps or the automated use of convergence acceleration tools made available in MCNP6 [1]. As an example, the TopOpt resolution of the problem given in section 3 requires ~10 hours of calculation/iteration/configuration on a powerful modern server (an AMD EPYC 9654 96-Core Processor), knowing that around a hundred iterations are necessary to converge. Solving a problem of type (1) therefore remains, despite the aforementioned improvements, intensive in calculation time.

[‡] This step represents a challenge in itself. As the sum of the volume fractions is 1 by definition in each voxel, there are therefore at each iteration $(M\text{-}1)^N$ possible modifications of the structure of the device to be tested. For the example given in section 3.3, for $N = 85$ and $M = 4$ e.g., there are therefore ~10^{40} modifications to test at each iteration, theoretically.

Once the optimal volume fractions of the materials are obtained in each voxel, there remains one last practical problem to solve. The volume fractions χ_{opt} are real numbers, which can take any possible value between 0 and 100%, continuously, in each voxel. To conformally manufacture such a structure, it would be necessary, for example, to prepare sandwiches of multi-material plates, of variable compositions and thicknesses, in each voxel, in order to reproduce this continuum. For projects where budget is not a limiting factor, such custom manufacturing is not infeasible. For a small project, on the other hand, the associated financial cost can be a problem. This will be particularly the case for the example presented in section 3. For such small project, we must find a way to simplify the χ_{opt} design without losing too much efficiency. To do this, we have developed a fairly simple procedure for filtering volume fractions. In each voxel where the volume fractions of the materials are not sufficiently close to 0% or 100%, i.e. in areas where a mix of materials is really necessary, the voxel in question is subdivided into subvoxels, each containing a single material. The choices of materials per subvoxel and their dimensions are then subject to a second optimization. This procedure, SIMP, will be used in section 3.

3 Example of application of the multi-material multi-constraint TopOpt procedure

In a recent communication, [7], we presented a first application of the multi-material topology optimization procedure described in section 2. This procedure was used to generate the optimal structure of a key component of a BNCT unit (Boron Neutron Capture Therapy) [(§)], called a Beam Shaping Assembly (BSA), which serves as its name indicates to shape the neutron field, in space and spectrum, sent to the patient. The structure of the BSA generated by TopOpt makes it possible to achieve treatment depths 30% greater than any other design obtained to date, illustrating the effectiveness of the method [7].

In this article, we will propose another example of practical application of this method, for the design of an epithermal neutron source for metrological applications. The interest of this example is its large number of design constraints, otherwise difficult to respect. We will note again section 3.3 that the performance of the moderator generated by TopOpt exceeds by 30-40% those obtained with a parametric optimization, although methodical.

3.1 Description and formalization of the problem to be solved

The T400 accelerator (IRSN, Cadarache, France) sends deuterons of up to 400 keV on a TiD target, to generate neutrons of ~3 MeV [8]. For its metrology studies, IRSN's Microirradiation, Neutron Metrology and Dosimetry Laboratory (LMDN) wishes to couple this accelerator to a moderator, in order to slow down the 3 MeV source neutrons generated down to the 0.5 eV – 10 keV range, and thus obtain a pure and intense epithermal neutron field. The design constraints of this future moderator are, however, complex:

Design objective. The dose rate generated at the exit of the moderator on a thin cylindrical dosimeter, 10 cm in diameter, positioned 50 cm from the exit face of the moderator on the beam axis, must be as intense as possible.

§ BNCT is a radiotherapy of interest for the treatment of diffuse and/or radioresistant cancers, during which a patient is exposed to a neutron field. Before treatment, patients absorb a Boron-10 vector, which binds preferentially to tumor cells. Neutrons are captured on this Boron-10, causing the emission of alpha and lithium nuclei with high linear energy transfer in cancerous tissues, which destroys them.

Purity constraint. This dose rate should be mainly epithermal. Its thermal component (E < 0.5 eV) must be less than ~3% and its fast component (E > 10 keV) must remain reasonable, ~10-15% max.

Dimensional constraints. Due to structural limitations (size of the platform which will support the moderator, maximum capacity of the overhead crane, etc.), the moderator must not weigh more than 3.5 t, and must not exceed 70 cm in radius and 130 cm in length.

Budget constraint. The budget available to build this moderator is limited. Consequently, the use of rare, expensive and/or difficult to source materials is excluded.

The design problem to be solved can thus be reformulated as follows:

$$\begin{aligned} &\max_{\mathbf{x}} D_{tot} \\ &\text{subject to} \quad D_{th}/D_{tot} \leq\sim 3\% \quad \text{(C1)} \quad (3) \\ &\qquad\qquad\quad D_{fast}/D_{tot} \leq C_{\max} \quad \text{(C2)} \\ &\qquad\qquad\quad P \leq P_{\max} \quad \text{(C3)} \end{aligned}$$

In (3), (C1)-(C3) are the aforementioned design constraints; D_{tot} is the neutron dose deposited on the dosimeter in 6 hours of operation of the T400 at 8 mA; D_{th} and D_{fast} are the thermal (E < 0.5 eV) and fast (E > 10 keV) components of this dose; C_{max} is the maximum admissible fast neutron contamination of the neutron field. For this study, D_{th}, D_{fast} and D_{tot} were calculated with the Monte-Carlo code MCNP6 [1] using a flux-dose function provided by the IRSN [9]. The energy and angle distribution of the d-d source neutrons used in the MCNP simulations was calculated using the TARGET code [9, 10]. P is the weight of the moderator structure and P_{max} the maximum admissible weight, here 3.5 tons.

3.2 Resolution by parametric optimization

Problem (3) is a complex optimization problem, the solution of which is difficult to intuit. Firstly, we tried to solve it tentatively, using parametric optimization procedures (ParamOpt). This approach is presented in this section, 3.2.

To solve problem (3), we must start by identifying materials likely to play an important role in the structure of the moderator. For this study, the materials selected were: (1) aluminum (2.7 g/cm^3), (2) PTFE (CF_2, 2.2 g/cm^3), (3) natural titanium (4.506 g/cm^3) and (4) natural lead (11.34 g/cm^3). The choice of this short-list is based in part on abundant existing literature, on the one hand, and on the other hand the result of numerous ParamOpt and TopOpt tests previously carried out with other materials. Compact epithermal moderators, similar to the one we wish to design for the T400, are key components of BNCT installations [11]. Their design has therefore already been the subject of a large number of published studies [11-18, etc.]. Nowadays, these designs almost all use fluorinated ceramics, the most used of which are AlF_3, MgF_2 and TiF_3 [11-17]. Some studies sometimes use custom-made materials, by sintering of AlF_3 and LiF powders, e.g. Fluental™ [19]. These dense fluorinated materials have the advantage of having low capture cross-sections and well-placed inelastic diffusion regimes to slow down fast neutrons towards the epithermal range in a compact volume. However, they are too expensive for the limited budget of the project (see *budget constraint* section 3.1). For the T400, these materials will therefore be replaced by an Al+PTFE mixture [18]. PTFE (Teflon™) is a fluorinated material that is slightly less efficient than ceramics, but much cheaper, and is therefore also used in BNCT [13-18]. To this

Al+PTFE mixture, we added titanium, cf. TiF_3 above, which serves as a filter for thermal and fast neutrons [17, 20], as well as lead, often used as a reflector and radiological protection in BNCT [13-18]. Finally, we added a natural Cadmium cover, of fixed thickness 0.5 mm, on the output face of the moderator, to more easily check the constraint (C1) of problem (3).

To solve (3) by ParamOpt, it is then necessary to intuit parameters **x**, in limited number to keep the calculation time admissible, (therefore) judiciously chosen to play a role in the structure of the moderator. Again drawing inspiration from the BNCT literature [11-18, etc.], the thus parameterized structure of the T400 ParamOpt moderator is presented in Fig. 1 (the finger glove of the T400, mainly made of aluminum, is in red). The ParamOpt moderator is assumed to be axially symmetrical, of truncated conical shape, with a moderation body in homogeneous Al+PTFE, a Pb reflector of thickness e_{Pb} and an exit window in Ti of thickness e_{Ti}, itself covered with a 0.5 mm sheet of Cd. The volume fraction of Al in the moderation body is denoted χ_{Al}. The total length of the moderator is H+L, where H is the length of the front part of the moderator, counted from the exit face of the T400, and L is the thickness of the rear part of the moderator. L is fixed, equal to 17 cm, because imposed by the shape of the T400 finger glove. Finally, the parameters R_{min} and R_{max} are the min. and max. radii of the moderator, with R_{max} set at 70 cm (see *dimensional constraints* section 3.1). Taking $R_{min} \leq R_{max}$ makes it possible to increase the number of configurations which verify the weight constraint (C3).

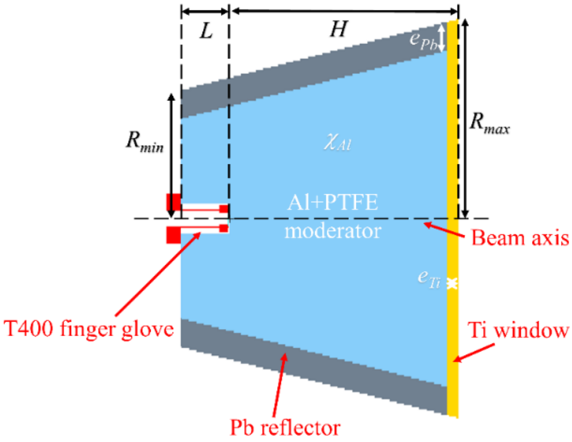

Fig. 1. Structure and parameters of the parametric moderator tested.

For this study, we varied: (1) H between 66 cm and 114 cm in steps of 6 cm. The max. boundary on H is imposed by the maximum total length H+L of the moderator, which must not exceed 130 cm (see *dimensional constraints* section 3.1); (2) R_{min} between 30 cm and 70 cm in steps of 5 cm; (3) χ_{Al} between 5% and 95% in steps of 5%; (4) e_{Pb} between 0 and 10 cm in steps of 5 cm; (5) e_{Ti} between 0 and 5 cm in steps of 1 cm. In the end, there are 27702 possible configurations, including 7543 which verify the weight constraint (C3) and must be simulated. Despite the apparent simplicity of the design chosen in Fig. 1, exploring these 7543 configurations to solve the parametric optimization problem required 4 weeks of calculation on 288 CPUs, using in addition a means of convergence acceleration (**).

** The large distance, 50 cm, between the exit face and the dosimeter requires taking a high number of source neutrons in the MCNP simulations to limit the stat. fluctuations on the doses to an acceptable level.

In table 1, we give the performances of the best parametric moderators obtained as a function of C_{max}, the maximum fast neutron contamination of the field, varied between 10% and 17% (see *purity constraint* section 3.1). We give in this table: (i) the relative thermal, epithermal, and fast components of the dose deposited on the dosimeter, D_{th}/D_{tot}, D_{ep}/D_{tot} and D_{fast}/D_{tot}; (ii) the total dose D_{tot} deposited on the dosimeter in 6 hours of operation of the T400 at 8 mA; (iii) and the weight P of the structure. We observe in Table 1 that there exists a continuum of structures satisfying the constraints (C1)-(C3). The choice of moderator will therefore have to be the subject of a compromise, essentially between the desired neutron field intensity D_{tot} and the contamination level C_{max} deemed acceptable.

Table 1. Performances and parameters of the best ParamOpt moderators, as a function of C_{max}.

C_{max} (%)	H (cm)	R_{min} (cm)	χ_{Al} (%)	e_{Ti} (cm)	e_{Pb} (cm)	D_{th}/D_{tot} (%)	D_{ep}/D_{tot} (%)	D_{fast}/D_{tot} (%)	D_{tot} (mSv)	P (t)
10	102	50	55	1	0	2.2	88.6	9.3	3.76	3.39
11	102	50	60	1	0	1.7	87.7	10.6	4.42	3.43
12	96	55	50	1	0	2.4	85.8	11.8	4.69	3.44
13	96	55	55	1	0	1.9	85.2	12.9	5.53	3.48
14	96	55	55	1	0	1.9	85.2	12.9	5.53	3.48
15	96	55	55	0	0	2.1	83.7	14.2	5.77	3.45
16	96	50	60	1	0	1.4	83.1	15.5	6.16	3.25
17	90	55	50	1	0	2.0	81.0	17.0	6.79	3.26

3.3 Resolution by topology optimization

Section 3.2, we showed that there are structures satisfying the constraints (C1)-(C3) of the problem (3). Some of these structures are promising, associated with high dose rates and reasonably fast contamination. However, can we do better? Are there even more efficient moderator structures?

Answering this question was one of the main objectives of the CNRS-IRSN CHEMINS project, cf. acknowledgments, which we solved using the topology optimization procedure presented above. To do this, as indicated in section 2, we discretized the volume of the moderator, here a cylinder of length $H+L$ and radius 70 cm, in N voxels, with $N = 80$ for $H = 78$ cm and $N = 85$ for $H = 84$ cm. These voxels are cylindrical rings of variable thicknesses and radii, shown in Fig. 2. Regarding the materials, we have kept part of the short-list used in section 3.2: Al, PTFE, and Ti [††]. We removed Pb from this list, also eliminated from the best parametric designs given in Table 1. On the other hand, we added to the list a seemingly anecdotal material, air. The addition of air in TopOpt calculations is crucial, as our previous studies have shown [2-4, 7]. Indeed, it makes it possible to generate voids in the structure of the moderator, necessary to control its weight when the latter approaches the P_{max} limit (here 3.5 t).

[††] In the first TopOpt calculations carried out to solve (3), we added many additional materials to this shortlist, in particular C, Cu, D_2O, Fe, Ni, PE, etc. However, over the course of iterations, these additional materials were gradually eliminated from the designs. As the TopOpt calculation time increases rapidly with M, we removed these materials from the list to save our computing resources.

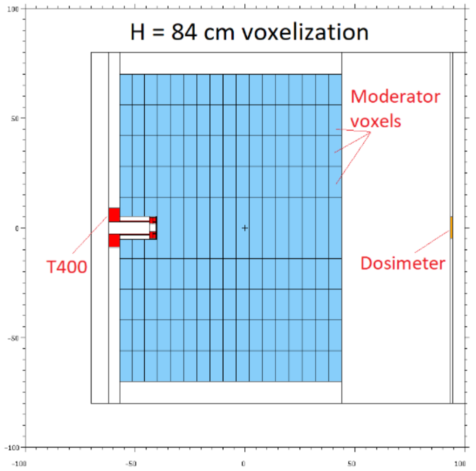

Fig. 2. Voxelization of the moderator for H = 84 cm. The T400 finger glove is in red, the voxelized volume of the moderator in blue and the target dosimeter in yellow.

The structures of two TopOpt + SIMP calculations are presented in Fig. 3 for H = 84 cm and C_{max} = 11% or 13%. These figures are sections passing through the axis of the beam. We observe that the TopOpt + SIMP procedure generates structures that combine a rear and radial reflector in PTFE (in blue) with an internal moderator consisting of an axial core in PTFE and an annular structure ("ring") composed mainly of aluminum (in red). In certain configurations, e.g. H84_C11 shown Fig. 3, this ring contains mixed Al+PTFE zones made up of plates alternating these two materials. The generated moderators all end with a titanium window (in yellow) with a radius of 70 cm and variable thickness (covered with a 0.5 mm thick Cadmium sheet). Finally, we observe that the TopOpt algorithm removes part of the rear PTFE reflector, replacing its most external cells - the least important - with air, in order to check the weight constraint without impacting performance.

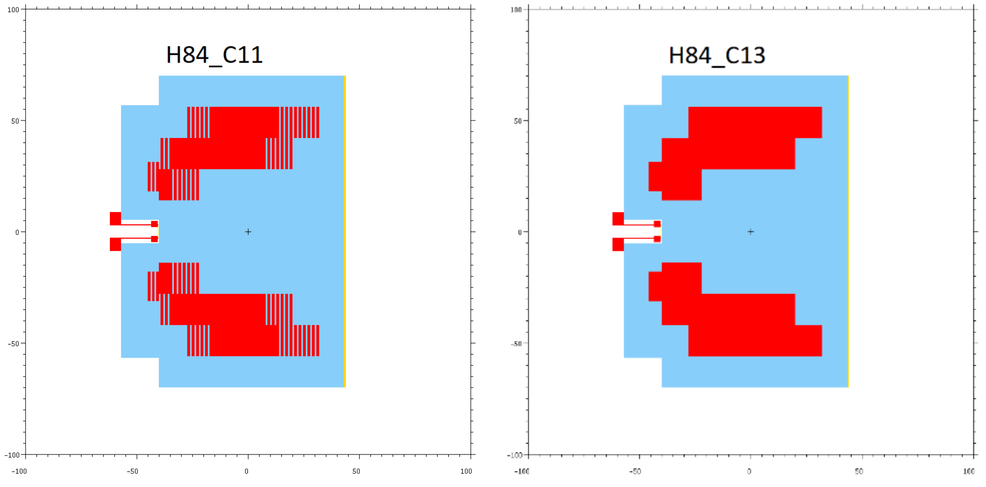

Fig 3. Examples of TopOpt + SIMP moderator structures, obtained for H = 84 cm and C_{max} = 11% (left, H84_C11) or 13% (right, H84_C13). Materials: air (white), Al (red), PTFE (blue), Ti (yellow).

The performances of the TopOpt structures, calculated for H = 78 or 84 cm, are given in Table 2 as a function of C_{max} (no TopOpt solution found for C_{max} = 10% with H = 78 and 84 cm). These moderators are named Hx_Cy, with x = H (cm) and y = 100.C_{max}. We observe in Table 2 that, at equal C_{max}, the TopOpt structures generate dose rates 30-40% higher than those generated by the best parametric moderators, cf. right column. TopOpt moderators are also more compact than their parametric counterparts, thanks to better use of available mass.

Table 2. Performance of TopOpt moderators as a function of C_{max}. We give in the right column the ratio D_{tot}(TopOpt) / D_{tot}(ParamOpt, see Table 1) at equal C_{max}.

C_{max} (%)	TopOpt Config.	D_{th}/D_{tot} (%)	D_{ep}/D_{tot} (%)	D_{fast}/D_{tot} (%)	D_{tot} (mSv)	P (t)	$D_{tot}(TopOpt)$ / $D_{tot}(ParOpt)$
11	H84_C11	3.0	86.0	11.0	5.62	3.45	1.27
12	H84_C12	2.8	85.7	11.5	6.66	3.45	1.42
13	H84_C13	2.4	85.1	12.4	7.92	3.47	1.43
14	= H84_C13	2.4	85.1	12.4	7.92	3.47	1.43
15	H84_C15	2.5	83.4	14.1	8.10	3.45	1.40
16	= H84_C15	2.5	83.4	14.1	8.10	3.45	1.31
17	H78_C17	2.2	81.3	16.5	8.72	3.27	1.28
	NO_AL	5.1	73.9	21.0	1.66		

The aluminum rings highlighted in red in Fig. 3 are a key feature introduced by the TopOpt algorithm in this application. Despite what may be implied by Fig. 3, these rings have substantial volumes and weights, for example approximately 1.3 tons for H84_C13. They are crucial to the design, and removing them significantly reduces performance. For example, in Table 2 we give the performance of design NO_AL, which involves replacing the aluminum ring from design H84_C13 with PTFE. This change resulted in a significant decrease, by a factor of approximately 5, in the field intensity, as well as an increase in thermal and fast neutron contamination. The TopOpt structures have been submitted to IRSN. After discussions, the design H84_C13 was chosen as it presents an optimal compromise between neutron field intensity, its contamination level, and the ease of manufacturing the structure. This design does not include mixed Al+PTFE zones. The geometry of this design has been forwarded to the IRSN's Microirradiation, Neutron Metrology and Dosimetry Laboratory (LMDN), which will oversee the construction process.

4 Conclusion

In this article, we present the development of a multi-material topology optimization algorithm capable of creating the best structure for a nuclear device. We applied this new tool to design an epithermal neutron moderator for metrological use, which will be deployed at the T400 facility of the Institute for Radiation Protection and Nuclear Safety (IRSN) in France. The chosen TopOpt moderator produces a dose rate 40% higher than that of the best equivalent parametric design, while also being more compact. When constructed, this moderator will be the first nuclear device designed using topology optimization, paving the way for a new approach to design in our fields.

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