NordDesign 2022
August 16-19, 2022
Kgs. Lyngby, Denmark

Material selection for extreme thermo-mechanical loads using design space projection: A concept study for an ultra-high power X-Ray source

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Abstract

Material selection is one of the key steps in the concept design phase. It may be challenging due to circular dependencies. An optimal choice of material depends on the yet-to-be-determined geometry and vice versa. Commonly used material selection methods like Ashby's chart (M.F.Ashby 1992) may not be applicable since it considers only one requirement at a time. Using the properties of materials as design variables and solving it as an optimization problem may lead to solutions that are practically infeasible materials. This paper proposes a novel method to select the material and size for a design problem using design space projection. The method involves formulating a mathematical model to evaluate the quantities of interest as a function of materials properties and key geometrical parameters. The quantities of interest are used to determine whether the thermal and mechanical requirements are satisfied. They are used in the method to create projected design spaces with good designs and are used as to tool to evaluate whether a given material and corresponding size would satisfy the requirements. The method is applied to the thermo-structural problem of target wheel design for an ultra-high power x-ray source with multiple requirements. The results indicate that the existing design configuration and materials of common x-ray tube targets could be potentially used for an ultra-high-power specification of 1.5 MW, with only the size and angular speed being scaled up. The paper also presents results from the application of the method to specific common materials to arrive at the smallest possible sizing of the target wheel. The results produced using the method indicate the theoretical feasibility of an x-ray target wheel design with MW scale power specifications and common materials, for novel applications like microbeam cancer therapy.

Keywords: design space projection, material selection, circular dependency, radiation therapy

1 Introduction

1.1 Motivation

Microbeam X-ray therapy is an emerging technique with enormous potential for cancer treatment, exhibiting less toxicity towards healthy tissues while being effective against cancer tissues (Slatkin DN et al. 1992). The source of microbeam X-rays, characterized by a high peak to valley dose ratio, has been only the synchrotrons so far. One of the key steps toward making the therapy mainstream is the development of compact sources of microbeam x-rays and several concepts have been attempted by researchers (Stefan Bartzsch et al. 2020). One of the concepts is described in further sections.

1.2 Material selection

Target wheel design for X-Ray tube design involves several constraints to ensure mechanical and thermal integrity and material selection is a key step in the concept design phase. While methods like Ashby's chart focus on single requirements like stiffness or stress, a complex thermo-mechanical loading on an x-ray target wheel needs multiple requirements on maximum temperature and stresses. The material properties that affect these requirements include thermal and mechanical properties like density, specific heat, and thermal conductivity. The target body material selection will be taken up in this work and the focal track is assumed to be tungsten. The requirements and the corresponding quantities of interest for the target design problem and the method of selecting material are explained in further sections.

1.3 Line focus X-Ray tubes

Line focus X-Ray tubes use the same concept as conventional X-Rays tubes, where an electron beam is made to hit a rotating target made of heavy metal and release X-Ray beams in the process. The modifications proposed include a high surface speed of the rotating target and a very thin width of the focal spot where the electron beam gets focussed to get high aspect ratio microbeams (Stefan Bartzsch and Uwe Oelfke 2017). This higher surface speed enables the target to achieve the power levels required for microbeam X-Ray therapy, while encountering lesser temperature rise, by transitioning into the heat capacity limit of the target material.

1.4 Proposed specification of the X-Ray tube

For a line-focus X-Ray tube to work for clinical applications, the concepts for the components of the electron source and high voltage supply have been developed by researchers for a power level of 1.5 MW hitting the target body as the pulse of several seconds (Johanna Winter et al. 2020). While the work assumed that the target body is working under the heat capacity limit, the details of the material and sizing of the target have not been arrived at in detail. Conventional X-Ray tubes, predominantly used in computational tomography, operate in the power range of a few hundred kilowatts (SIEMENS Healthineers AG 2020). The challenge of scaling up the target body for this order of magnitude higher power is taken up in this work. A schematic of an x-ray source is shown in figure 1.

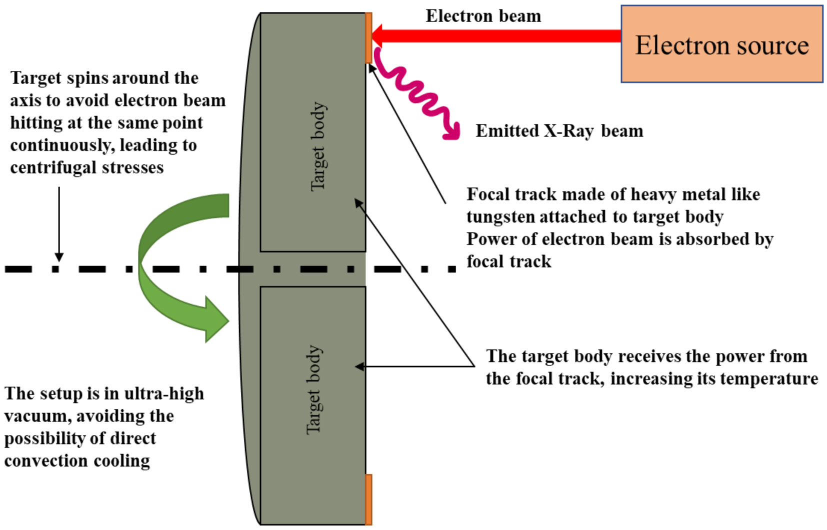

Figure 1: Cross-section of an X-Ray target wheel with electron beam source and rotation axis

2 Method

2.1 Design space projections

Solution space engineering, as laid out in Zimmermann et al. (2017), is a method that enables, the translation of system-level requirements to the requirements of the component level or design variables. The process considers a design as a set of design variable inputs and evaluates each design based on a set of quantities of interest and evaluation criteria. The solutions spaces are generated from the design spaces, by choosing design points with methods like sampling. The designs which pass the evaluation criteria for all quantities of interest are good designs and the intervals of the design variables which create good designs are solution spaces. In this work, the design spaces are projected on plots of suitable design variable choices to obtain the feasible design space for the key thermophysical properties and geometric design variables. The method starts with the schematic of the system dependency graph, where the relationship between the quantities of the interest and design variables is represented. The next two section covers the details of the system for the target body design.

2.2 Quantities of interest and design variables

The study uses four categories of design variables namely thermal properties design variables, geometric design variables, operational design variables and mechanical properties design variables. The names and symbols of them are given in table 1 along with their domain of variation considered in the study. The domain for material properties is chosen based on the common material properties which are potential candidates for a target design. The operational design variables are chosen around the nominal design requirement suggested by the line focus X-Ray tube system in the work by Johanna Winter et al. (2020). The three quantities of interest (QoI) and their definitions are listed in table 2. The first QoI r_melt_ft is to ensure that the focal track temperature is below the melting point of the focal track material. The second QoI r_melt_t is to ensure that the target body temperature is below the melting point of the target material, the selection of which is the focus of the study. The third QoI ry_t is to ensure that the mechanical stress is below the yield strength of the target material.

Table 1. Design variables

Design variables	symbols	design space
Power	P	1.3 to 1.5 MW
outer radius	r_o	0.05 to 2 m
height of target at minimum radius	h_0	0.03 to 2 m
angular spinning speed	w	25 to 5000 rad/s
time of pulse	t _op	1 to 3 sec
Melting point of target body material	T_melt_t	1000 to 4000 K
thermal conductivity of target material	k_t	5 to 1500 W/m-K
Specific heat of target material	Cp_t	5 to 1500 J/kg-K
Density of target material	rho_t	1000 to 25000 kg/m^3
Poisson's ratio of target material	nu_t	0.15 to 0.5
Yield strength of target material	σ_{y_t}	300 to 1500 Mpa

Table 2. Quantities of interest and definition

Quantities of Interest	symbol	definition	Requirement
Reserve against melting of focal track	r_melt_ft	T_peak / T_melt_ft	<1
Reserve against melting of target	r_melt_t	T_surface_d_t / T_melt_t	<1
Yield stress reserve of the target body	r_yt	$\sigma_{max}/ \sigma_{y\_t}$	<1

The relationship between the design variables and the QoI is depicted in the dependency graph in figure 3. The intermediate variables involved in the dependency are listed in table 3.

Table 3. Intermediate variables

Intermediate variables	symbols
Temperature increase in the focal spot	deltaT
Peak temperature in the target body	T_surface_d_t
Maximum temperature of the focal track	T_peak
Melting point of the focal track	T_melt_ft
Maximum vonmises stress in target body	σ_{max}

2.3 System model

2.3.1 Assumptions

The quantities of interest are computed using analytical models explained in the upcoming sections, considering a cylindrical target of finite radius and thickness. Even though the target body is subjected to both thermal and mechanical loads, the locations of maximum stress and maximum temperature are close to the inner and outer radius, respectively. Based on this minimal risk of high-stress zones occurring in high-temperature regions, constant mechanical properties are used in the work. And with the purpose of using analytical solutions for the temperature distribution in the target, constant thermal properties at a nominal temperature are used.

The configuration assumed for the study is a cylindrical target body with a thin layer of tungsten as a focal track where the electron beam is irradiated upon. The setup is shown in figure 2. The thickness of the target body is assumed to reduce exponentially (exponent m) from the centre height of h_0 at the minimum radius r_i to a minimum thickness h_min of 0.03 m at the outer radius. The orange layer represents the thin layer of tungsten focal track on the circumference of the target body. The governing equation for height h(r) at a given radius r is given as equation 2.1. This has been incorporated with the intention of reducing the mass at the outer radii and reducing the stress. The thermal solution for the study is, however, done assuming a thickness and inner radius, both equal to the value of 0.03 m. This approach is done to aid the use of analytical solutions for temperature distribution. The real temperature reached for the exponential thickness variation is expected to be lower, thus making it a conservative approach. The electron beam is assumed to irradiate the circumference.

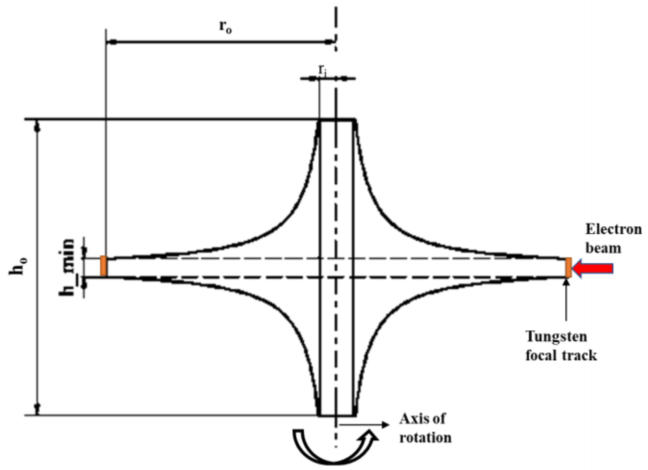

Figure 2: Target and irradiation

$$h(r) = h_0\left({r}/{r_i}\right)^m \quad (2.1)$$

2.3.2 Mathematical model

The stress on the target body is evaluated using the analytical model developed by Veil Yildirim (2018) to compute the radial stress (σ_r) and circumferential stress (σ_c) at any point as a function of radius r at that point. The effective von-mises stress (σ_v) is computed using equation 2.2 for every radius r. The maximum stress in the target body σ_{max} is the maximum von-mises stress across all radii (Equation 2.3).

$$\sigma_v(r) = \sqrt{\sigma_r^2(r) + \sigma_c^2(r) - \sigma_r(r)\sigma_c(r)} \quad (2.2)$$

$$\sigma_{max} = \max(\sigma_v(r)), \text{ for all } r \in (r_i, r_o) \quad (2.3)$$

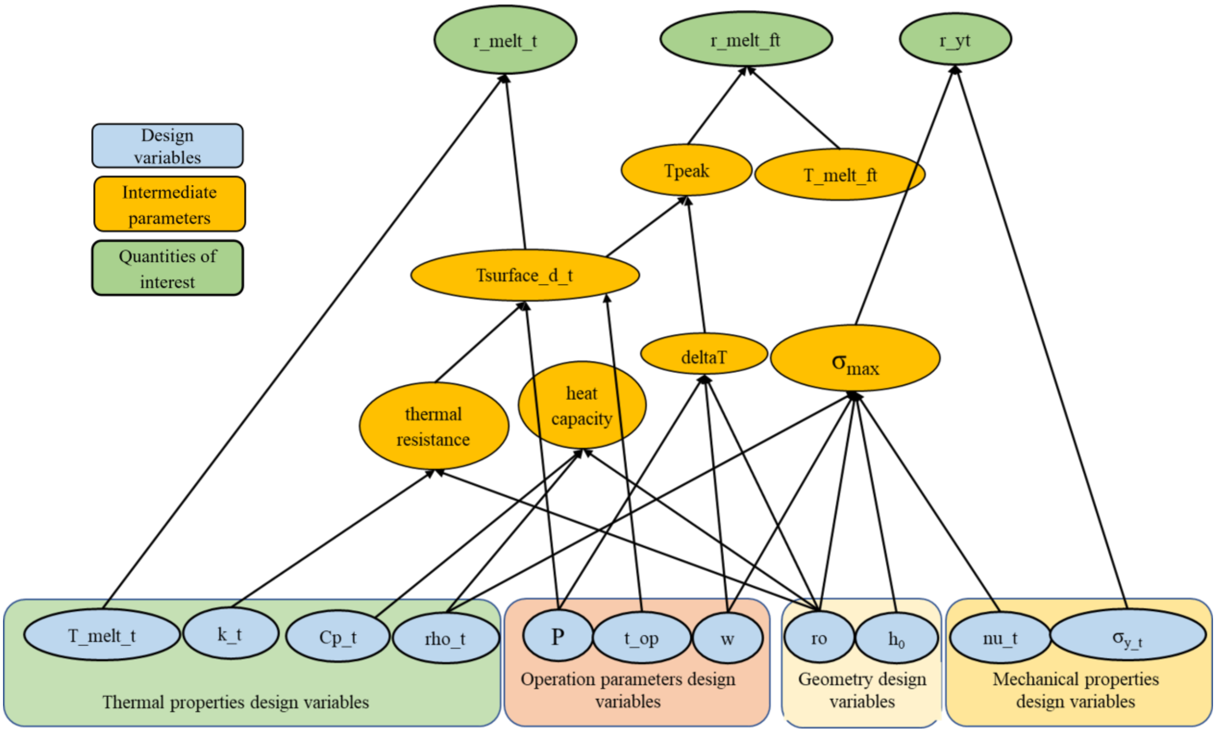

Figure 3: Dependency graph for the target body design problem

The temperature of the target is computed using two steps. The maximum bulk temperature of the target body, T_surface_d_t is computed from the analytical solutions of the Fourier's equation applied for a cylinder of uniform heat flux on the circumference (Frank P. Incropera et al. 2007). The local temperature rise deltaT on the focal track is computed using the heat balance of the infinitesimal focal track element (Stefan Bartzsch & Uwe Oelfke 2017), evaluated at the depth of maximum absorption of electrons. The maximum temperature of the focal track T_peak is computed as the sum of both, as written in equation 2.4.

$$T\_peak = deltaT + T\_surface\_d\_t \quad (2.4)$$

3 Results

3.1 Design space projections

The projected design spaces are generated by evaluating designs based on the values of quantities of interest and their requirements. The plots are generated among the design variables of choice, by projecting the design points from the entire domain of variation of all other design variables. The good designs are represented by green dots and designs which violate other quantities of interest are represented by legend shown in figure 4. The lack of green dots in an area represents an absence of good design, in that domain of the two variables in the plot, irrespective of the value of the other design variables.

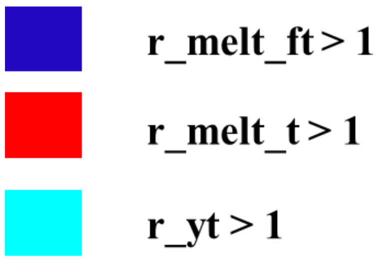

Figure 4: Colour code for violations in Quantities of interest

3.1.1 Design space projections of material properties

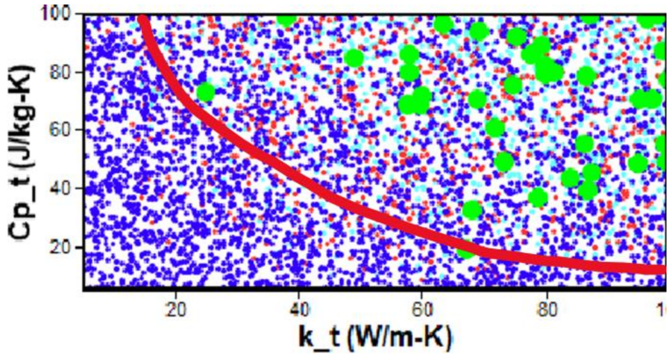

Figure 5: Projected design space with good designs in green dots (thermal conductivity vs specific heat)

As depicted in the dependency graph, the surface temperature of the target, T_surface_d_t has an inverse relation with the heat capacity and direct relation with the thermal resistance of the target. They are both in turn directly and inversely related to the specific heat and thermal conductivity, respectively. This leads to the inference that the thermal properties of specific heat and conductivity need to be more than a minimum, either simultaneously or individually. The region below which they do not yield any good designs is marked by a red curve in figure 5.

Given heat capacity is a function of not just the heat capacity but also the volume of the target and density of the target, a similar relationship exists between specific heat and both the geometric parameter of radius as well as the density, as depicted in figure 6. The target needs to be larger and larger as the specific heat gets lower and lower and the material needs to be denser and denser as the specific heat gets lower, as marked by the red curves in figure 6.

Figure 7 explains the relationship between yield strength and spinning speed. The stress varies as the square of the angular speed and the same is explained by the higher possible angular speed as the strength increases since the material can withstand higher stresses. Also, implied is the fact that irrespective of the material strength, there is an upper limit of angular speed of operation. Hence, to achieve the required surface speed, a minimum radius becomes necessary, as explained by the dependence of all quantities of interest on the outer radius.

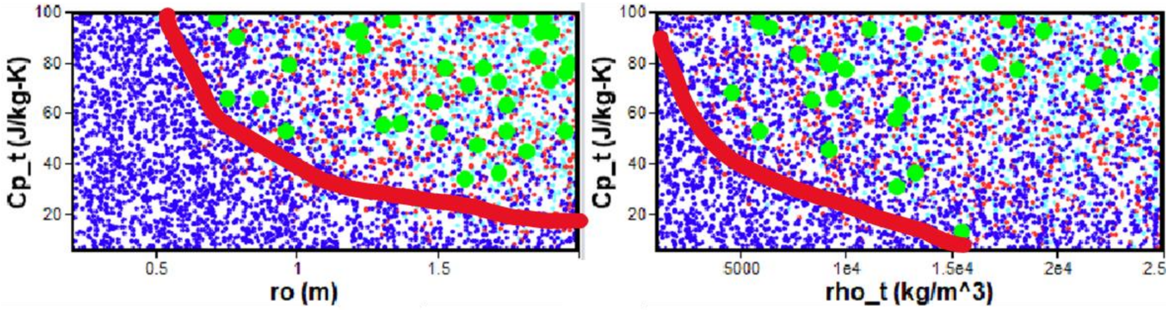

Figure 6: Projected design space with good designs in green dots (Outer radius vs specific heat on the left and density vs specific heat on the right)

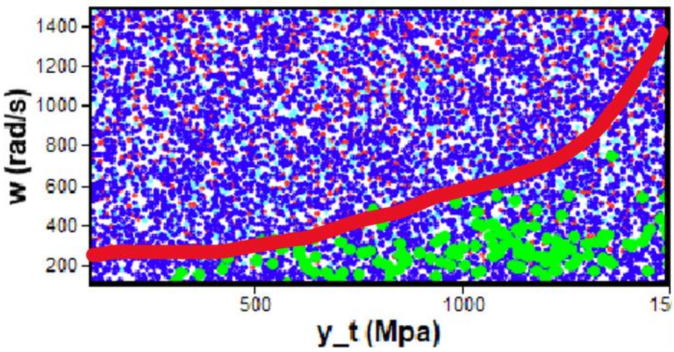

Figure 7: Projected design space with good designs in green dots (yield strength vs angular speed)

3.1.2 Material selection with design space projections

The projected design spaces explained in the previous section will be used to position specific materials in the design space. Figure 8 explains the nature of the lower limit of thermal properties relative to the materials titanium (Titanium, Royal society of chemistry 2022), steel (Stainless steel: Tables of Technical Properties 2007), molybdenum alloy called TZM (Plansee SE, Molybdenum, 2021) and tungsten (Plansee SE, Tungsten, 2021). The plot on the left marks the red curve limit for a maximum allowed radius of 0.5 m, while the curve on the right marks

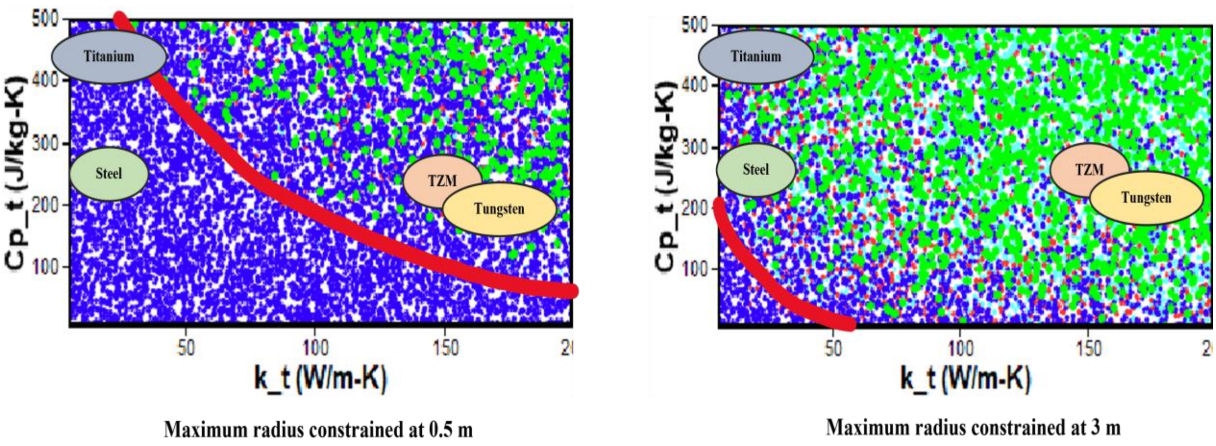

Figure 8: Projected design space with good designs in green dots (thermal conductivity vs specific heat)

the same for a maximum radius of 3 m. Materials with poorer thermal properties namely Titanium and Steel are not feasible choices for smaller radius but enter feasible design space once the radius is allowed to be larger. Materials with good thermal properties are in good design space, in both plots. Target made with superior thermal properties and higher densities can be invariably smaller. A similar argument is applicable for the relationship between specific heat and density as shown in figure 9. High density and high specific heat materials TZM and tungsten are in good design space in both the radius constraints while steel and titanium are feasible only with the higher radius constraint.

Figure 10 shows the relationship between radius and density for thermal properties capped at 500 and 1500 (SI units). For lower thermal properties, the minimum required radius is higher than that of the higher thermal properties case as we found earlier in figure 6. Also, the use of lighter materials like aluminium (Aluminium, Royal society of chemistry 2022) inevitably calls for use of a bigger radius if the thermal properties are inferior. If the thermal properties are superior, density has very less influence on the minimum radius requirement, as seen in the right curve.

4 Case studies

The section takes up the design with two chosen material candidates TZM and tungsten and arrives at the smallest possible target for the given requirements. Figure 11 shows the relationship between geometric design variable radius with angular speed for TZM material. As explained in the distribution of green dots the smallest possible radius is 0.4 m. Any smaller radius will result in the reduction of heat capacity leading to higher peak temperatures (shown by dark blue dots) and any higher radius will lead to more stresses (shown by magenta dots). A similar trend is shown for tungsten is figure 12. The minimum possible radius for Tungsten is around 0.4 m as well, explained by their similar thermal conductivities and product of density and specific heat.

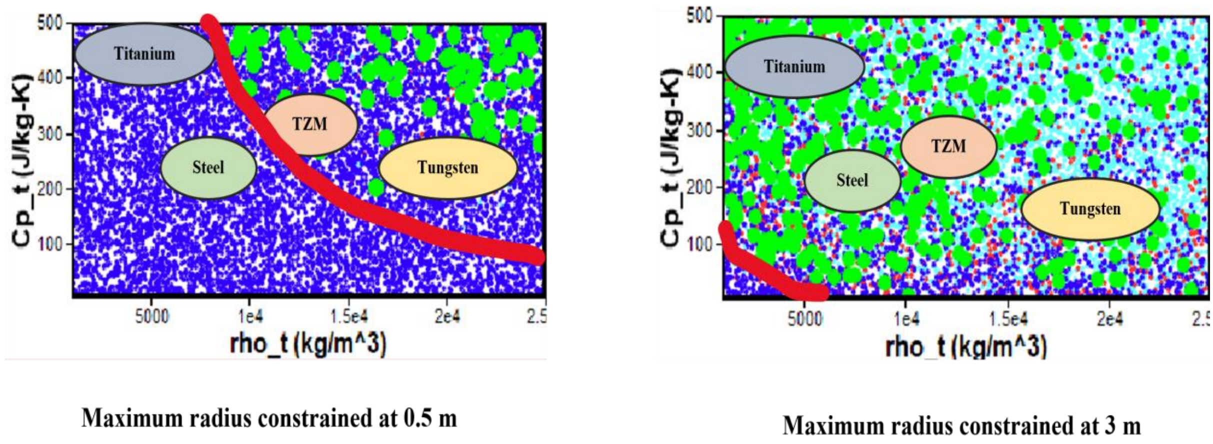

Figure 9: Projected design space with good designs in green dots. (Density vs specific heat)

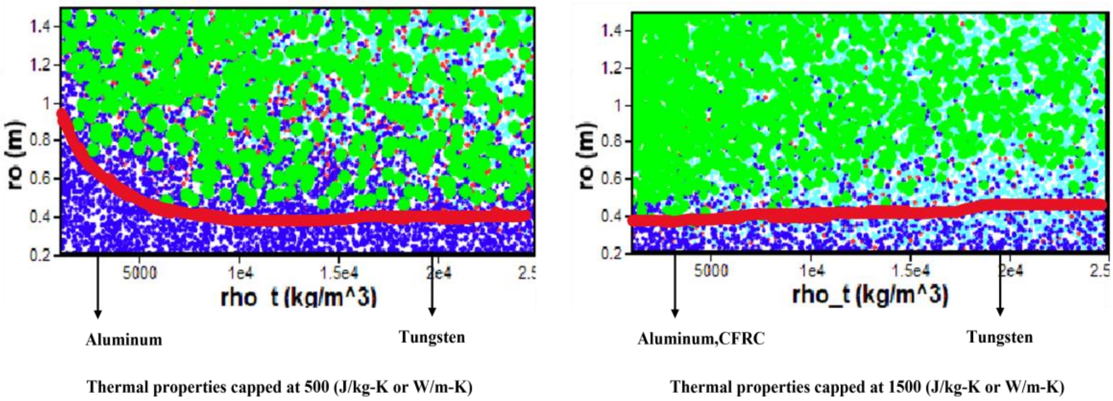

Figure 10: Projected design space with good designs in green dots. (Density vs outer radius)

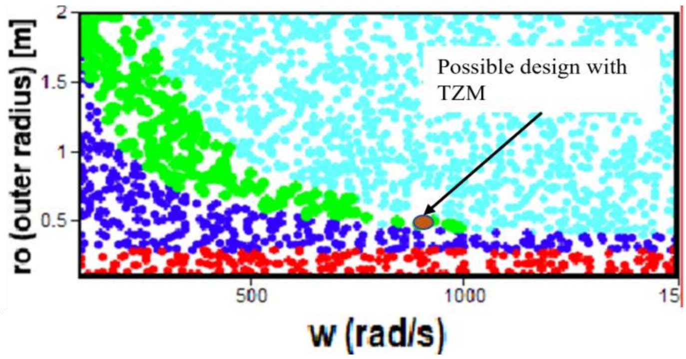

Figure 11: Projected design space with good designs in green dots for TZM (Angular speed vs outer radius)

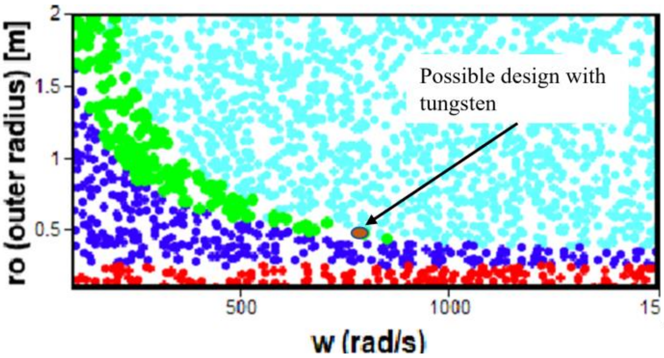

Figure 12: Projected design space with good designs in green dots for tungsten (Angular speed vs outer radius)

5 Summary

The use of the design space projection method has helped to arrive at a domain of thermophysical properties, from which materials could be chosen for the design of a target for a power of 1.5 MW. The resulting projected design spaces were used to infer that the design necessarily must be above a critical radius for any thermo-physical property combination possible and the minimum requirement on thermal properties of materials required for any size and material density possible. The minimum possible radius for the new power requirement was also found to be 0.4 m, for two commonly used materials in X-Ray tubes of the state of the art, TZM and tungsten.

6 Outlook

The paper has computed the theoretical feasibility of using the existing design configuration of X-Ray tube targets and commonly used materials for application in microbeam therapy with ultra-high power. The detailed design of the target needs to be carried out, with the materials having the thermo-physical properties found as feasible in this work, to assess the real temperatures and stress levels. Added to that, factors to be considered in the mathematical model include temperature-dependent thermo-physical properties and radiation cooling of the target to get closer to realistic results. The potential extension of the method to arrive at the thermo-physical properties and size limits, considering cooling would be further beneficial. For instance, incorporating an algorithm which can compute the numerical values of the lowest possible thermal properties and strength possible for a given maximum radius of the design allowed is an improvement for the method. The addition will help in quickly evaluating new material choices or combinations of materials such as matrix materials.

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