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Developing a Design Optimization Methodology for the Thermal-Hydraulic Evaluation for a High Temperature Reactor During a DLOCA

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Abstract. Methods of implementing uncertainty within nuclear reactor modelling have traditionally been achieved via worst case scenario uncertainty quantification. This article investigates how this practice can be expanded to provide data on the driving factors behind the temperatures experienced during accident conditions via a global sensitivity analysis. The second part of the article investigates how a stochastic optimization technique can be included within the design process to provide the most cost-effective core geometry which meets the temperature constraints of the fuel and the reactor pressure vessel. The third study investigates the impact of how uncertainty reduction can be used in combination with the stochastic optimization technique to provide further design optimization.

1. Introduction

Historically, nuclear energy systems have been designed by government sponsored research establishments which enabled the country to gain a lead within the nuclear market. As the technology matured, mainly through light water reactors, the export potential has been significant, and this has created highly skilled jobs and export potential. Several countries, such as the UK and France have privatized (and partially privatized) these assets, which has led to companies which are commonly seen today such as Westinghouse [1] and EDF energy. Today, due to the availability to nuclear design tools and a highly skilled labor market, nuclear designs are now open to small startups which are trying to revolutionize the future of nuclear reactors through Generation IV designs and Small Modular Reactors (SMRs) [2], [3].

With a generation of design engineers embracing the freedom of new ideas and new modeling methods, this provides the opportunity to change the way which the design process is implemented. One exciting area of new development is the use of design sensitivity and optimization tools. From a regulatory perspective it is a requirement for the designer to provide evidence that under all circumstances the reactor is safe to operate. This is historically achieved through a "Worst case scenario" approach, where conservative design variables are chosen to represent the worst case physically possible. This method is particularly attractive as it is easy to implement, and the computational power is low as only a minimal number of simulations are required.

As nuclear systems are complicated, the variables within the system are often not independent of one another. This means that the prediction of worse case scenarios becomes challenging and new methods of identifying the impacts of changes on the system are required. As modern computational power has developed, uncertainty and optimization tools are being developed to support these engineering requirements as this will improve the design process. As nuclear energy develops, these tools should be used to enhance the safety of nuclear systems and minimize the cost.

This article aims to provide modern uncertainty and design optimization tools on the High Temperature Engineering Test Reactor (HTTR) [4] which is owned and operated by Japan Atomic Energy Agency (JAEA). The optimization process occurs when simulating a Depressurize Forced Loss of Coolant Accident (DLOCA). Within this accident scenario, there are two key factors, the maximum fuel temperature and the maximum Reactor Pressure Vessel (RPV). The maximum fuel temperature is based upon the TRi-structural ISOtropic (TRISO) fuels design limit, where the structural integrity of the silicon carbide layer starts to deteriorate at ~1600 °C, therefore, JAEA have a maximum fuel temperature design limit of 1495 °C [5]. The maximum RPV temperature is determined by the type of steel used within the design, if breached, the steel will start graphitizing and the structural integrity of the steel is reduced. The RPV is made of SUS304 steel which has a design limit of 550 °C [5]. The maximum fuel and RPV temperature occur at opposing conditions, where the minimal thermal conductivity of the core provides the highest fuel temperature and conversely for the maximum RPV temperature.

This article takes the form of providing a 1D heat transfer model of the HTTR where a code to code comparison between JAEA's heat transfer software TAC-NC [6] is undertaken. After this a sensitivity analysis is performed with regards to the design variables of the reactor. Following this, a design optimization procedure is undertaken using genetic algorithm to determine the optimum design geometry based upon minimizing the cost of the design while maintaining the safety-based temperature constraints. The final study combines the sensitivity study with the optimization procedure as an uncertainty reduction optimization study is performed.

2. DLOCA in the high temperature engineering test reactor

High temperature reactors are renowned for their passive safety features which have been well documented. One such source of this information is the HTTR, where a DLOCA was performed at 9MWth. Prior to this, JAEA had modelled the DLOCA scenario using their code suite to determine the maximum temperatures experienced. Within open literature, JAEA have published a full power DLOCA to provide the maximum fuel and RPV temperature at day 660 and day zero of the HTTRs operation [5] (beginning of life and end of life). This work aims to reproduce these results by providing a similar analysis by producing a 1D heat transfer model for the HTTR in Matlab. This is achieved by creating models representing the conditions of the HTTR at these dates using the engineering first principles in TAC2D [7], TAC-NC's predecessor.

2.1. Model description

Within JAEA's model a worst-case approach has been taken towards the parameters of both the maximum fuel and RPV temperature. The HTTR is shown in Figure 1 where the heat transfer problem occurs from the center of the core outwards towards the exterior. At the exterior the HTTR's auxiliary cooling system provides the boundary condition of 90 °C immediately after the accident. Up until the point of the boundary, the heat transfer across the core is calculated by radiation and conduction through each material and a 1 mm gap between each component.

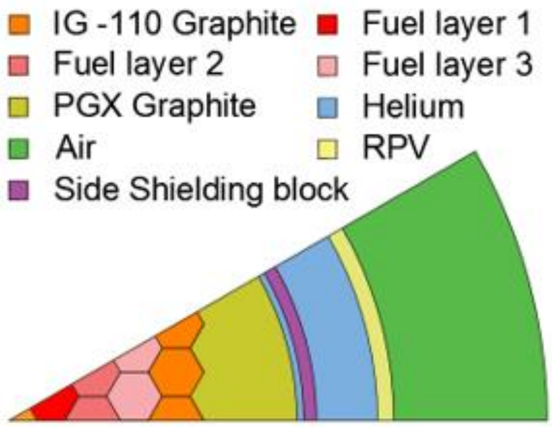

Figure 1. HTTR radial representation of the materials across the core. Within the modelling procedure the hexagonal shapes are approximated by using equal volume cylinders to provide a length for the heat transfer path.

The model provides the heat transfer methods shown in eq 1-3.

$$Q_{conduction} = \frac{2\,\pi\,R_i\,H\,K(T_i - T_o)}{\Delta g} \tag{1}$$

$$Q_{convection} = 2\,\pi\,R_i\,H\,h_{coff}\,(T_i - T_o) \tag{2}$$

$$Q_{radiation} = \frac{2\,\pi\,R_i\,H\,\sigma\,({T_i}^4 - {T_o}^4)}{\frac{1}{\epsilon_i} + \left(\frac{1}{\epsilon_o} - 1\right)\left(\frac{R_i}{R_o}\right)} \tag{3}$$

Where subscripts i and o represent inside and outside of the gap areas surfaces, H represents the height of the section, σ the Boltzmann constant, T as temperature, R as radius, Δg as gap length, h_{coff} as the heat transfer coefficient.

Following on from these equations TAC2D provides the following formula to determine the surface temperatures between gaps as follows.

$$T_i = B(To_V - T_o) + Ti_V \tag{4}$$

$$T_o = \frac{To_V(NB + 1) + NTi_V}{NB + 1 + N} \tag{5}$$

Where B and N are defined in eq. 6 & 7, and K represents the thermal conductivity of the material.

$$B = \frac{K_o A_o L_i}{K_i A_i L_o} \tag{6}$$

$$N = \frac{K_g A_g L_o}{K_o A_o \Delta g}\left(1\,\frac{\sigma \Delta g({T_i}^2 + {T_o}^2)(T_i + T_o)}{K_g\left(\frac{1}{\epsilon_i} + \frac{1}{\epsilon_o} - 1\right)}\right) \tag{7}$$

To emphasize the different conditions of the thermal conductivities of some of the materials, the fuel layers thermal conductivity at day zero and day 660 is shown in Figure 2.

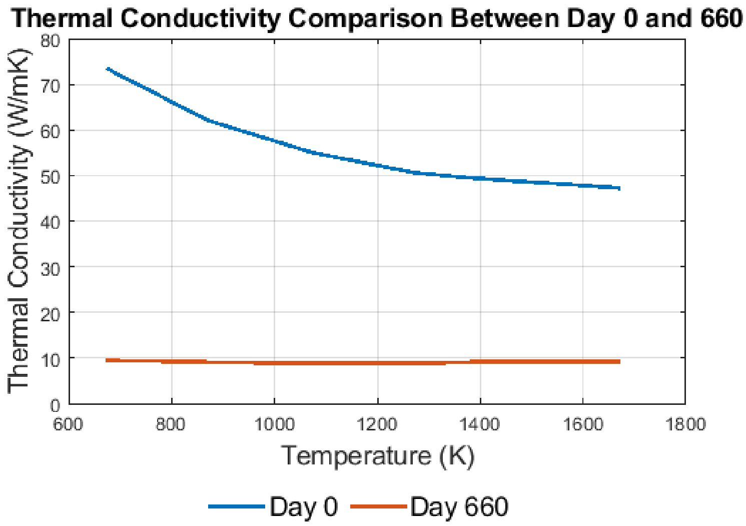

Figure 2. Thermal conductivity of the fuel layers at day zero and day 660

The thermal conductivities in Figure 2 are based upon worse case scenarios, where a 20% safety margin has been added to each case [5]. The significant reduction in the thermal conductivity provides a restricted heat transfer path across the gemometry and therefore provides the higher maximum fuel temperatures experienced. The power profiles at the different time periods for the fuel layers are shown in Table 1.

Table 1. Power fractions for the fuel blocks at day zero and day 660

		Fraction of the total power		
	Day	Layer 1	Layer 2	Layer 3
Power block 1 (top)	0	0.0319	0.0331	0.0967
	660	0.0458	0.0467	0.1313
Power block 2	0	0.0605	0.0623	0.1702
	660	0.0584	0.0606	0.1647
Power block 3	0	0.0607	0.0570	0.1586
	660	0.0492	0.0510	0.1368
Power block 4	0	0.0331	0.0343	0.0959
	660	0.0332	0.0332	0.0873
Power block 5	0	0.0214	0.0222	0.0622
	660	0.0222	0.0222	0.0577

2.2. Model validation
To validate the model a code-to-code comparison is produced between TAC-NC and the model produced during the worst-case accident faults. As these faults occur at different times, the maximum temperatures experienced are shown in Figure 3 & 4.

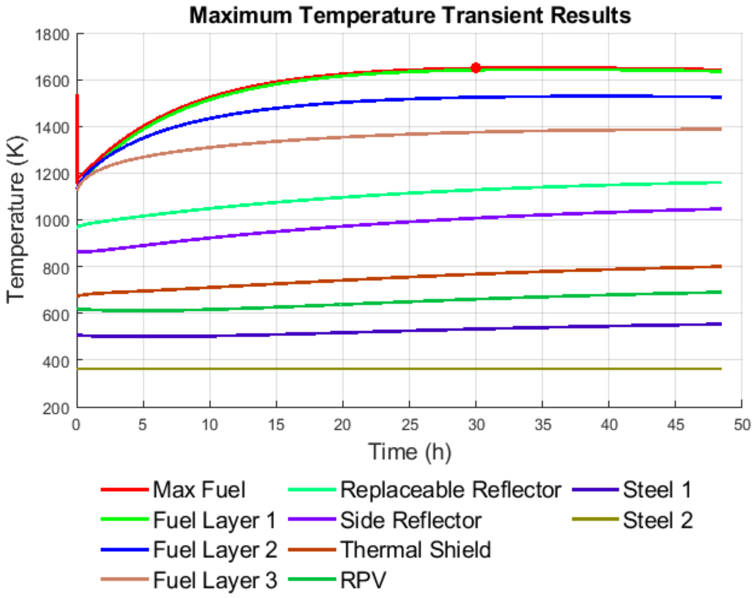

Figure 3. Maximum fuel temperature of the model compared to JAEA's value which is represented as a red dot.

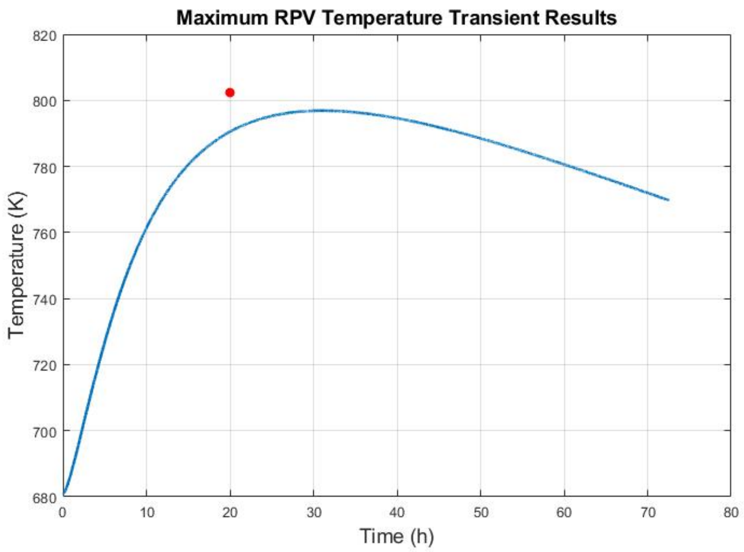

Figure 4. Maximum RPV temperature of the model compared to JAEA's value which is represented as a red dot.

Figure 3 provides a full temperature evaluation of each material. The model can accurately represent the maximum fuel temperature during the transient, with the maximum discrepancy being 10 K. From Figure 4, there are some slight deviations from TAC-NC which is caused by the lack of natural circulation used within the model provided in this work which means that immediately after the transient the coolant within the fuel blocks is circulated to the RPV, causing a slightly quicker heat up of the RPV.

As a conclusion, the model can produce similar results to TAC-NC under the worst-case assumptions.

3. Sensitivity study of a DLOCA in the HTTR

Uncertainty arises from the deviation of the model from the practical application. This can occur through various means and these should all be considered when quantifying the total system uncertainty as this can have an impact on critical safety procedures.

The nuclear industry invests heavily in manufacturing processes to reduce the uncertainty of components or materials varying significantly from their predicted value; however, uncertainty will always be present within the model. Within this case study the uncertainties are grouped as material properties and thermophysical properties. Material properties are based upon machine tolerances of parameters, such as the density of graphite materials. Thermophysical properties represent the uncertainty of the thermophysical data. These unknowns have been determined from the literature and are depicted in Tables 2 & 3.

Table 2. Uncertainties used for the materials case [8] [5] which were represented as a uniform distribution.

Part	Nominal value	Tolerance	Units
Fuel compact inside diameter	10	0.1	mm
Fuel compact outside diameter	26	0.1	mm
Graphite sleeve inside diameter	26.25	0.1	mm
Coolant channel inside diameter	34	0.1	mm
Coolant channel outside diameter	41	0.1	mm
IG110 graphite	1.75	0.04	g/cm^3
PGX graphite	1.73	0.04	g/cm^3
Initial helium pressure	40	3.50%	Bar
Inlet temperature	395	14	°C
Gap width	1	100%	mm
Emissivity graphite	0.8	25%	n.a.
Emissivity steel	0.8	25%	n.a.

It should be noted that JAEA does not provide any uncertainty data within regards to the volumetric heat capacity of the graphite, so this has been artificially included.

A global sensitivity analysis aims to determine the output variance based upon the input uncertainty; this is particularly useful within the design process as this method can highlight the most affective design parameters on certain input conditions. The global sensitivity analysis chosen was Sobol' indices (S_i) [9] which is a ratio of the conditional expectance of the input parameter over the total variance of the output Var(Y) as shown in eq. 8.

$$S_i = \frac{Var_{X_{\sim i}}\left(E_{X_{\sim i}}(Y|X_i)\right)}{Var(Y)} \tag{8}$$

Where ∼i means the expected values are calculated for all other variables except i. One of the benefits of this method comes from the ability to include combinations of each input parameter, to determine the total index (T_i) and thus determine the combined effect.

$$T_i = 1 - \frac{Var_{X_{\sim i}}\left(E_{X_i}(Y \mid X_{\sim i})\right)}{Var(Y)} \tag{9}$$

The test used OpenCossan's [10] Monte Carlo simulation to determine the output variances for each of the input variables and OpenCossan calculated Sobol's indices and the total index. The Monte Carlo simulation used 290K samples.

Table 3. Uncertainties for the thermophysical properties [5] which were represented as a uniform distribution. Where ∝ means proportional to.

Uncertainties	Nominal value	Uncertainty (%)	Unit
Reactor power	30	2.50%	MWth
Thermal conductivity fuel layers	∝ Temperature	20%	W/mK
Specific heat capacity fuel layers	∝ Temperature	10%	J/m^3K
Thermal conductivity RR	∝ Temperature	20%	W/mK
Specific heat capacity RR	∝ Temperature	10%	J/m^3K
Thermal conductivity SR	∝ Temperature	20%	W/mK
Specific heat capacity PR	∝ Temperature	10%	J/m^3K

3.1. Results of the sensitivity analysis of the HTTR

The sensitivity analysis was performed to determine the parameters which have the highest impact on the maximum fuel and RPV temperatures. Within this analysis a single simulation was performed, which provided Sobol's indices for each parameter, which provides the individual contribution for each parameter. It was determined that the total index variance was almost identical to the first index and therefore the combined interactions between uncertainty are not a dominant factor for the sensitivity of the system. If these indices were significantly different, the total index would be the most suitable to use.

For clarity, these are displayed in two graphs but represent the first indices of the maximum fuel and RPV temperature. From Figure 5, the manufacturing tolerances provide very little impact on the maximum temperatures experienced. The highest impact parameter is the emissivity of steel is the largest driving factor for the RPV temperature, this is because the heat leaving the RPV to the outside steel is determined nearly independently through radiation.

From Figure 6, the thermal conductivities are, as expected, the main contributors for the maximum fuel temperatures.

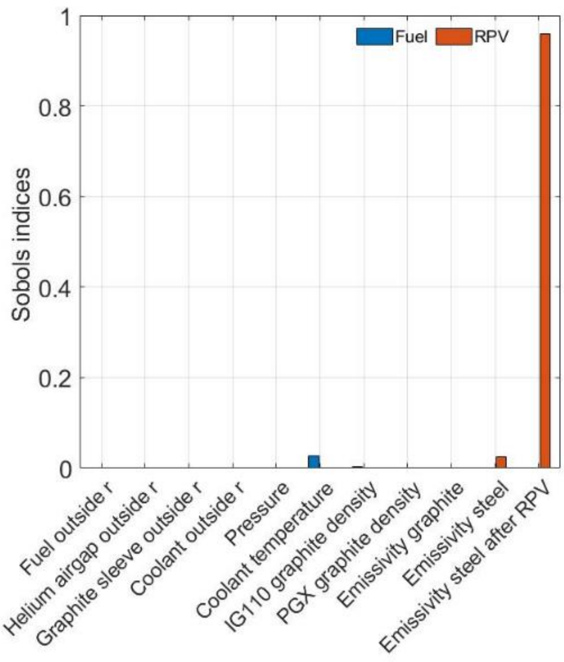

Figure 5. Materials Sobol's indices during the DLOCA for the maximum fuel and RPV temperatures. Where r denotes the radius.

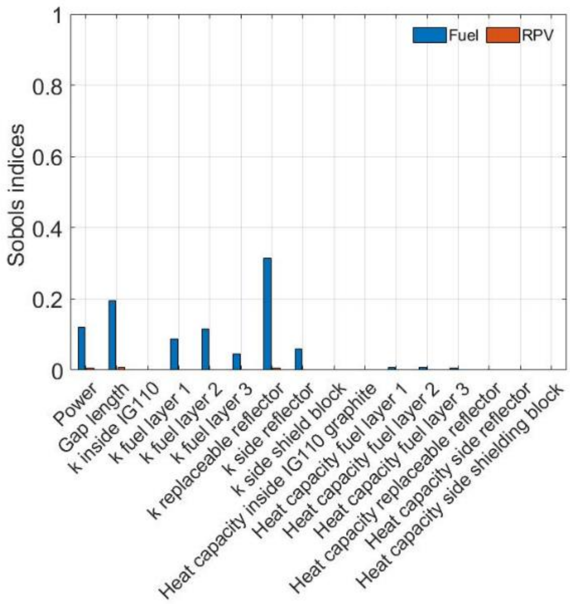

Figure 6. Thermophysical Sobol's indices during the DLOCA for the maximum fuel and RPV temperatures. Where k denotes the thermal conductivity.

4. Optimization procedures for the HTTR Geometry during a DLOCA

With modern techniques it is possible to reduce the overall cost of the design based upon automated stochastic global optimization methods such as Genetic Algorithm (GA) [11]. GA is an artificial learning technique which follows the process of Figure 7. The initial population is a coarse range of the input parameters, these are then evaluated to determine the best "score" based on the object function, in the case cost and any selection which does not meet the constraints is discarded. The highest scoring designs have their design variables crossed between other high scoring selections; this allows for GA to determine the highest impact parameters on the object function. After the crossover, the design variables can mutate, providing a finer range of the design variables until the optimum solution is found.

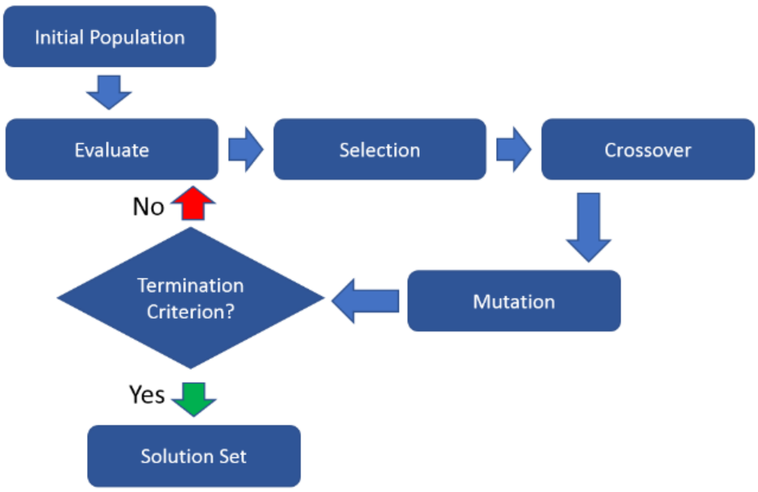

Figure 7. Genetic Algorithm solver flowchart

The design variables which are edited relate to the size of the reactor, with the aim of finding the optimal radial geometry. The variables, a, X2, X3 and X4 are shown in Figure 8 and eq. 9.

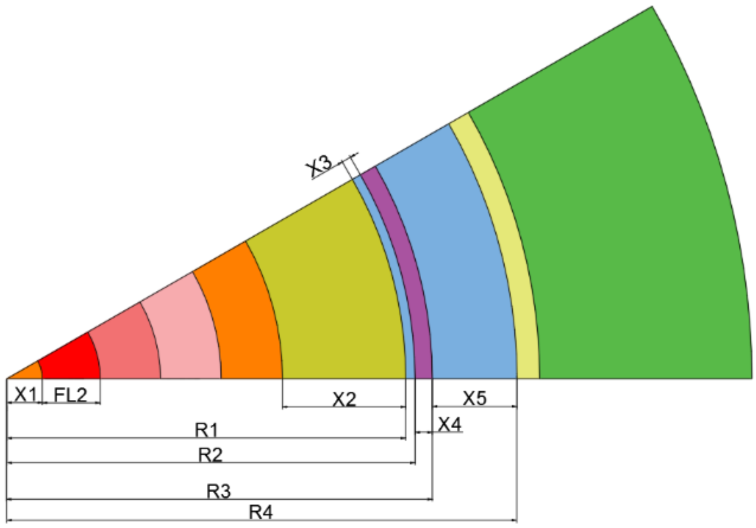

Figure 8. HTTR design variables X2, X3 and X4 highlighted.

Each of the fuel layers and replaceable reflector use of the same value of a, this is to retain the hexagonal lattice withing prismatic HTR cores. The value of X1 is determined via eq. 10.

$$\sqrt{\frac{3\sqrt{3}}{2\pi}a^2} = X1 \tag{10}$$

X2 represents the replaceable reflector width and with X3 being the inside helium channel. To retain the same inlet flowrate, the volume of helium is kept the same, so X5 increases in size proportionally to the design variable X3. X4 is the thickness of the side shielding block. The nominal values of these parameters and the upper and lower bounds for GA can be found in Table 4. The uncertainty within the model uses the worst-case scenario method for each of the parameters presented within Table 2 and Table 3 which was determined by performing a local sensitivity analysis using a one-at-a-time (OAT) technique to determine if the maximum or minimum value should be used for the worse case analysis.

The cost of the reactor must be estimated based upon realistic material costs as shown in Table 5 which have been obtained from a recent report on the U-Battery, a similar HTR reactor type [12]. The graphite in the HTTR uses IG110 graphite, which is purified, this increases the cost compared to the PGX graphite. The steel within this case represents the cost of RPV steel, which is significantly higher due to maintenance and fabrication costs. The cost of the core is based upon open literature with the materials of each section shown in Table 6 it should be noted that this excludes fuel, licensing and manufacturing costs which are assumed to be uniform for all designs.

Table 4. Arbitrary Design variables used for GA

Part	Variable	Nominal (cm)	Lower bound (cm)	Upper bound (cm)
Fuel block	a	20.78	18.70	22.86
Side reflector	X2	66.5	33.25	99.75
Helium gap	X3	5	2.5	7.5
Side shielding block	X4	9.3	4.65	13.95

The design variables for GA were selected to provide an input range for the GA and therefore these do not consider external factors which might be considered within the design phase such as radiation damage.

The limiting constrains of the maximum fuel and RPV temperature were set to 1495 °C and 550 °C respectively as to maintain the original constraints from JAEA. The object function of GA as shown in eq. 11 aimed to minimize the design cost with the tolerance set is 10^{-5} with a maximum amount of 200 iterations for convergence.

$$Min = Cost_{IG110} + Cost_{PGX} + Cost_{RPV\ steel} + Cost_{SSB} \tag{11}$$

Table 5. Costs of materials used in GA

Material	Cost $/Kg	Original design costs (M$)
IG110 graphite	77	1.76
PGX graphite	53	5.52
RPV Steel	42	13.85
Side shielding block steel	35	1.08

The overall nominal cost of core is $22.22 M. The smallest core will result in the cheapest core, however, as the core size shrinks, the RPV temperature increases and GA will have to find the optimal size at the minimal cost.

Table 6. Geometry material descriptions and the nominal geometry on the HTTR

Part	Material	Installed dimensions	
		Inside	Outside
Central graphite block	IG110 graphite	n.a.	0.191
Fuel layers	IG110 graphite	0.191	1.156
Replaceable reflector	IG110 graphite	1.156	1.485
Side reflector	PGX graphite	1.485	2.15
Side shielding block	Steel/PGX 0.47/0.53	2.2	2.293
Steel	Steel	2.75	2.872

4.1. Results of the optimization analysis of the HTTR

GA was provided with the boundaries in Table 4 and was tasked with determining the optimal geometry (lowest cost) yet remains within the constraints of the maximum temperatures of 1495 °C and 550 °C. The determined design is shown in Figure 9.

From Figure 9 the optimal solution for the geometry of the HTTR. GA has used a combination of reducing a and X2 to provide the main volume reduction of the core and thus saving per unit. The helium thickness (X3) is reduced to help reduce the cost of the expensive thermal shield (X4) where this volume has been minimalized. The overall cost of GA's design is $18.02 M, which is a 18.9% cost reduction over the original design. To convert the cylindrical geometry back to the hexagonal form, the total volume of the hexagonal region would be divided equally amongst the hexagons to provide the area of a single hexagon.

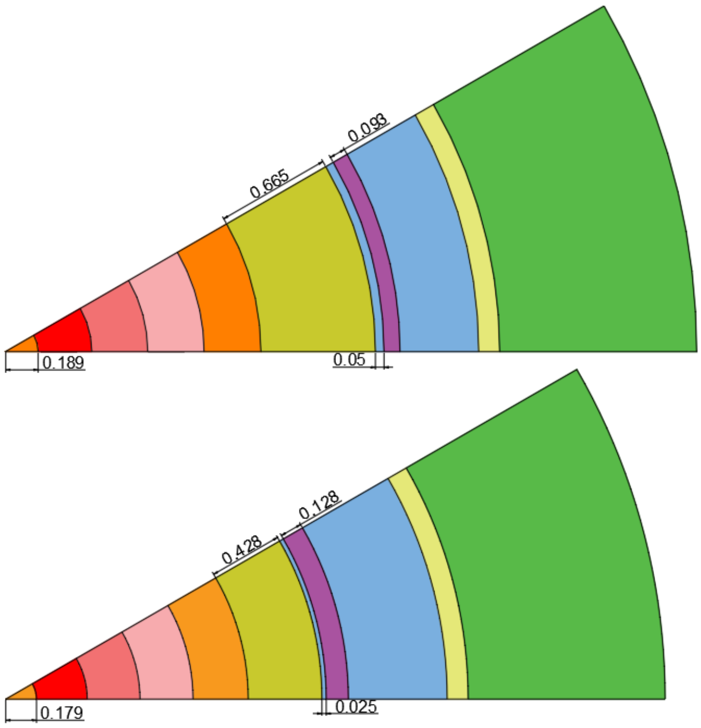

Figure 9. Top; The original HTTR geometry. Bottom; GA's optimized geometry.
All geometry in meters.

To be assured that this new design meets the safety criteria the new DLOCA temperature profiles are provided within Figure 10 and Figure 11. It should be noted that the limiting factor within this design is the maximum RPV temperature.

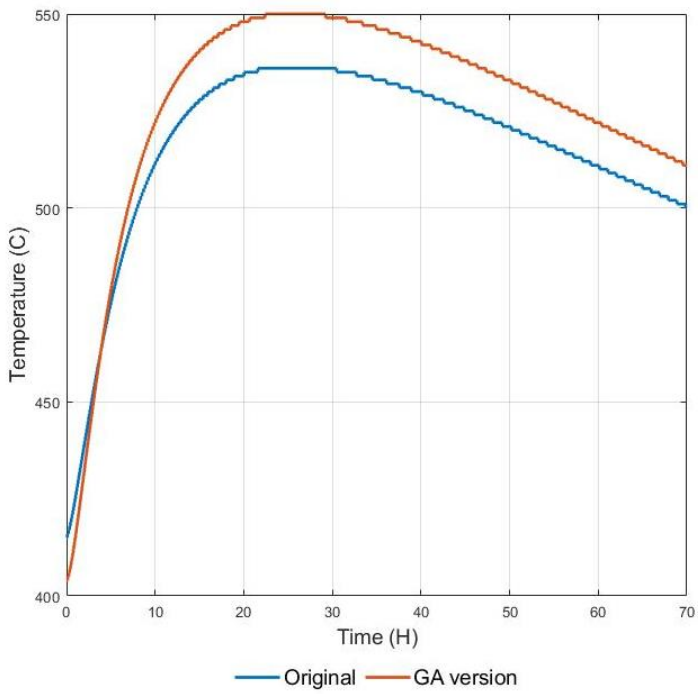

Figure 10. GA models DLOCA transient maximum RPV temperature.

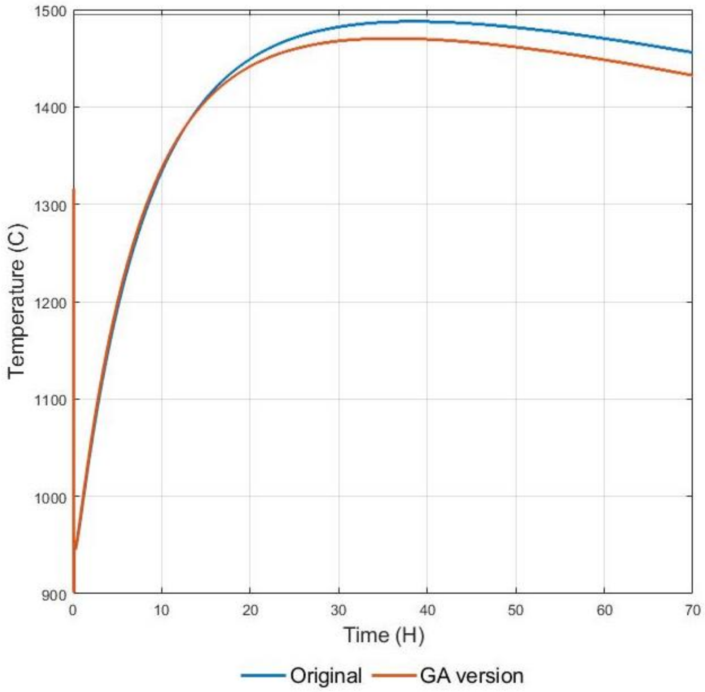

Figure 11. GA models DLOCA transient maximum fuel temperature.

GA has found a reduced cost design based upon the original design criterion which can meet the exact design constraints of set by JAEA. The process of using GA is relatively simple, due to the software being easy to use in parallel which makes this optimization technique easily applicable to the design of reactors, without the requirement for large amounts of computational time.

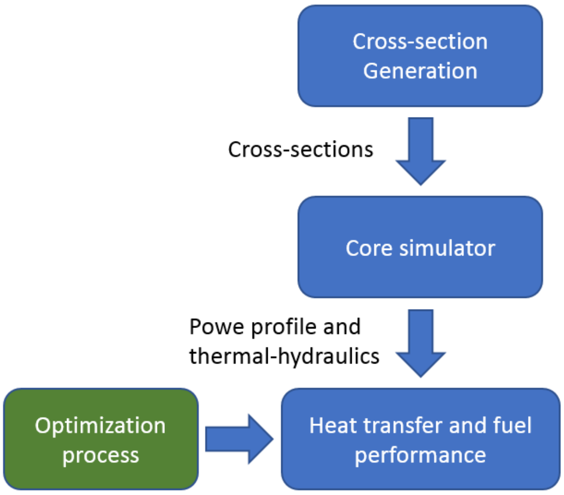

Figure 12. Current modelling methodology.

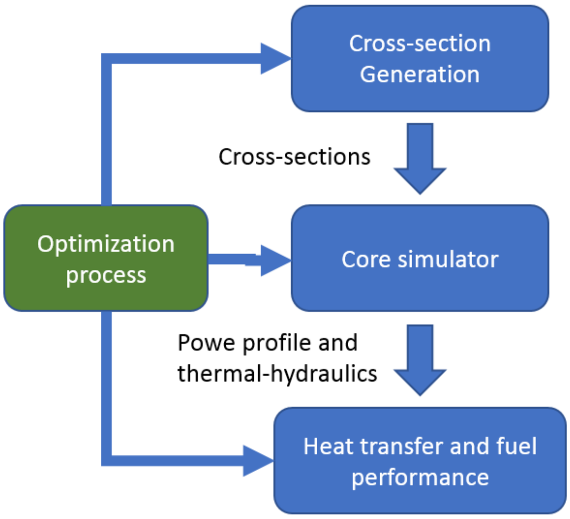

Figure 13. New proposed modelling methodology.

It should be noted that this study is limited, as the changes in the geometrical parameters of the design will have an impact into the performance of the design. This section has highlighted that GA can be used as a powerful tool within the design phase, however, to achieve a full system understanding of the new design, this must be incorporated within the modelling structure of reactors shown in Figure 12. To accomplish this, uncertainty and optimization tools are regularly used as methods of coupling software together, as in the case of OpenCossan. To achieve this, OpenCossan would need to be linked to other design software in parallel, as depicted by Figure 13. The drawbacks of this method would be incurred due to the computational power required; however, this can easily be managed by only running each software for high scoring designs.

5. Uncertainty reduction opimization procedures for the HTTR during a DLOCA

Section IV identified that GA can provide a design at a lower cost, however, this new design is limited by the maximum temperature of the RPV. To further refine these techniques, an uncertainty reduction study has been performed, where the global sensitivity analysis determined the highest impact parameter on the maximum RPV temperature is the emissivity of the steel proceeding the RPV. The steel proceeding the RPV is important as the distance between the RPV and the containment vessel is large and the conducting medium is air, which means most of the heat transfer is provided by radiation. JAEA models this emissivity as a conservative 0.6 during the worst-case scenario modelling of a DLOCA for the RPV temperature. There are methods to increase this emissivity, such as painting the containment building with a matt black paint or changing the material to provide a higher emissivity. This next study aimed to determine if the overall costs of the design could be reduced by reducing the uncertainty of this material.

5.1. Results of the reduced uncertainty optimization of the HTTR

GA was once again used for a gradually reduced uncertainty of the emissivity proceeding the RPV. The results of the impact on the total cost are depicted in Figure 14.

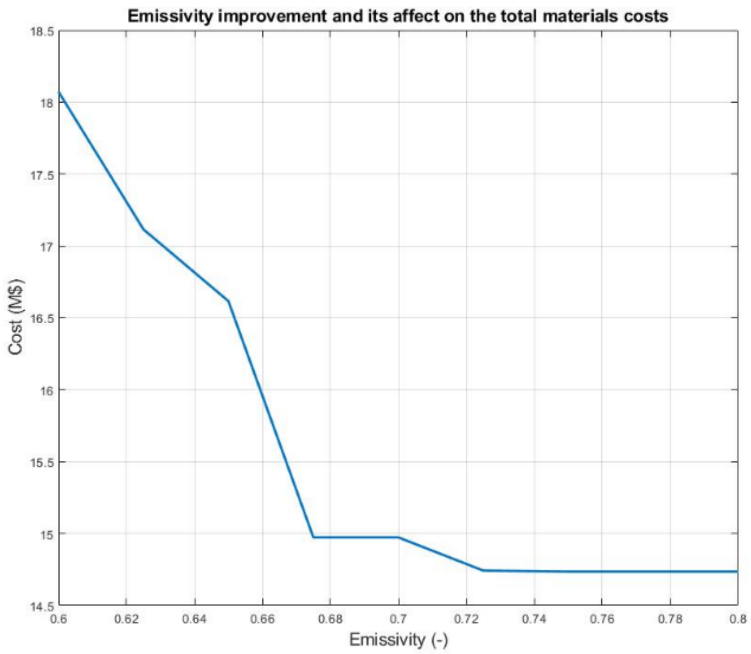

Figure 14. Design costs as the emissivity of the steel proceeding the RPV is reduced

From Figure 14, GA has identified that the design costs can be reduced to 14.75 M$ with an emissivity of 0.72 at which point any further reduction sees no benefit. This represents a further 18% cost reduction from the optimal design within section IV. This was an interesting study as GA not only predicted an optimal design, but also provided a target emissivity for the design which is useful for the design process. For completeness, the optimal geometry model geometry for the lowest cost design with reduced uncertainty is shown in Figure 15.

This study can be continued further for other design parameters; however, this is beyond the scope for this article. It should be noted that GA requires a new simulation for each value of the emissivity used, this is more computationally expensive than the method used within section IV, so, these simulations work well alongside the global sensitivity analysis.

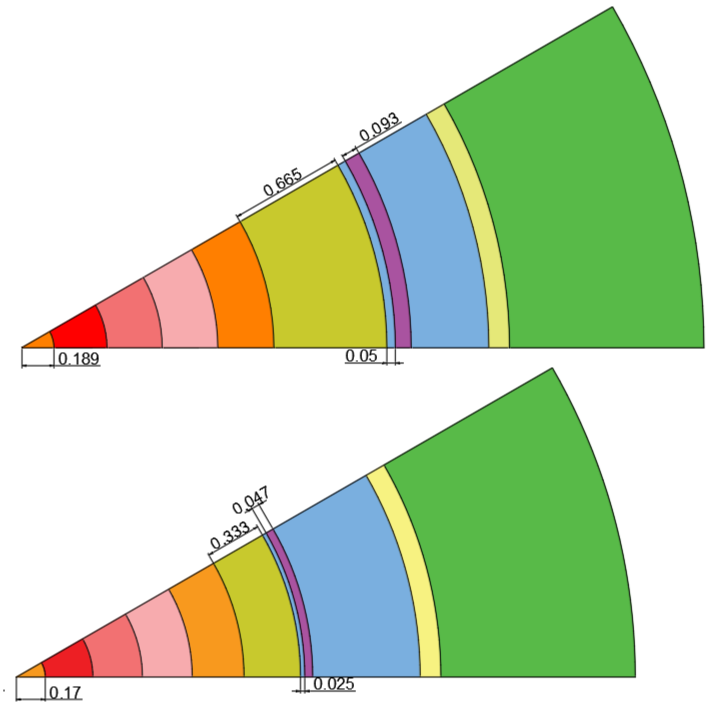

Figure 15. Top; Original model dimensions. Bottom; Optimal cost with increased emissivity of the RPV steel geometry

6. Conclusion

This article aimed to provide a methodology to incorporate design uncertainty and optimization software for the design of high temperature reactors with an aim of reducing the capital costs. This was initially achieved via a global sensitivity analysis which provided a method of identifying the highest impact parameters for the maximum temperatures experienced. This study provided the impact of each of the parameters, thus enabling for further insight into the design process.

The second study investigated how GA can be used to determine the optimal geometrical parameters of the design. This process enabled a smaller design to be obtained, which came in at a reduced cost yet remained below the safety-imposed design constrains. This study highlighted that this methodology works well, however, there are limitations as a full system approach should be used to understand the impact of the new chosen design. A method to implement this by using an interlinked system has been developed, however, this would require further work to determine the true potential of this software and the drawbacks with regards to computational requirements.

The third analysis combined the results from the sensitivity study and the GA to provide an uncertainty reduction investigation with regards to the emissivity of the steel proceeding the RPV. This was a very useful study as this highlighted that GA can also provide methods to optimize the material choice with defined targets to meet with regards to material properties.

This work has highlighted the benefits of including uncertainty and optimization software within the design process. This can be a powerful tool for HTR design manufacturers to optimize the design and provide vital safety specific data for regulatory approval. The practicality of such a software depends on the speed at which the relevant calculations can be performed, so this approach might not be beneficial for high fidelity methods due to the computational requirements. From a practical perspective, these methods could easily be applied for design refinement using the current approach, however, this is likely to be an interesting topic within the future, with long term benefits for all reactor designs.

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