Multi-objective, multi-physics optimization of 3D mixed-oxide LWR fuel assembly designs using the MOJADE algorithm

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Abstract

Optimization problems in the research literature are typically simplified and/or heavily constrained and focus on a single set of physical processes. Real-world nuclear engineering problems feature competing multi-physics phenomena and require equally complex analysis. To prove its usefulness in this area, optimization must demonstrate an ability to handle many competing objectives whilst accurately simulating the reactor environment. This paper applies the MOJADE optimization algorithm to two design problems, a 3D PWR Supercell and a 3D BWR fuel assembly, evaluating performance objectives related to neutronics and thermal hydraulics simultaneously, using the concept of Pareto dominance. In both cases, MOJADE was able to find competitive or non-dominated designs compared to baseline solutions generated from the literature and required no control parameter tuning or training time. Analysis revealed that MOJADE can identify key variables which impact objective performance, demonstrating the algorithm's ability to provide new insight to complex 3D problems featuring multi-physics analysis.

1. Introduction

Nuclear reactor fuel assembly design, like many engineering design problems, is an exercise in balancing a series of trade-offs between a variety of constraints and objectives. However, unlike other fields, the design process involves a large number of variables that interact in a non-linear manner. Optimization techniques offer the engineer a capability to explore these trade-offs in a methodical manner where conventional judgement alone is insufficient.

Optimization attempts to determine which combination of variables produces the best solutions with regard to the pre-defined performance objectives. Examples of optimization techniques applied to nuclear engineering fuel loading patterns include dynamic programming (Stout and Robinson, 1973), particle swarm optimization (Ahmad and Ahmad, 2018) and genetic algorithms (Parks, 1996). Some of the most successful techniques belong to a class of 'metaheuristics' (Glover, 1986), which are algorithms that use feedback information from the search in iteration to determine how the algorithm will search in the next iteration. Evolutionary algorithms (EAs) (Coello Coello et al., 2007), which include the aforementioned genetic algorithms, and differential evolution (DE) (Storn and Price, 1997), are part of this class. In EAs, a set of possible solutions is stored as a population. The population is then modified through mimicking the natural mammalian reproduction process of selection, crossover and mutation, to attempt to create offspring (a new set or generation of solutions) which are superior to their parents. Over a number of generations, the population then converges towards the most

optimal solution for single-objective problems, or a set of solutions for multi-objective problems.

For multi-objective problems, which consider two or more objectives simultaneously, the set of most optimal solutions is known as the Pareto-front. On the Pareto-front, no solution is dominated by any other, which means that no solution is superior to another in one objective without simultaneously being inferior in another. Whilst the true Pareto-front of a problem is seldom found in real-life problems (which would, in theory, require the exhaustive evaluation of all possible solutions), an effective multi-objective optimization algorithm can find a Pareto-front which is a sufficient approximation of the true one. The main problems of optimization using metaheuristic algorithms include the amount of time needed to determine optimal control parameters to a particular problem (either for the algorithm itself or on the user-defined parameters of the algorithm), and premature convergence, which occurs when the algorithm becomes trapped with a set of solutions that are superior to nearby solutions in the search space, but do not represent a global optimum. For multi-modal problems with high dimensionality this is a significant problem. In complex problems it is also difficult to know when you have converged on the true Pareto-front, and therefore having some real-world data to serve as a reference point is highly desirable.

Both problems tackled in this paper are multi-objective, and no weighting was given to any of the objectives; nor was any objective constrained in order to treat the problem as a series of sequential single-objective problems. This is in order to avoid contaminating the results with factors that are mostly subjective and based on the designer's judgement (Parks, 1996). Furthermore, the problems are based on real-world multi-physics fuel assembly design challenges concerning two of the latest reactor designs on the market: the European Pressurized Reactor (EPR) by Orano and the Advanced Boiling Water Reactor (ABWR) by Hitachi GE. Optimization was performed using the multi-objective DE algorithm MOJADE, which has already demonstrated both its effectiveness and its insensitivity (discussed in Section 2 below) to different nuclear engineering fuel assembly optimization problems (Charles and Parks, 2018). MOJADE was combined with a development version of the analysis package WIMS (Lindley et al., 2015) to evaluate the reactor physics and thermal hydraulics performance of the algorithm-generated solutions.

The rest of the paper is laid out as follows. Section 2 explains the concept of differential evolution and the multi-objective form of the JADE algorithm, developed previously in (Charles and Parks, 2018). Sections 3 and 4 detail the two complex and realistic problems in the nuclear engineering design of LWR fuel assemblies on which the algorithm was tested. The first seeks to optimize a 2×2 supercell of Uranium Oxide and Mixed Oxide (UOX – MOX) assemblies relating to the EPR design; the second a 3D BWR fuel assembly relating to the ABWR design. The results of these two computational experiments are detailed in Sections 5.1 and 5.2 respectively. The paper concludes with a summary of the main findings and their implications for future work in Section 6.

2. Differential evolution and the MOJADE algorithm

Differential evolution is a form of optimization that works by combining good solutions to produce superior solutions, just like the concept of evolution in biology. Each solution is ranked according to how well it performs against the objectives of the problem. New solutions are generated by taking the difference between the variables of existing solutions (parents) and using them to modify another solution. This difference is scaled or 'mutated' using a mutation strategy, which is often unique to different DE algorithms. In JADE (Zhang and Sanderson,

2009), this mutation strategy is referred to as “DE/current-to-pbest/1” and will always use a random member of a superior subset of the population (the ‘best’ solutions) as one of the parent solutions. In addition, a second difference is added which uses the difference between a random member of the current population and an archive of ‘worst’ solutions. The intention here is to utilize the best solutions to make the algorithm elitist / ‘greedy’ to encourage convergence on areas of optimality, but to also maintain diversity within the population through the inclusion of poor solutions to avoid the previously mentioned phenomenon of premature convergence. “DE/current-to-pbest/1” is detailed in Eq. (1):

$$v_{i,g} = x_{i,g} + F_i \times (x_{best,g}^p - x_{i,g}) + F_i \times (x_{r1,g} - \bar{x}_{r2,g}) \quad (1)$$

where $v_{i,g}$ is the mutated solution, $x_{i,g}$ is a current member of the population, $x_{r1,g}$ is a randomly chosen member of the population, $\bar{x}_{r2,g}$ is a randomly chosen solution from an archive of ‘worst’ solutions, $x_{best,g}^p$ is a solution from an archive of ‘best’ solutions, and F_i is a weighting factor. The mutated solution $v_{i,g}$ then undergoes crossover (discrete recombination) with the original solution $x_{i,g}$, where some variables are changed to those of the mutated solution and others are left with the values in the original solution, to create a new test solution, $u_{i,g}$. This test solution is evaluated against the problem objectives and compared to the original. If it is superior, then it replaces the original solution and the original is placed in the archive of ‘worst’ solutions. If it is inferior, then it is discarded.

For other DE algorithms and other evolutionary algorithms, the likelihood of mutation and crossover occurring is typically set by the user and can drastically affect the performance of the algorithm depending on the values used. In JADE, the setting of these parameters is handled by the algorithm itself, and these probabilities are sampled from distributions, the mean values of which are determined by previous successful solutions. This allows the algorithm to use feedback from the search process to adjust its own control parameters, and significantly reduces the amount of training time needed to ‘tune’ the algorithm on new problems.

MOJADE is a multi-objective adaptation of the JADE differential evolution algorithm, first developed by Zhang and Sanderson (2009). MOJADE was developed to investigate the performance of DE algorithms on optimization problems in nuclear engineering, and was first presented in (Charles and Parks, 2017), where it was shown to outperform a conventional genetic algorithm. It has since been shown to be effective on more complex problems and its performance is relatively insensitive to changes in its control parameters (Charles and Parks, 2018), making it a suitable choice for the multi-physics design problems under consideration. MOJADE was implemented in C++ and has two major modifications to allow optimization within a multi-objective environment. Firstly, selection and ranking use the concept of dominance to allow for representation of the Pareto-front. This makes the subset of ‘best’ solutions a list of currently non-dominated solutions (i.e. the current Pareto-front within a generation). Secondly, the archive only accepts dominated solutions but features an additional separate archive of new solutions which are Pareto-equivalent (which neither dominate nor are dominated). Further details of MOJADE and its pseudocode can be found in (Charles and Parks, 2018).

3. EPR test problem

3.1. *The EPR*

The UK European Pressurized Reactor or EPR is a Pressurized Water Reactor (PWR), designed by Framatome and Electricité de France (EDF) for construction and operation in the UK (Orano & EDF, 2007). It has a rated thermal power of 4500 MW and an electrical power of around 1630 MW. It was designed to improve over existing technology in a number of ways, including core damage frequency, plant availability, load following capability, and an ability to load up to 50 % of the core with MOX fuel assemblies. As part of the UK's Generic Design Assessment regulatory process with the Office of Nuclear Regulation, documents were made publicly available and contain significant details pertaining to the design and operation of the UK EPR (Orano & EDF, 2007). From these it is possible to construct a representative model of the EPR reactor core fuel assemblies.

3.2. *WIMS and the ARTHUR subchannel module*

The lattice reactor physics code WIMS is used to solve the neutron transport equation, to produce the flux map for the supercell and to calculate individual pin powers. A development version of WIMS was used for this work to include the recently developed 'ARTHUR' subchannel module, which is due to be released in the Quality Assured (QA) release of WIMS 11 (Tollit et al., 2018). Based on established approaches such as the COBRA code series (Pacific Northwest Laboratory, 1983), ARTHUR provides an integrated thermal hydraulics solver capable of modelling at the fuel assembly average resolution and also at a pin-by-pin / channel-by-channel resolution. ARTHUR solves the energy conservation equation for pins, coupled to coolant channel mass, momentum and energy conservation equations. Using an integrated solver avoids the difficulties involved in attempting to couple two separate codes together, and has potential benefits in avoiding the increased computational loads associated with coupled codes. Coupled codes require each code to either pause during runtime to await the output of the other (requiring continued memory usage), or to exit completely and restart once the other code has finished (increasing the read / write demand). Integrated codes, on the other hand, continue without interruption.

Some features of the ARTHUR module as implemented in this work include:

- The Finite Volume Method to solve for enthalpy, axial mass flow rate and pressure drop;
- The pin conduction model includes user-specified material properties and fuel-cladding-gap heat transfer, featuring the Dittus (Dittus & Boelter, 1985) and Thom (Thom et al., 1965) heat transfer correlations;
- Electric Power Research Institute (EPRI) (Lellouche & Zolotar, 1982) models are used for sub-cooled boiling and vapour slip;
- The Blasius friction model and two-phase factors (Blasius, 1913);
- The EPRI correlation (Reddy & Fighetti, 1983) is used for Critical Heat Flux prediction.

ARTHUR solves for thermal hydraulics using the power profile generated by the MERLIN module, a homogeneous SP3 approximation solver. New material densities and temperatures are then used to update the appropriate cross-sections for the model, and the process repeats until some kind of convergence criterion has been achieved (e.g. on temperature, k-infinity, or a hard iteration limit).

3.3. Test problem

This investigation uses a 2×2 supercell of UK EPR-type fuel assemblies with translational (top-bottom, left-right) boundary conditions around all four radial edges, and vacuum boundaries at the top and bottom. The supercell consists of two UO₂ fuel assemblies and two MOX fuel assemblies arranged in a checkerboard pattern, as shown in Figure 1, without axial reflector. All assemblies are fresh fuel, with the exact MOX compositions and uranium enrichments depending on the supercell created. This model therefore represents a UK EPR core of 50% MOX assembly loading.

Figure 1 – EPR supercell of 2 MOX fuel assemblies and 2 UOX fuel assemblies arranged in a 2×2 grid. Yellow pins are Guide Tubes, grey pins are UOX, green pins are MOX type 1, orange pins are MOX type 2, red pins are MOX type 3.

The design problem concerns optimizing the distribution of plutonium and gadolinium within the MOX and UO₂ fuel assemblies to optimize the following objectives:

1. Maximize the amount of plutonium in the assembly (MOXT) at beginning of life
2. Minimize the Power Peaking Factor (PPF) over the life of the assembly
3. Maximize the minimum Departure from Nucleate Boiling Ratio (DNBR) encountered over the life of the assembly¹

These objectives were chosen as they represent desirable performance and safety criteria for nuclear fuel assemblies. To achieve these objectives, the algorithm generates different sets of 2×2 assemblies with three types of MOX pin with varying MOX pin amounts. These supercells are then evaluated using the WIMS reactor physics code in order to determine their performance against the objectives. The algorithm then selects which supercell designs are

¹ Operating closer to the departure from nucleate boiling point increases the amount of heat transfer and is therefore more beneficial from a performance standpoint. However, in this study the DNBR is used purely as a safety criterion and hence is maximized, in order to determine the minimum safety margin that exists for this design, which would inform the design engineer on how much potential safety margin they have to work with when considering other factors.

allowed to proceed to the next generation, and the process repeats until a generation limit has been reached. Through a process of trial-and-error, a generation limit of 50 was chosen for this problem, as by then the Pareto-front had been most clearly established and was no longer undergoing significant change from generation to generation.

To offset the additional reactivity and potential for power asymmetry within the reactor produced by including plutonium, the algorithm has the ability to substitute MOX pins and UO₂ pins with gadolinium oxide pins of up to 10 wt% gadolinium. There is no upper limit to the number of gadolinia pins that can be placed, but the presence of gadolinia in the MOX assembly necessarily reduces the amount of Pu contained within the assembly. Therefore, it provides another means of balancing the trade-offs between the objectives.

The supercell was depleted to 15 GWd/t as a simplified representation of the length of a single PWR cycle. In real-world operation, assemblies do not have a fixed uniform burnup as the radial and axial power-shapes are not completely flat. In addition, the shuffling of fuel during reloading will place fresh fuel next to once- or twice-burnt fuel. However, for the purposes of the study, a fixed burnup is used as a proof-of-concept for the applicability of the methodology to real-world engineering problems. A rating of 38 MW/t was assumed for all evaluated assemblies when calculating depletion. Burnup was performed in 4 steps: an initial depletion of 1×10^{-12} MWd/t during which saturated quantities of Xe135 are calculated and added to fuel materials, to represent xenon equilibrium with fresh fuel. Following this, there is an increment to 1 GWd/t, then increments to 8 GWd/t and finally 15 GWd/t. These steps were chosen after a trial-and-error investigation to determine a sufficient resolution to accurately model burnup to 15 GWd/t whilst minimizing the number of steps (and hence the computational cost). Each depletion step consisted of a neutronics / thermal hydraulics solver loop to include the thermal-hydraulic effects and recalculate the PPF and DNBR objective values for every depletion step, in order to evaluate these objectives over the life of the assembly.

To include thermal-hydraulic feedback affecting criticality, WIMS was executed iteratively a number of times to allow convergence between neutronics and thermal hydraulics. Through testing, it was found that an iteration of 2 cycles was sufficient to reliably give good agreement between cycles of around 500 pcm. This is also justified by the nature of the problem, which is to search a very large possible search space for potentially good solutions, and not to claim that a detailed design evaluation has been performed on every solution. Furthermore, for generated solutions that have extremely heterogeneous layouts (such as large gradients of plutonium concentration within the MOX assembly), the resulting PPF- and DNBR-evaluated objectives are likely to be too poor for the solution to be selected for the next generation, let alone for the solution to be on the Pareto-front. It is therefore not worth the additional computational effort required to fully converge the multi-physics simulations.

The model was set up using material and design data sourced from the Pre-Construction Safety report, specifically Chapter 4 – Reactor and Core Design (EDF, 2012), which sets out the physical dimensions for the supercell (Table 1), as well as material data such as the plutonium vector (Table 2) and coolant properties (Table 3). Material property data were sourced from (IAEA, 2006). Some properties will be changed by the algorithm; these are highlighted in Table 2.

Table 1 – PWR fuel assembly properties

Parameter	Value
Core height (active)	4.2 m
Assembly layout	17 × 17
Pin pitch	1.2598 cm
Fuel pellet radius	0.40956 cm
Fuel pin radius	0.4751 cm
Number of fuel pins	265
Guide tube radius	0.5725 cm
Guide tube radius + cladding	0.6225 cm
Number of guide tubes	24
Gap between fuel assemblies	0.08 cm

Table 2 – PWR material properties

Parameter	Value
Fuel temperature starting estimate	600 °C
UO ₂ pin composition	Uranium dioxide
Uranium vector (wt%)	U234 – 0.04 % U235 – 5 % U238 – 94.96 % (algorithm controlled)
Plutonium vector (wt%)	Pu238 – 4 % Pu239 – 50 % Pu240 – 23 % Pu241 – 12 % Pu242 – 9.5 % Am241 – 1.5 %
MOX pin composition	Uranium / plutonium dioxide (algorithm controlled)
Maximum wt% Pu per MOX pin	20 %
MOX pin U235 enrichment (wt%)	0.2 %
UO ₂ -gadolinium pin composition	Gadolinia / uranium dioxide (algorithm controlled)
Gadolinium vector (wt%)	Gd152 – 0.2 % Gd154 – 2.18 % Gd155 – 14.8 % Gd156 – 20.47 % Gd157 – 15.65 % Gd158 – 24.84 % Gd160 – 21.86 %
Maximum gadolinia per Gd-UO ₂ pin (wt%)	10 %
Gadolinia pin U235 enrichment	2.6 %
Cladding material	Zircaloy-4 ²
Coolant material	Borated water (700 ppm, based on EPR Cycle 1 nominal power with xenon equilibrium (EDF, 2012))

² The UK EPR uses Zircaloy M5, but this is approximated to Zircaloy-4 as correlations for thermal conductivity

Table 3 – EPR coolant properties

Parameter	Value
Coolant inlet temperature	295.6 °C
Coolant velocity	500 cm / s
Core inlet pressure	155 bar

Both the MOX and UO₂ assemblies were assumed to have 1/8th symmetry, giving 40 unique pin positions for each assembly. When generating the initial population, a maximum of five pins per 1/8th of each assembly can be gadolinium pins. However, during the optimization process, there is no upper limit on how many pins can be gadolinium, as this is naturally counterbalanced by the objective of maximizing the amount of plutonium contained within the MOX assembly. Three types of MOX pin are allowed with plutonium oxide concentrations up to 20 wt% per pin. The U235 enrichment for MOX pins is kept fixed at 0.2 wt%, but for UO₂ pins it can vary up to 5 wt%. MOX pins are confined to the MOX assembly and UO₂ pins are confined to the UO₂ assembly to preserve heterogeneity – only gadolinium pins can be placed in both assemblies. The value of each design variable for each assembly is determined by the MOJADE algorithm in its function to generate solutions which most optimally satisfy the objectives.

3.4. Moderator Temperature Coefficient constraint

All solutions generated by the algorithm were constrained to have a negative Moderator Temperature Coefficient (MTC) of reactivity, which is typical for LWRs under nominal conditions. This constraint is imposed before the solution is evaluated against the objectives in order to reduce computational running time. Solutions which fail to satisfy the MTC constraint are rejected outright and new solutions which do satisfy the constraint are generated to replace them. The MTC was not selected as an objective to optimize, as requiring it to be minimized could have resulted in unrealistic assembly designs: a negative MTC is desirable but a large negative value of MTC places unacceptable demands on the reactivity control system, particularly for certain cool-down accident scenarios such as a mainline steam break. The MTC is primarily affected by the moderator-to-fuel ratio and increases with the amount of fuel in the reactor (e.g. increasing the wt% Pu in the MOX pins). Therefore, due to the objectives of the study, the MTC value was not expected to be excessively negative. In the UK EPR, the MTC ranges between –20 and ~–80 pcm/°C.

3.5. Baseline comparison

In order to provide some indication as to the effectiveness of the optimization algorithm, a comparison solution was generated based on data from the publicly available literature on the EPR design in (EDF, 2012). Some assumptions were necessary as not all the necessary data is publicly available. These include:

- No gadolinia pins were included in the baseline design. In the available literature, the EPR is described as being capable of handling up to 50 % MOX assemblies, although core layout pictures only depict up to a 30 % loading, with the MOX assemblies surrounded by UOX

are more easily accessible. Since the main differences between the two are concerned with fuel performance and not neutronics or thermal hydraulics, this was judged as an acceptable simplification.

assemblies with varying numbers of gadolinia pins. The majority of assemblies surrounding MOX assemblies do not have gadolinia pins in the layouts provided.

- Region averages of plutonium content were assumed for each of the three MOX pin types. In the baseline design, a maximum limit of 7.44 wt% Pu per fuel rod is applied to comply with fabrication limits and also to limit the impact on the void coefficient³, according to (EDF, 2012). For designs generated by the algorithm, this limit was changed to 20 wt% (consistent with other studies, e.g. (Lattarulo et al., 2014)) in order to examine the effect of pins with higher wt% Pu. Given this study is a demonstration of the capabilities of the algorithm and the resulting trade-offs between objectives, and is not intended to provide new assembly designs that would necessarily be suitable for manufacture and deployment, this was deemed to be an acceptable constraint relaxation. The supercell baseline design layout is presented in Figure 2, which shows the values of wt% Pu within the MOX pins that are normally controlled by the optimization algorithm.

Figure 2 – Baseline EPR supercell. 3 wt% Pu in MOX type 1, 6 wt% Pu in MOX type 2, 7 wt% Pu in MOX type 3.

This model was evaluated using the same methodology as algorithm-generated solutions are evaluated under, and its objective values were used to provide a baseline comparison.

³ Increasing the Pu content in MOX assemblies increases the void coefficient due to the peak in thermal capture of Pu239 at ~0.3eV, which encourages hardening of the spectrum.

4. ABWR test problem

4.1. The ABWR

The ABWR is the latest design of generation III+ reactor in operation by GE Hitachi Nuclear Energy. It has a rated full power of 1350 MWe (Hitachi, 2014). Currently in operation at three sites in Japan, there have been numerous plans to construct additional reactors in Japan, Taiwan, the United States and in the UK. Unfortunately, all of these projects have either been suspended or cancelled for financial reasons, with the UK project being the latest to face cancellation (BBC News, 2019). However, the design remains a possible future reactor choice. As BWRs differ substantially in operation to PWRs with more complicated thermal hydraulics (the primary coolant undergoing a phase change inside the core), they offer unique problems on which to test the performance of our design optimization framework, utilizing multi-physics software. Two of these features, which were modelled in the problem, are detailed below.

Firstly, due to the primary coolant phase change, the axial fuel composition of BWR fuel pins is generally more heterogeneous than PWR fuel pins. BWRs can utilize partial-length rods to decrease the amount of fuel in the upper regions of the core, which offsets the increased neutron mean free path in steam and reduces the likelihood of U238 in the fuel absorbing a neutron and creating Pu239. The pressure drop is also reduced, potentially allowing for more fuel rods or a larger fuel rod diameter.

Secondly, water rods placed in the centre of the bundle increase the moderation effect, decrease the maximum local power factor and reduce the magnitude of the void coefficient of reactivity by increasing the fuel-to-moderator ratio (Bozzola, 1982).

4.2. Test problem

Figure 3 – $\frac{1}{4}$ (lower right) of an ABWR cell, featuring one fuel bundle, adapted from (Hitachi-GE, 2017).

As before, the same development version of the lattice reactor physics code WIMS is used to determine the flux profile and individual pin powers, along with the integrated thermal hydraulics solver. This test problem concerns a single BWR fuel assembly (Figure 3), modelled as three 10×10 grids of fuel pins and two water rods, with reflective boundary conditions, to represent three axial layers of a 3D fuel bundle inside the reactor core (Figure 4). Three layers were chosen as a compromise between accuracy and computational speed.

Figure 4 – Three axial layers comprising the 3D representation of an ABWR assembly used in this study, showing water rods and partial-length fuel rods (full-length fuel rods not shown here), adapted from (Hitachi-GE, 2017).

Each axial layer is first solved for the neutron flux using the Method of Characteristics. These layers are then merged to form a 3D model which is solved for the neutron flux in 3D using the simplified spherical harmonics method (Gelbard et al., 1959), with reflective boundaries along the radial edges and vacuum boundaries at the top and bottom. The 3D flux solution is used to determine the thermal-hydraulic feedback, which then updates the material properties (density and temperature) for the axial slices, and the process continues until convergence on k -effective is achieved. This model allows simulation of both full- and partial-length fuel rods within the assembly.

Tie-rods, tie-plates, end plugs and springs, the assembly shroud, grid spacers, the control blade and axial reflectors are not modelled here. This problem is intended to showcase the concept of linking optimization methods to complex multi-physics problems, but not to undertake the detailed analysis that would be required in perfecting the design. Therefore, these omissions are deemed acceptable for the current scope, as they would only serve to increase the accuracy of the solution, and not affect the ability of the algorithm to optimize.

Convergence between thermal hydraulics and neutronics is realised for every test assembly within the multi-physics software. Unlike the looser coupling used in the previous PWR problem, the software continues to run until the difference between k -infinity of the neutronics from one iteration is at least within 100 pcm of the previous iteration. It should be emphasized that this level of convergence is not suitable for detailed design work, although may be appropriate for ranging studies performed at the conceptual design stage.

The test problem concerns optimization of the design of heterogeneous BWR fuel within the assembly, with the following objectives:

1. Minimize the gadolinium concentration within the assembly
2. Maximize the amount of plutonium in the assembly
3. Minimize the PPF in the assembly
4. Maximize the minimum Critical Heat Flux (CHF) Ratio in the assembly

For BWRs a priority safety criterion for thermal hydraulics is to prevent dryout from occurring within the coolant channels and uses the Critical Power Ratio (CPR). This happens when the CHF Ratio (CHFR) is exceeded and the annular flow regime within the channel dissipates to expose the fuel pin to vapour coolant only. This leads to highly reduced heat transfer and potential breaching of thermal limits. The standard method in safety analysis involves determining the correlation between the boiling length (the distance between the

dryout point and the point at which the quality is zero, i.e. sub-cooled boiling is no longer possible) and the critical quality (Hench & Gillis, 1981). This is in contrast to PWR thermal hydraulics where local conditions, such as heat flux, dominate the process. In ARTHUR, the CHF correlation is selected by the user, and the option chosen for this study was the EPRI correlation, which was designed with both PWR and BWR applications in mind (Reddy and Fighetti, 1983), has demonstrated good agreement with experimental results (Chen et al., 1984), and is considered to be sufficient for steady-state BWR analysis (Ferroni et al., 2009). It is used here to calculate a CHFR, which will be a performance objective to maximize and is not intended to represent the CPR.

According to the literature, the ABWR is capable of handling a 100 % MOX core (Ihara et al., 2009; Hitachi, 2017). It is therefore assumed, for the purposes of this investigation, that all the fuel pins, whether full- or partial-length, are MOX pins. Three different concentrations of MOX pin are allowed, up to 20 wt% Pu each, and one type of partial-length rod MOX concentration is allowed. The optimization algorithm can vary the distribution and number of each type of full-length MOX pin and partial-length pin across the assembly (although the position and number of water rods is kept constant). All fuel pins (full-length and partial-length) have one radius, which is allowed to vary from 0.3 to 0.55 cm and has a fixed cladding thickness of 0.066 cm. Each of the two water rods is modelled in the lattice code simply as four separate water rods in a 2×2 configuration, with a radius of 0.5325 cm each, to conserve mass.⁴ The control blade is not modelled. The layout is as shown previously in Figure 3. The assemblies are evaluated as before using the multi-physics software in order to determine their performance against the objectives, which determines which designs will be chosen for the next generation. This process repeats until a generation limit of 50 is reached.

In the same manner as for the PWR problem, physical (Table 4), material (Table 5) and coolant properties (Table 6) were sourced from the ABWR Pre-Construction Safety Report, specifically Chapter 11 – Reactor Core (Hitachi-GE, 2017a) as well as (IAEA, 2011) and (Peakman et al., 2019). Some material property data was sourced from (IAEA, 2006). Some properties will be changed by the optimization algorithm; these are highlighted in Table 5.

⁴ The thermal hydraulics module in the development version of WIMS used in this study did not feature cross-channel mixing (i.e. the coolant in a channel surrounding one fuel pin does not mix with neighbouring channels). Therefore modelling a single water rod as four separate rods does not have the same thermal-hydraulic implications here as it would in real life.

Table 4 – BWR fuel assembly properties

Parameter	Value
Core height (active)	3.810 m
Partial-rod length	2.540 m (due to three axial layers modelled)
Assembly layout	10 × 10
Pin pitch	1.295 cm
Fuel pin radius	0.3 – 0.55 cm (algorithm controlled)
Fuel cladding thickness	0.066 cm
Number of fuel pins	92 (49 with ½ assembly symmetry)
Water pin radius (Each modelled as 4 smaller pins in a 2 × 2 configuration)	1.161 cm, modelled as 4 pins of radius 0.5325 cm each

Table 5 – BWR material properties

Parameter	Value
Fuel temperature starting estimate	600 °C
Plutonium vector (wt%)	Pu238 – 4 % Pu239 – 50 % Pu240 – 23 % Pu241 – 12 % Pu242 – 9.5 % Am241 – 1.5 %
MOX pin composition	Uranium / plutonium dioxide (algorithm controlled)
Maximum wt% Pu per MOX pin	20 %
MOX pin U235 enrichment (wt%)	0.07 – 5 % (algorithm controlled)
Cladding material	Zircaloy-2
Coolant material	Non-borated water

Table 6 - BWR coolant properties

Parameter	Value
Coolant inlet temperature	278 °C
Coolant mass flowrate per assembly	16,628.44 kg/s
Core pressure	71.7 bar

Assemblies were assumed to have ½ symmetry, giving 49 unique pin positions per assembly. No limit was placed on the number of partial-length pins since the total amount of plutonium in the assembly is reduced if a partial-length rod is used, which reduces the performance against objective 2.

4.3. Void Coefficient constraint

All solutions generated by the algorithm were constrained to have a negative Void Coefficient (VC) of reactivity. Solutions which fail to satisfy the VC constraint are rejected outright and new solutions which do satisfy the constraint are generated to replace them.

4.4. Baseline comparison

As before, a baseline was generated using available data from the literature. However, as there was no information available for the design of MOX ABWR assemblies, the baseline comparison is for a UO₂-only ABWR assembly, which features a uniform enrichment of 4.9 wt% and zero partial-length rods. The radius of the fuel pins was 0.447 cm. The radius of the equivalent water rods was kept at 0.5325 cm.

5. Results and discussion

5.1. EPR test results

The Pareto-front solutions from 20 independent runs of the design optimization process were recorded and an overall Pareto-front against all three objectives was identified. Figure 5 and Figure 6 show the performance of PPF vs –MOXT and –DNBR vs –MOXT respectively, with the baseline design included for comparison (orange). Since all objectives are to be minimized, the lower left quadrant is the most optimal “ideal” location for each graph, although in reality it may not be possible to reach this. Solutions where all MOX pins have at least 15 wt% plutonium are coloured in red. Solutions where all MOX pins have less than 10 wt% plutonium are blue, and solutions which have MOX pin plutonium concentrations between 10 and 15 wt% are coloured in green. For Figure 6, the horizontal line denotes where the DNBR limit is breached and solutions above this line exceed the CHF. In real-world analysis, this cutoff is usually placed lower (for example, the UK EPR uses a DNBR limit of 1.21 for high pressure accidents, and a limit of 1.12 for low pressure accidents). In Figure 6, the line is purely there for reference to the CHF and is not a comment on the suitability of solutions against real-world DNBR limits.

Figure 5 – PPF vs –MOXT for Pareto-front solutions from the EPR problem.

Figure 6 – –DNBR vs –MOXT for Pareto-front solutions for the EPR problem.

As Figure 5 and Figure 6 show, the optimization algorithm was able to find a variety of solutions which feature higher values of plutonium content, solutions which have lower PPF values, and solutions which have higher margins to CHF (–DNBR). The outlier solution on Figure 6 has a –DNBR value of ~ -0.55 , clearly unacceptable for any real-world application. It also shows that the algorithm was not able to find a Pareto-front solution with a MOXT value of greater than 23 that also had a DNBR greater than one. This suggests a limit on the maximum plutonium content permissible without performing other design changes, such as increasing the pin pitch to increase the moderator-to-fuel ratio and soften the spectrum, as well as improving thermal-hydraulic conditions.

It can also be seen from these graphs that the algorithm may have produced solutions that dominate the reference solution. However, this cannot be conclusively determined from these

2D graphs alone. This highlights an additional challenge posed by multi-objective problems: how to visualize multi-dimensional data.

For problems with more than two objectives, displaying the results showing the trade-off between various objectives in a clear manner is not straightforward. One solution to this is to use Parallel Coordinates (PC), developed by Inselberg (1985). By mapping multi-variate relations into indexed subsets, this constrains the display of information to a two-dimensional space. What is then produced is a series of polylines, which represent individual Pareto-front solutions on a 2D graph with multiple y-axes separated equidistantly. Each y-axis represents a variable, and where the line crosses that axis denotes the value of that variable for that solution (likewise, if the y-axis represents the value of an objective, the intersection denotes that solution's performance against that objective). Visualizing complex multi-dimensional data in this way can reveal commonalities between solutions and trends in the plotted data, which can lead to greater understanding of the nature of trade-offs and the features of highly performing solutions.

The Pareto-front solutions formed from the 20 independent runs on this problem are displayed using the Parallel Coordinates software Xdat (Xdat, 2019) in Figure 8. In this figure, the first 40 y-axes represent the plutonium concentrations within the MOX assemblies. The second set of 40 y-axes then show the pins for the UOX assemblies. Pins are numbered according to Figure 7.

									40
								38	39
							35	36	37
							33	34	
					28	29	30	31	32
					23	24	25	26	27
			18	19	20		21	22	
		10	11	12	13	14	15	16	17
1	2	3	4	5	6	7	8	9	

Figure 7 – Numbering of pins in EPR assemblies with 1/8th symmetry.

In both cases, negative values on the y-axes indicate the gadolinium content in the pin. The objective values of –MOXT, PPF and –DNBR for each Pareto-front solution are shown on the right-hand side of Figure 8, inverted so that the ‘best’ solutions are at the top. The same colour scheme used for the previous graphs is used here. The highlighted black line corresponds to the one solution found that dominates (has better values of all three objectives than) the baseline design. Figure 9 shows the dominating supercell design.

Figure 8 – Parallel Coordinates plot of each Pareto-front solution for the EPR problem and corresponding objective values, with the dominating solution highlighted in black.

Figure 9 – Supercell design of the one solution found that dominates the EPR baseline design (Figure 2). Numbers inside the assemblies denote wt% Pu.

5.2. Discussion of EPR test results

Figures 5, 6 and 8 show results which are typical of such optimization problems. MOX assemblies which contain high amounts of plutonium naturally do better at the $-MOXT$ objective, but perform worse against PPF and $-DNBR$ than their low $-MOXT$ counterparts, and there appears to be a direct correlation between PPF and $-DNBR$ as one would expect. Whilst the Pareto-front contains a wide variety of wt% Pu pin compositions, there do not appear to be large differences in the three wt% Pu MOX pin types determined for each solution (the largest difference between MOX pin types in a single solution was 6.87 wt% compared to 4 wt% for the baseline). Filtering these to focus on the one solution that dominates the baseline design and the two supercell layouts in Figure 2 and Figure 9, we can see the range of wt% Pu MOX pins has been further decreased to between 7 and 9 wt% Pu. The lower wt% Pu pins have been moved into the central locations to reduce the radial power peaking. No gadolinium pins have been used in the MOX or UOX assemblies, and this trend in the results is discussed further below.

The problem did not contain a specific objective for k-effective, as has been the case in other optimization studies, as setting a ‘target’ would introduce subjectivity into the results based on the target chosen. As a result, the employment of gadolinium in designs created by the optimization algorithm was solely to improve performance against the objectives of reducing PPF and maximizing DNBR over the life of the assembly. Since placement of gadolinium inside the MOX assemblies would negatively affect the performance against the objective of maximizing the amount of plutonium inside those assemblies, most solutions on the Pareto-

front feature very few, if any, gadolinia pins inside the MOX assemblies. (This can be seen in Figure 8, with the average number of gadolinia pins inside MOX assemblies amongst the Pareto-front solutions being just 0.02 per 1/8th assembly due to symmetry.) However, as Figure 8 shows, many Pareto-front solutions do feature gadolinium inside the UOX assemblies.

Figure 10 shows the average amount of gadolinium per pin in the supercell versus the change in k-effective over one cycle, using the same colour-coded wt% Pu MOX assemblies as before. As one would expect, there is a general trend for supercells with higher average gadolinia contents to have a smaller reduction in k-effective over the course of depletion, as the presence of burnable poisons suppresses reactivity at the beginning of life, enabling more fissile material to be loaded into the core in order to increase the cycle length. The design with the highest gadolinia content (highlighted in the black circle on the graph) has one of the high estimated wt% Pu MOX values, with no gadolinia pins in the MOX assembly (but 6 per 1/8th UOX assembly) and objective values of –19.36, 1.26 and –1.16 for –MOXT, PPF and –DNBR, respectively. In comparison, other high wt% Pu MOX designs feature larger reactivity swings, and, in some cases, worse PPF, –DNBR, or –MOXT values. This highlights the benefit of careful selection of objectives and variables: optimization can yield additional information about the search space without requiring separate sensitivity studies for each variable, potentially reducing time and cost on the project. In this case, designs using gadolinium are produced which reduce reactivity swings, PPF and DNBR without requiring a specific objective to include gadolinium or an objective (or constraint) to reach a target k-effective.

Figure 10 – Average wt% Gd per pin inside the MOX assemblies for the EPR problem Pareto-front solutions vs their corresponding reduction in k-effective for a burnup of 0–15 GWd/t.

It should be noted that, whilst the baseline comparison did not feature gadolinia poison, UK-EPR reactor fuel assemblies do in real life, with designs featuring 8, 12 or 16 gadolinia rods per UOX assembly. In a potential future study designed to optimize EPR fuel assemblies, gadolinia would need to be included in the baseline comparison case in order to properly evaluate any objective relating to k-effective.

5.3. EPR test conclusions

As well as demonstrating the continued applicability of multi-objective optimization to multi-physics nuclear engineering problems, this study serves to reinforce the following benefits of non-dominated multi-objective optimization:

1. Multi-objective optimization can reveal additional information about the search space, even outside of the pre-set objectives, and can assist engineers in managing trade-offs through identifying important variables such as gadolinium distribution.
2. The multi-objective optimization algorithm MOJADE is capable of generating designs of four PWR assemblies arranged in a 2×2 supercell, with 40 MOX pin locations and compositions and 40 UOX pin locations and compositions, that result in Pareto-equivalent objective performance to the established baseline design or perform better across all objectives throughout the depletion of the assembly.

5.4. ABWR test results

With four objectives, projection onto 2D graphs would reveal little about the nature of the Pareto-front. However, Parallel Coordinates can again be used to visualize and analyse the results. Figure 11 shows a PC plot of the four objectives using data from a single optimization run. The blue lines are the starting population, created randomly using the CPU clock at initialization as the random seed. The red lines are the resultant Pareto-front solutions after 50 generations of the MOJADE algorithm. The green line is the baseline solution provided for comparison.

Figure 11 – Parallel Coordinates plot of the objective performance of Pareto-front solutions from one run on the ABWR problem.

It is shown in Figure 11 that the algorithm has definitely been able to improve on the starting population and find a Pareto-front. It can also be seen that the found Pareto-front solutions improve on the two safety related objectives – PPF and CHFR, whilst increasing the MOX content and minimizing (relative to other solutions) the gadolinium content. This demonstrates

that the optimization algorithm is able to identify solutions which can be said to be superior to the baseline.

Visualizing the full Pareto-front of 20 independent optimization runs becomes impractical even when using PC, due to the number of Pareto-front solutions⁵. Other features of the Pareto-front include a smaller pin radius on average of ~ 0.34 cm with a standard deviation of 0.02 cm, compared to the baseline of 0.447 cm. This indicates the algorithm favoured increasing the moderator-to-fuel ratio at the cost of smaller fuel elements and hence less overall plutonium in the assembly (although this was not explicitly reflected in the $-MOXT$ objective since it was based on a wt%). This clearly contributed to the improved performance against PPF and particularly $-CHFR$, where every solution was able to improve on the baseline. Figure 12 shows the frequency in % of each pin in an assembly (numbered 1 to 49, as shown in Figure 12) either being a partial-length rod or a gadolinium rod.

Figure 12 – Frequency of a gadolinium rod (blue) or a partial-length rod (red) featured (left) for each of the possible 49 unique pin positions in the ABWR test assembly (right) in the Pareto-front solutions found in 20 independent optimization runs. Pin position 33 is highlighted in yellow.

Figure 12 shows that the Pareto-front solutions make use of partial-length rods up to 15 % of the time for each pin, and no location was particularly favourable to being a partial-length rod. As for gadolinium rods, the central pin (pin 33) location was most commonly (22 % of the time) found to be gadolinium. In the real world, the central pin is often a partial-length fuel rod, and gadolinium is dispersed in the assemblies with axial heterogeneity (Bozzola, 1982) as a means of reducing excess reactivity at the beginning of life, rather than a means of reducing the PPF. Nevertheless, MOJADE clearly used both partial-length rods and gadolinium rods in an attempt to improve the objectives relating to power peaking and thermal hydraulics, and evidently found that placing a Gd or a partial-length rod in the central pin reduces power peaking.

⁵ As the number of competing objectives increases, the number of trade-offs increases and the likelihood that one solution is non-dominated decreases. With four objectives it is more likely that solutions are Pareto-equivalent rather than dominating/dominated.

5.5. ABWR test conclusions

The algorithm MOJADE was able to tackle a fully 3D optimization problem featuring 10 different types of rods and 49 different rod locations, and generated a set of designs, which when considering the overall Pareto-front from 20 independent runs, improved on the PPF and CHFR of the baseline solution in 87 % of cases. Analysis showed that MOJADE used the optional gadolinium and partial-length rods to reduce power peaking in the central assembly regions as it attempted to optimize the thermal-hydraulic objectives.

6. Conclusions

This study serves to show that multi-objective algorithms can be applied successfully to nuclear engineering design optimization problems with realistic levels of complexity, utilizing multi-physics analysis methods to identify solutions which have the potential to outperform reference designs. It has been demonstrated that when combined with some of the latest coupled multi-physics codes, MOJADE is still capable of converging on optimized designs and operates in a multi-objective manner by exploring the trade-offs involved using optional non-fuel elements. For the EPR problem, MOJADE optimized both UOX and MOX assemblies simultaneously considering thermal hydraulics, depletion and burnable poison non-fuel elements. A solution that dominates the reference design was found, and analysis also showed that the results gave insight into using gadolinium to reduce reactivity changes over the cycle. For the ABWR problem, a single BWR fuel assembly was optimized using a tight coupling of neutronics and thermal hydraulics and considering both gadolinium and partial-length rods as non-fuel elements. In both cases, a Pareto-front and dominating solutions compared to baseline solutions based on the available literature were found.

This study is not intended to identify superior designs to either the current EPR or ABWR designs or to point out deficiencies in the existing designs, but rather to illustrate how multi-objective optimization can be applied to complex 3D multi-physics problems to provide insight into the search space which can inform the design process. Further work could look at establishing the convergence criteria necessary for the MOJADE algorithm to have optimal performance, as well as further testing on real-world problems for which complete data about existing fuel assembly designs is publicly available.

7. Data availability statement

To the best of the authors' knowledge, this paper and references herein contain all the data needed to reproduce and validate the results presented.

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