Parametric neutronics analyses of lattice geometry and coolant candidates for a soluble-boron-free civil marine SMR core using micro-heterogeneous duplex fuel

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Abstract

Civilian marine reactors face a unique set of design challenges in addition to the usual irradiation and thermal-hydraulic limits affecting all reactors. These include requirements for a small core size, long core lifetime, a 20% cap on fissile loading, and limitations on the use of soluble boron. One way to achieve higher burnup/longer core life is to alter the neutron spectrum by changing the hydrogen-to-heavy-metal ratio, thus increasing the conversion of fertile isotopes in the fuel. In this reactor physics study, we optimize the two-dimensional lattice geometry of a 333 MWth soluble-boron-free marine PWR for 18% ^{235}U enriched micro-heterogeneous ThO_2-UO_2 duplex fuel and 15% ^{235}U enriched homogeneously mixed all-UO_2 fuel. We consider two types of coolant: H_2O and mixed 80% D_2O + 20% H_2O. We aim to observe in which spectrum discharge burnup is maximized in order to improve uranium utilization, while satisfying the constraint on moderator temperature coefficient. It is observed that higher discharge burnup for the candidate fuels is achievable by using either a wetter lattice or a much drier lattice than normal, while epithermal lattices are distinctly inferior performers. The thorium-rich duplex fuel exhibits higher discharge burnup potential than the all-UO_2 fuel for all moderation regimes for both coolants. The candidate fuels exhibit higher initial reactivity and discharge burnup with the mixed D_2O-H_2O coolant than with the H_2O coolant in the under-moderated regime, whereas these values are lower for the D_2O-H_2O coolant in the over-moderated regime.

Keywords: Civil marine propulsion, Small modular reactor, Soluble-boron-free operation, Micro-heterogeneous thorium-based duplex fuel, Lattice geometry optimization, Achievable discharge burnup, Initial reactivity, Conversion ratio, Moderator temperature coefficient.

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1. Introduction

Perhaps surprisingly, interest is presently being shown in the possible application of nuclear energy in marine propulsion and this topic has recently received renewed attention after many years of apparent neglect (Hirdaris et al., 2014, Ragheb, 2012, Carlton et al., 2011, Sawyer et al., 2008). Since 2002 there has been a resurgence of reconsidering the technical and economic feasibility of technology options for marine nuclear propulsion due to the environmental concerns and changes in market economics. A nuclear-powered ship – be it a surface ship or a submarine – receives its propulsion energy from a nuclear power plant on board, and can be dubbed an "atomic engine" (Ragheb, 2012). The main advantages of nuclear marine propulsion are that atomic engines do not consume hydrocarbon-based fuel and oxygen, and produce no exhaust gas (Ragheb, 2012). Atomic engines are reliable, compact sources of energy that can operate for years without new fuel (Hirdaris et al., 2014). These benefits have motivated the development of atomic engines without too much concern regarding cost (Hirdaris et al., 2014, Carlton et al., 2011, Sawyer et al., 2008). The employment of advanced reactors and a careful concentration on cost-conscious design can result in nuclear marine propulsion systems that are economically superior to conventional energy systems.

In an effort to decarbonise energy production and concerns about the effects of climate change, there is growing interest in the possibility of using nuclear propulsion systems (Kramer, 1962). Maritime shipping accounts for $\sim$3% of global CO_2 emissions, and could account for 15-30% of all CO_2 emissions permitted in 2050 as economic growth in the developing world increases the volume of international commerce. The current global shipping industry emits roughly 1Gt CO_2 about a third more than current aviation emissions. Without significant policy action, future projections of global maritime shipping emissions suggest that we are likely to be on a path that would lead to global shipping emissions of $\sim$3 Gt CO_2 in 2050. This would represent almost a threefold increase on today's levels (1Gt CO_2). Diesel shipping poses serious threats to the environment both on inland waterways and on the ocean. Most large ships emit significant amounts of sulphur and nitrous oxides from the combustion of heavy fuel oil, and it is expected that maritime sources will soon account for the majority of all SO_x and NO_x emissions in Europe (Otto, 2013, Hirdaris et al., 2014). These pollutants are solely responsible for additional health costs of tens of billions of euros associated with heavy maritime traffic (Otto, 2013, Schinas and Stefanakos, 2012). Since nuclear fission produces no direct emissions, it clearly enjoys key environmental advantages over current diesel engines.

Considering the non-proliferation issues associated with naval reactors, a major loophole has been created by the Non-Proliferation Treaty (NPT) of nuclear weapons which allows a non-nuclear-weapon country to avoid international safeguards governing highly enriched weapon-grade fissile materials if it claims that the materials will be used for a nuclear marine propulsion program (McCord, 2013, Harvey, 2010). Therefore, a non-nuclear-weapon country can produce or stockpile weapons-grade highly enriched uranium (HEU) for a nuclear marine propulsion core to be constructed in the future, which can then potentially be used for the production of nuclear weapons. Concerns regarding nuclear weapons proliferation have significantly increased since some countries have sought to develop new nuclear energy programs, and it is well known that these countries can use centrifuges to make HEU more easily than previously assumed (McCord, 2013, Ma and Von Hippel, 2001). However, in recent times, there have been significant technological advances in low enrichment uranium (LEU) fuel systems and efforts made to improve LEU fuel technology in major universities and R&D departments of leading nuclear laboratories (Alam, 2018). Therefore, in light of the proliferation concerns, there is a strong motivation to examine the design of marine reactor cores with the low-enriched uranium (LEU) fuel candidates.

There are several engineering challenges unique to civil marine reactors (Ragheb, 2012). Civil marine reactors must additionally be capable of operating with long refueling intervals and low fissile loadings (Hirdaris et al., 2014), which makes it fundamentally different from land-based nuclear plant system. In previous studies (Alam, 2018, Alam et al., 2019) we have examined the feasibility of micro-heterogeneous ThO_2-UO_2 duplex fuel and all-UO_2 fuel for civil marine propulsion. We sought to design 333 MW thermal power cores that will operate with long refueling intervals of (at least) 15 effective-full-power-years (EFPY). We focus on PWR technology since this is the most common reactor in the world today, with a proven record of maritime operation. PWRs are robust and proven reactors for aircraft carrier and submarine propulsion. Therefore, a PWR type small modular reactor (SMR) is considered in this study. In addition, for reasons of operational simplicity, there is no soluble boron used in naval reactors. The elimination of soluble boron offers several advantages for reactor cores. Most of these advantages are realized through significant core simplification (removal of pipes, pumping, and purification systems), space saving, the removal of the corrosive effects of soluble boron over the long core life, and from improved safety effects, improvement of the moderator temperature coefficient and elimination of an entire class of boron dilution accidents (Kim et al., 1998). Additionally, there is concern that if a ship relying on soluble boron for reactivity control were to sink, the dilution of the coolant with seawater could cause a criticality accident (Kusunoki et al., 2000).

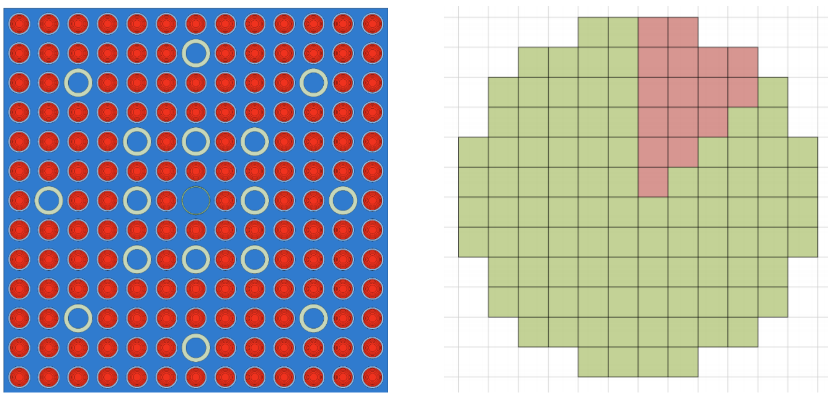
In this study, we seek to optimize the two-dimensional lattice geometry of a 333 MWth SBF marine PWR, with an emphasis on the initial reactivity, achievable discharge burnup and conversion ratio, using 18% ^{235}U enriched micro-heterogeneous ThO_2-UO_2 duplex fuel and 15% ^{235}U enriched homogeneously mixed all-UO_2 fuel. One way to achieve higher burnup/longer core life is to alter the neutron spectrum by changing the hydrogen-to-heavy-metal ratio (H/HM), thus increasing the conversion of fertile isotopes in the fuel (Otto, 2013, Xu, 2003, Alam et al., 2016). We have considered two types of coolant: H_2O and a mixture of 80% D_2O + 20% H_2O. To date, mixing light and heavy D_2O waters as a "mixed coolant" isn't practically employed (Nagy et al., 2014), although some proposed reactor designs, such as Spectral Shift Control Reactor (SSCR) (Engelder, 1961) and the Mixed Moderator PWR (MPWR) (Tochihara et al., 1998) considered this technique. In addition, for the H_2O coolant, important contributions are made by an MIT study (Xu, 2003), where optimization of the PWR lattice is performed for a range of H/HM. This study explored how many different independent variables affect discharge burnup and what types of H/HM are most effective for maximizing burnup. However, this analysis assumed licensing limits of 5% enrichment with soluble boron system.

There is a significant gap in assessing the effect of neutron spectrum variation over burnup, especially for SBF, SMR cores (Alam, 2018, Otto, 2013, Ippolito, 1990). Therefore, the main objective of this parametric neutronic study is to observe the effects of varying the neutron spectrum under different degrees of moderation in order to maximize the attainable discharge burnup (thereby improving uranium utilisation) while maintaining a negative moderator temperature coefficient (MTC). It is important to address that since the scope of this paper is limited to "parametric neutronic analyses", the safety issues (thermal-hydraulics, fuel performance) are out of the scope of this paper.

2. Design methods

2.1. Reference subassembly sizing

Our subassembly sizing calculations use a 13×13 assembly design. For purposes of comparison, we began by considering a standard Westinghouse 4-loop PWR core, which has a fueled core area of 8.9 m^2 and uses 193 assemblies with 264 pins in a 17×17 array (Winters, 2004). We found that the marine reactor requires a fueled core area of 3 m^2, a 67% reduction in area (Alam, 2018, Alam et al., 2015, Otto, 2013). If 112 assemblies with a 13×13 pin array are used, we achieve this size reduction while reducing the freedom for subassembly design and core design equally (a 42% reduction in pins per assembly and a 42% reduction in assemblies per core). Fortuitously, 112 is a 'magic number' of squares that can be formed into the approximate shape of a circle (Fig. 1b). Thus, we begin with 112 assemblies with a 13×13 arrangement. In a Westinghouse 17×17 assembly, there are 24 control pins and one instrument tube (8.7% of pin locations). We maintain a similar ratio in our design, while preserving octant symmetry to help reduce power peaking, so we have 16 control pins (9.5% of pin locations) and 153 fueled pins.



(a) (b)

Fig. 1. Subassembly sizing: (a) 13×13 assembly geometry layout; (b) Schematic of a 112-assembly core, with one octant highlighted.

2.2. Computational methods

The subassembly design analysis employed the WIMS-10 lattice physics code using nuclear data from the JEF 2.2 database available from the IAEA (Newton et al., 2008). For each burnup step, WIMS completes a 172-group 'fine' solution to the transport equation in a smeared geometry. It then refines this solution using a few-group calculation in a precise geometry. In this study, we used a 6 energy group structure, as shown in Table 1. It is important to address the calculation route for WIMS. In our study, WIMS module HEAD sets up cross-sections in library groups and PRES/CACTUS/RES sequence does a subgroup calculation of resonance shielding, where PRES sets up subgroup cross-sections at the fuel temperature, CACTUS calculates the subgroup fluxes by Method of Characteristics (MoC) and RES completes the subgroup calculation of resonance shielding. Multicell collision probability equations is solved by PERSEUS/PIP sequence. PERSEUS calculates multicell collision probabilities for the full problem in the geometry and PIP calculates neutron spectra for each material. The condensed cross-sections and flux spectrum calculated by COND module. BURNUP module carries out depletion of fuel at specified rating and timestep.

Group	1	2	3	4	5	6
Upper fine group	1	23	46	93	136	153
Lower fine group	22	45	92	135	152	172
Upper (eV)	19.64×10^{6}	820.85×10^{3}	9.12×10^{3}	4.00	625×10^{-3}	140×10^{-3}
Lower (eV)	820.85×10^{3}	9.12×10^{3}	4.00	625×10^{-3}	140×10^{-3}	110×10^{-6}

Table 1. 6-group WIMS energy structure.

2.3. Fuel selection

There have been several past studies of homogeneously mixed Th/UO_2 fuel (Galperin et al., 2002) and heterogeneous seed-blanket arrangements (Kazimi et al., 1999, Todosow et al., 2005, Clayton, 1993). Homogeneously mixed Th/UO_2 fuel only yields promising performance in a single-batch core when the ^{235}U enrichment exceeds 20% (Galperin et al., 2002, Otto, 2013). Previous studies have indicated that thorium's advantages are best realized in micro-heterogeneous and heterogeneous geometries (MacDonald and Lee, 2004), but heterogeneous seed-blanket arrangements rely on being able to remove the seed region and replace it mid-life with fresh fuel (Kazimi et al., 1999, Todosow et al., 2005, Clayton, 1993), which is not compatible with single-batch operation. In contrast, the ability of duplex fuel to exploit the potential benefits of thorium in the context of a single-batch, low enriched uranium, SBF, long-life, small modular reactor (SMR) core is yet to be fully explored (Zhao, 2001, MacDonald and Lee, 2004). Therefore, in this study we evaluate the performance of micro-heterogeneous ThO_2-UO_2 duplex fuel[1], loaded in a single-batch strategy. To provide a basis for comparison we also evaluate the performance of homogeneously mixed all-UO_2 fuel.

[1]We use the term 'duplex' to refer to the micro-heterogeneous ThO_2-UO_2 duplex fuel throughout this paper.

2.4. Design of fissile loading

In ThO_2-UO_2 duplex fuel, the UO_2 and ThO_2 components are not blended together (as in homogeneous fuel) but are discretely interspersed on small distance scales (Alam et al., 2019, Shwageraus et al., 2004, Alam et al., 2018c,d). In our case, an individual fuel pin is composed of a UO_2 centre surrounded by an annulus of pure ThO_2, as shown in Fig. 2.

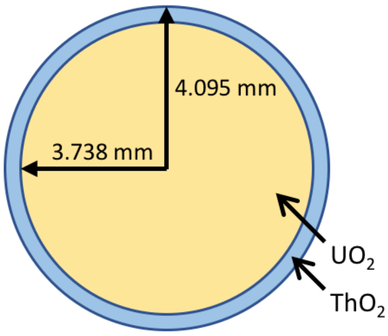
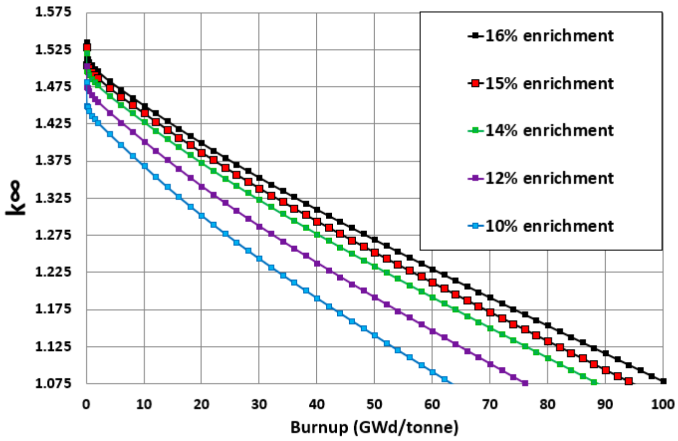


Fig. 2. Configuration of the micro-heterogeneous duplex ThO_2-UO_2 fuel.

It was assumed in the sizing analysis that the irradiation tolerance of the fuel (100 GWd/tonne) is the primary limiting factor in the core design. According to an MIT study (Xu, 2003), smaller cores are more sensitive to higher neutron leakage than that of the commercial PWR. As an example, for constant power density, a 500 MWth core will exhibit approximately twice leakage than that of the 3500 MWth core. The smaller core (500 MWth) will lose 7%, If the latter (3500 MWth) loses 3.5%. Furthermore, a recent SMR neutronic study by Oak Ridge National Lab (Brown et al., 2017) showed that $\sim$400 MWth SMR exhibits 6–8% leakage depending on the core loading patters and other input parameters. Since WIMS calculations assume an infinitely-large core and a small core is prone to larger leakage, we have assumed 7.5% leakage in this study.

In conventional PWR reactor, 4% leakage is considered while considering 2D lattice-level calculations (Alam, 2018). We have estimated from our core sizing analyses that considering our marine propulsion SMR core (Power = 333 MWth, Volume = 5.3 m^3), leakage of 7.5% is considered conservative. This leakage has been checked with 3D whole-core nodal diffusion code PANTHER (Hutt, 1992). In the assembly level analysis for fresh fuel in WIMS (which assumes an infinitely-large core), discharge burnup is 95 GWd/tonne considering 7.5% leakage, while whole-core exhibits the average burnup of 97 GWd/tonne, which proves that 7.5% leakage is conservative for our SMR core design. The discharge burnup is therefore estimated from the point on the assembly burnup curve where the infinite multiplication factor, k_∞, is 1.075.

The fissile loadings of the duplex and UO_2 fuels were determined from enrichment sensitivity studies, seeking values that keep the core critical for a burnup of $\sim$95 GWd/tonne. It is clear from Figs. 3a and 3b that, in order to achieve the target discharge burnup, initial enrichments of 15% and 18% ^{235}U are required for the UO_2 and duplex fuels, respectively. The duplex fuel requires higher enrichment than the all-UO_2 fuel due, in part, to the lower



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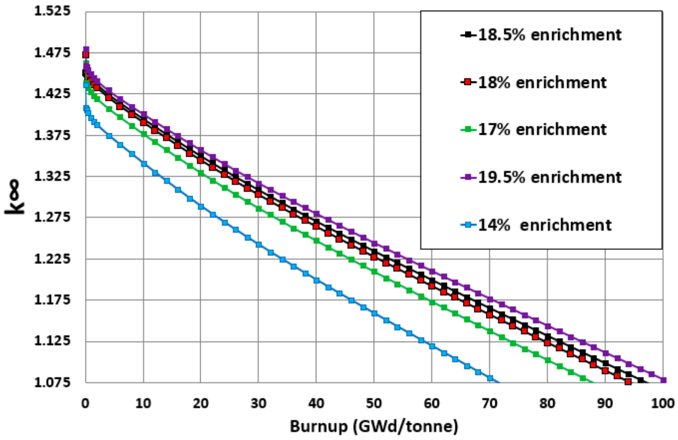


(b)

Fig. 3. Fuel depletion calculations for various fissile loadings: (a) UO_2 fuel; (b) Duplex fuel.

volume of UO_2 in the fuel and, in part, to the higher thermal absorption cross-section of the fertile ^{232}Th.

Lattice physics calculations for the assemblies were performed in previous studies (Almutairi et al., 2018, Alam et al., 2018b,a) using the deterministic transport code WIMS, the Monte Carlo (MC) code Serpent (Leppänen and Pusa, 2009) and the hybrid MC code MONK (Long et al., 2015). For both candidate fuels, excellent agreement (∼100–350 pcm) was observed between the codes, giving reassurance that WIMS can be used to provide reliable lattice physics results for SBF marine propulsion cores at much reduced computational cost compared to the MC code Serpent and hybrid MC code MONK.

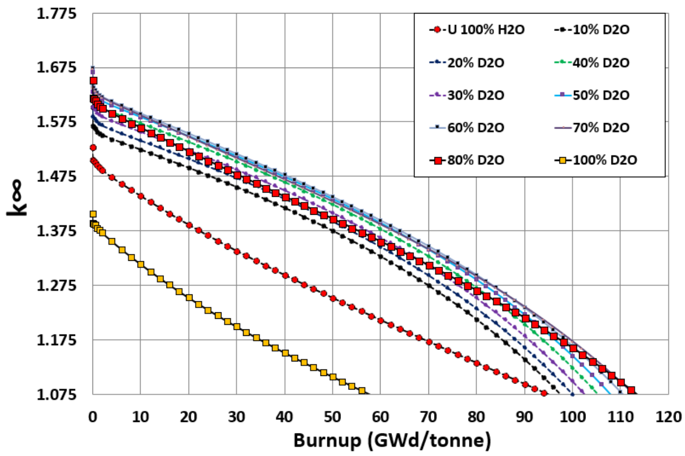
2.5. Coolant molecular ratios

Next, we use mixtures of light and heavy water at molecular ratios ranging from 0% to 100% D_2O with both candidate fuels. Figs. 4a and 4b show that both fuels achieve the highest discharge burnup with the 80% D_2O + 20% H_2O mixed coolant. Neutron capture in D_2O-H_2O dominates when it is more than 80% D_2O due to the substantial degradation in the thermal neutron utilization arising from the reduced presence of hydrogen atoms.n This necessarily provides the highest uranium utilization, making this coolant composition the natural choice to take forward in this study. As expected, since deuterium is not as efficient a neutron moderator as hydrogen, the neutron spectrum was found to be increasingly hardened and the resonance flux relatively higher as the D_2O percentage in the moderator increased.

The reference design parameters of the proposed marine core are shown in Table 2 (Alam, 2018).

Parameter	Value
Thermal power (MWth)	333.33
Minimum desired lifetime (years)	15
Assembly size	13×13
Control rods per assembly	16
Pin pitch (mm)	12.65
Fuel pellet diameter (mm)	8.19
Cladding thickness (mm)	0.605
Gap thickness (mm)	0.0498
Number of assemblies	112
Fuel height (m)	1.79
Core diameter (m)	1.97
Pitch/diameter ratio	1.33
Hydrogen-to-heavy metal (H/HM) ratio	3.99
Assembly side length (cm)	16.45
Assembly area (m^2)	0.03
Power density (MW/m^3)	63
Average linear rating (kW/m)	10

Table 2. Reference design parameters of proposed marine core.



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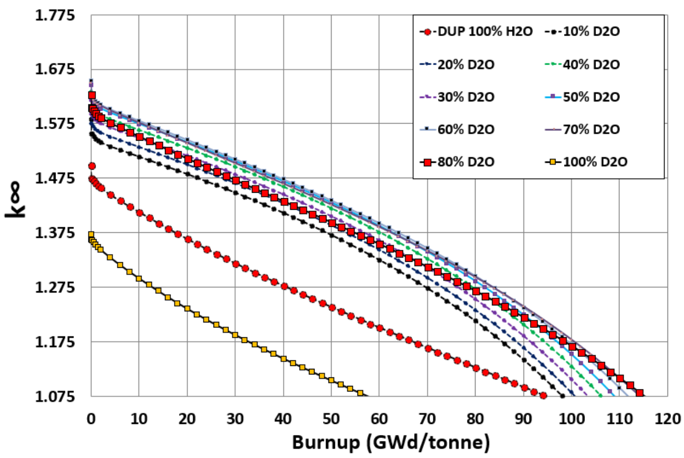


(b)

Fig. 4. Fuel depletion calculations for varying molecular ratios of light and heavy water: (a) 15% ^{235}U enriched UO_2 fuel; (b) 18% ^{235}U enriched duplex fuel.

3. Lattice geometry optimization and moderation effects

The main objective of this parametric study is to observe the effects of varying the neutron spectrum under different degrees of moderation in order to maximize the attainable discharge burnup and secure improved uranium utilization while maintaining a negative MTC. Since the achievable burnup is dependent on the hydrogen-to-heavy-metal ratio (H/HM) for H_2O coolant, and on the deuterium-hydrogen/heavy-metal ratio (DH/HM) for mixed D_2O-H_2O coolant, we optimize these ratios by changing: (1) the fuel rod diameter; (2) the pin pitch; and (3) the coolant density. Together, these parameters determine the reactor's H/HM and DH/HM ratios, and hence have a crucial effect on the neutron energy spectrum.

Our strategy for this study of moderation effects is the following: by varying the H/HM and DH/HM ratio in a core, we can find the most suitable operating range with respect to achievable discharge burnup for a given initial enrichment for the candidate fuels. Optimizing moderation to achieve long core life requires a balance to be struck between three main factors (Alam, 2018):

(a) Early in life, it is desirable to encourage a higher neutron capture rate in the fertile components of the fuel, suppressing initial reactivity and enhancing the breeding of new fissile material.
(b) Late in life, it is necessary to reduce captures in the fertile components of the fuel so as to increase the core reactivity, which helps in preventing the core from losing criticality.
(c) And throughout all stages of life, it is necessary to maintain a sufficiently negative MTC to ensure stable operation.

In this study, we have defined the following:

1. The fast region to correspond to a H/HM or DH/HM < 0.50, the epithermal region to H/HM or DH/HM between 0.50 and 2.88, and the thermal region to H/HM or DH/HM > 2.88 (Xu and Driscoll, 1997, Alam, 2018).
2. We refer to the region below the optimal (point of highest discharge burnup) H/HM or DH/HM as 'under-moderated' and the region above the optimum as 'over-moderated'.
3. The reference values of pin pitch = 12.65 mm, fuel pin diameter = 9.50 mm, coolant density = 0.707 g/cm^3 (for H_2O) and 1.0832 g/cm^3 (for 80% D_2O + 20% H_2O).

We use 'D_2O' as a short-hand label for the 80% D_2O + 20% H_2O coolant[2].

3.1. Initial reactivity

The focus here is on the beginning-of-life (BOL) k_∞ of poison-free fuel lattices at hot full power and xenon-free conditions. We have investigated BOL k_∞ by varying the coolant density, fuel pin diameter and pin pitch over wide ranges with other parameters held constant. These resulting plots provide information on several points of interest.

Fig. 5a shows that an increase in H/HM leads to a higher BOL k_∞ for both the duplex and all-UO_2 fuels up to some value of H/HM. Due to the increased presence of hydrogen

[2] 80% D_2O + 20% H_2O coolant is referred to interchangeably as 'mixed coolant' and 'D_2O'.

atoms, neutrons are better thermalized (Fig. 5b) up to H/HM $\approx$ 15 for H_2O coolant. k_∞ peaks at this H/HM value and tends to decrease thereafter. In the over-moderated region, k_∞ decreases as H/HM increases since the large capture cross-section of water begins to dominate the effect of improved neutron thermalization (Xu and Driscoll, 1997). It should be noted that our reference marine PWR lattice has H/HM and DH/HM values of 3.99 and 5.0, respectively and therefore is not optimal if trying to maximize BOL k_∞.

Figs. 6a and 6b show that the variation of BOL k_∞ for the candidate fuels is similar with the D_2O-H_2O coolant for similar reasons. k_∞ peaks at around DH/HM $\approx$ 10. Neutron absorption in mixed D_2O-H_2O coolant begins to play a dominant role at a lower value of DH/HM (compared to H/HM for the H_2O coolant) due to the substantial degradation in the thermal neutron utilization arising from the reduced presence of hydrogen atoms.

Figs. 5a and 6a show that the peak value of k_∞ is lower for the duplex fuel than the all-UO_2 fuel for both coolants. This is because ^{232}Th has a higher absorption cross-section than ^{238}U. The peak k_∞ of both candidate fuels with the D_2O-H_2O coolant is $\sim$2% higher than with the H_2O coolant in the under-moderated region, due to the presence of large volumes (80%) of D_2O and its small neutron capture cross-section compared to H_2O coolant.

Fig. 7 shows the BOL normalized neutron flux ratio (the ratio of the flux in the mixed coolant to that in the H_2O coolant) for UO_2 fuel. It suggests that the mixed coolant yields a softer spectrum than the H_2O coolant. The ratio in the thermal range is $\sim$1.65–1.70, meaning that flux values in the thermal range are $\sim$65–70% softer for the mixed coolant. Thus, the peak k_∞ values are higher for the mixed coolant due to better neutron thermalization compared to the H_2O coolant.

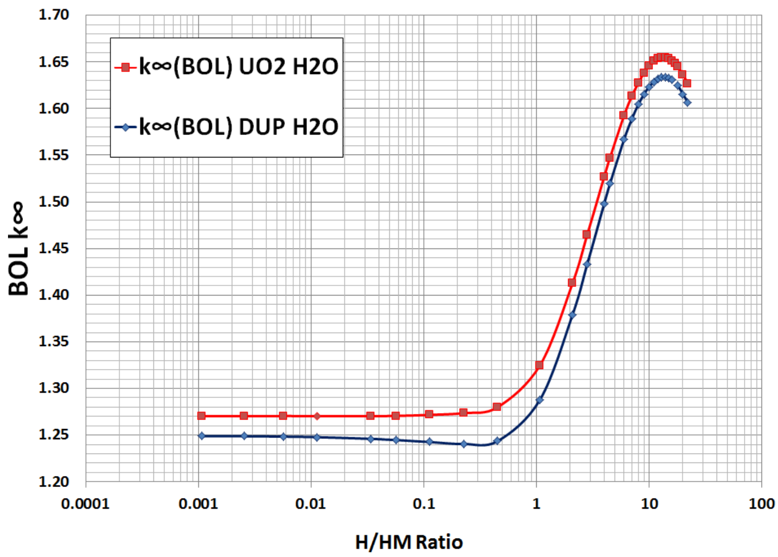
Things are different in the over-moderated region, where neutron capture in the mixed coolant dominates capture in H_2O. Fig. 8 show that BOL k_∞ values for the mixed coolant become lower than corresponding values for the H_2O coolant towards the upper end of this region.

The sensitivity of BOL k_∞ to varying fuel pin diameter (over the range 4.79–9.50 mm), while keeping the pin pitch and coolant density constant (at reference values), was investigated. Fig. 9 shows the peak BOL k_∞ values of the UO_2 and duplex fuels with H_2O coolant occur at H/HM = 14 and 16, respectively. Due to the presence of a strong thermal absorber (^{232}Th), the peak k_∞ of duplex fuel is 4% less than for the UO_2 fuel, which is beneficial from the perspective of reactivity control.

In contrast, it can be seen for the mixed coolant that peak BOL k_∞ values are reached for DH/HM $\approx$ 8. At high H/HM and DH/HM ratios, BOL k_∞ values for the H_2O coolant are higher compared to those for the D_2O coolant for both the candidate fuels. This is due to the dominance of the elastic scattering cross-section of hydrogen (which is 5 times greater than that of deuterium in the slowing-down energy range).

Finally, we increased the pin pitch (over the range 9.51–23.08 mm) while keeping the fuel diameter and coolant density constant at reference values. Fig. 10 shows that the peak BOL k_∞ of the all-UO_2 fuel is 1.2% and 1.8% higher than that for the duplex fuel for the D_2O and H_2O coolants, respectively. Both candidate fuels reach peak BOL k_∞ values at an H/HM value of 14 and a DH/HM value of 9 for the D_2O and H_2O coolants, respectively.

From a neutronics viewpoint it can be anticipated that with decreases in H/HM or DH/HM



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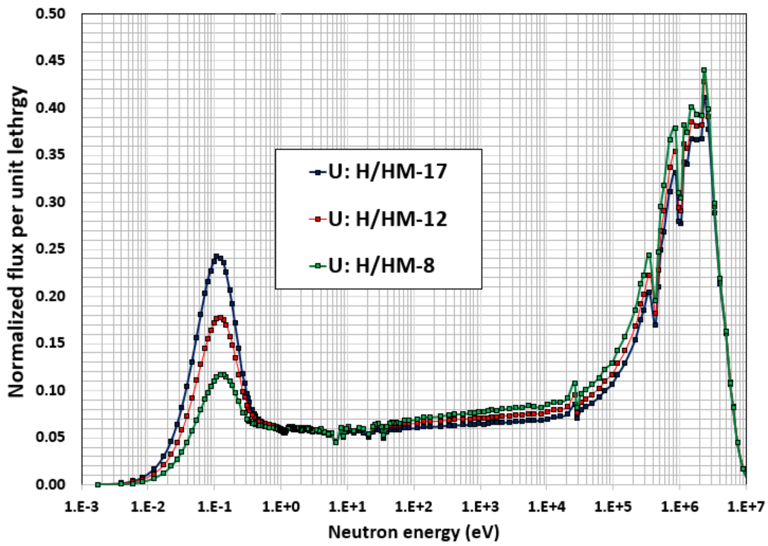
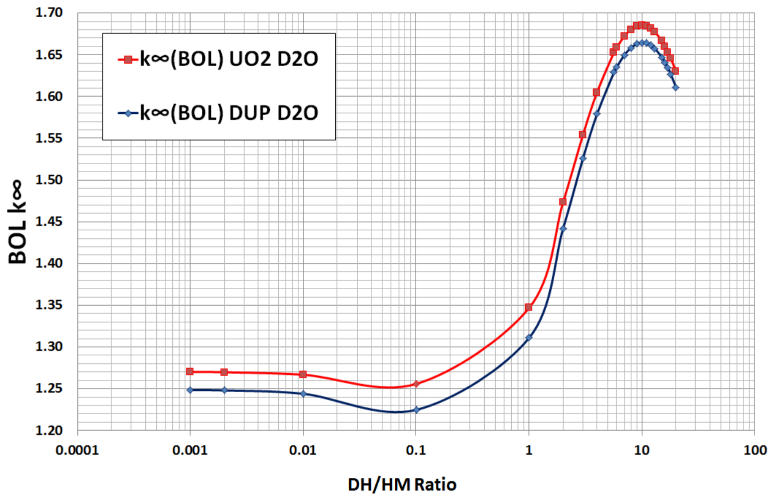


(b)

Fig. 5. (a) Initial k_∞ as a function of H/HM by varying coolant density. (b) Neutron spectra normalized per unit flux at BOL by varying H_2O density for UO_2 fuel – H/HM values of 8, 12 and 17 are shown.



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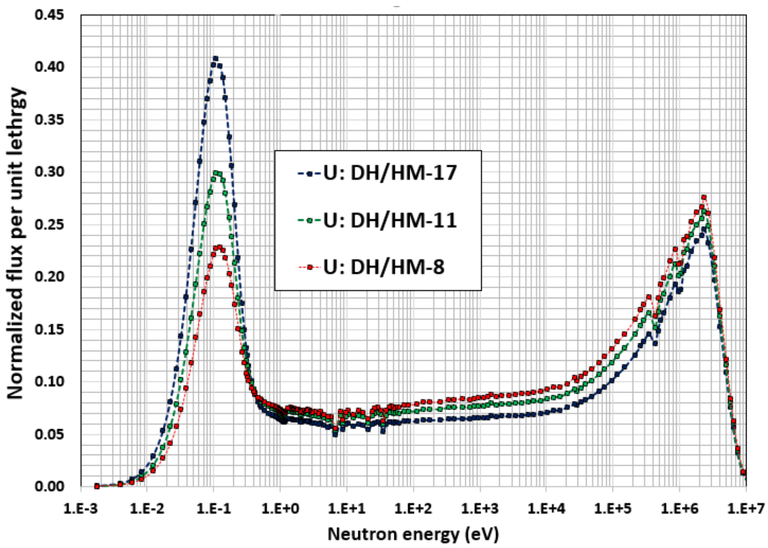

(b)

Fig. 6. (a) Initial k_∞ as a function of DH/HM by varying coolant density. (b) Neutron spectra normalized per unit flux at BOL by varying D_2O-H_2O density for UO_2 fuel – DH/HM values of 8, 11 and 17 are shown.

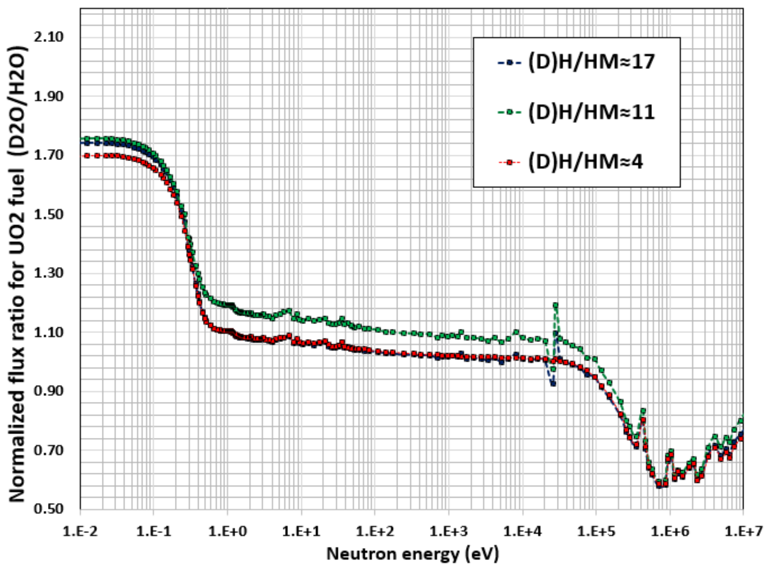

Fig. 7. Normalized neutron flux ratios (D_2O-H_2O:H_2O coolant) for UO_2 fuel at BOL.

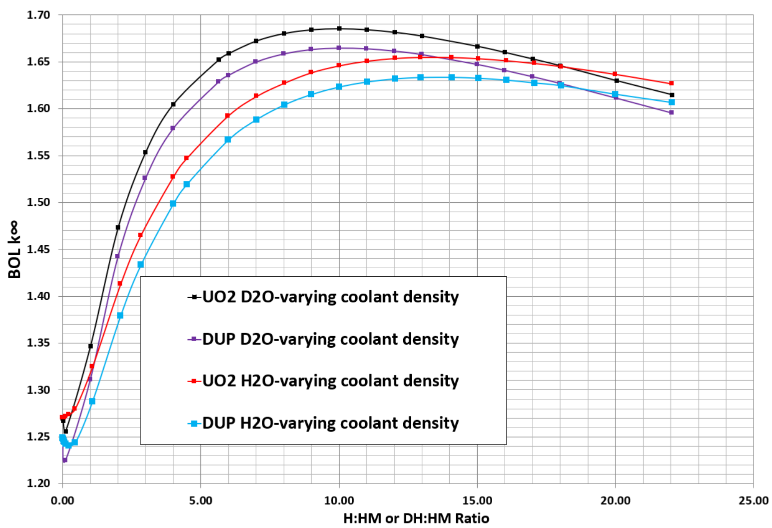

Fig. 8. BOL k_∞ as a function of H/HM or DH/HM for all-UO_2 and duplex fuels by varying coolant density.

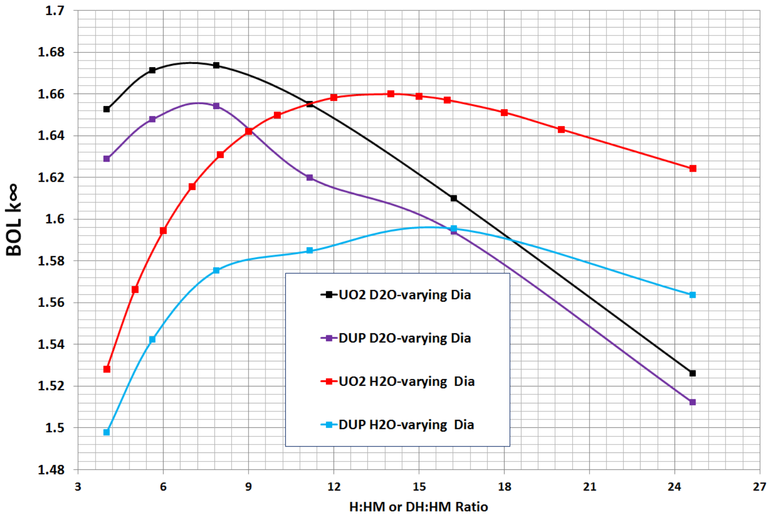

Fig. 9. BOL k_∞ as a function of H/HM or DH/HM by varying fuel diameter (standard pitch).

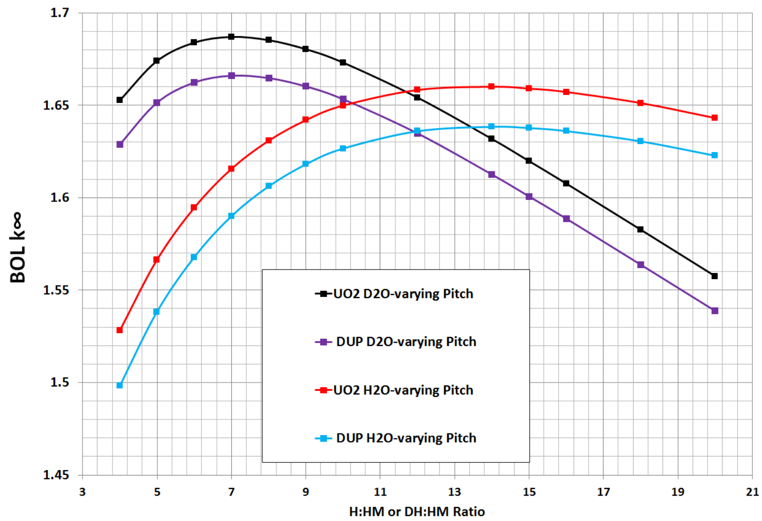

Fig. 10. BOL k_∞ as a function of H/HM or DH/HM by varying pitch (standard fuel diameter).

below the optimal ratios, the neutron migration length increases so that the lattice becomes ever more homogenized. The hardening of the neutron spectrum increases the resonance absorption in ^{238}U relative to ^{235}U. Thus a monotonic decrease in k_∞ with decreasing H/HM and DH/HM is observed.

Control requirements are largely determined by the initial reactivity, and this parametric study suggests that wetter lattices need more control. It can be concluded that BOL k_∞ is higher for the all-UO_2 fuel for both coolants, which will certainly exacerbate the reactivity control requirements for SBF operation. Conversely, the duplex candidate fuel will require less burnable absorber than the all-UO_2 fuel for reactivity suppression. Since the D_2O coolant provides higher peak BOL k_∞ for both fuels, it will require greater poison loading for reactivity suppression, although this disadvantage may be offset by the higher achievable discharge burnup that results. Since soluble boron isn't used for reactivity control, it is required to use integral fuel burnable absorber (IFBA) burnable poison as traditional poison like gadolinia and/or erbia wasnt efficient enough (Alam, 2018, Alam et al., 2015). Therefore, a high-thickness ZrB_2 IFBA poison coating is considered in order to achieve the crucial self-shielding effect, investigating coatings of 150 µm (Alam, 2018). In our IFBA assembly design, 150 µm adhesive coating of zirconium diboride is coated onto the outer surface of a UO_2 pellet. For the duplex fuel case, IFBA layers are applied on the outer surface of the ThO_2 region. In order to suppress high initial and through-life reactivity swing, we used boron 95% enriched in ^{10}B throughout in order to increase neutronic effectiveness. In boron 95% enriched with ^{10}B, the ratio of the absorption to total cross-section $\sigma_a/\sigma_t = 0.95$, and therefore boron is an approximately black absorber. When incorporated into ZrB_2 (density: 6.5 g/cm^3), it has a macroscopic absorption cross-section of $\Sigma = 297$ cm^{-1}, and therefore a mean free path λ of $\sim$34 µm (Otto, 2013, Alam, 2018, Alam et al., 2015). As a result, 150 µm coating has poison layer with thickness greater than 3λ and these high-thickness poison layers can therefore intercept at least $\sim$95% of incident neutrons. In addition, the existing subassembly design has 16 guide-tubes for loading control rods and a standard 16-rod rod cluster control assembly (RCCA) of B_4C is used. In our 112-assembly marine PWR core, 3 banks of control rods (A, B and C) are used for power maneuvering and 3 other banks (SA, SB and SC) are used for shutdown. A total of 36 rod cluster control assemblies each of 16 rods are used. Finally, B_4C control rod bank banks are used for obtaining criticality over life (Alam, 2018).

3.2. Achievable discharge burnup

We now examine the reactivity-limited achievable discharge burnup (B_D) as a function of H/HM and DH/HM. B_D is defined from the burnup value on the depletion curve (k_∞ vs. burnup) where $k_\infty = 1$, i.e. leakage is not considered in this analysis. The sensitivity of B_D is observed for varying coolant density, fuel pin diameter and pin pitch. Figs. 11 and 12 show that the duplex fuel can achieve up to $\sim$2% more discharge burnup compared to the UO_2 fuel for both coolants by varying fuel pin diameter (over the range 4.79 mm–9.50 mm) and pin pitch (over the range 12.65–23.08 mm).

In contrast, the duplex fuel can achieve $\sim$7% higher discharge burnup than the UO_2 fuel by varying the coolant density (over the ranges 2.0×10^{-3}–3.90 g/cm^3 (for H_2O) and

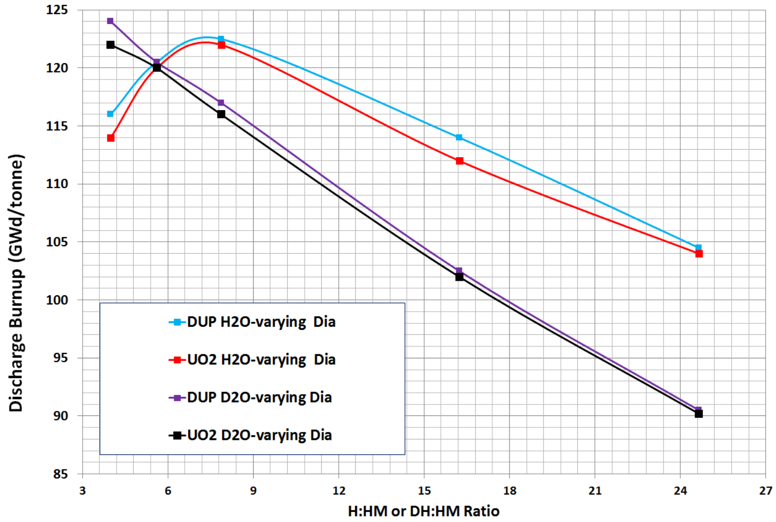

Fig. 11. B_D as a function of H/HM or DH/HM by varying fuel diameter (standard pitch).

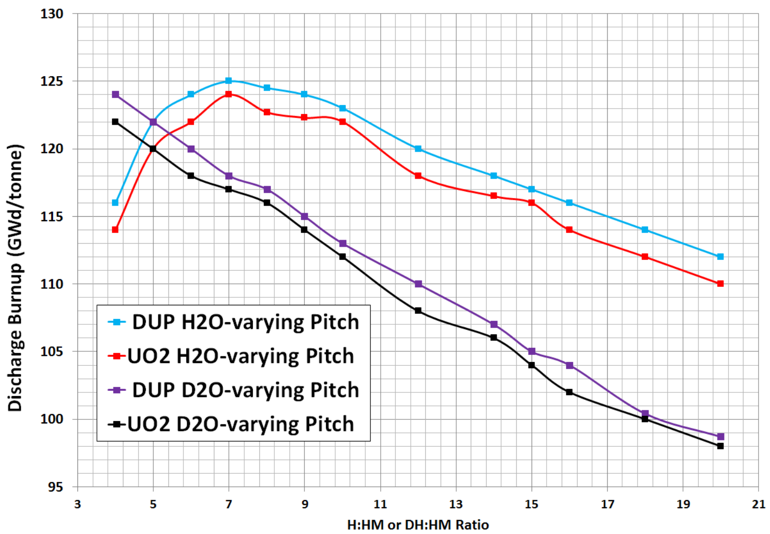

Fig. 12. B_D as a function of H/HM or DH/HM by varying pitch (standard fuel diameter).

1.92×10^{-4}–3.84 g/cm^3 (for the mixed coolant)), as shown in Fig. 13. This is due to the improved 'fertile-capture-to-fissile-absorption ratio' of duplex fuel (Fig. 14), which is advantageous for achieving better fissile accumulation potential and thus leads to higher discharge burnups.

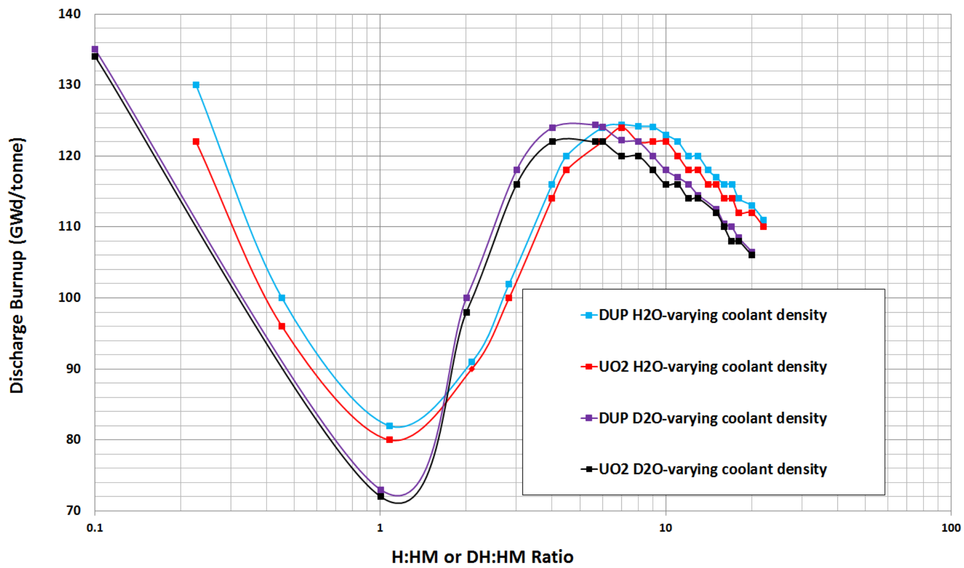

Fig. 13. B_D as a function of H/HM and DH/HM ratio by varying coolant density.

A slight asymmetry in B_D for various lattice optimizations can be observed. This is to be expected since the reactor physics is not entirely determined by H/HM or DH/HM. For instance, an assembly with large fuel elements and a large pitch may have the same moderator/fuel ratio as a standard assembly, but since the assembly dimensions in terms of neutron mean-free-paths are different, the neutronic behavior will not be identical in the two assemblies.

Figs. 11 and 12 show that, for values of (D)H/HM < 5 achieved by varying the fuel diameter or pin pitch, discharge burnups up to $\sim$8% higher are obtained with the mixed coolant. For (D)H/HM values > 5, the H_2O coolant yields higher values of B_D, with the peak occurring for H/HM ≈ 7.

Fig. 13, which illustrates the effect on B_D of varying the coolant density, shows that higher B_D values are achieved with the mixed coolant for (D)H/HM values in the range from $\sim$2 to 6. The highest B_D values are achieved with a hard spectrum ((D)H/HM $\ll 1$). For both coolants there is also a local maximum in B_D for each fuel at DH/HM ≈ 5 (D_2O-H_2O) and H/HM ≈ 7 (H_2O).

For all these lattice optimizations (varying the coolant density, fuel pin diameter and pin pitch), the duplex fuel consistently offers higher achievable discharge burnups for all moderation regimes for both coolants. It can achieve B_D values of 125 GWd/tonne with H_2O (H/HM = 7) and 124 GWd/tonne with D_2O-H_2O (DH/HM = 4), respectively, which represent $\sim$7% increases in B_D compared to a reference lattice.

Although higher discharge burnups can be achieved with a hard spectrum ((D)H/HM $\ll$

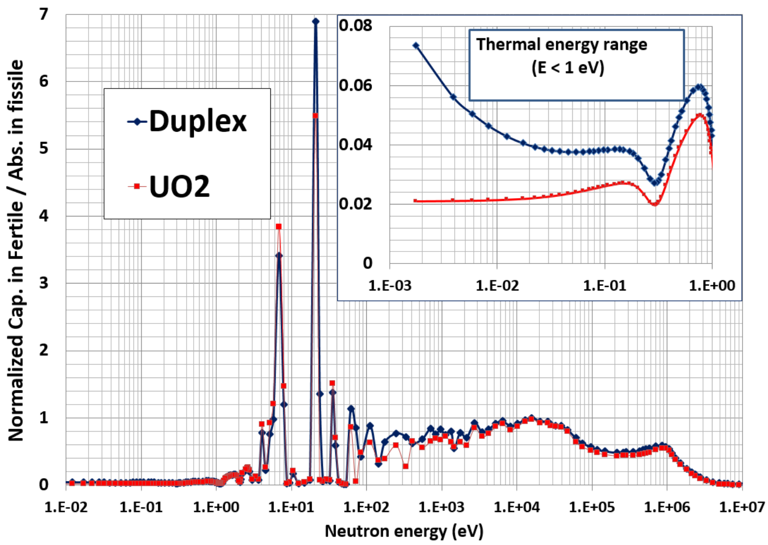

Fig. 14. Fertile-capture:fissile-absorption ratios at BOL.

1), the analysis of initial reactivity in Sect. 3.1 showed BOL k_∞ values are significantly lower in this moderation regime.

3.3. Conversion ratio

The relationship between discharge burnup and initial reactivity can be explained using the concept of conversion ratio (CR), which measures the ratio of the fuel's end-of-life (EOL) and BOL fissile content. The variation of the 'achievable discharge burnup' can be understood using the linear reactivity model (Driscoll et al., 1990). Using this model, the discharge burnup in single-batch operation is determined by the initial reactivity and the slope of the k_∞-burnup characteristic, which is proportional to (1/CR) (Xu and Driscoll, 1997). Here, the BOL CR is calculated as a function of (D)H/HM by varying coolant densities while keeping the fuel diameter and pin pitch constant (at reference values) over the range of moderation regimes. It can be observed from Fig. 15 that overall the CR decreases as (D)H/HM increases, implying that the net fissile content declines faster with increasing moderation. By looking at the figures for initial reactivity (Figs. 8, 9 and 10) and CR (Fig. 15), the behavior of 'achievable discharge burnup' (Figs. 11, 12 and 13) is elucidated. In the thermal range, there is a peak in B_D, the location of which is to the right of the peak for BOL k_∞. In the epithermal range, B_D exhibits a minimum due to the trade-off between reduced BOL k_∞ and improved CR. For H_2O and D_2O-H_2O cooled lattices, it is not worthwhile to operate in the epithermal range under the constraint of a once-through fuel cycle. In the fast range, the effect of CR is dominant since the initial reactivity is nearly constant.

Fig. 16 shows that for UO_2 fuel the neutron spectrum is gradually hardened for lower H/HM values, as expected. Since a harder spectrum facilitates the efficient conversion of fertile to fissile material, CR values are higher in the fast region than in the thermal region (as shown in Fig. 15).

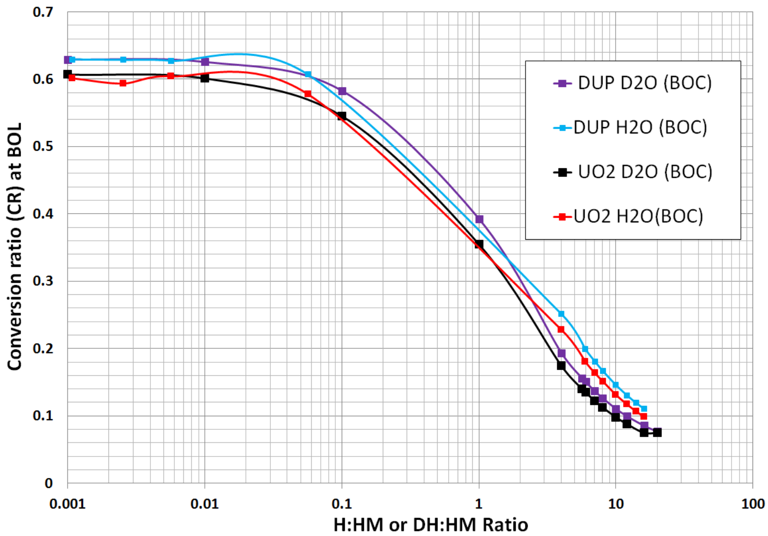

Fig. 15. BOL conversion ratio as a function of H/HM or DH/HM by varying coolant density.

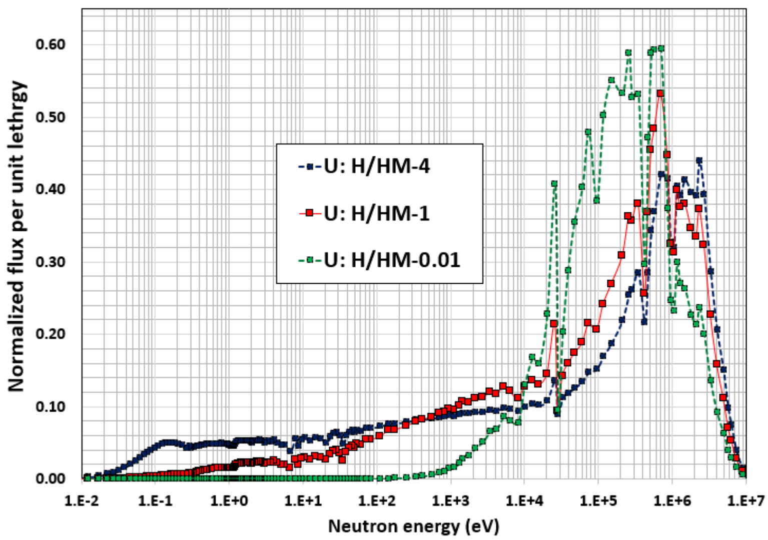

Fig. 16. Normalized flux per unit lethargy at BOL for UO_2 fuel at different H/HM by varying coolant density – H/HM values of 0.01, 1 and 4 are shown.

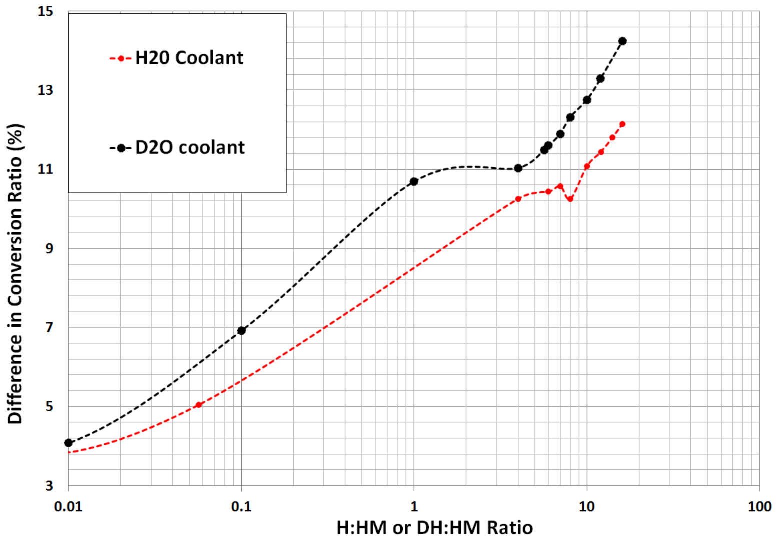

Fig. 17. Difference (%) in conversion ratio between duplex and UO_2 fuels as a function of H/HM or DH/HM by varying coolant density.

A higher CR is often a design goal. Fig. 17 shows that the CR of the duplex fuel is ∼3%, ∼8% and ∼10% higher than that of the all-UO_2 fuel in the fast, epithermal and thermal energy ranges, respectively, for both coolants, thus explaining the higher discharge burnup capability of the duplex fuel.

For both fuels, CR is higher for the mixed coolant in the under-moderated region but these values fall dramatically in the over-moderated region (DH/HM > 6), and in that moderation regime are exceeded by the CR values for the H_2O coolant.

The higher CR of the duplex fuel could facilitate a longer core life, which is a desirable feature for our marine core. The higher CR also results in a smaller reactivity swing between BOL and EOL, which makes the task of reactivity control of the SBF core easier.

4. Evaluation of the MTC and Safety Perspective

It is important to observe the effect of the H/HM and DH/HM on MTC and how temperature changes in the moderator affect overall reactivity. In our SBF marine core, since the coolant is also the moderator, an increase in reactor power will heat the moderator and reduce the density of moderator atoms via thermal expansion. Thus, an increase in temperature reduces the H/HM and DH/HM values. This affects the core's reactivity primarily through two distinct, but antagonistic mechanisms (Otto, 2013, Xu, 2003):

1. As the density of moderator decreases, the neutrons have fewer elastic collisions before entering the fuel. They are more likely to enter the fuel in the epithermal energy range and be absorbed in the fuel's resonances. This decreases the resonance escape probability and thus lowers k_∞.
2. As the density of the moderator decreases, thermal neutrons are less likely to be parasitically captured in the moderator. This increases the thermal utilization factor

and thus also k_∞.

This has important consequences for reactivity stability and inherent safety. When the first effect outweighs the second, the reactor is under-moderated, and an increase in temperature will decrease reactivity and stabilize the reactor. However, if the second effect outweighs the first, the reactor is over-moderated, and a temperature rise will further increase reactivity and power, leading to positive feedback. Any 'optimization' of the lattice geometry must not breach this threshold and undermine this inherent stability.

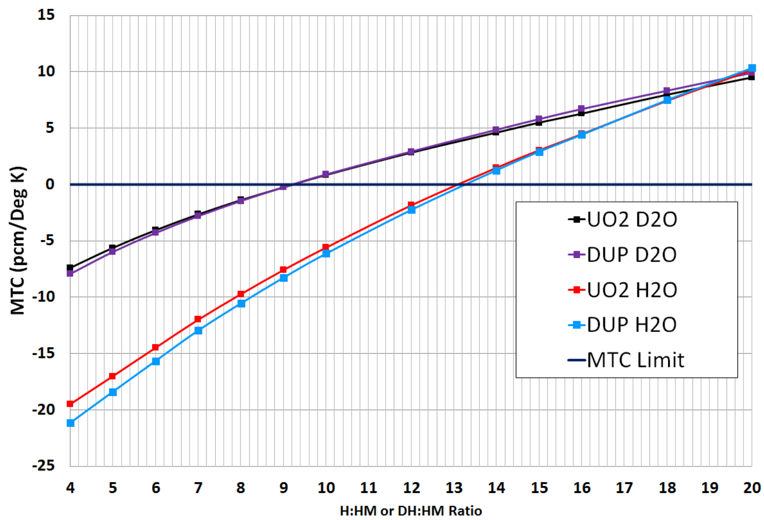

Fig. 18. MTC as a function of H/HM or DH/HM by varying pin pitch.

To evaluate α_M, the MTC, we calculate the BOL reactivity (ρ) for an assembly in two different conditions: first, at the standard moderator temperature (T) of 580 K, and second, with a moderator temperature ($T + \Delta T$) of 590 K (and an appropriately adjusted water density). Taking $\alpha_M \approx \Delta\rho/\Delta T$, we plot α_M against (D)H/HM in Fig. 18. MTC was investigated by varying pin pitch (over the ranges 11.54–19.94 mm (for H_2O) and 12.65–23.08 mm (for the mixed coolant)), while keeping the fuel pin diameter and coolant density constant at reference values.

SBF operation offers potential safety in the presence of negative MTC over the entire core life. Fig. 18 shows that except at very high (D)H/HM values the MTC is lower (more negative) for the H_2O coolant. For both fuels, the upper limit on DH/HM (for negative MTC) for the mixed coolant is $\sim$9 and on H/HM for H_2O it is $\sim$13. For both coolants, for (D)H/HM values giving negative MTC, the MTC of the duplex fuel is slightly more negative than that of the UO_2 fuel, more so for H_2O.

It is important addressing that since this neutronic study has been performed for the poison-free candidate fuels, the power peaking factors (PPF) won't represent the true values as higher burnable poison loading and control rods will be required to suppress the reactivity for this SBF operation (Alam, 2018, Alam et al., 2015). High thickness IFBA provides different PPF values than the poison-free fuel and might deteriorate the PPFs . Therefore, PPF hasn't been considered in this paper. In addition, peak cladding temperature calculation for the poison-free fuels will be misleading since it is required to perform safety analyses for the hottest channel to observe whether all operational safety criteria are met (Alam, 2018, Oliveira, 2016, Todreas and Kazimi, 2012). Through-life hottest channel is identified by finding the pin with the highest power (Todreas and Kazimi, 2012), which is seriously influenced by burnable poison and control rods. Therefore, peak cladding temperature hasnt been considered in this parametric neutronic analyses of poison-free fuels. However, in order to confirm that all the thermal-hydraulic safety constraints are satisfied for both the candidate fuels, 3D neutronic/thermal-hydraulic hot channel analysis has been performed and our study confirmed that thermal-hydraulic design requirements for both the candidate fuels can be met (Alam, 2018).

5. Conclusions

This parametric neutronics study shows that, for the candidate fuels for use in a SBF, civil marine SMR core considered

- A higher discharge burnup is achievable in either a wetter-than-normal or much dryer-than-normal lattice, while epithermal lattices are distinctly inferior performers.
- D_2O-H_2O coolant is effective for the drier lattices in terms of achieving higher discharge burnup, whereas H_2O coolant is effective for the wetter lattices.
- Candidate fuels with D_2O-H_2O coolant would require higher poison loadings than with H_2O coolant due to their higher initial reactivity.
- The duplex fuel configuration offers higher discharge burnup potential for all moderation regimes for both coolants due to its higher conversion ratio.
- The duplex fuel lattice would also require less burnable absorber to suppress initial excess reactivity than the all-UO_2 fuel.

Future work will include the consideration of alternative cladding materials (e.g. ODS-type steel and SiC) for very high burnup fuels and coupled neutronic-thermal-hydraulic studies for heavy water coolants. Since power density is an important figure of merit and characterizes design performance of marine propulsion cores, future work will also focus on the design of a high power density core that fulfills the objective of providing 15 EFPY life.

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