COMILLAS
UNIVERSIDAD PONTIFICIA
ICAI

GRADO EN INGENIERÍA Y TECNOLOGÍAS INDUSTRIALES

TRABAJO FIN DE GRADO

ANALYSIS OF MSRs AS OPPOSED TO OTHER TECHNOLOGIES TO SOLVE ENERGY NEEDS

Autor: Pablo Vereda Gorgé

Director: Youping Chen

Madrid

I, hereby, declare that I am the only author of the project report with title:

Analysis of MSRs as opposed to other technologies to solve energy needs

which has been submitted to ICAI College of Engineering of Comillas Pontifical University in the academic year 2021/22. This project is original, has not been submitted before for any other purpose and has not been copied from any other source either fully or partially. All information sources used have been rightly acknowledged

Sgd.: Pablo Vereda Gorgé Date: 13/06/2022

I authorize the submission of this project

PROJECT SUPERVISOR

Sgd.: Youping Chen Date: …14…/ …06…/ …2022…

“For those who believe, no explanation is necessary; for those who do not believe, no explanation will suffice.”

Michio Kaku

Acknowledgement

I would like to thank Dr. Youping Chen and Dr. Yang Li for assisting me on this project. I would also like to thank my family; without them this would not have been possible.

ANÁLISIS DE MSRs EN CONTRAPOSICIÓN CON OTRAS ENERGÍAS PARA RESOLVER LAS NECESIDADES ENERGÉTICAS

Autor: Vereda Gorgé, Pablo.
Director: Chen, Youping.
Entidad Colaboradora: ICAI – Universidad Pontificia de Comillas.

RESUMEN DEL PROYECTO

La conductividad térmica del dióxido de torio se ha simulado utilizando el programa LAMMPS y NEMD. Los modelos eran más grandes que otros encontrados en la literatura y el valor para el más grande fue de 12.9 W/m-k. Además, se desarrolló un análisis de los MSR considerando los requisitos de combustible y la gestión de residuos comparándolo con otras tecnologías.

Palabras clave: MSR, torio, dióxido de torio, LAMMPS, NEMD, energía nuclear, fisión, energía, transporte térmico, renovables, GN, residuos nucleares, PWR.

1. Introducción

Es del interés de gobiernos y sociedades regular otros posibles combustibles nucleares y desarrollar sus ciclos y procesamiento, incluso si es solo para prepararse contra escenarios extremos donde no se puede garantizar el suministro. Esto es dado la importancia que el único estándar actual de la industria para el combustible nuclear tiene hoy en día. El torio se puede utilizar en un ciclo de fisión nuclear conocido como el ciclo Th-U para producir energía y es 3-4 veces más abundante que el uranio además de presentar otras ventajas importantes.

Posiblemente, la tecnología más prometedora que hace uso del ciclo Th-U es el MSR (Reactor de Sal Fundida) desarrollado por primera vez en la década de 1950 hasta finales de la década de 1970 en el ORNL (Oak Ridge National Laboratory) [1]. En una primera instancia, fue parte del programa estadounidense conocido como ARE (Aircraft Reactor Experiment) que intentaba desarrollar un reactor nuclear con capacidad de propulsar un avión. Para ello, el MSR era muy atractivo principalmente por su tamaño compacto, uno de los mayores inconvenientes que tienen los reactores nucleares tradicionales y comercializados. Los MSR presentan una seguridad superior, residuos con vidas medias mucho más cortas, capacidades intrínsecas de seguimiento de carga y un mayor uso del combustible proporcionado en comparación con los PWR (reactores de agua a presión) y BWR (reactores de agua en ebullición), entre otras virtudes que vienen con inconvenientes ya que el procesamiento químico es complejo.

2. Descripción del proyecto

En primer lugar, la conductividad térmica del dióxido de torio se estima por medio de NEMD. Los modelos utilizados son más grandes que los desarrollados previamente por Park et. al [2] y, por lo tanto, se espera que se reduzca la dispersión fonón-fonón, un fenómeno conocido por reducir potencialmente la conductividad térmica. A continuación, se demuestra y evalúa la limitación térmica de los combustibles nucleares de estado sólido. Se proporciona una solución teórica seguida de otras numéricas.

Los MSR se analizan en términos de consumo de combustible y producción y gestión de residuos para luego compararse con un PWR tradicional. El gas natural se evalúa por ser considerado uno de los mejores combustibles fósiles disponibles y una vez más se evalúan los requisitos de combustible y la producción de residuos. Por último, se considera el papel que juegan las energías renovables en comparación con los MSR y se determina una estimación del mismo.

1. Metodología

3.1 Simulación de conductividad térmica del ThO2

Para ejecutar la simulación, primero se debe crear un modelo con la geometría que se va a evaluar, esta geometría contendrá los átomos en sus posiciones correspondientes. Se ha desarrollado un código de MATLAB para la generación del modelo.

En primer lugar, se necesita el número de átomos de O y Th junto con su distribución en la estructura cristalina y el tamaño de esta. Una vez que esto se conoce, se puede definir la celda unitaria (como se muestra en la Figura 1) y la geometría final será un múltiplo de esa unidad para cada una de las dimensiones espaciales. Un ejemplo de la geometría final se muestra en la Figura 2.

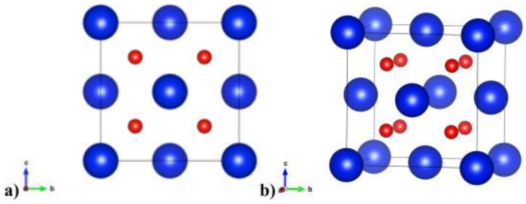

Figura 1: Celda unitaria del dióxido de torio [2].

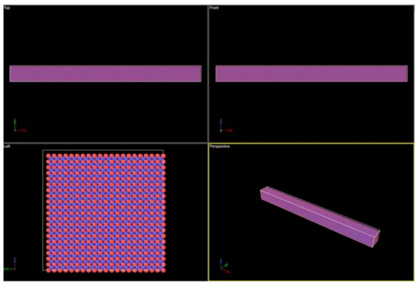

Figura 2: Ejemplo de un modelo generado con MATLAB. Imagen del autor.

Una vez que se genera un modelo válido, las condiciones para la simulación deben establecerse en un archivo que se pueda ejecutar en LAMMPS. Es necesario definir los parámetros básicos, como las unidades que se utilizan, las condiciones de contorno, las dimensiones consideradas o el potencial interatómico.

En segundo lugar, las regiones se definen para crear una fuente de calor en el centro, dos disipadores de calor, uno en cada extremo, y dos regiones intermedias donde se medirán las temperaturas. La temperatura se puede calcular como la energía cinética promedio de los átomos, no como una traslacional, sino como el resultado promedio de la vibración de átomos individuales o grupos de átomos a lo largo del tiempo.

3.2 Análisis de MSR

El cuello de botella térmico se demuestra en un modelo simple mediante la obtención de la expresión para el perfil de temperatura en las diferentes regiones de un elemento combustible y la posterior evaluación de valores numéricos.

El consumo de combustible y la producción de residuos se estiman para una planta de energía de 1 GWe durante 1 año de operación. Esto se hace para tres escenarios diferentes considerando que la planta hace uso de un PWR, un MSR o gas natural. Con este fin, la energía liberada por fisión o por combustión se consideró junto con sus subproductos.

Para los residuos producidos por ambos reactores se consideran las tecnologías en las que se basan. Por ejemplo, en las tecnologías MSR sólo el material fisionable entra en el núcleo y ningún otro material fértil o subproductos de fisión quedan contaminados o atrapados [1].

3. Resultados

Una vez que la simulación LAMMPS se ha ejecutado y alcanzado el régimen estacionario, se genera el perfil de temperatura. Con esto, se obtiene la pendiente después de aislar una de las ramas como se muestra en la Figura 3, y se evalúa la conductividad térmica. Los resultados de las conductividades térmicas obtenidas para diferentes geometrías se muestran en la Tabla 1.

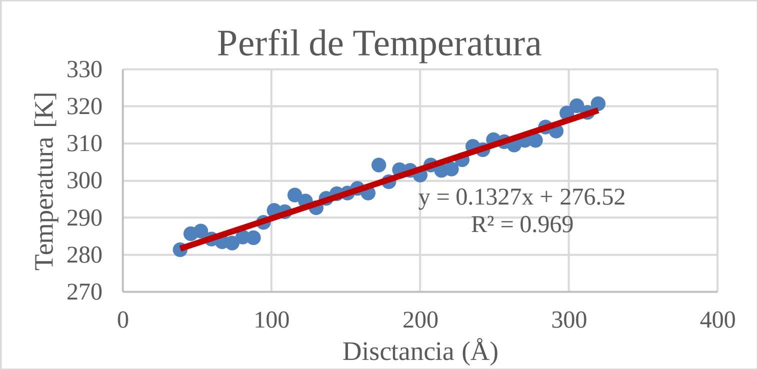

Figura 3: Ejemplo de la línea de tendencia. Imagen del autor.

El modelo para el perfil de temperatura en un elemento combustible mostró que la temperatura es mucho más alta en el elemento combustible que en el contacto con el refrigerante. Se estima que esto resulta en un aumento de hasta el 3.23% en la eficiencia para cambios relativamente pequeños (aproximadamente de 2 unidades) en la conductividad térmica del combustible.

Tabla 1: Resultados obtenidos para la conductividad térmica de ThO_2 a temperatura ambiente

Dimensiones [Å]	Conductividad térmica [W/m-K]
[420, 18, 18]	11.5850
[700, 56, 56]	12.7533
[840, 56, 56]	12.8820

Tabla 3: Costo de combustible y residuos por año para una planta de energía de 1 GWe en los tres escenarios considerados.

	Costo de combustible por año	Costo de residuo por año
PWR	$34.61 M	$5.24 M
MSR	US$ 43.28 K	$261.8 K
NG	$356.94 M	US$ 3.2 M

Los resultados de los requisitos de combustibles y gestión de residuos para las centrales eléctricas PWR, MSR y GN (gas natural) de 1 GWe se resumen en la Tabla 3.

4. Conclusiones

Las conductividades térmicas obtenidas en las simulaciones son inferiores a las estimadas por Park et al. [3] para estructuras más pequeñas, sin embargo, no se espera que los resultados sean completamente precisos, sino una aproximación debido a que dependen de los potenciales interatómicos. Con este fin, se estima que en el peor de los casos ThO_2 se comportará aproximadamente como UO_2.

Los MSR en cuanto a recursos y residuos demuestran ser una opción muy interesante en la que vale la pena invertir y desarrollar. El cuello de botella de fusión del combustible puede ser y es una limitación y una preocupación de seguridad. Los reactores de sal fundida son el único diseño Gen-IV que supera completamente esto ya que el combustible está en forma líquida.

Finalmente, se estima que las energías renovables no serán suficientes en el futuro dado las tecnologías con las que contamos y aún se requieren métodos de producción de energía muy competitivos, en este escenario se demuestra que los MSR son una de las mejores alternativas dado que se logre el pleno desarrollo y aprobación en los próximos años.

2. Referencias

[1] J. R. Engel, W. R. Grimes, W. A. Rhoades and J. F. Dearing, "MOLTEN-SALT REACTORS FOR EFFICIENT NUCLEAR FUEL UTILIZATION WITHOUT PLUTONIUM SEPARATION," Oak Ridge, 1978.

[2] Ashley Shields, David Santos-Carballal, Nora H. de Leeuw, "A density functional theory study of uranium-doped thoria and uranium adatoms on the major surfaces of thorium dioxide," Journal of Nuclear Materials, pp. 99-111, 2016.

[3] J. Park, "Thermal transport in thorium dioxide," 2018. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S1738573317306101.

ANALYSIS OF MSRs AS OPPOSED TO OTHER TECHNOLOGIES TO SOLVE ENERGY NEEDS

Author: Vereda Gorge, Pablo.
Supervisor: Chen, Youping.
Collaborating Entity: ICAI College of Engineering, Comillas Pontifical University.

ABSTRACT

The thermal conductivity of thorium dioxide was simulated using the program LAMMPS and NEMD. The models were bigger than others found in the literature and the values for the biggest one was found to be 12.9 W/m-k. An analysis of MSRs was then developed considering fuel requirements and waste management comparing it to other technologies.

Keywords: MSR, thorium, thorium dioxide, LAMMPS, NEMD, nuclear energy, fission, energy, thermal transport, renewables, NG, nuclear waste, PWR.

3. Introduction

It is in the best interest of governments and societies to regulate other possible nuclear fuels and develop their cycles and processing even if it just to prepare for extreme scenarios where supply cannot be guaranteed, given the importance that the one and only current industry standard for nuclear fuel has today. Thorium can be used in a nuclear fission cycle known as the Th-U cycle to produce energy and it is 3-4 times more abundant than Uranium alongside with other major advantages.

Possibly, the most promising technology that makes use of the Th-U cycle is the MSR (Molten Salt Reactor) first developed in the 1950s through the late 1970s at the ORNL (Oak Ridge National Laboratory) [1]. In a first instance, it was part of the US program known as the ARE (Aircraft Reactor Experiment) where a nuclear reactor suitable to power an aircraft was to be developed. To this end, the MSR was very attractive mainly due to its compact size, one of the mayor drawbacks that traditional and commercialized nuclear reactors have. MSRs present superior safety, waste with much shorter half-lives, autonomous load following capabilities and higher fuel usage when compared to common PWRs (Pressurized Water Reactors) and BWR (Boiling Water Reactors) among other virtues that comes with drawbacks as the chemical processing is complex.

4. Project description

First, the thermal conductivity of thorium dioxide is estimated by means of NEMD. The models used are bigger than the ones previously developed by Park et. al [2] and thus phonon-phonon scattering, a phenomenon known to potentially reduce thermal conductivity is expected to be reduced. Next, the thermal limitation of solid-state nuclear fuels is demonstrated and evaluated. A theoretical solution followed by numerical ones are provided.

MSRs are then analyzed in terms of fuel consumption and waste production and management to then be compared to a traditional PWR. NG is then evaluated as being considered one of the best fossil fuels available and once again fuel requirements and waste production are evaluated. Finally, the role that renewable energies play when compared to MSRs is considered and an estimation of the same is determined.

5. Methodology

3.1 ThO2 thermal conductivity simulation

To run the simulation, first a model needs to be created with the geometry that is to be evaluated, this geometry will contain the atoms in their corresponding positions. A MATLAB code was used for the model generation.

Firstly, the number of O and Th atoms along with their distribution in the lattice and the lattice constant are needed. Once this is known, the unit cell can be defined (as it is shown in Figure 1) and the final geometry will be a multiple of that unit for each of the spatial dimensions. An example of the final geometry is shown in Figure 2.

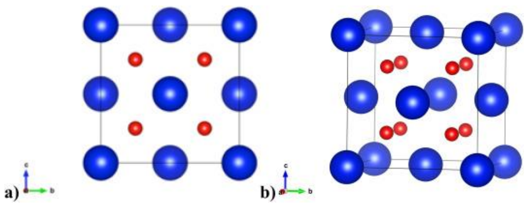

Figure 1: Thorium dioxide unit cell [2].

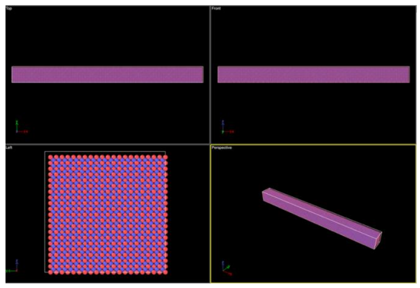

Figure 2: Example of a model generated with MATLAB. Image by the author.

Once a valid model is generated the conditions for the simulation need to be stablished in a file that can be executed in LAMMPS. Some basic parameters need to be defined, such as the units being used, the boundary conditions, the dimensions considered or the interatomic potential.

Secondly, regions are defined to create a heat source at the center, two heat sinks, one at each end, and two intermediate regions where the temperatures will be measured. The temperature can then be calculated as the average kinetic energy of the atoms, not a translational one, but the average result of the vibration of either individual or clusters of atoms over time.

3.2 MSRs analysis

The thermal bottleneck is demonstrated in a simple model by means of obtaining the expression for the temperature profile in the different regions of a fuel element and evaluating numerical values.

Fuel consumption and waste production is estimated for a 1 GWe power plant during a 1-year operation. This is done for three different scenarios considering that the plant makes use of a PWR, a MSR or natural gas. To this end, the energy released per fission or per combustion was considered alongside their byproducts. For the waste produced by both reactors the technologies that they are based on are considered. For instance, in MSR technologies only the fissile material goes into de core and no other fertile material and fission byproducts are contaminated or trapped [1].

6. Results

Once the LAMMPS simulation has run and reached steady state, the temperature profile is generated. With this, the slope is obtained after isolating one of the branches as shown by Figure 3, and the thermal conductivity is evaluated. Results for thermal conductivities obtained for different geometries are shown by Table 1.

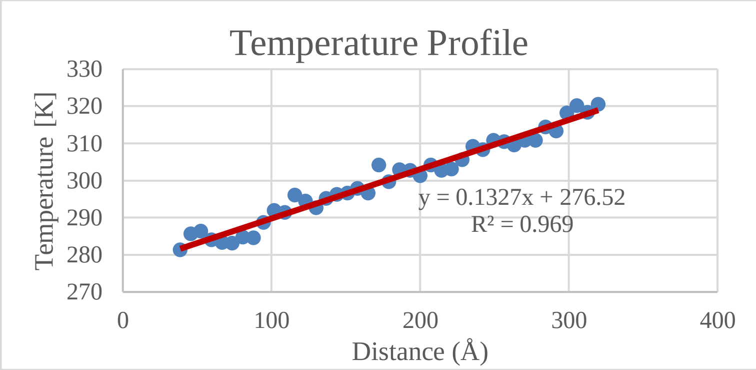

Figure 3: Example of the trendline. Image by the author.

The model for the temperature profile in a fuel element showed that temperature is much higher at the fuel element that at the interface with the coolant. This is estimated to result in up to 3.23% increase in the efficiency for relatively small changes (about 2 units) in the thermal conductivity.

Table 1: Results obtained for thoria thermal conductivity at room temperature

Dimensions [Å]	Thermal conductivity [W/m-K]
[420, 18, 18]	11.5850
[700, 56, 56]	12.7533
[840, 56, 56]	12.8820

Table 3: Cost for fuel and waste per year for a 1 GWe power plant in the three scenarios.

	Fuel cost per year	Waste cost per year
PWR	$34.61 M	$5.24 M
MSR	$43.28 K	$261.8 K
NG	$356.94 M	$3.2M

Results for fuel and waste management for the PWR, MSR and NG (natural gas based) power plants are summarized on Table 3.

7. Conclusions

The thermal conductivities obtained by the simulations are lower than those estimated by Park et al. [3], however results are not expected to be completely precise, but an approximation due to them being dependent on the interatomic potentials. It is estimated that in a worst-case scenario thoria will behave about as uranium dioxide.

Resource wise and waste-wise MSRs prove to be a very interesting option worth investing in and developing. The meltdown bottleneck can be and is a limitation and a safety concern, MSRs are the only Gen-IV design that completely overcome this as the fuel is in liquid form.

Finally, renewables are estimated to not suffice in the future as technology stands today and very competitive energy producing methods are still required, in this scenario MSRs are proved to be one of the best alternatives given that full development and approval are achieved in the following years.

8. References

[1] J. R. Engel, W. R. Grimes, W. A. Rhoades and J. F. Dearing, "MOLTEN-SALT REACTORS FOR EFFICIENT NUCLEAR FUEL UTILIZATION WITHOUT PLUTONIUM SEPARATION," Oak Ridge, 1978.

[2] Ashley Shields, David Santos-Carballal, Nora H. de Leeuw, "A density functional theory study of uranium-doped thoria and uranium adatoms on the major surfaces of thorium dioxide," Journal of Nuclear Materials, pp. 99-111, 2016.

[3] J. Park, "Thermal transport in thorium dioxide," 2018. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S1738573317306101.

TABLE OF CONTENTS

FIGURES

TABLES

1 INTRODUCTION

Nuclear energy remains to be one of if not the best alternative to fossil fuels even after other technologies for energy production and storage have been developed and implemented. This is due to its proven security, reliability and low cost as nuclear reactors can operate for decades and use very little fuel. In addition to that, nuclear technology can substitute reliably and at a reasonable cost big fossil fuel engines such as those found on ships, or generator sets that power isolated communities that are not connected to the main electric grid. The same simply cannot be said about wind and solar technologies not even in combination with state-of-the-art battery technologies or other energy storing methods (water pumping, hydraulic lifting…). At the current nuclear fuel consumption, the world supply of viable uranium (the most common nuclear fuel) is expected to last for another 80 years. Although it could also be extracted along with other valued materials from sea water as some studies suggest [1], and nuclear reactors use a higher percentage of the fuel as technology advances [2], the current demand should be expected to grow at a high rate during the following decades and prices for viable uranium to be much higher than they currently are. This can prevent further implementation of this technology and a revival of fossil fuels for energy generation.

It is in the best interest of governments and societies to regulate other possible nuclear fuels and develop their cycles and processing even if it just to prepare for extreme scenarios where supply cannot be guaranteed, given the importance that the one and only current industry standard for nuclear fuel has today. Thorium can be used in a nuclear fission cycle known as the ^{232}Th-^{233}U cycle to produce energy and it is 3-4 times more abundant than Uranium alongside with other major advantages.

Possibly, the most promising technology that makes use of the ^{232}Th-^{233}U cycle is the MSR (Molten Salt Reactor) first developed in the 1950s through the late 1970s at the ORNL (Oak Ridge National Laboratory). In a first instance, it was part of the US program known as the ARE (Aircraft Reactor Experiment) where a nuclear reactor suitable to power an aircraft was to be developed. To this end, the MSR was very attractive mainly due to its compact size, one of the mayor drawbacks that traditional and commercialized nuclear reactors have. MSRs present superior safety, waste with much shorter half-life, autonomous load following capabilities and higher fuel usage when compared to common PWRs (Pressurized Water Reactors) and BWR (Boiling Water Reactors) among other virtues that do not come without drawbacks as it will be discussed.

2 TECHNOLOGY DESCRIPTIONS

MD (Molecular Dynamics) is a computer simulation method that uses the equations derived from the science known as lattice dynamics to predict the end result of laboratory experiments or materials properties. LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) implements MD and it is used to simulate how materials will behave under certain conditions. For instance, it can be used to estimate the Young's modulus of a certain metal, or its thermal conductivity by knowing its composition, lattice structure, and interatomic potential of the elements involved.

3 STATE OF THE ART AND JUSTIFICATION

One important parameter when exploring nuclear fuels for existing reactor technologies is its thermal conductivity. This property has an important role in the reactor thermals and thus its feasibility, efficiency and expected life. It can be estimated with computer simulations before investing more resources into getting more accurate results from laboratory experiments or actual testing. Some molecular dynamics simulations for ThO_2 can be found in the literature, possibly the most significant being the ones by Ma et al. [3] and Park et al. [4]. However, only the latter made use of NEMD (Non-Equilibrium Molecular Dynamics) and simulated a larger structure that allows for a reduced phonon-phonon scattering. Still, the values obtained differ a lot from one another and from other experimental results, ranging the thermal conductivity of thoria (ThO_2) between 7 and 18 W/m-k at room temperature.

4 OBJECTIVES

The first objective of this work is to use molecular dynamics to simulate a heat flux in thorium dioxide to generate a temperature profile and from that predict its thermal conductivity. NEMD will be used, and the structures simulated will be larger and those found in the Parker et al. work allowing for more precise results under the same conditions. Not only that, but if the thermal conductivities obtained are similar, it will add consistency to the predictions made by Park for a non-phonon-phonon scattering scenario. Alongside with this first objective, a mathematical model will be developed to demonstrate the importance of the fuel's thermal conductivity in the reactor that is not demonstrated in the similar works and that will serve to link the first part of this analysis to the second.

Finally, MSRs will be reviewed and analyzed. Although there is substantial literature on MSRs it is limited to describing it, examine some of its virtues and drawbacks as compared to traditional nuclear technology, researching the on-line reprocessing unit, or reporting the technology readiness (actual designs and operation reports may also be found). This project has as an objective to determine how it stands today as compared to other technologies (not only conventional nuclear reactors), what a real-world application of this technology may mean, or in what fields it may end up being implemented in a first instance. The latter will focus on fuel economy and waste that result as a byproduct of regular operation for energy or heat production.

5 ThO_2 THERMAL CONDUCTIVITY SIMULATION

5.1 METHODOLOGY

Molecular dynamics allows for the simulation of materials under given conditions using mathematical models developed by lattice dynamics. This unlocks the possibility to recreate certain laboratory experiments on computer programs such as LAMMPS (the one used for this simulation). Although, the precision of the results obtained will heavily depend on the model being used, the kind of experiment trying to simulate, or certain parameters that are not perfectly defined for all materials such as the interatomic potential; some examples show that very good predictions can be achieved. In the case of thoria thermal conductivity several values are given in the literature obtained from both laboratory experiments and molecular dynamics simulations, nonetheless they do differ a lot from one another. Though an exact value would be the ideal scenario, that was not the objective of these simulations, but a prediction of what the value could be, and more importantly, whether that value would be higher, similar, or lower than that of UO_2. This simple statement can give a good idea on some of the factors involved in investing in ThO_2 as a new standard for nuclear fuel. It was predicted in all simulations that the thermal conductivity of thorium dioxide is higher than that of uranium dioxide as shown by Park et al. [4], and this prediction suggests that thoria could have several advantages as opposed to UO_2, such as smaller dimensioning required, superior safety or allow for more fuel consumption before replacing it completely as will be detailed later.

5.1.1 MODEL GENERATION

To run the simulation, first a model needs to be created with the geometry that is to be evaluated, this geometry will contain the atoms in their corresponding positions. Instead of creating a “Basis” (with material properties) and a “gen” (that distributes the atoms and creates the structure), a MATLAB code shown in Appendix A was used for the model generation.

First, the number of O and Th atoms along with their distribution in the lattice and the lattice constant are needed. Once this is known, the unit cell can be defined (as it is shown in Figure 1) and the final geometry will be a multiple of that unit for each of the spatial dimensions.

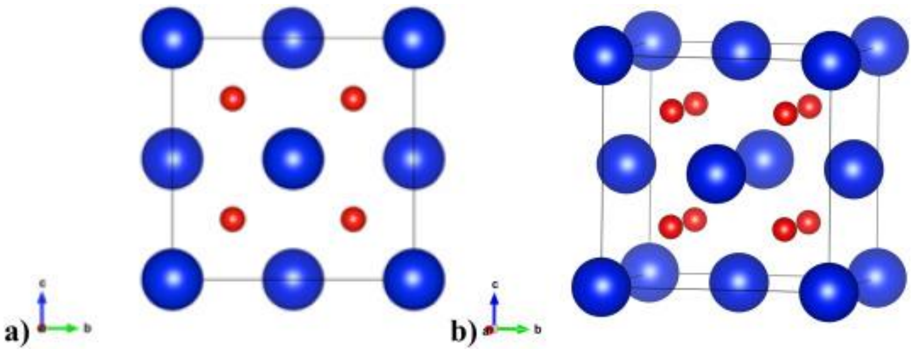

Figure 1: Thorium dioxide unit cell [5].

Once the previous is defined, the MATLAB code generates a file that can be opened with the program Ovito to visualize the structure as shown in Figure 2. The boundary for this geometry is set to be slightly larger than the geometry itself to prevent some problems that might occur, as due to how the model will be treated in the edges, it might result in some of the atoms overlapping with one another, resulting in an error during the computation.

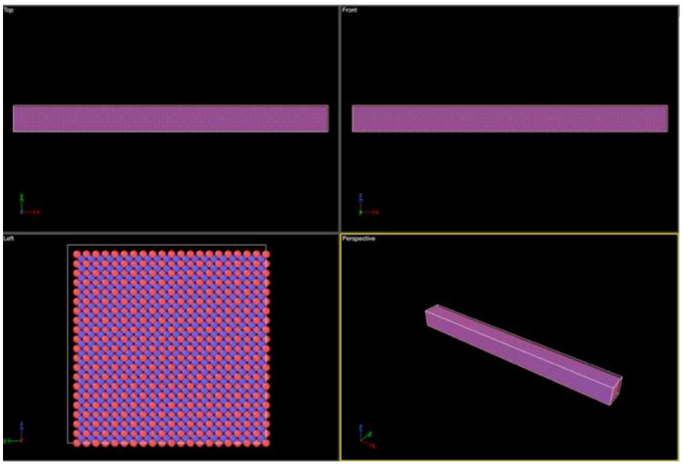

Figure 2: Example of a model generated with MATLAB. Image by the author.

5.1.2 LAMMPS INPUT

Once a valid model is generated the conditions for the simulation need to be defined in a file that can be executed in LAMMPS. First, some basic parameters need to be defined, such as the units being used, the boundary conditions, the dimensions considered or the interatomic potential.

Simulations were made using “atomic” style, however very low thermal conductivities were obtained (in the realm of 0.5 to 2 W/m-K), this may be due to how the interatomic potentials are defined in the file selected however this should not have resulted in a problem. Finally, the systems were simulated using “full” for the atom style, resulting in closer to previously predicted values.

The boundary condition used is the default (p p p), and it imposes that the boundaries are “in touch” with one another, that is, atoms can exit one end of the boundary and enter at the other end.

For the interatomic potential, the ones obtained by Cooper et al. [6] for actinide oxides were used. This is possibly to be the most important parameter used as the quality of the interatomic potentials used will directly determine the quality of the simulation since they represent the physical basis of the elements simulated. They were selected and not calculated as it is not the objective of the present work to obtain more high-quality results for interatomic potentials than the previously calculated.

Next, regions are defined to create a heat source at the center, two heat sinks, one at each end, and two intermediate regions where the temperatures will be measured. If the geometry is set to be centered, the definition of the different regions may be defined as shown by Figure 3. The last line shown in the previously mentioned image can be used to double check that there is no overlapping as that will result in an error. The temperature can then be calculated as the average kinetic energy of the atoms, not a translational one, but the average result of the vibration of either individual or clusters of atoms over time.

```
#  define groups
   region     1 block -15 15 EDGE EDGE EDGE EDGE units box
   region     2 block -205 -190 EDGE EDGE EDGE EDGE units box
   region     3 block 190 205  EDGE EDGE EDGE EDGE units box
   region     4 block EDGE -205 EDGE EDGE EDGE EDGE units box
   region     5 block 205 EDGE EDGE EDGE EDGE EDGE units box

   group          source region 1
   group          sinkone region 2
   group          sinktwo region 3
   group          B1 region 4
   group          B2 region 5
   group          free subtract all B1 B2

  # delete_atoms overlap 0.1 all all
```

Figure 3: Example of group definition. Image by the author.

Phonon-phonon scattering can have a significant effect in these types of simulations as they usually operate at room temperature or above. In this temperature range, Umklapp phonon-phonon scattering intervenes as opposed to “normal” phonon-phonon scattering. This has to be noted as Umklapp phonon-phonon scattering may result in a reduced effective thermal conductivity as crystal momentum is not conserved. Following this phenomenon, a significant phonon source as may be the one considered in the simulation as the heat source or a beam of light, may produce phonons with high enough energy as to split into two different ones. As the crystal momentum conservation does not apply, residual energy different from the two resulting phonons will be produced consequently. This effect may be represented by E. 1.

E. 1 $$\mathbf{q_1} = \mathbf{q_2} + \mathbf{q_3} + \mathbf{G}$$

This has to be noted as Umklapp phonon-phonon scattering may result in a reduced effective thermal conductivity since crystal momentum is not conserved. If it were to be conserved, the net heat source from the heat source to the heat sink would not be affected. However, the residual heat may have any direction, that includes an opposite direction to that of the general flow, increasing the temperature locally and effectively reducing the overall thermal conductivity. This effect can be illustrated as represented by Figure 4. Notice that this effect will not always reduce thermal conductivity, on the other hand, it may never increase it as the resistance of the material for the passing of any phonon will be the same but phonon going on the opposite direction is understood in the results as a higher resistance.

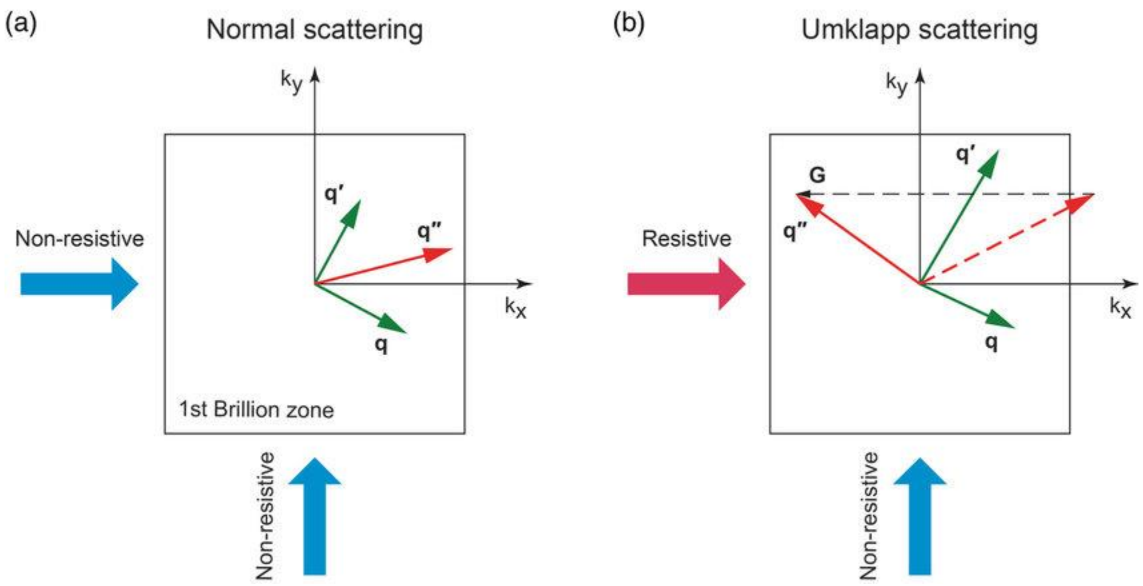

Figure 4: Normal and Umklapp scattering representation [7]

Once the temperatures are measured, a temperature profile can be obtained, that along with the heat flux that is added to the system, can be used to determine the thermal conductivity applying Fourier's Law (E. 2).

Although a simpler system with only one heat source and one heat sink (like the one shown in Figure 5) can be used to determine the same, similar conditions to those simulated by Park et al. [4] are trying to be reproduced. In this regard, the system is also elevated to 500 K and then the temperature is reduced to room temperature using isenthalpic ensemble and microcanonical ensemble.

E. 2 $$\boldsymbol{q} = -k\nabla T$$

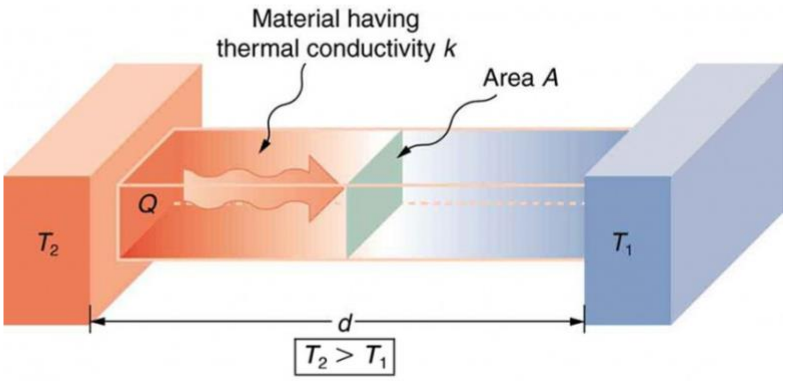

Figure 5: Schematic of the direct method [8].

Finally, the heat source and heat sinks are applied to the regions previously defined to be consistent with those of Figure 6. The temperatures are then measured by calculating the average kinetic energy of the atoms and averaging them over the number of timesteps defined.

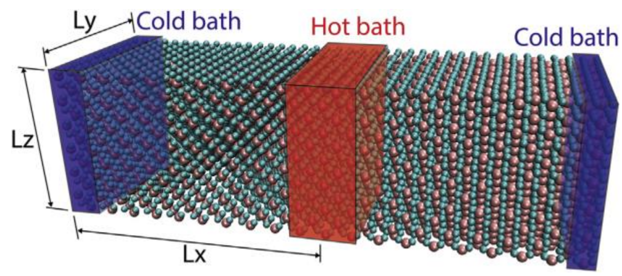

Figure 6: Schematic of the system simulated [4].

5.2 RESULTS

After the simulation has run, a file with temperatures corresponding to the normalized length (x/total length) is generated. The normalized length can be transformed into actual position for the temperature with the total length of the sample; and the temperature profile can be obtained as shown in Figure 7. One of the branches of the temperature profile is selected and the values are adjusted into a trendline (Figure 8), the slope of this trendline is used to calculate ∇T in E. 2.

The reader can realize a relatively large drop in between the first temperature measured and the second one, as well as in between the last temperature to the right and the second to last. This is due to the temperature in the wall being fixed at each end. These two points are to be removed in order to obtain an accurate thermal conductivity as shown by the result of the simulation.

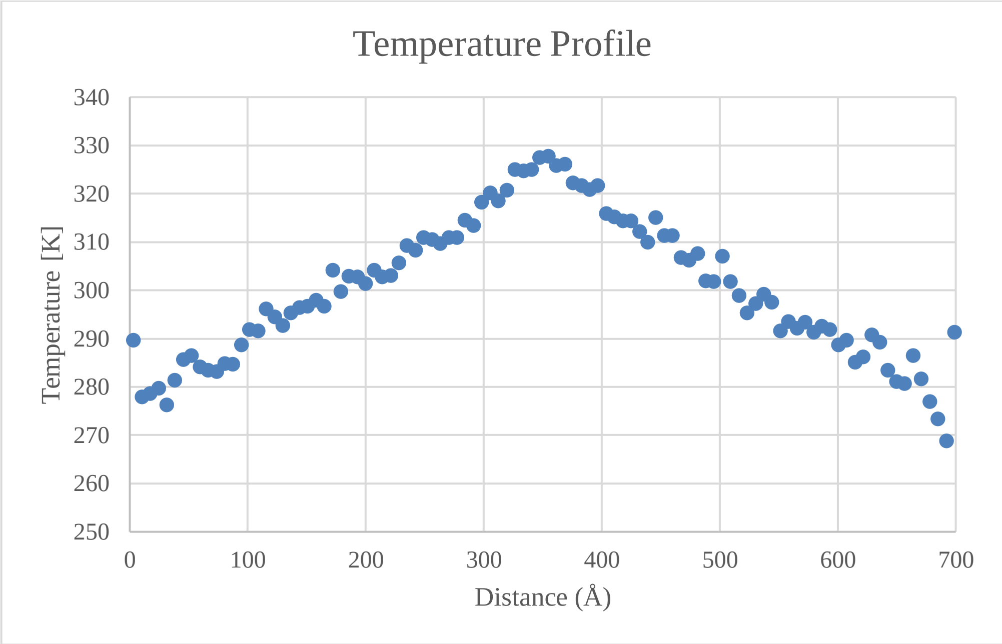

Figure 7: Example of the temperature profile. Image by the author.

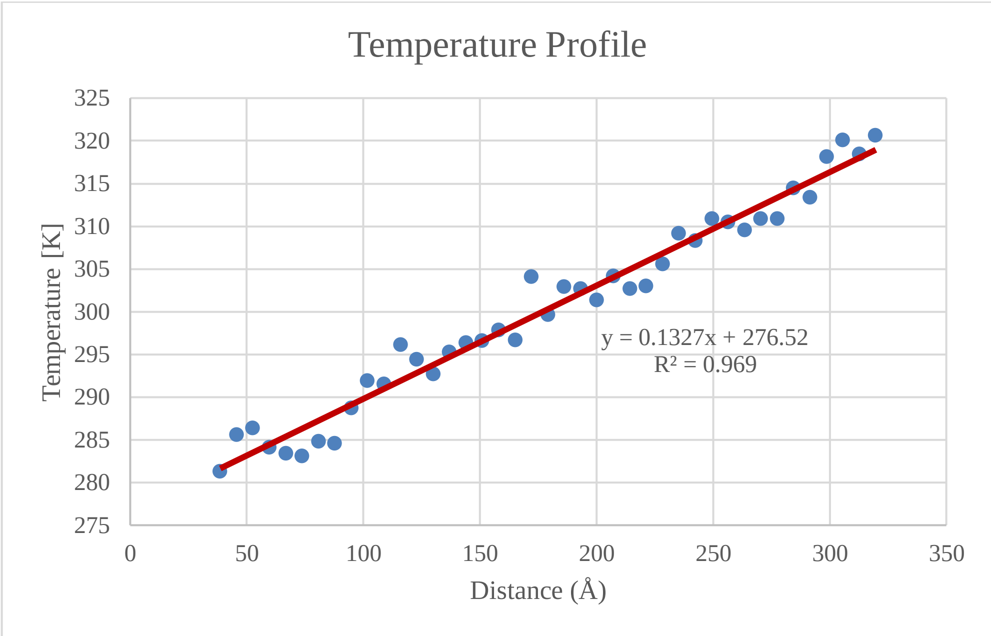

Figure 8: Example of the trendline. Image by the author.

Once ∇T is known along with the heat added to the system, the thermal conductivity can be evaluated. The thermal conductivities obtained for different geometries are shown in Table 1.

Table 1: Results obtained for thoria thermal conductivity at room temperature

Dimensions [Å]	Thermal conductivity [W/m-K]
[420, 18, 18]	11.5850
[700, 56, 56]	12.7533
[840, 56, 56]	12.8820

5.3 DISCUSSION

Even though the results are reasonable, they are far from those other reported by similar NEMD simulations. To be more specific the values shown in Table 1 get close to 13 W/m-K while those reported are between 8 and 16 W/m^2-K (closer to the last value as the dimensions of the model increase, due to reduced phonon-phonon scattering [6]). Additionally, the thermal conductivities obtained by Park et al. at equal x-length and similar cross-section (420x11.2x11.2 angstrom) are about 3 units higher when compared to the ones obtained here. On the bigger geometries this 3 units difference persists as thermal conductivities reported by those simulation topped at about 15.9 and here, they do so at 12.9 W/m-K. Taking a look at the same results for uranium dioxide, reveals that still those are higher than the ones obtained with the simulations of this work, reaching 14.9 W/m-K.

The difference in the results may be due to the interatomic potential used since all other parameters were set to be either the same or very similar. Machined-learning is being applied to calculate more accurate interatomic potentials using quantum-mechanical calculations and high order numerical regression. The accuracy of the potentials obtained through ML can be significantly improved by augmenting the database used and they allow for more efficient calculations [9]. Although promising, these new calculation methods applied remain to be very accurate interpolations of values dependent on quantum physics calculations, so they are not and will not be completely accurate. Last of all, it should be recalled that, as stated at the beginning of this report, complete accuracy is not the objective here, but to have a good idea of what to expect before moving forward to a real-world application of what it is being simulated.

6 ANALYSIS OF MSRS

6.1 THE THERMAL BOTTLENECK

Nuclear fuels can come in many forms, but most of the commercialized nuclear fuels come in the form of pellets (Figure 9), plates or pebbles (Figure 10). These have in common that the fuel is encapsulated inside come kind of cladding to protect it, containing it from leaking if melting occurs, or contain fission gasses (mainly xenon and krypton) that occur as a byproduct of the reaction. The thermals of the simplest out of the before mentioned shapes that nuclear fuel may come in (plates), will be analyzed next. Thus, the geometry in questions is shown by Figure 11 and Figure 12.

Figure 9: Nuclear fuel pellets assembly. Image by Westinghouse Electric.

UO_2 is commonly used as fuel today in commercial nuclear power plants, so this is the compound analyzed along with its fuel cycle. The volumetric internal heat generation rate (due to fission) is assumed to be uniform and not all relevant details are considered in this model (such as the gap that usually exists in between the fuel and the cladding) as this model is accurate and detailed enough for the purposes of this work.

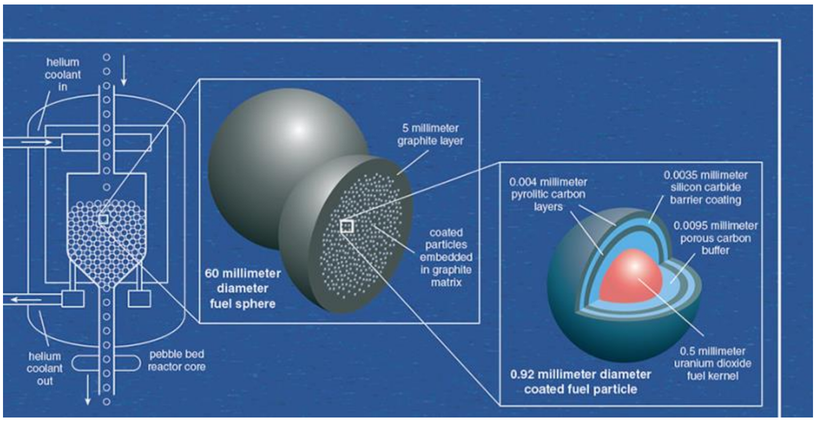

Figure 10: Nuclear fuel pebble and pebble bed (left). Image by Tom Dunne.

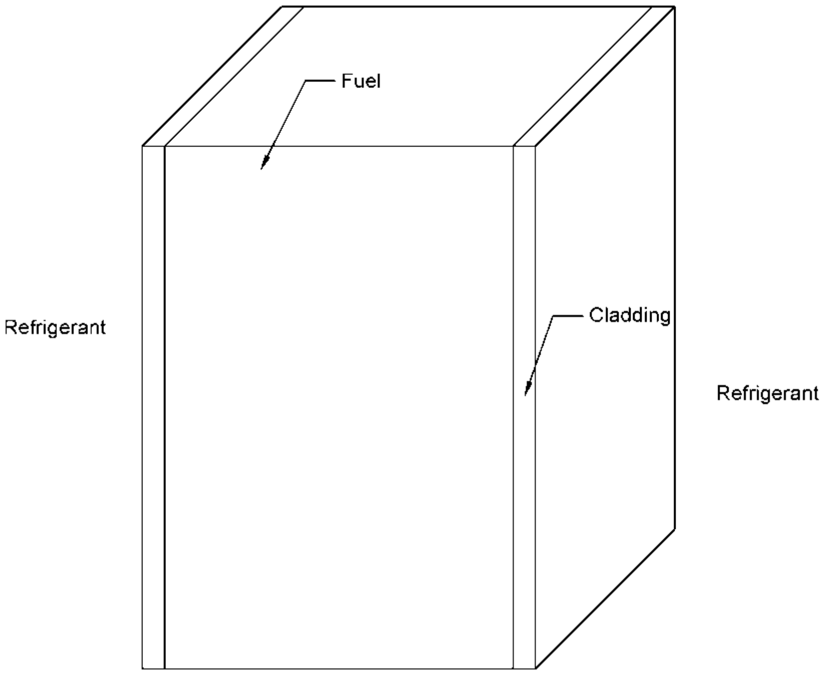

Figure 11: Fuel plate to be analyzed. Image by the author

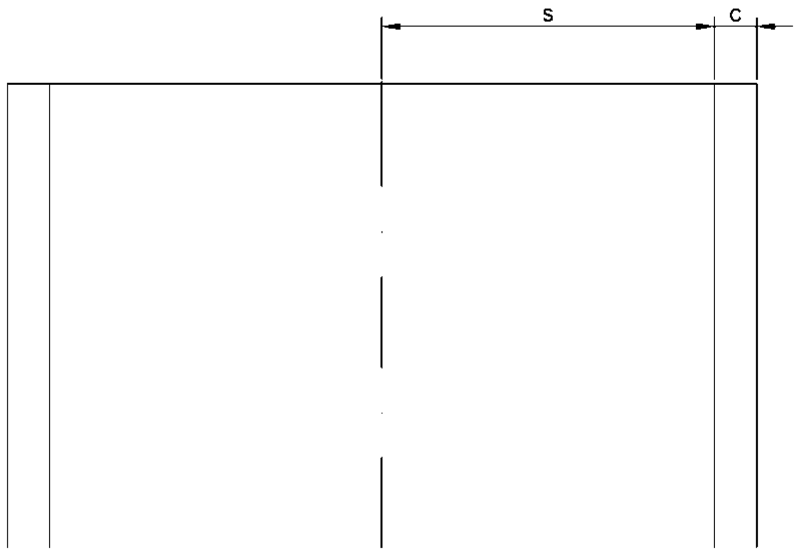

Figure 12: Detail for the nomenclatures used for fuel and cladding dimensions. Image by the author

If the heat equation (E. 3) is considered for the model represented by Figures 9 and 10, and the assumption made before about heat generation being uniform, 3 different zones can be recognized. The first, where the fuel is located and fission is taking place, a second one would be that for the cladding and the third one is located throughout the refrigerant and the temperature profile approaches the bulk temperature of the refrigerant. The model is made to be steady state and the plate can be assumed to be semi-infite, so only the x direction of the temperature profile is considered.

E. 3

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} + \frac{\dot{q}}{k} = \frac{\rho C_p}{k}\frac{\partial T}{\partial t}$$

Parameters considered are given on Table 2. If the first part is considered, the heat equation for that part is as follows:

E. 4
$$\frac{d^2T}{dx^2} + \frac{\dot{q}'''}{k} = 0 \quad \forall\, x\ \in [0, s]$$

Once T is obtained from the differential equation (E. 4), boundary conditions have to be stablished to determine the constants. The maximum temperature is found at x=0 and that also means that dT/dx in that point must be zero. The temperature expression for this first region is then given by:

E. 5
$$T = -\frac{\dot{q}'''}{2k_f} x^2 + T_m \quad \forall\, x\ \in [0, s]$$

Table 2: Parameters considered

Parameter	Definition
s	Half width of the fuel
c	Thickness of the cladding
k_f	Thermal conductivity of the fuel
k_{cl}	Thermal conductivity of the cladding
T_{inf}	Coolant bulk temperature
T_m	Maximum temperature of the fuel
T_1	Maximum temperature in the cladding or at the interface fuel-cladding
T_2	External temperature of the cladding
$\dot{q}'''$	Volumetric heat generation rate in the fuel

The expression that can be used to obtain the temperature profile inside of the cladding is the same as the one of E. 4 but without volumetric heat generation. Finally, the boundary conditions can be obtained by imposing that the heat flux is the same throughout all the cladding and equal at both sides of the interfaces fuel-cladding and cladding-refrigerant. The solution is then as follows:

E. 6 $$T = -\frac{\dot{q}'''s}{k_{cl}}x + T_m - \frac{\dot{q}'''s^2}{2k_f} + \frac{\dot{q}'''s^2}{k_{cl}} \quad \forall\, x \in [s, s+c]$$

The shape for the temperature profiles at the fuel and cladding are represented in Figure 13. The maximum temperature is found at the center of the fuel, and it is a design limitation since a meltdown of the fuel is not considered and will result in a shutdown. The smaller the fuel pellets then, the lower this will be limitation since the cladding surface temperature will be closer to the maximum temperature.

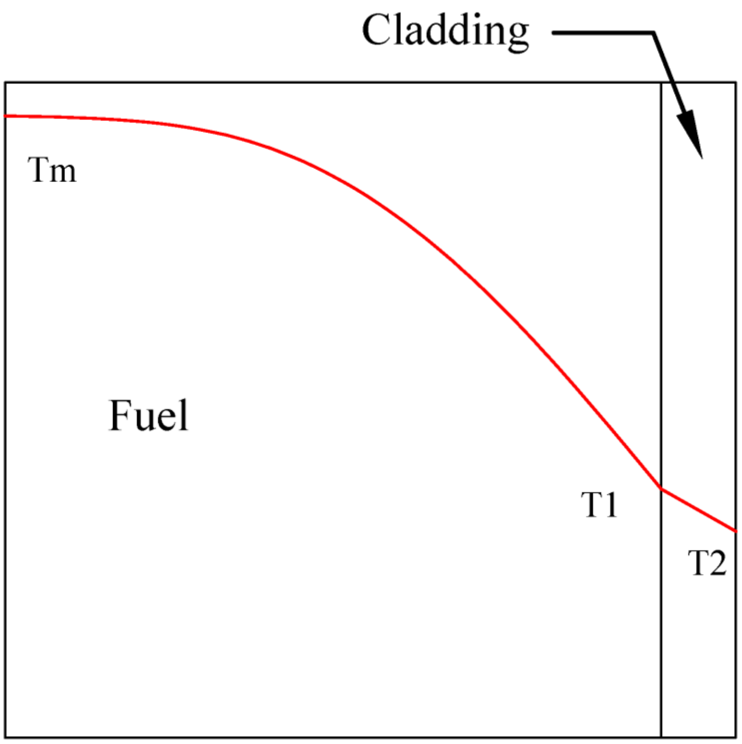

Figure 13: General shape for the temperature profile of a semi-infinite nuclear fuel plate. Image by the author

The heat generated using this model (solid fuel), must travel through the UO_2 and then through the cladding before it can be extracted and used in a power cycle. If the fission rate increases because of over moderation (which was the case for the RBMK design [10]) the fuel is generated at a faster rate than it is extracted, and the temperature increases inside of the assembly. Not only this, but radioactive fission byproducts get trapped inside of the material generating residual heat after the service life.

Numeric solutions for the specified geometry are represented in Figure 14 and Figure 15, the MATLAB code for them and the thermal model can be found in Appendix C. For these two solutions all parameters are the same except for the thermal conductivity of the fuel. In the first case it was set to be 10 W/m-K and in the second 12 W/m-k. A difference of 2 units, which is about the difference for the thermal conductivity of UO_2 as opposed to that of ThO_2, being the latter the larger of the two. This relatively small difference results in outer temperatures of the cladding of about 451 K and 481 K respectively. A 30-degree difference that is very substantial given that the temperature at which heat is added to the power cycle is a fundamental parameter. This concept is demonstrated in its simplest manner by the Carnot efficiency equation (E. 7) and following it, for this case the difference in efficiency is: 21.98%-18.75% = 3.23%. It is a safe prediction to assume that if this thermal isolation in between where fission occurs, and heat is extracted much higher efficiencies could be achieved.

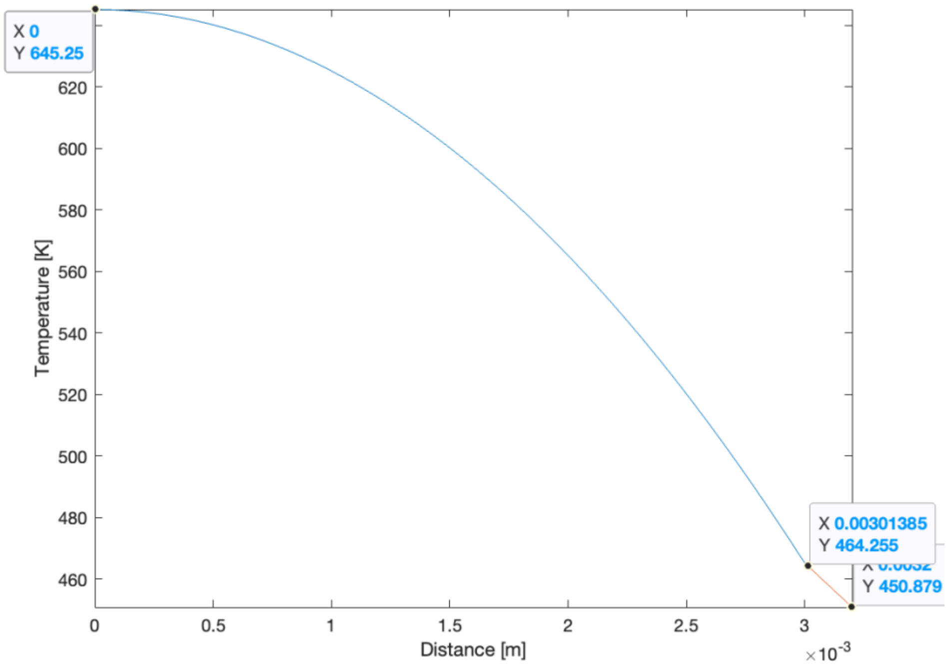

Figure 14: Numeric solution for the temperature profile 1. Image by the author.

E. 7

$$\eta_{Carnot} = 1 - \frac{T_{cold}}{T_{hot}}$$

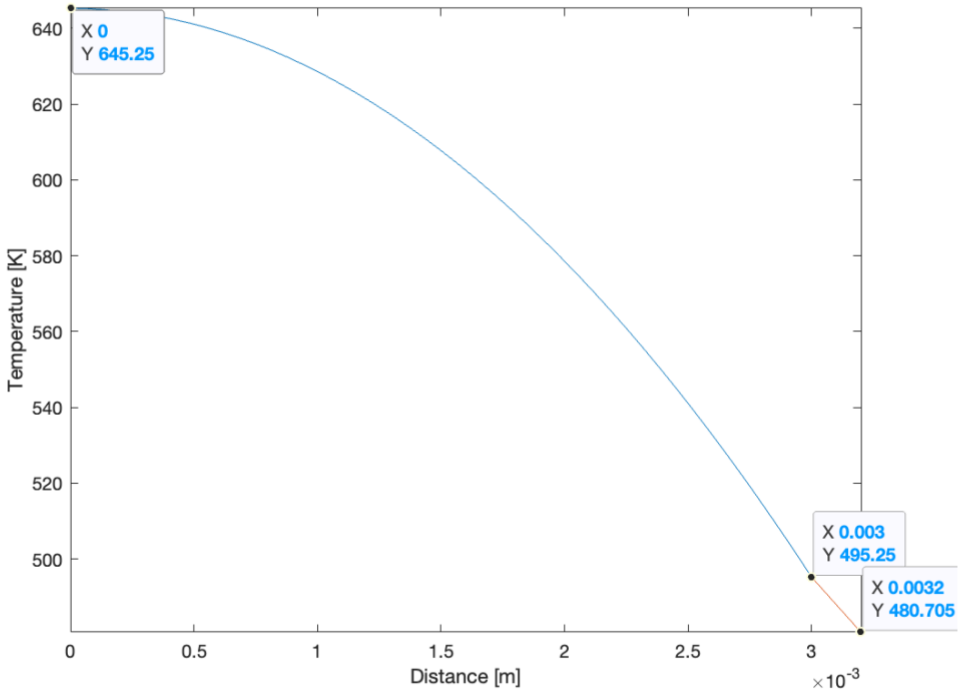

Figure 15: Numeric solution for the temperature profile 2. Image by the author.

6.2 MSRs TECHNOLOGY DESCRIPTION AND OTHER GEN-IV DESIGNS

MSRs is a nomenclature used for any technology that produces nuclei fissions and uses molten salt as the refrigerant and the fuel may or may not be dissolved in it. There are many ways of implementing these concepts into real world applications whether that will be for a breeding or an energy production operation. One main concept currently being considered is the one shown by Figure 16. The designs usually consider a core which is much hotter and where fission is taking place and a blanket that surrounds it. In the blanket, excess neutrons are absorbed for fissile uranium breeding from fertile thorium following E. 8 and as represented in Figure 17. Pa-233 must be constantly removed from the blanket to let it “mature” (beta decay) to fissile U-233, failing to do so will result in Pa-233 absorbing more neutrons and increasing Pa-233 losses (thus fissile material) and reducing neutron economy.

E. 8 $$ {}^{232}_{90}\mathrm{Th} \xrightarrow{+n} {}^{233}_{90}\mathrm{Th} \xrightarrow{\beta^-} {}^{233}_{91}\mathrm{Pa} \xrightarrow{\beta^-} {}^{233}_{92}\mathrm{U} $$

There are many benefits related to size and safety when MSRs are considered compared to traditional BWR, PWR or any other technology being currently implemented such as a big negative and void coefficients. As temperature raises, the salt expands, the density of the fuel decreases and the reactivity decreases. Moreover, some behaviors that are inherent to this design simplify otherwise major problems to overcome in today’s working technology. The capacity of the salt to vary its volume as temperature changes allows for load following capabilities, something possible with current technologies but very hard to implement and not very flexible [11]. The worst accidents in nuclear energy production history were caused by a meltdown of the core, such event is not a problem in this design, as the fuel is in liquid form during regular operation. Finally, the fuel is always in a homogeneous mix, this is possibly the best assumption that reactor designers can make. Since the fuel is not encapsulated in pellets, fission products can be removed during operation and complete or a much higher burnup can be achieved. So, with smaller inventories of fissile or fertile materials much more energy can be produced.

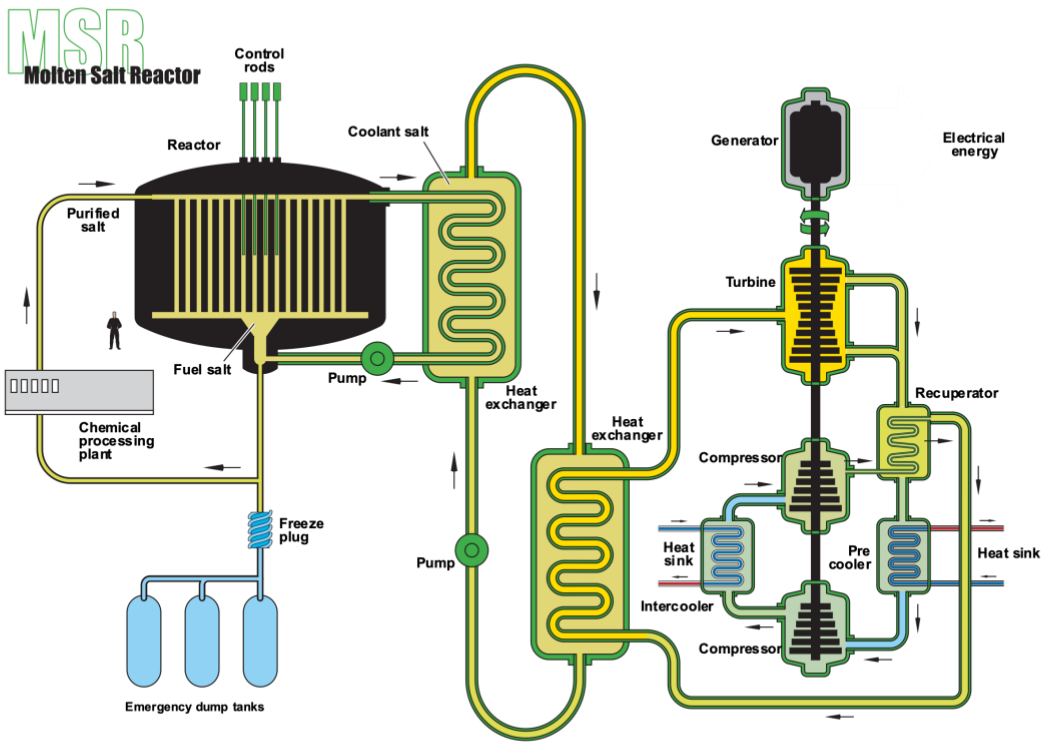

Figure 16: Graphite-moderated Molten Salt Reactor scheme [12]

Although most of the advantages previously mentioned are good enough by themselves for companies and governments to invest in this technology, they will not be discussed in the present work. Instead, an analysis on fuel economy alone will be carried out. When all benefits are discarded in favor of commodity an answer will be given for how much is that commodity worth.

Gen-IV reactors include designs that implement cooling in the form of light water, helium, lead-bismuth, sodium, and fluoride salt (the one analyzed here). All these designs except for the MSR operate with solid state fuels, some of them do make use of a pebble bed like the one represented on Figure 10 that reminds more and more of a liquid form. This implies that the thermal barrier previously commented still applies, and not a full online reprocessing is possible (although the pebble bed design does allow for some degree of processing). Three of the six designs being developed operate in the fast neutron range thus are usually conceived either to breed fissile nuclear fuel or burn other elements that do not fission in the thermal range, such as the actinides with long lives produced as waste in traditional reactors, or new ones that may operate in the thermal spectrum.

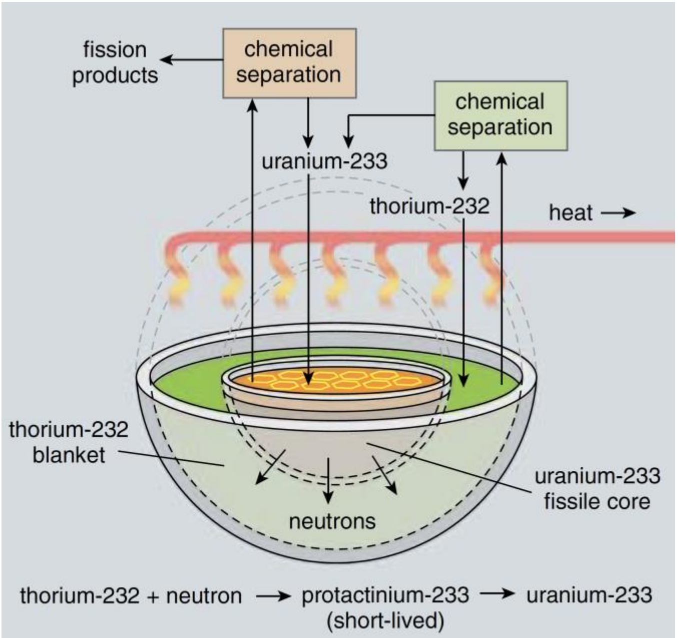

Figure 17: Thorium powered MSR blanket [13]

6.3 ECONOMIC IMPLICATIONS OF FUELS AND ITS STATES

6.3.1 TRADITIONAL REACTOR FUEL ANALYSIS

Energy released per U-235, or U-233 fission is usually assumed to be about 200 MeV, and about 210 MeV for Pu-239 [14]. Once this has been considered, the energy in joules released by 1g of U-235 can be estimated as given by E. 9.

E. 9

$$Q = \frac{N_A}{\text{Molecular Weight}} \times (\text{Energy released per fission}) \times (\text{Percentage of the fuel that is used})$$

Enrichment for commercial nuclear fuel is maxed at 5% by the Nuclear Regulatory Commission (NRC). Additionally, about 1% of U-235 is found in the composition of nuclear pellets at their end life, assuming that the Pu-239 bred from U-239 doesn't produce any of the fissions and that no mass is lost, the percentage of fissile material spent can be approximated as 4/5=80%. Finally, the energy releases per gram of U-235 can be estimated as follows:

$$Q = \frac{6.023 \cdot 10^{23} \left(\frac{\cancel{\text{nuclei}}}{\cancel{\text{mole}}}\right)}{235.044 \left(\frac{\text{g}}{\cancel{\text{mole}}}\right)} \left(200 \left(\frac{\cancel{\text{MeV}}}{\cancel{\text{nuclei}}}\right) \cdot 1.6022 \cdot 10^{-13} \left(\frac{\text{J}}{\cancel{\text{MeV}}}\right)\right) (0.80)$$
$$= 6.5681 \cdot 10^{10} \frac{\text{Joules}}{\text{gram of U} - 235}$$

A 1 GW nuclear plant will need to produce 3153.6 TJ of energy during a 1-year operation if a 100% efficiency is considered. That amount of energy would require about 480.14 kg of U-235 or 9602.8 kg of bulk U-238 for a 5% enrichment (10894 kg of fuel when it comes in the form of uranium dioxide). If a 33% efficiency is considered [15] for the whole process from heat released by fissions to net energy production, then the mass of enriched uranium required will be 202080 kg (1455 kg of U-235).

Natural uranium is estimated to cost $32.5 per pound ($71.72 per kg) by the U.S. Energy Information Administration [16] and the price for 1 kg of separative work (SWU) $99.54 as claimed by the same administration. 7.14 kg of natural uranium need to be processed for every kg of enriched uranium required. Other costs like processing into the end product or transportation of the enriched uranium are not considered.

U-235 found in natural U-238 accounts for 0.72%, since 1455 kg of U-235 are needed, 202083.33 kg of natural uranium are needed and have to go through an enrichment process. To sum up, the cost for a 1-year worth of fuel for 1 GW nuclear plant using PWRs is estimated to be:

$$\begin{aligned}\mathrm{Cost} &= \mathrm{Cost\ of\ bulk\ material\ (U-238) + Cost\ of\ enrichment} \\ &= 202.08 \cdot 10^3(\$71.72 + \$99.54) = \$34.608\ \mathrm{M/year}\end{aligned}$$

6.3.2 MSR FUEL ANALYSIS

As opposed to a traditional reactor, a MSR will usually take advantage of the thorium cycle. Thorium is much more common on Earth, and it is extracted accidentally as a byproduct of mining other materials. Moreover, thorium is used as a fertile nuclear fuel to breed other element actually fissile, that is U-233. The equivalent to doing this with the traditional uranium cycle would be to breed fissile Pu-239 from U-238, instead of only using the fissile U-235, but that may cause the proliferation of nuclear weapon grade Pu which usually wants to be avoided at all costs.

Figure 18 shows fission cross-sections (probability that fission will occur) for different elements in the thermal and up to the beginning of fast neutrons spectrum. The thermal spectrum is the one of interest as most nuclear reactors operate in that range (they are also referred to as thermal reactors). Thermal neutrons are those with an energy less that 5eV. As it can be seen on Figure 18, U-233 has an even better cross-section profile than U-233 so it is an easy element for reactor designers to work with. Note that Figure 18 represents fission cross-sections and not absorption cross-sections (the latter is shown by Figure 19)

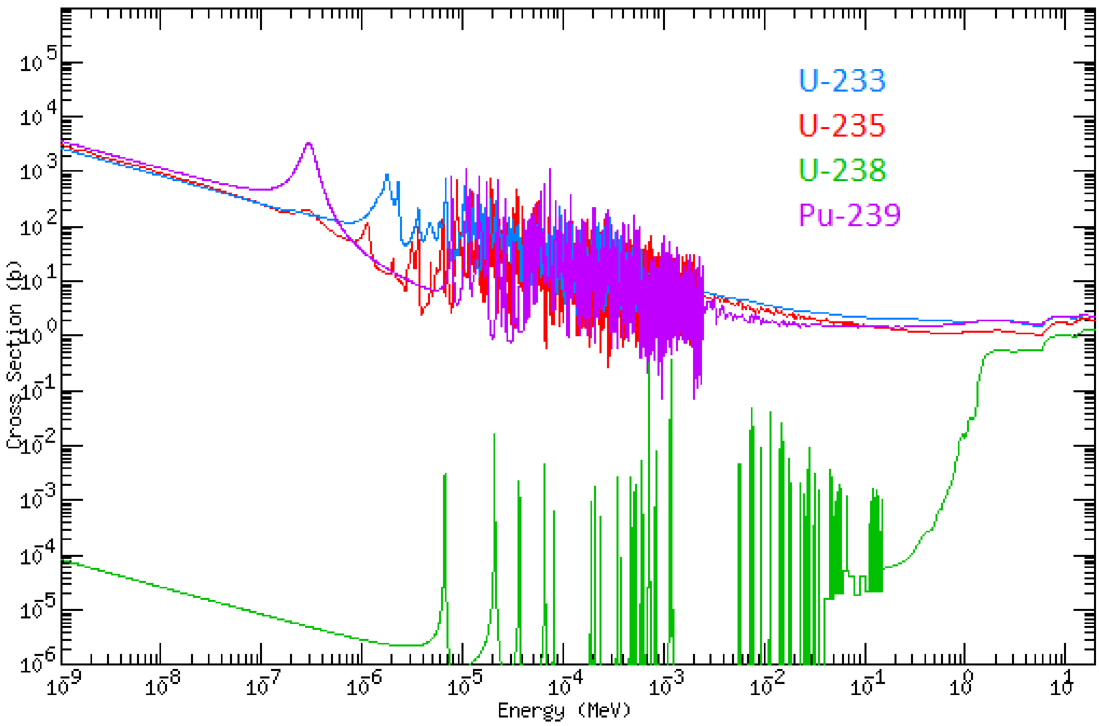

Figure 18: Fission cross-sections [17]

The energy released per gram of U-233 can be calculated in a similar manner as it was previously calculated for U-235. However, since now a MSRs is the technology of choice to extract the energy from the heat released by fission, and online reprocessing is possible, all heat is directly transferred to the coolant (fuel is dissolved in the salt) and theoretically all U-233 can be used for fission. The energy in Joules released per gram of U-233 is then as follows:

$$Q = \frac{6.023 \cdot 10^{23} \left(\frac{\cancel{nuclei}}{\cancel{mole}}\right)}{233.04 \left(\frac{g}{\cancel{mole}}\right)} \left(200 \left(\frac{\cancel{MeV}}{\cancel{nuclei}}\right) \cdot 1.6022 \cdot 10^{-13} \left(\frac{J}{\cancel{MeV}}\right)\right) \quad (1)$$

$$= 8.2807 \cdot 10^{10} \frac{\text{Joules}}{\text{gram of U} - 233}$$

This relatively subtle change of the fuel and its state makes for a major difference of 17.126 GW/gram of fissile material (26.08% increase). Not only that, but other more notable advantages invisible for the inexpert eye such as an always homogenous mix (some parts of the fuel aren't more used up than others since it is in liquid form) along with naturalizing the meltdown can be found.

An initial inventory of fissile material will most likely be needed for a reactor of these characteristics, but plutonium found in waste nuclear fuels stored usually underground or close by to currently operating NPPs (Nuclear Power Plants) can be used for this purpose. Once startup is achieved, U-233 releases about 2.48 neutrons for every fission, so reactor designers can account for an initial inventory of Pu that allows for refueling of Th alone, at least for the design life. The initial inventory is very low when compared to the rest of the fuel and has a very low impact when usual design lives are considered (>40 years), so it will not be considered.

As opposed to previously stablished, in these reactors all fuel can be used for fission, not only the fissile part of it. Theoretically, all Th-232 can be converted to U-233 by neutron absorption and later "maturing" (beta decay). Nonetheless, a loss of Pa-233 by neutron absorption will be considered accounting for 40% of all the fertile Th used (again this Pa loss can be accounted for in the initial inventory, so that refueling of fissile material will not be necessary).

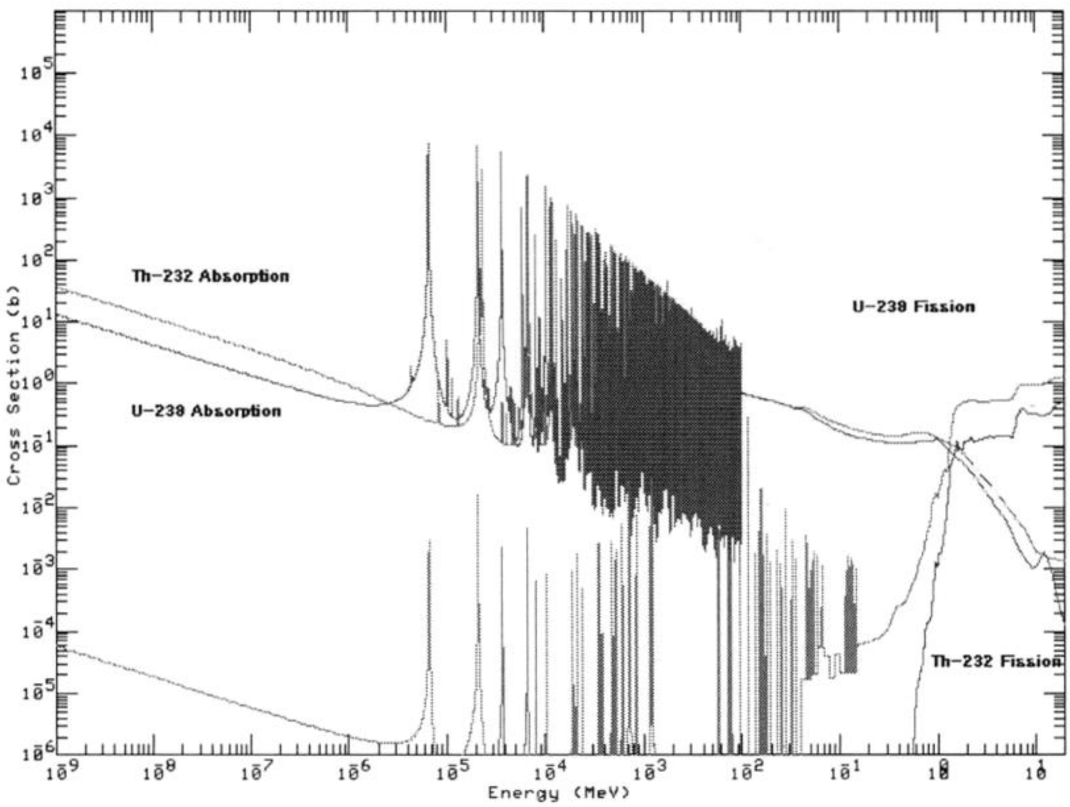

Figure 19: Absorption cross-sections [18]

The same 1 GW nuclear power plant previously studied will need 380.84 kg of U-233 this time for a 100% efficiency. MSRs allowed for 44% efficiency back when they were being experimented with at the ORNL in the 1970s [19] so this will be assumed to be the efficiency from heat production by fission to electricity generation. 865.54 kg of U-233 will be needed for the efficiency considered (44%), this yields 1442.6 kg of Th-232 needed as a 40% protactinium loss was assumed.

Once again other factors such as transportation costs for the thorium (much cheaper than for the enriched uranium) and transformation into the end product will not be considered. Finally, the price for Th-232 is accepted to be $30 per kg [20] and the cost for a 1-year worth of fuel for a 1 GW nuclear power plant making use of one or several MSRs is estimated to be:

$$\text{Cost} = \text{Cost of bulk material (Th} - 232) = 1442.6\,\cancel{\text{kg}} \cdot \frac{\$30}{\cancel{\text{kg}}} = \$43.277\ \text{K}$$

To conclude, not only way less material is needed, but it is much cheaper, it does not require further mining operations that the ones currently being developed, and it does not require enrichment processes. This enrichment is incorporated into the energy production process and although the chemistry required for the online reprocessing is challenging, it was proved to be possible and will hardly add more difficulty to the current designs that operate at very high pressures and do require of a containment vessel.

This difference in the fuel cost will be reflected as an annuity for new projects considering both designs and will result in a +$34.565 M in favor of the MSR design. Fuel expenditure is considered at the end of year 40 to account for possible problems that may occur during transportation or installation during the design life of the power plant. Annual costs in fuel for the two different technologies may be drawn as presented by Figure 20 and Figure 21:

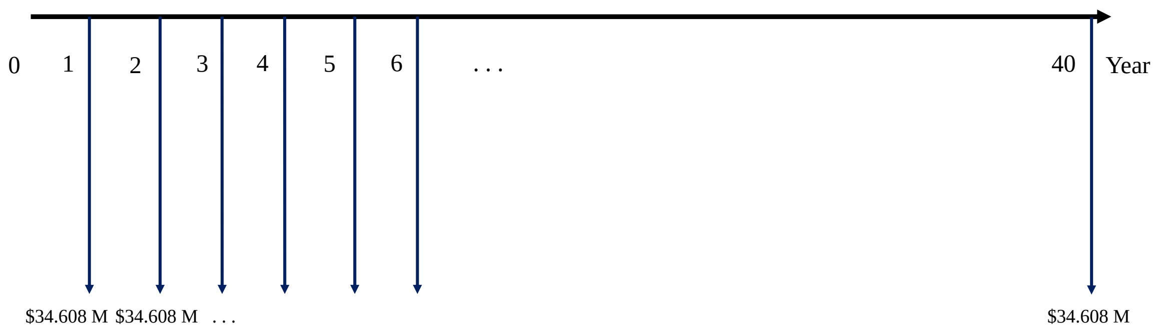

Figure 20: Cash flow diagram representing fuel annuity cost for a traditional PWR (1GW). Image by the author

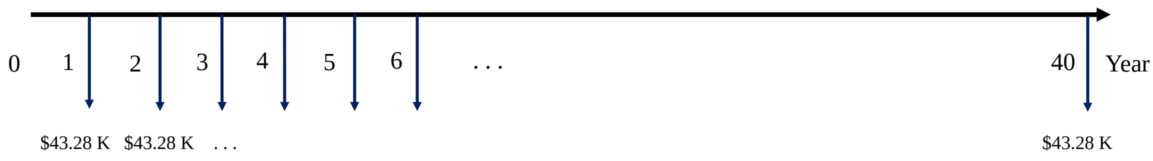

Figure 21: Cash flow diagram representing fuel annuity cost for a MSR (1GW). Image by the author

Finally, when both are compared to one another the cash flow comparing both investments may be represented as follows, where the “benefits” represent the savings in fuel annually:

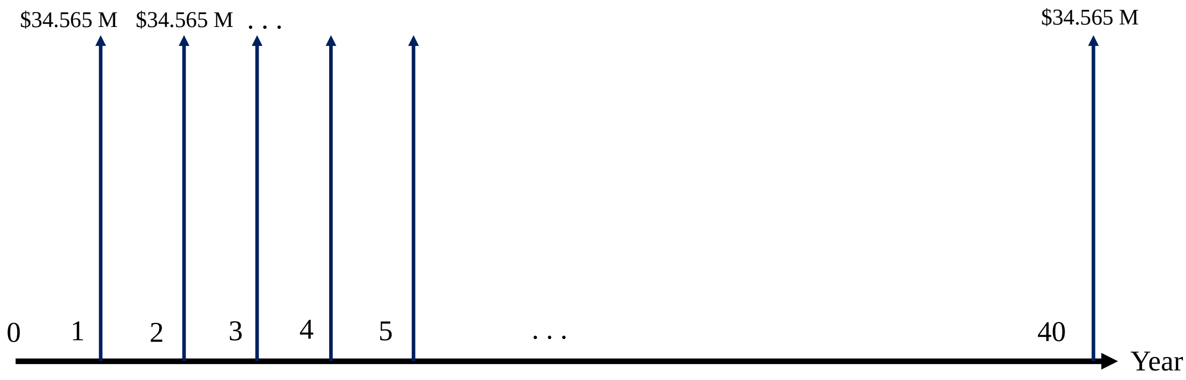

Figure 22: Cash flow diagram representing fuel annuity savings for a MSR (1GW). Image by the author

This annual difference may be brought to the present by using E. 10 to obtain a factor that can be used to directly convert the annuity into a present worth. N represents the number of years the annuity lasts and i the interest rate. N=40 and the interest rate, i, is assumed to be similar to other construction loans [21], thus it is assumed to be 3% including fees. Tables for economic factors were used to obtain the value: (P/A,i=4%,40) = 19.793. The present worth of the annual saving is then found to be $684.14 M.

E. 10 $$(P/A,i,N) = [(1+i)^N - 1]/[i(1+i)^N]$$

6.4 WASTE ANALYSIS

6.4.1 TRADITIONAL REACTOR WASTE ANALYSIS

The average reactions that take place as a result of U-235 fission are given by E. 11 and E. 12. In average, about 2.43 neutrons are released per fission [15] with this and taking into account the energy of 1 amu (931.5 MeV [22]) then mass balance can be applied to determine the amount of fission wastes:

$$\text{Average mass of fission products} = (235 + 1 - 2.43)\text{amu} - \frac{200\ \cancel{\text{MeV}}}{931.5\frac{\cancel{\text{MeV}}}{\text{amu}}}$$

$$= 233.355\ \text{amu}$$

This accounts for 233.355/235=99.3% of the U-235 that results in fission. It has to be noted though that not all interactions result in a fission reaction, some of them involve neutron absorption resulting in other actinides with long half-lives. But it is safe to assume that most of them do. On the other hand, as the core is composed of a lot of material (a lot of mass) once the encapsulation and the U-238 are considered, these do have to be treated as radioactive waste.

E. 11 $${}^{1}_{0}\text{n} + {}^{235}_{92}\text{U} \rightarrow {}^{141}_{56}\text{Ba} + {}^{92}_{36}\text{Kr} + 3\,{}^{1}_{0}\text{n}$$

E. 12 $${}^{1}_{0}\text{n} + {}^{235}_{92}\text{U} \rightarrow {}^{140}_{54}\text{Xe} + {}^{94}_{38}\text{Sr} + 2\,{}^{1}_{0}\text{n}$$

If the previous 1 GW nuclear power plant is considered, then (0.8)(0.993)(1455) = 1155.852 kg of fission products are produced every year, and 202080 kg of highly radioactive material not taking into account the mass of the cladding and the encapsulation (noble gasses released by fission and trapped in the encapsulation are considered). Some elements found in these residues (actinides) are known to have a half-life of over a thousand years [13] and most of it is trapped in a solid crystalline structure inside of the cladding. In addition, as some Pu may be found in the residues, governments have to keep a close eye on them as criminal organizations or other questionable governments may use it for war purposes. For this purpose, companies aren't usually allowed to manage residues by themselves during all the required time and are instead taxed by governments for them to do so.

6.4.2 MSR WASTE ANALYSIS

A similar process can be developed for U-233 fission. The average reaction is given by E. 13. Average neutron release is estimated to be 2.50 by the IAEA [23] (very similar to that of U-235 reaction) and once again mass balance can be applied to determine the amount of fission wastes:

$$\text{Average mass of fission products} = (233 + 1 - 2.50)\text{amu} - \frac{200\ \cancel{\text{MeV}}}{931.5\frac{\cancel{\text{MeV}}}{\text{amu}}}$$

$$= 231.285\ \text{amu}$$

E. 13 $${}_{0}^{1}\text{n} + {}_{92}^{233}\text{U} \rightarrow {}_{54}^{137}\text{Xe} + {}_{38}^{94}\text{Sr} + 3{}_{0}^{1}\text{n}$$

The result accounts for 231.185/233=99.26% of the U-233 that results in a fission reaction. This time the different concept in which MSRs are based on shines again. As it was previously demonstrated only the material suitable for fission is brought inside of the reactor (aside from the molten salt that is already inside of it or used to bring it in). Theoretically only (0.9926)(380.84)/0.44 = 865.55 kg is produced, however the piping system of the primary loop that is in contact with the highly radioactive material is expected to have to be replaced at least every year before some more knowledge on radiation damage for piping suitable materials is acquired [19]. But these would not present long disintegration half-lives and thus would only be radioactive for relatively short periods of times specially if water treated. Additionally, the protactinium losses previously considered (neutron absorption) may result in other actinides that would have to be considered. With these, the potential mass of relatively long lived radioactive material can go up to 865.55 + (0.4)(1442.6) = 1442.6 kg.

To sum up, the 1 GW nuclear power plant with a MSR studied will potentially produce in the realm of 955.16/202080 ~ 0.7138% of the nuclear waste, as compared to the same using a traditional reactor considering the ones with long half-lives (>100 years). This number was estimated by Hargraves et al. [13] to be (2.86%)(0.17) = 0.4857%. Moreover, the elements with longer half-lives were concluded to top at around the 300 years (until they reach natural radioactivity levels once) by the same article.

It is not easy to account for how much it costs to take care of nuclear waste. Although the concept is simple (dig a deep hole in a secure location and place it inside), the U.S. government has failed to do so (after successfully collecting the money they estimated that it was necessary to do so). The money already paid by U.S. citizens to their government to build a secure location and take responsibility for the nuclear waste produced for energy production purposes alone (>$40 billion dollars) is ignored, and only what they are currently paying yearly (in the form of a fine) is considered, that is, $0.5 billion dollars a year [24]. This amount of money can be divided by the number of GW of nuclear power installed in the US to obtain a good estimate of yearly cost for waste management for a 1 GW traditional power plant. In the U.S. there were 95.492 GW of nuclear generation capacity installed by the end of 2021 [25]. That yields $5.236 M/year per GW of nuclear energy production for waste management costs.

Variance from the results obtained concerning proportions of radioactive wastes is accepted and instead of using the ~0.7% obtained previously, a 5% will be taken. If only 40 years of operations is considered for the project, and the fine for waste management is to be passed on to the next project then the comparative cash flow for waste management may look as shown by Figure 23.

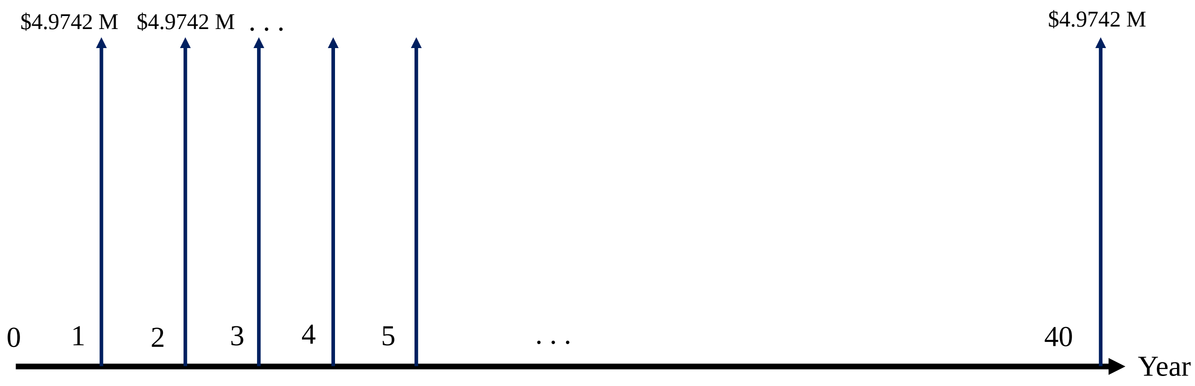

Figure 23: Comparative cash flow showing benefits for expenditure on waste management of MSR as opposed to traditional reactors. Image by the author

Note that as only a 40-year timeline is considered the added benefits of shorter half-lives that MSR's wastes have as opposed to traditional reactors (~300 years vs > 1000 years) is not considered.

This annuity accounts for $4.9742(P/F,i=4%,40) = ($4.9742)(19.793) = $98.4543 M. This result although not that significant when compared to the previously calculated on fuel expenditure ($684.14 M) should be accounted for, especially if not only money is considered , but also potential risks for managing and transporting much higher amounts of radioactive material. However, the latter is not considered in this work.

7 FOSSIL FUELS

7.1 FUEL ANALYSIS

As archaic as it may seem in some countries the fact of investing in new projects involving fossil fuels, it is a reality that many countries still do not have any regulations on them nor any plan to impose them. In this scenario, companies or governments interested in building a power plant may consider all alternatives and choose the cheapest.

Energy production through means of burning fossil fuels is very well known and highly efficient power cycles have been developed. For this analysis, natural gas will be considered as it is arguably one the cheapest, cleanest, and most abundant alternatives. Energy release by natural gas (composed mainly of CH4) follows E. 14. The energy released per kg of CH4 is between 50 and 55 MJ [26], being 52.5 MJ the value of choice.

E. 14
$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O + \text{Energy}$$

For the same power installed considered before, 1 GW and same energy produced per year, 3153.6 TJ, 1.1617 M metric tons of natural gas will be needed for a 57% efficiency [27] from heat to energy production. Prices for natural are taken as of February 2021 in the U.S. Even though this is an undoubtedly high price for natural gas, it is a penalty stablished for the fact of it being a limited resource which price fluctuates a lot. The price for the required amount of NG needed is then:

$$\frac{\$9.33}{\cancel{1000\,\text{ft}^3}\ \frac{28.3168\,\cancel{\text{m}^3}}{\cancel{1000\,\text{ft}^3}}}\ 0.717^{-1}\frac{\cancel{\text{m}^3}}{\text{kg}}\ \text{NG} = \$0.46\ \text{kg}^{-1}\ \text{NG}$$

$$\$0.46\ \text{kg}^{-1}\ (1.0538 \cdot 10^9)\text{kg} = \$484.27\ \text{M}$$

This is a considerable high price for a year's worth of fuel even if only compared to a traditional reactor ($34.608 M). But even if a one of the lowest prices for NG in the last decade is chosen ($2.71), the price is still much higher ($484.27 M (2.71))/(9.33) = $140.66 M). It should be considered that the construction costs are much lower, and construction times are shorter for NG power plants as opposed to nuclear power plants. In addition to this, the value given by the energy production flexibility has to be kept in mind. On the other hand, design lives for these kinds of power plants are usually between 25-30 years as claimed by the energy production company Sargent & Lundy. If all of the aforementioned are to be reflected in a 5 years' worth of fuel in profits (a conservative assumption), and the fuel for the first year is considered to be a part of the initial investment (just as before) then the cash flow diagram comparing the previously studied 1 GW traditional nuclear power plant with the now evaluated 1 GW NG power plant may look as shown by Figure 24

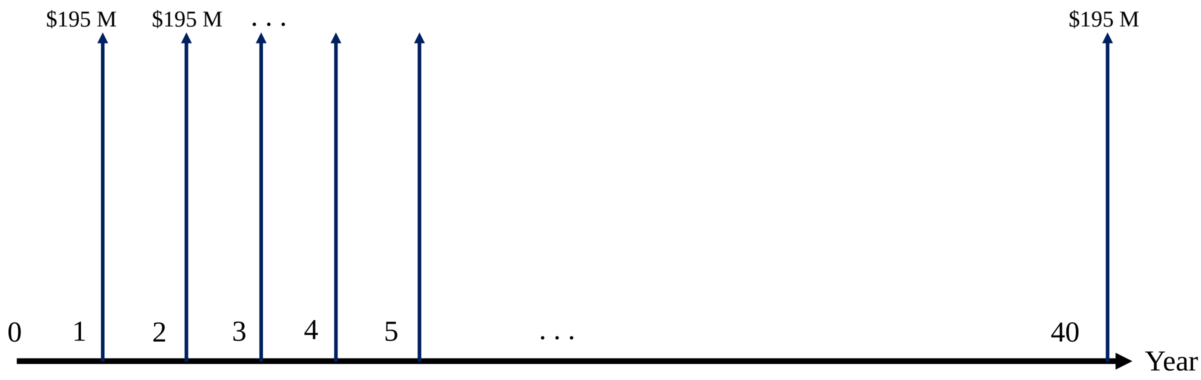

Figure 24: Annual savings in fuel for 1 GWe electricity when traditional reactors are used instead of NG. Image by the author

To account for the assumptions made first the cash flow diagram represented by Figure 25. Next the present worth at year 6 of the 34-year annuity was calculated (P/A,34,4%) and that value was transformed to present value at year 0 to then be annualized for the 40 years of the project (P/F,6,4%) (A/P,40,4%), this results in $229.6 M.

The average price between the high and low previously detailed is used and refueling at the end of year 40 is considered to regard for possible shipment losses or damages during the working life (just as before).

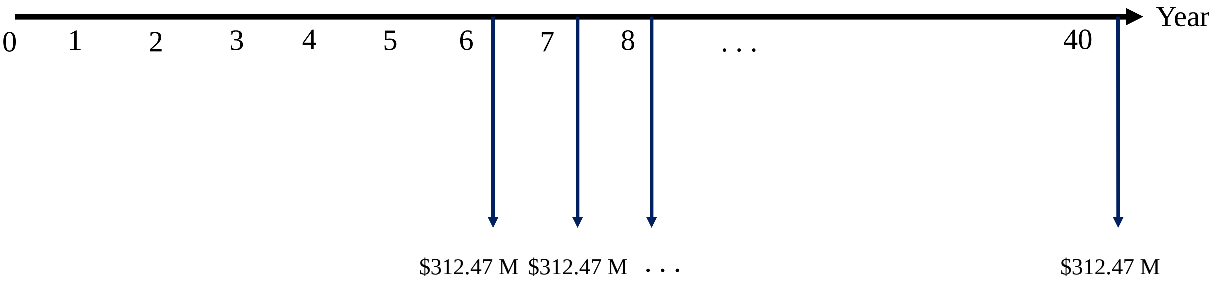

Figure 25: Annual expenditure in fuel for a 1 GW NG power plant after assumptions. Image by the author

$195 M/year may seem like a huge difference, and possibly enough to at least wonder why all private companies aren't just investing in nuclear power plants. All factors aren't considered here as it is not the objective of this work, for instance, the initial investment for a nuclear power plant is much higher and it takes longer to make a profit. Furthermore, insurances for nuclear power plants can be very high ($450 M/year [28]). It is not the aim of this work to consider all economic factors and speculations, but to evaluate the options resource wise and their time value.

7.2 WASTE ANALYSIS

As previously stated, many countries in the world don't regulate emissions, however, the impact that using a technology must be considered even if it is only to have regrets about the waste being dumped into the atmosphere.

Applying mass balance to E. 14 it can be determined that for every kg of CH_4 burnt, 2.75 kg of CO_2 are released to the atmosphere. The amount of CO_2 per year released by the 1 GW NG power plant is evaluated to be 3.1945 million metric tons. If taxation is imposed on these emissions, either directly or in the form of sanctions imposed by the so-called developed countries then the cost of these emissions can be estimated.

Taxation in the EU varies from 0 to over $30 dollars per metric ton of CO_2 produced depending on the country [29]. If a symbolic penalty of 1$ per metric ton of CO_2 is accepted, then about \$3.2 M dollar will have to be paid annually for “waste management”. This would directly add up to the previously calculated \$229.6 M previously calculated as it does not benefit from the assumptions made.

8 RENEWABLE ENERGIES

To determine whether one technology or a different one should be used; the question should be made first if both technologies serve the same or different purposes. This way it can be determined if it makes any sense to confront them to one another. Main renewables energies are usually considered to be solar, wind, hydropower and geothermal. It is a safe assumption to make, given the focus of this work, that all engineering projects involving producing energy from renewable sources should move forward even if costs are much higher. However, the system doesn’t allow for this, as technologies compete against one another and are or not developed usually based on how profitable they are. This is to say that what matters usually is how many dollars can be made from them for every unit energy produced (and not how many dollars it costs per unit of energy produced).

It is obvious that there has been a huge interest in making these renewable energies profitable, even if it was at the cost of leaving aside very promising technologies. As a result, some countries such as Spain have made it mandatory that new buildings that meet certain characteristic have PV solar panels installed [30] (this is not only the case for E.U. countries, but some states such as California have similar mandates). This has produced an increased interest in knowing if the grid and how it is regulated (traditionally designed to receive high amounts of energy from a few points), is prepared to receive much smaller amounts of energy from thousands of points. Additionally, there is an interest in knowing how the demand curve would look like after the supply curve from solar energy is subtracted.

Gómez Navarro et al. [31] predicted the shape of supply and excess power to be as shown by Figure 26. If the PV production is subtracted from the demand curves, a bimodal demand curve can be visualized, with the two peaks being about 9 p.m. and before sunrise. If this model can be escalated (assuming it is correct, then it is correct to do so) reliable sources of energies will have to be forced to produce high amounts of energies during night hours and maybe even shut down during the day. This conclusion would make reliable power plants non-profitable during their design life unless they are highly incentivized. In this scenario, a reliable power plant that can highly reduce its power output during the day and can produce reliably very high amounts of energy during the night at very low and fixed costs would be the best investment.

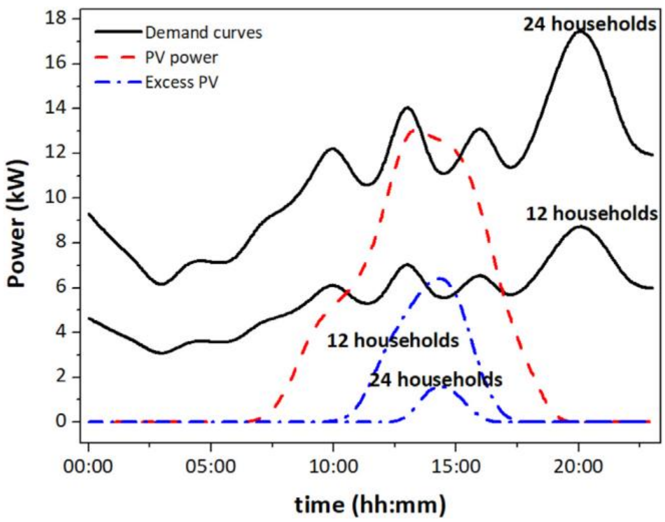

Figure 26: Predicted supply and demand curves for 24 and 12 households with PV energy production [31]

Out of the possible options that technology allows or could allow and that are low resource consuming, MSRs are possibly one of the best as it has been demonstrated. Wind energy will only produce a similar effect where, at certain times, power input to the grid will not be necessary or even penalized. And although others such as hydropower or geothermal may be an option, they are not available everywhere on earth and environmental impact, specially of hydropower may prove too concerning. Not only that, but they are also simply not as reliable.

Energy storage alternatives are not considered as an alternative at least as technology stands today. Possibly the two most popular energy storage methods are pumped hydroelectric and batteries. Pumped hydroelectric is not considered as geography doesn't always allow for it, or it is directly not possible due to the lack of a water source (considerably big river, lake, or access to the ocean). And although it might be reasonable to store about 10% of daily energy needs in batteries, some other alternative energy sources will still be needed for many tasks as renewables and batteries can't produce or store enough energy per unit mass. One of the best battery technologies currently available in terms of performance and cycle life are Li-ion batteries. These have an energy density that tops at 265 Wh/kg [32], one can see the limitations that these have by noticing energy densities for common fuels such as diesel (11.6 kWh/kg). Ideally, the best way to optimize resources would be to develop and implement a technology that can be used in as many applications as possible. For instance, MSRs other than allowing for a resilient electric grid, could power container ships, cargo trains, mining operations… Finally, synthetic fuels (hydrogen, ammonia, e-diesel…) could be considered as a good alternative, but these play in favor of nuclear technology as they are very energy intensive to produce and would multiply energy needs, leaving no other options but to use every zero-emission energy production method that one may think of.

To sum up, by taking it to the extreme and considering that solar were the most competitive energy of all, it was predicted that much more competitive energy production methods than the ones we have today will be needed if very high prices at certain hours or incentives want to be prevented (especially if zero emissions wants to be achieved at some point). MSRs could potentially fill that role, but most importantly, it is estimated that both technologies are not mutually exclusive and that they can prove much more useful if used together. Moreover, there are many energy-intensive applications (mining, off-shore operations, space missions …) that can hardly be done using renewable energies and it is not realistic to think that the main grid can be extended to them.

9 DISCUSSION

The thermal conductivity of thoria was simulated and the values obtained average at 12.4 W/m-k, however the most significant is the one obtained for the longest geometry (12.9 W/m-K) in the x-direction as the phenomenon known as phonon-phonon scattering has a significant effect in reducing the thermal conductivity. As the geometries simulated are larger, results should be closer to reality, are they are usually very small as of now (in the nanometer scale). It can be deduced that these larger dimensions allow for a reduced phonon-phonon scattering at the thermal conductivity is observed to increase as implied by the simulations. The thermal conductivities obtained are in the range of others estimated for the same material but does not match with the most similar simulations. Moreover, it is lower when compared to similar simulations of uranium dioxide, suggesting that significant difference in the thermal conductivities of these two materials may not be observed during operation.

The thermal barrier in nuclear fuel used for commercial nuclear reactors was analyzed and proved to be a drawback, as it does not allow for heat to escape from the inside of the fuel and to the refrigerant. It was estimated that up to a 3.23% increase in efficiency can be achieved just by increasing the thermal conductivity of the fuel by about 2 units. This barrier can directly be overpassed by MSRs as the fuel is in a liquid stated and thus it melting down is not a reason to worry about, the same cannot be said about other Gen-IV reactors being researched.

A traditional PWR powering a 1 GWe power plant will consume 202080 kg of enriched uranium (5% enrichment) for conventional 33% efficiency that these reactors have. This is opposed to the 1442.6 kg of Th that would be required for an MSRs making use of the thorium cycle and for the same energy generation at a 44% efficiency. This efficiency was considered as proved to be possible back in the 1970s.

Waste produced for the traditional pressurized water reactor was estimated to be 20280 kg of radioactive material for the 1-year operation. On the other hand, for the same operation and one more time for a 1-year service a MSRs will produce 9551.6 kg. This las number is considering some other materials that may not have been accounted for by multiplying the estimated wastes by 10.

Similar procedures were followed for a power plant burning natural gas instead, and it was found that considerably more fuel would be required and much more wastes would be produced. This was to be expected given the energy densities of both fuels. However, this was calculated as a cost only of the raw material, and no other factors such as transportation or installation were considered. The results are summarized on Table 3. The average value for NG price between the high and low previously mentioned were considered for the results shown.

Table 3: Cost for fuel and waste per year for a 1 GWe power plant in the three scenarios considered.

	Fuel cost per year	Waste cost per year
PWR	\$34.61 M	\$5.24 M
MSR	\$43.28 K	\$261.8 K
NG	\$356.94 M	\$3.2M

Considerable savings of resources can be observed. The difference is of 3 orders of magnitude for fuel cost between PWRs and MSRs, this same difference is of 4 orders of magnitude for a NG burning power plant. When waste costs are considered, similar differences are found, this time being in the 10 times from one another.

Renewable energies will need reliable and very competitive energy sources as they are expected to be pushed back to operate at their maximum capacity during a fraction of the time than they currently do. If this prediction is correct, current power plants would not be able to make a profit during their design life. It is not trivial that both technologies would actually compete with one another but really complement each other. From the perspective of this work, it makes sense that all renewable-energies-based projects should move forward specially if they have very long design lives. This is because they require no fuel and produce little to no waste unless they cannot be recycled.

10 CONCLUSIONS AND FUTURE WORK

NEMD simulations were made to estimate the thermal conductivity of thorium dioxide. The values obtained are lower than those found by comparable simulations, and they suggest that the thermal conductivity may not be as high as some simulations predict. Results from these simulations highly depend on the interatomic potentials used and as science stands today it is not possible to obtain completely accurate results. The objective was not to obtain completely accurate values but to determine the realm of the possible values. Additionally, the results imply similar thermal conductivities to that of uranium dioxide, so in the worst-case scenario, if thoria were to be used as nuclear fuel in a solid form it is estimated that it will have similar thermal performance to currently used fuel.

The thermal barrier of nuclear fuels that come in a solid state was demonstrated. The temperature at the center was shown to be much higher than the one measured at the interface with the cladding or with the coolant. A theoretical model was provided, and then numerical solutions were given. The efficiency was shown to be very related to the overall efficiency of the nuclear power plant. Sudden and big increases of the rate of fissions and thus the temperature will cause the fuel to melt down, as it does not have time to evacuate that heat. This has been the reason for major nuclear accidents.

Gen-IV reactors provide many advantages, operating at higher temperatures, and allowing for increased efficiencies. Some of them operate at low pressures providing key safety advantages. 3 of the 6 designs operate in the fast spectrum, so they do not compete for the positions that MSRs may occupy. Finally, MSRs are the only ones that operate with fuel in a liquid form, completely removing the thermal barrier discussed, and allow for online fuel processing.

MSRs' fuel requirements and waste management were analyzed and compared with those of a traditional PWR. This comparison was then converted into what it represents in terms of dollars. Major benefits for using MSRs were found, however, it is hard to argue that they can compete with already up-and-running power plants as they have already been amortized and some of them are expected to be able to operate for 40 more years by the IAEA (this is known as Long Term Operation).

A similar comparison was made for nuclear technology and a natural gas-based power plant. The results once again show no reason in terms of fuel cost and waste management to make new investments in fossil fuel-based energy production projects (regulations aside). However, it must be noted that many other factors have to be considered, so it is the responsibility of more technologically advanced countries to make these other factors easy to overcome if a fossil fuel renaissance wants to be avoided.

Finally, it was concluded that renewable energies may not have to be considered up against nuclear technology when new investments on energy production are brought up, as they serve different purposes aside from the basic energy production. Supply must be guaranteed at every moment and at a cheap price. Additionally, development of new technologies that can serve many purposes has to be considered.

11 BIBLIOGRAPHY

[1] K. Dungan, G. Butler, F.R. Livens, L.M. Warren,, "Uranium from seawater – Infinite resource or improbable aspiration?," *Progress in Nuclear Energy,,* vol. 99, pp. 81-85, 2017.

[2] Ali Bamshad, Omid Safarzadeh,, "Effects of the move towards Gen IV reactors in capacity expansion planning by total generation cost and environmental impact optimization," *Nuclear Engineering and Technology,* vol. 53, no. 4, pp. 1369-1377, 2021.

[3] Jiang-Jiang Ma, Ji-Guang Du, Ming-Jie Wan, Gang Jiang, "Molecular dynamics study on thermal properties of ThO2 doped with U and Pu in high temperature range," *Journal of Alloys and Compounds,* vol. 627, pp. 476-482, 2015.

[4] J. Park, "Thermal transport in thorium dioxide," 2018. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S1738573317306101.

[5] Ashley Shields, David Santos-Carballal, Nora H. de Leeuw, "A density functional theory study of uranium-doped thoria and uranium adatoms on the major surfaces of thorium dioxide," *Journal of Nuclear Materials,* pp. 99-111, 2016.

[6] M W D Cooper, M J D Rushton, R W Grimes, "A many-body potential approach to modelling the thermomechanical properties of actinide oxides," *Journal of Physics: Condensed matter,* vol. 26, no. 10, 2014.

[7] Ding, Zhiwei & Zhou, Jiawei & Song, Bai & Li, Mingda & Liu, Te-Huan & Chen, Gang, "Umklapp scattering is not necessarily resistive," *Physical Review B,* 2018.

[8] Sima Samadianfard and Vahab Toufigh, "Energy Use and Thermal Performance of Rammed-Earth Materials," *Journal of Materials in Civil Engineering,* vol. 32, no. 10, 2020.

[9] Y. Mishin, "Machine-learning interatomic potential for material science," *Condensed Matter*, vol. 214, 2021.

[10] "INSAG-7 The Chernobyl Accident: Updating of INSAG-1," INTERNATIONAL ATOMIC ENERGY AGENCY, Viena, 1992.

[11] Thomas James Dolan, Molten Salt Reactors and Thorium Energy.

[12] Carlos H. Yamaguchi, Giovanni L. Stefani and Thiago A. Santos, "A general overview of generation IV molten salt reactor (MSR) and the use of thorium as fuel," ASSOCIAÇAO BRASILEIRA DE ENERGIA NUCLEAR, Belo Horizonte, 2017.

[13] R. Hargraves and R. Moir, "Liquid Fluoride Thorium Reactors: An old idea in nuclear power gets reexamined," *American Scientist,* vol. 98}, pp. 304--313, 2010.

[14] "world-nuclear.org," [Online]. Available: https://world-nuclear.org/information-library/nuclear-fuel-cycle/introduction/physics-of-nuclear-energy.aspx#:~:text=The%20total%20binding%20energy%20released,about%20210%20MeV*%20per%20fission.. [Accessed 2022].

[15] Paul Breeze, "Nuclear Power," in *Power Generation Technologies (Third Edition),* Newnes, 2019, pp. 399-429.

[16] "eia.gov," 2022. [Online]. Available: https://www.eia.gov/uranium/marketing/. [Accessed 2022].

[17] Soiamaat, "commons.wikimedia.org/," 2017. [Online]. Available: https://commons.wikimedia.org/wiki/File:Fission_cross_section_of_4_nuclides.png. [Accessed 2022].

[18] Bae, Kang-Mok & Kim, Myung Hyun, "Assemblies for PWR (I)-Nuclear Design and Fuel Cycle Economy," *uclear Engineering and Technology,* vol. 37, 2005.

[19] J. R. Engel, W. R. Grimes, W. A. Rhoades and J. F. Dearing, "MOLTEN-SALT REACTORS FOR EFFICIENT NUCLEAR FUEL UTILIZATION WITHOUT PLUTONIUM SEPARATION," Oak Ridge, 1978.

[20] "power-eng.com," 2019. [Online]. Available: https://www.power-eng.com/nuclear/reactors/is-thorium-the-fuel-of-the-future-to-revitalize-nuclear/#gref. [Accessed 2022].

[21] "phoenixandpartners.co.uk," [Online]. Available: https://phoenixandpartners.co.uk/commercial-construction-loans-guide/.

[22] Galen J. Suppes, Truman S. Storvick, "Chapter 8 - The Future in Nuclear Power," in *Sustainable Power Technologies and Infrastructure*, 2016, pp. 247-343.

[23] "www-nds.iaea.org," 2019. [Online]. Available: https://www-nds.iaea.org/sgnucdat/a6.htm. [Accessed 2022].

[24] "earth.stanford.edu," [Online]. Available: https://earth.stanford.edu/news/steep-costs-nuclear-waste-us#gs.2g9g46.

[25] "www.eia.gov," 2022. [Online]. Available: https://www.eia.gov/energyexplained/nuclear/us-nuclear-industry.php. [Accessed 2022].

[26] "world-nuclear.org," [Online]. Available: https://world-nuclear.org/information-library/facts-and-figures/heat-values-of-various-fuels.aspx.

[27] Kenneth Storm, "Chapter 6 - Combined cycle power plant (1×1) labor estimate,," in *Industrial Construction Estimating Manual*, Gulf Professional Publishing, 2020, pp. 95-159.

[28] "nrc.gov," 2022. [Online]. Available: https://www.nrc.gov/reading-rm/doc-collections/fact-sheets/nuclear-insurance.html. [Accessed 2022].

[29] "taxfoundation.org," [Online]. Available: https://taxfoundation.org/carbon-taxes-in-europe-2021/.

[30] "Documento Básico HE Ahorro de energía," Dirección General de Arquitectura, Vivienda y Suelo del Ministerio de Fomento, Madrid, 2019.

[31] Tomás Gómez-Navarro, Tommaso Brazzini, David Alfonso-Solar, Carlos Vargas-Salgado, "Analysis of the potential for PV rooftop prosumer production: Technical, economic and environmental assessment for the city of Valencia (Spain)," *Renewable Energy,* vol. 174, pp. 372-381, 2021.

[32] "cei.washington.edu," 2021. [Online]. Available: https://www.cei.washington.edu/education/science-of-solar/battery-technology/. [Accessed 2022].

[33] Mario Pagliaro, Francesco Meneguzzo, "Lithium battery reusing and recycling: A circular economy insight," *Heliyon,* vol. 5, no. 6, 2019.

APPENDIX A: MATLAB CODE USED TO GENERATE THE MODELS

```
Atom ID
clc, clear, close all;
lat_p=input('lattice parameter (A): ');
x_len=input ('x(A): ');
y_len=input ('y(A): ');
z_len=input ('z(A): '); % r=input('radius (A): ');
N=ceil(max([x_len,y_len,z_len])/lat_p);
corners=(0:lat_p:N*lat_p)';
faces=(0.5*lat_p:lat_p:(N+0.5)*lat_p)'; % N+0.5 so the is no problem with ovitto
interior=(0.25*lat_p:0.5*lat_p:(N+0.25)*lat_p)';
[X,Y,Z]=meshgrid(corners, corners, corners);
Xpos=X(:); % make the matix a column
Ypos=Y(:);
Zpos=Z(:);
[X,Y,Z]=meshgrid(faces, faces, corners);
Xpos=[Xpos;X(:)];
Ypos=[Ypos;Y(:)];
Zpos=[Zpos;Z(:)];
[X,Y,Z]=meshgrid(faces, corners, faces);
Xpos=[Xpos;X(:)];
Ypos=[Ypos;Y(:)];
Zpos=[Zpos;Z(:)];
[X,Y,Z]=meshgrid(corners, faces, faces);
Xpos=[Xpos;X(:)];
Ypos=[Ypos;Y(:)];
Zpos=[Zpos;Z(:)];

X=Xpos;
Y=Ypos;
Z=Zpos;


X_del=find(X>x_len);
Y_del=find(Y>y_len);
Z_del=find(Z>z_len);

coords=[X,Y,Z];
coords([X_del;Y_del;Z_del],:)= []; % delete what is not necessary

X=coords(:,1)-x_len/2;
Y=coords(:,2)-y_len/2;
Z=coords(:,3)-z_len/2;

[X2,Y2,Z2]=meshgrid(interior, interior, interior);
```

```
Xpos2=[X2(:)];
Ypos2=[Y2(:)];
Zpos2=[Z2(:)];

X2=Xpos2;
Y2=Ypos2;
Z2=Zpos2;


X_del2=find(X2>x_len);
Y_del2=find(Y2>y_len);
Z_del2=find(Z2>z_len);

coords=[X2,Y2,Z2];
coords([X_del2;Y_del2;Z_del2],:)= []; % delete what is not necessary

X2=coords(:,1)-x_len/2;
Y2=coords(:,2)-y_len/2;
Z2=coords(:,3)-z_len/2;

scatter3(X,Y,Z,'filled');
hold on
scatter3(X2,Y2,Z2,'filled','red')
hold off
xlabel('X');
ylabel('Y');
zlabel('Z');


% atomic data file format
mass1=232.04000000;
mass2=15.99900000;
Xtotal=[X;X2];
Ytotal=[Y;Y2];
Ztotal=[Z;Z2];
atomID=(1:length(Xtotal))';
atom_type=ones(length(X),1);
zeros1=zeros(length(Xtotal),1)
atom_type=[atom_type;2*ones(length(X2),1)];

mkdir('LAMMPS RUN');
filename= 'LAMMPS RUN/data.ThO2';

fid1= fopen (filename, 'w');
fprintf(fid1, 'FileComment: ThO2, lattice constant=%g\n',lat_p);
fprintf(fid1, '%d atoms\n', atomID(end));
fprintf(fid1, '2 atom types\n');
fprintf(fid1, '%f %f xlo xhi\n', -max(Xtotal), max(Xtotal)+lat_p/2);
fprintf(fid1, '%f %f ylo yhi\n', -max(Ytotal), max(Ytotal)+lat_p/2);
fprintf(fid1, '%f %f zlo zhi\n', -max(Ztotal), max(Ztotal)+lat_p/2);
fprintf(fid1,'\n');
fprintf(fid1, '%s\n', 'Masses');
fprintf(fid1, '%s\n', '');
fprintf(fid1,'\t\t1 %12.8f\n',mass1);
```

```
fprintf(fid1,'\t\t2 %12.8f\n',mass2);
fprintf(fid1,'Atoms\n');
fprintf(fid1,'\n');
fprintf(fid1,'%d %d %d %d.%d %f %f
%f\n',[atomID,zeros1,atom_type,zeros1,zeros1,Xtotal,Ytotal,Ztotal]');
fclose(fid1);


% full data file format
mass1=232.04000000;
mass2=15.99900000;
Xtotal=[X;X2];
Ytotal=[Y;Y2];
Ztotal=[Z;Z2];
atomID=(1:length(Xtotal))';
atom_type=ones(length(X),1);
zeros1=zeros(length(Xtotal),1)
atom_type=[atom_type;2*ones(length(X2),1)];

mkdir('LAMMPS RUN');
filename= 'LAMMPS RUN/data.ThO2';

fid1= fopen (filename, 'w');
fprintf(fid1, 'FileComment: ThO2, lattice constant=%g\n',lat_p);
fprintf(fid1, '%d atoms\n', atomID(end));
fprintf(fid1, '2 atom types\n');
fprintf(fid1, '%f %f xlo xhi\n', -max(Xtotal), max(Xtotal)+lat_p/2);
fprintf(fid1, '%f %f ylo yhi\n', -max(Ytotal), max(Ytotal)+lat_p/2);
fprintf(fid1, '%f %f zlo zhi\n', -max(Ztotal), max(Ztotal)+lat_p/2);
fprintf(fid1,'\n');
fprintf(fid1, '%s\n', 'Masses');
fprintf(fid1, '%s\n', '');
fprintf(fid1,'\t\t1 %12.8f\n',mass1);
fprintf(fid1,'\t\t2 %12.8f\n',mass2);
fprintf(fid1,'Atoms\n');
fprintf(fid1,'\n');
fprintf(fid1,'%d %d %f %f %f\n',[atomID,atom_type,Xtotal,Ytotal,Ztotal]');
fclose(fid1);
```

APPENDIX B: SAMPLE LAMMPS INPUT FILE

```
#   ThO2 simulation

     units metal
     dimension   3
     boundary    p p p

     atom_style     full
     neighbor       2.5 bin
     neigh_modify   delay 5

       # import ThO2 structure
     read_data      data.ThO2
        variable Th equal 1
        variable O equal 2

        # set charges
        set type $O charge -1.1104
        set type ${Th} charge 2.2208

       # define interatomic potential via coulombic and embed_UO2.fs tabulation
        kspace_style pppm 1.0e-5
        variable SR_CUTOFF equal 11.0
        pair_style hybrid/overlay coul/long 11 eam/alloy
        pair_coeff   *    *    coul/long
        pair_coeff   *    *    eam/alloy CeThUNpPuAmCmO.eam.alloy O Th


  #  define groups
     region      1 block -10 10 EDGE EDGE EDGE EDGE units box
     region     2 block -200 -10 EDGE EDGE EDGE EDGE units box
     region      3 block 10 200  EDGE EDGE EDGE EDGE units box
     region     4 block EDGE -200 EDGE EDGE EDGE EDGE units box
        region     5 block 200 EDGE EDGE EDGE EDGE EDGE units box

        group          source region 1
        group          sinkone region 2
        group          sinktwo region 3
        group          B1 region 4
        group          B2 region 5
        group          free subtract all B1 B2




  #  initial velocities
      compute       1 all temp
```

```
timestep     0.001
   thermo 1000
   thermo_style custom step temp press


dump    1 all custom 10000 dump.xyz id type x y z

#fix     NVE all nve
   #run 20000
   #unfix NVE

   #set the temperature of the environment
   fix NPH all npt temp 500 500 1.0 iso 1.0 1.0 10.0
   run   60000
   unfix NPH

   fix NVE all nve
   fix 4 free langevin 500.0 500.0 1.0 699483
   run   60000
   unfix 4
   unfix NVE

   fix NPH all npt temp 300 300 1.0 iso 1.0 1.0 10.0
   run   60000
   unfix NPH

   fix NVE all nve
   fix 4 free langevin 300.0 300.0 1.0 699483
   run   60000
   unfix 4
   unfix NVE

   undump 1

#direct method
fix          NVE free nve
   fix         1 source heat 1 0.5
   fix         2 sinkone heat 1 -0.5
   fix         3 sinktwo heat 1 -0.5


   #output temperature distribution to tmp.profile
   compute      KE all ke/atom
   compute cc1 all chunk/atom bin/1d x lower 0.01 units reduced
   fix         5 all ave/chunk 1 10000 100000 cc1 temp file tmp.profile

   #writing restart file every 20000 steps
restart   500000 restart.*

run    2000000
```

APPENDIX C: TEMPERATURE PROFILE MODEL

```
# General derivation
clc; clear; close all;
syms q_v k_f x s T_s C_1 C_2
% I FUEL REGION
d2T_f=q_v/k_f;
dT_f=int(d2T_f,x,x,s)+C_1;
T_f=int(dT_f,x,x,s)+C_2;

% dT(x=0)=0
b1=subs(dT_f,x,0);
eqnb1 = b1==0;
C_1=solve(eqnb1,C_1)

% T(x=s)=T_s
b2=subs(T_f,x,s);
eqnb1 = b2==T_s;
C_2=solve(eqnb1,C_2)


d2T_f=-q_v/k_f;
dT_f=int(d2T_f,x,x,s)+C_1
T_f=int(dT_f,x,x,s)+C_2

%T_m & T_s
T_m=subs(T_f,x,0)
T_s=subs(T_f,x,s)

syms c T_c C_3 C_4 k_cl
% II Cladding Region

d2T_cl=0;
dT_cl=int(d2T_cl,x,x,s)+C_3;
T_cl=int(dT_cl,x,x,s)+C_4;

% T_cl(x=s)=T_s
b3=subs(T_cl,x,s);
eqnb3 = b3==T_s;
C_4=solve(eqnb3,C_4)

% T_cl(x=s+c)=T_c
b4=subs(T_cl,x,(s+c));
eqnb4 = b4==T_c;
C_3=solve(eqnb4,C_3)

C_4=T_s
C_3=(C_4-T_c)/c

d2T_cl=0;
```

```
dT_cl=int(d2T_cl,x,x,s)+C_3
T_cl=int(dT_cl,x,x,s)+C_4

syms h T_inf
% heat flux at x=s
q_s1=-k_f*subs(dT_f,x,s) % >0, generated
q_s2=-k_cl*subs(dT_cl,x,s) % <0, absorved

q_c1=-k_cl*subs(dT_cl,x,(s+c))
q_c2=-h*(T_c-T_inf)


syms T_m
% SUMMARY
eqn1 = T_m==subs(T_f,x,0)
eqn2 = q_s1+q_s2==0
eqn3 = q_c1+q_c2==0

% PARAMETERS: q_v,k_f,k_cl,s,c,T_m,T_s,T_c,T_inf,h

% Sample solution
syms c s Tm q kf kcl x h Tinf
T_fuel=-q/(2*kf)*x^2+Tm
T_cladding=-q*s/(kcl)*x+Tm-q*s^2/(2*kf)+q*s^2/(kcl)


clc; clear; close all;
syms x
q=400e6;
s=(0.30)*1e-2;
c=(0.02)*1e-2;
kf=10;
kcl=16.7;
Tinf=315.6+274.15;
Tm=371.1+274.15;



T_fuel=-q/(2*kf)*x^2+Tm;
T_cladding=-q*s/(kcl)*x+Tm-q*s^2/(2*kf)+q*s^2/(kcl);
fplot(T_fuel,[0,s])
hold on
fplot(T_cladding,[s,s+c])
xlabel("Distance [m]")
ylabel("Temperature [K]")

clc; clear; close all;
syms x
q=400e6;
s=(0.30)*1e-2;
c=(0.02)*1e-2;
kf=12;
kcl=16.5;
Tinf=315+274.15;
```

```
Tm=371.1+274.15;




T_fuel=-q/(2*kf)*x^2+Tm;
T_cladding=-q*s/(kcl)*x+Tm-q*s^2/(2*kf)+q*s^2/(kcl);
fplot(T_fuel,[0,s])
hold on
fplot(T_cladding,[s,s+c])
xlabel("Distance [m]")
ylabel("Temperature [K]")
```

APPENDIX D: SDGS ALIGNMENT

SDG number 9, "Build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation". This project promotes a resilient infrastructure that is not merely based on economic benefit, but efficient resource wise and that can be maintained over time. Not only that, but it does so primarily by specifically enhancing scientific research (target 9.5) on an inclusive technology that can be implemented anywhere in the world and can be affordable for all. MSRs were proved to be highly efficient, and require very little raw material, for huge amounts of energy production when compared to other available technologies that require of fuel (any non-renewable). The thermal conductivity of thoria was estimated and the way that this property may directly significantly affect performance of a nuclear reactor was demonstrated. It was estimated (by consistent assumptions) that renewable energies alone will not suffice if a truly resilient infrastructure wants to be built.

Quantification of the impact of the contribution to SDG number 9:

- Efficiency of a nuclear can be increased by as much as 3.23% with relatively small changes of the nuclear fuel thermal conductivity at high temperatures (about 2 W/m^2-k).
- In an electric grid where all households contribute to it by means of PV energy production and taking into account the current power generation technologies available in the EU and the US, 3.1945 million of metric tons of CO2 will be released to the atmosphere for every GWe consumed for flexible generation (that is big generation changes during short periods of time).

SDG number 7, "Ensure access to affordable, reliable, sustainable and modern energy for all". More exactly target 7.1 aims at ensuring universal and affordable energy. If cheap energy for all wants to be accomplished, then energy production methods that do not make use of huge amounts of limited resources should be avoided. Not only this, but very large amounts of energy will have to be produced in a reliable and consistent manner. MSRs allow for this possibility even more so than traditional nuclear technology does and it does so by also allowing load following capabilities. Although the technology is complex and potentially expensive to develop, the amounts of energy generated can make up for it in the long term. Additionally, it does not require of any water source for refrigeration and can be built pretty much anywhere that it may be needed, even ships. Mobile power plants in the form of containers or ships can be designed using this technology allowing for cheap energy in remote places. On the other hand, it would be complicated to have these reactors completely ready and approved by regulators before the deadline of this target (2030), however if all factors are to be considered, there really aren't any possibilities that could make this target achievable by that deadline as of today. Sustainability of MSRs is guaranteed as they required very little fuel and due to on-line reprocessing capabilities can produce much less radioactive waste. The longest lasting of these fuels are estimated to only must be stored at secured locations for a few hundred years instead of over a thousand that current nuclear wastes require.

Quantification of the impact of the contribution to SDG number 7:

- Costs for fuel in MSRs are estimated to save $34.608 M per year in fuel for a 1 GW power plant when compared to a PWR based power plant with the same capacity.
- Nuclear waste for a MSRs-based power plant is estimated to account for less than 0.5% of the waste produced by traditional PWR, before irradiated materials from the pumping system used in the primary loop is accounted for. This may be directly translated into up to 95.5% in savings for waste management when compared to the traditional nuclear fuel usage and cycle standard.
- Costs for fuel in MSRs are estimated to save $29.608 M per year in fuel for a 1 GW power plant when compared to another that burns natural gas instead and has an efficiency of 57%.
- Uranium mining and enrichment operations aren't necessary for MSRs.

SDG number 13, "Take urgent action to combat climate change and its impacts". This urgent action demands that big changes be made in short periods of time. Time is possibly the most determining factor for this goal, as it implies that more money, planning and resources will need to be mobilized. In order, to reduce these to a minimum, alternatives that allow for cost diversification have to be given more importance so that every industry can collaborate in a common goal more efficiently. Target 13.3 advices for education, early warning, and awareness-rising among others. This work does just that, by directly anticipating what current technology allows and will allow for and educating on alternatives that can lead countries to accomplish the SDG. MSRs functioning was reviewed, and fuel economy explained and compared to current reactors. Awareness was raised about costs of taking care of current nuclear waste and what that number may be reduced to if MSRs were developed. This work anticipates what the production and demand curves may look like in the future if heavy investment in renewables is carried out, and that current projects may prove not profitable in their design life if large incentives aren't provided.

Quantification of the impact of the contribution to SDG number 12:

- Nuclear waste for MSRs do not require safe storage for more than a thousand years, instead, only a about 3 hundred years is necessary.
- MSRs require much less raw material, and do not require further enrichment operations. It is estimated that 1442.6 kg of Th would be needed every year for a 1 GWe MSRs as opposed to the 202080 kg for the same 1 GWe traditional reactor. This implies that 200637.4 kg of raw material can be reduced for the same amount of energy production.
- When the same assumptions were made for the same 1 GWe power plant burning natural gas instead, 1.1617 million metric tons of raw material were needed. In other words, given the huge difference and rounding up, the same 1.1617 million metric tons of raw material needed can be reduced for the same amount of energy production.

APPENDIX E: ECONOMIC ANALYSIS

LAMMPS is an open-source (it does not require a license) program that allows to save costs by first exploring possible results before investing more money into more precise laboratory experiments. If the results show bellow necessary properties, further investment is prevented.

The cost for 1 hour of consulting work done by a young engineer without years of experience is accepted to be $50 (HubSpot). The case here is 5 hours a week, for 7 months, plus 25 hours for the composition of the document. Additionally, 1 hour a week of mentoring is accounted for, this is estimated to have a cost similar to that of a senior consultant or $100 per hour.

Rent for the office is considered to be similar to that of living in an apartment close to UF, and thus it is taken as $500 a month. A total of 7 months were dedicated to this although not exclusively, so $300 will be assumed on this topic.

Interactive Supercomputing rents supercomputer usage for $2.77 an hour. About, 23 simulations where made. Given that some of them failed since they did not reach steady state and took less time, the average time per simulation ended up being about 3 days.

Once these factors are considered, costs are summarized on Table 4. $18.7 K is a very low price considering that actual laboratory experiments where machinery is usually very expensive, requires calibration and very specific qualification are avoided. Moreover, the savings that projects like these may have if implemented in fuel savings alone are absurd compared to how much they cots in terms of resources and money.

Table 4: Costs analysis

Item	Quantity	Price per item [$]	Total Cost [$]
Direct costs			
Direct materials required for the service			
Supercomputer usage per hour	1656	2.77	4587.12
Labor required for the service			
Consulting hour	165	50	8250
Mentoring	28	100	2800
Indirect costs			
Cleaning fees	7	100	700
Rent and utilities (internet included)	7	300	2100
Amortization (laptop)	7	41.67	291.67
			$ 18728.79