Simulation of fission reactions in pressurised water reactors

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Developing and optimizing established power-producing systems is a promising solution to the ongoing energy crisis and could be essential for a more sustainable future. This project therefore aims to examine a specific type of nuclear power reactor, PWR, by simulating the fission reactions within them. The primary objective of this study is to investigate the influence of key factors; namely, temperature, reactivity, and control rod absorption on energy production within PWRs, to explore potential possibilities for energy optimization. A simplified 2D simulation model, based on reaction dynamics, was constructed to investigate this question. Our findings reveal a noteworthy correlation between reactivity and temperature, establishing the possibility of achieving a stable reactor state. Furthermore, the results indicate the existence of multiple outlet temperatures capable of sustaining steady states, which is achieved by varying control rod absorption rates. This implies that there is a possibility of energy optimization by changing this specific parameter. However, due to the simplifications and limitations of the project, further research has to be conducted to reach more reliable conclusions, which are discussed in the discussion part.

I. INTRODUCTION

As the global population grows and the energy demand increases due to the advancement of technology, sustainable energy production becomes increasingly crucial [1]. One promising solution to this challenge is the exploration and development of already-known power-producing technologies. Optimizing established systems, such as nuclear reactors, could potentially improve the ongoing energy crisis. In this context, developing a simulation for nuclear fission reactions can prove to be a valuable tool for advancing and optimizing nuclear energy production.

A. Background

A pressurized nuclear reactor (PWR) is a type of nuclear reactor in which the primary coolant is high-pressure water [2]. The heat within the reactor is generated when a collision between a neutron and a nucleus result in a fission reaction, releasing energy and subsequently heating the coolant. The fission is described by the two-step formula:

$$^{235}_{92}U + ^{1}_{0}n \longrightarrow ^{236}_{92}U \tag{1}$$

$$^{236}_{92}U \xrightarrow{85\%} ^{92}_{36}Kr + ^{141}_{56}Ba + 3^{1}_{0}n + 200MeV \tag{2}$$

The heated coolant then transfers its thermal energy to low-pressure water, which is turned into steam that drives a steam turbine, which then generates electricity. PWRs are generally stable due to a self-regulating mechanism whereby the reactivity in the reactor decreases as the temperature of the coolant increases [3].

To prevent the reactor from reaching too high a temperature, control rods are inserted into it [4]. These control rods are coated with different materials that continuously absorb neutrons, reducing the fission rate and consequently lowering the energy released from the reactions. This is essential to avoid complications such as explosions and to maintain a steady state. The absorption process depends on the exposed surface of the control rod and its absorption rate, which varies depending on which material is being used.

As mentioned, the control rods ensure a stable system and the stability of a PWR can be described with the multiplication factor, K. K is a ratio based on the change of the total number of neutrons from one time step compared to the previous one:

$$K = \frac{n_{t+1}}{n_t} \tag{3}$$

Where n_t is the total number of neutrons at time step t. The multiplication factor is also how reactivity is measured in a nuclear reactor. When the multiplication factor is equal to 1, which is called the critical reactivity, the reactor is stable. This is necessary to achieve a steady state. If the factor is less than 1, the system will decay and the fission reactions will eventually stop, and if it is greater than 1, the reactor becomes unstable and will eventually explode. It is therefore essential to continuously monitor the reactivity in the reactor.

B. Project Purpose

This project aims to develop a simplified simulation of the fission reactions occurring within a PWR to potentially achieve a better understanding of the process. Specifically, it aims to assess how reactivity and temperature change over time and the relationship between them. Furthermore, the project seeks to examine the possibility of optimizing energy production by exploring

multiple steady states through modifications to the absorption rate of the control rods. The research questions can therefore be formulated as;

1. Research questions

1. How do the temperature and reactivity change over time at a specific steady state, and what is the correlation between them?
2. Is it possible to optimize energy production by altering the control rods' absorption rate?

II. METHOD

A. Project model

Since the purpose of this project is to simulate a real PWR, it is important to base the dynamics of the model on suitable formulas. However, PWRs are complex systems, so for this project, simplifications had to be done. See Appendix A for the full limitation list. The most relevant part to establish is the energy balance of the system which is essential to estimate the energy yield of the simulation. The most interesting part is the energy that is being released in each fission reaction. The fission reaction (1,2) was therefore simplified as

$$1_{92}U^{235} + 1_0n^1 \xrightarrow{85\%} F_p + 3_0n^1 + E \tag{4}$$

where F_p are the fission products and E is the released energy. The energy released from the fission reaction is used to heat the water in the reactor. The energy balance can therefore be simplified as

$$E = m_r c_{H_2O}(T_o - T_i) - c_{H_2O} m_i (T_r - T_i) \tag{5}$$

where m_r is the water mass in the reactor, m_i is the water mass of the incoming water at each time step, T_o is the temperature of the water exiting the reactor, T_i is the temperature of the incoming water, T_r is the temperature inside the reactor and c_{H_2O} is the specific heat capacity for water. Assuming a homogeneous mixture within the reactor, the temperature of the water exiting the reactor, T_o, is equivalent to the temperature within the reactor itself, T_r. To estimate the temperature of the water in the reactor equation 4 can be rewritten as;

$$T_r = \frac{E}{c_{H_2O}(m_r - m_i)} + T_i \tag{6}$$

This equation is evaluated for each time step which means that E and T_r depend on the number of neutrons colliding with uranium atoms at each time step. The probability of collision is in turn dependent on the number of active neutrons and their positions and can be formulated as

$$n_{t+1} = n_t + 3 \cdot C_n \cdot p_r - a_n \tag{7}$$

Where, at each time step t, n_t is the total number of active neutrons in the reactor, a_n is the number of absorbed neutrons by the control rods, C_n is the number of collisions between neutrons and uranium atoms [4] and p_r is the reaction probability whenever a collision occurs.

As mentioned in section I A the number of neutrons that are absorbed by the control rods depends on the absorption rate as well as the surface control rod area. To accurately model a continuous absorption of neutrons the two factors were translated into a probability as,

$$a_c(t+1) \;=\; min(A_c,\; a_c(t) \;*\; 1.002) \tag{8}$$

$$a_c(0) = 0.01 \tag{9}$$

where a_c is the current probability that neutrons are absorbed and the term 1.002 emulates the insertion of the control rods. A_c is a set value and depicts the maximum absorption probability. When enough time steps have been executed the probability of absorption will be equal to A_c, which implies that the control rods are fully inserted and the absorption probability will stay constant throughout the rest of the run. A_c is therefore used to describe the control rod absorption rate in this project, and is the parameter that will be studied by manual testing to find an interval where a steady-state is reached.

1. Simulation model

As mentioned above, the number of collisions depends on the position of each neutron and uranium atom as well as the reaction probability. A reaction will happen if, and only if, the neutron is close enough to a uranium atom, which means that it is essential to keep track of each particle's position. This is achieved by partitioning the simulation world and storing the atoms in a hash table based on the partitioning. This way, finding collision "candidates" is fast. Once the neutrons are within the radius of the uranium atom, the fission reaction will occur with an initial probability of $p_r = 85\%$, to emulate Equation 2.

To be able to simulate the continuous process of nuclear fission, the process is discretized, where the system is updated at each time step. The update consists of six different parts: absorption, movement, collision, temperature adjustment, reaction probability adjustment, and adjustment of control rods. Absorption is modeled as a probability that the neutrons collide with the control rods. The probability itself depends on the fraction of the control rods that are submerged in the water. At each time step, the position of the neutrons are updated in order to facilitate collision with the stationary atoms. After updating their positions, the neutrons are checked against any adjacent atoms to see if any collisions have occurred. Each collision has a certain probability to split the atom, generating new neutrons and energy according to Equation 3. The generated energy is then used to

adjust the temperature by heating the coolant, and the new temperature is determined using a weighted mean of the coolant and the incoming flow of water. The reaction probability p_r is adjusted based on the increase or decrease in temperature as $p_r = 0.85 \cdot \frac{T_i}{T_r}$. At the beginning of the simulation, the control rods are pulled out of the reactor in order to kick start the chain reaction. The control rods are then inserted slightly every time step until a set value is reached.

2. *Parameters*

To get relevant results the following parameters were used in the simulation. The values are partly retrieved from literature and partly calculated, view Appendix B.

Parameter	Value	Source
E	200 MeV	[5]
T_i	561 K	[6]
c_{H_2O}	4184 J/kgK	[7]
m_r	59,47 m^3	[8]
m_i	4,97 m^3/s	[8]
uranium-235 nucleus radius	7.5 fm	[9]
neutron radius	0.8 fm	[10]
Δt	5 as	B
Reactor operating pressure	155 bar	[8]

TABLE I. Parameters for fission simulation.

III. RESULTS

The results in this section were obtained from the simulation model, using the initial values presented in Table I.

Figure 1 shows how the average temperature and reactivity vary as the absorption rate is increased, where the dashed lines represent the working temperature in the reactor AP1000 and the critical reactivity, which are equal to 597.85 K [8] and one, respectively. As seen, an interval of absorption rates seems to result in a critical reactivity, while their corresponding temperatures differ.

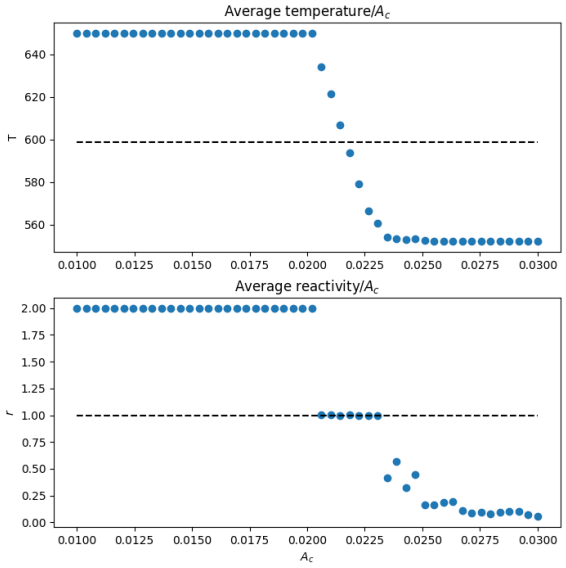

FIG. 1. Average temperature and reactivity as a function of the absorption rate when run for 10000 time steps. The first 1000 time steps are ignored to remove any transients. The maximum temperature is set to 650 K, and all runs that exceed this threshold are set to 650 K and a reactivity of 2. As seen, there is an interval of A_c that result in a reactivity of unity.

Figures 2 and 3 display how the reactivity and temperature change after each time step. In Figure 2 we see how reactivity decreases as temperature increases at the beginning of the simulation, and how both temperature and reactivity stabilize over time. Figure 3 shows a more detailed view of temperature and reactivity. From this, it is possible to see how reactivity and temperature follow each other at a steady state.

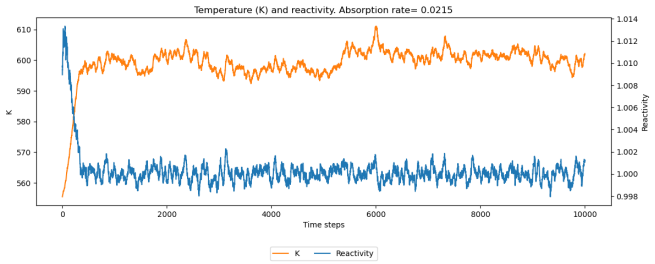

FIG. 2. Temperature in K, and reactivity measured in $\frac{n_{t+1}}{n_t}$ as a function of time steps. Absorption rate = 0.0215. Both the temperature and reactivity quickly reaches a steady-state.

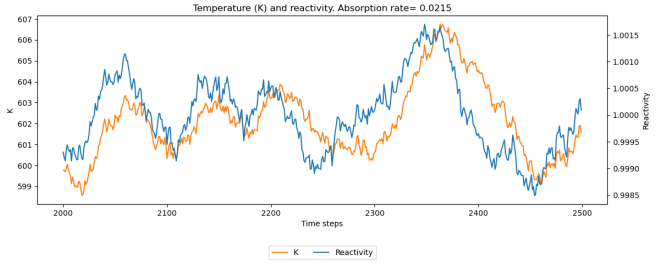

FIG. 3. Zoomed in view of the dynamics of Figure 2 between the time steps 2000 and 2500. As seen, the temperature and reactivity follows each other in an oscillating manner.

A. Long term steady state

To see how the model performs over longer time intervals simulation were run for several values of A_c. Figure 4 shows longer time dynamics of the model with absorption rate set at 0.0215. Both the average reactivity and temperature oscillate around a fixed value during the entire run. Table II shows the average reactivities and temperatures over 100000 time steps. Within the interval 0.021 - 0.023, a small increase in absorption rate keeps the reactivity close to 1, while the same increase from 0.023 to 0.0235 drastically decreases reactivity to around 0.5.

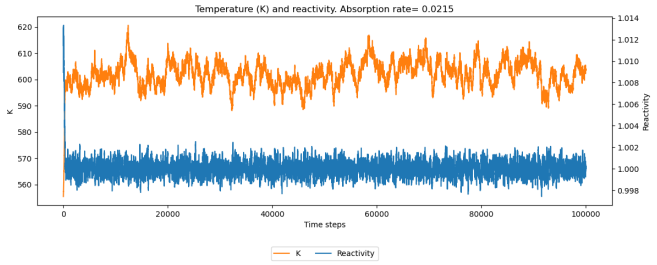

FIG. 4. The dynamics of the model with absorption rate 0.0215 measured over 100000 time steps. The dynamics keep their steady-states throughout the run.

A_c	Reactivity	T_o	ΔT
0.021	1.000007	620.85	68.85
0.0215	1.000009	602.96	50.96
0.022	1.000016	586.57	34.57
0.0225	1.000024	571.62	19.62
0.023	0.503437	555.01	3.01

TABLE II. Outcomes after 100000 time steps when varying A_c between 0.021 and 0.023, all values are averaged over all but the first 1000 steps.

IV. DISCUSSION

A. Discussion of results

As Figure 1 shows, multiple values of absorption rates seem to result in a steady-state for the given time period with different corresponding temperatures. This could imply that it is possible for the system to have multiple steady-state temperatures, which is of relevance due to the direct correlation between power production and moderator temperature as explained in section II A. However, the measured reactivities differ slightly from the de facto steady-state value, i.e. one. Even though these differences are relatively small (around 10^{-5}), there exists a risk that these blow up when running the simulation for an extended period of time. However, due to the small magnitude of these errors, they could also be a result of the finite time interval of the simulation, and not a true steady-state value.

Furthermore, some seemingly stable absorption rates result in temperatures higher than the boiling point of water at 155 bar (617 K). The model does not account for the reactor dynamics that arise in relation to boiling coolant, and as such, these results should be interpreted with caution. Since there seems to exist an interval of control rod absorption values, A_c, for which the system reaches a steady-state, ranging from 0.021 to 0.0225, one should be able to optimize the energy production by tuning this value. Another observation is that the temperatures of the steady-states seem to be centered around the working temperature of AP 1000 [8], which could be used as a measurement of the validity of the model.

When looking closer at the behaviour of temperature and reactivity at steady state, the temperature seems to follow the reactivity closely, as shown in Figure 3. This seems reasonable, as the temperature is directly defined by the number of collisions, which have increased when reactivity is higher. The relationship also show some oscillating behavior, which indeed could be confirmed from Figure 4, where obvious oscillations are shown. This could be interpreted as a sign of self-regulation within the system where the reactivity acts as a positive feedback for the temperature, while the temperature in turn acts as a negative feedback for the reactivity.

B. Discussion of Method

This simulation models the decrease in reaction probability with increasing temperature as a ratio between current temperature and T_i. While this captures the concept of negative reactivity feedback, its magnitude is not based on any scientific research. There exists some information regarding the change in reactivity with increasing temperature. However, it is given for

the system as a whole, and did not fit the setup of this project.

It is important to mention that the process of nuclear fission is very complex with many constituent parts that affect each other. Thus, it is difficult to estimate the effect of excluding some parameters, e.g. the void coefficient or Doppler effect, in the model.

The model represents a very small area of a PWR ($10^{-24}m^2$). As such, every single interaction plays a bigger role and this could be a determining factor in why the temperature and reactivity is so noisy in Figure 3. A bigger model would place less emphasis on individual interactions which could lead to less noisy results.

The parameters chosen were picked from relevant literature, but it was difficult to find one single set of values that fit together. This was in part due to the simplifications and assumptions made early in modeling. More research is needed to find a set of values accurately representing an existing reactor, possibly with modifications to the model.

In particular, the density of the uranium atoms is too high. The lattice parameters of uranium 235 is on the order of 10^{-10} meters [11]. Taking the size of the simulated area into account there are way to many atoms present. This could account for the very rapid time scales of the simulation.

V. CONCLUSION AND OUTLOOK

Based on the results found, a couple of conclusions can be drawn. Firstly, it should be possible to optimize the energy production by altering the control rods' absorption rate. In our simulations, the optimal absorption rate is found to be 0.0215, which yields the highest steady-state temperature without reaching the boiling point. Secondly, at absorption rates where a steady-state is reached, the temperature and reactivity closely follow each other, oscillating around the steady state without leaving it, which is an expected behaviour due to the self-regulating nature of pressurized water reactors.

This project has demonstrated the potential for evaluating well-established power-producing technologies and found the significance of identifying multiple steady states as a potential tool for optimizing nuclear energy. However, due to the scale and limitations of the project, more research has to be conducted to get more reliable results. It would be interesting to recreate the simulation under more realistic conditions and on a larger scale to examine if the same conclusions can be reached. Particularly, exploring specific dynamics, such as the Doppler effect, which were not addressed in this project, through dedicated simulations would be necessary. If similar conclusions are reached, the simulations could be a helpful tool to aid the energy crisis. Hopefully, this project will, at the very least, inspire others to pursue this quest.

VI. CONTRIBUTIONS STATEMENT

The group has been working closely together throughout the project. No member was assigned a specific role for the project. From the initial preparations and research, every member played an important role to ensure a comprehensive understanding of the theoretical foundations. During the formulation of the chosen method, all members explored diverse strategies and structures to guarantee an optimal model. Each team member made significant contributions to both the model's development and the composition of this report. Before summarizing the results, the team conducted thorough discussions, incorporating various perspectives. The resultant sections were then collaboratively written by all members, reflecting the collaborative approach of the project.

Appendix A: Limitations

As mentioned above, several simplifications were done in order to reduce the complexity of the simulation. The model only handles fission with U_{235}, and no regard is given to the combination of various isotopes typically found in real-world nuclear reactors (such as U_{238}). The neutrons are assumed to quickly slow down to a speed at which reaction with U_{235} is probable. In practice, this means that the neutrons move at a constant speed in the simulation.

The model also simplifies the way in which energy generation is calculated. In reality, the majority of the energy released during fission comes from the kinetic energy of the fission products, and these slow down as they pass through the coolant, thereby heating it up. This process is not instant. However, in the model, the energy from the fission reactions is instantly transferred to the water as described in Equation 6. As such, despite the neutrons having a non-zero velocity, they are modeled without kinetic energy.

Appendix B: Calculations

1. Time scale

The radius of a radium nuclei is 7.5 $l.u$ in simulation, and $7.5 \cdot 10^{-15} m$ in reality.

$$\begin{aligned} r_U &= 7.5 \cdot 10^{-15} m = 0.75\ l.u \\ \Leftrightarrow 1\ l.u &= 10^{-14} m \\ v = 1\ l.u/ts &= 10^{-14}\ m/ts \end{aligned}$$

for thermal neutrons $v \approx 2 \cdot 10^3\ m/s$.

$$\begin{aligned} 10^{-14}\ x &= 2 \cdot 10^3 \\ \Leftrightarrow x &= 2 \cdot 10^{17} \end{aligned}$$

one time step is $1/x\ s = 5 \cdot 10^{-18} s = 5as$

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