Modeling Radiation-Induced Molecular Decomposition of Water using a Simple Molecular Mechanics Force Field Model

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Code available at: https://github.com/rigpin2014/Chem279_FinalProject

Abstract

This study investigates a theory for molecular decomposition of water via neutron-induced radiolytic decomposition in a nuclear reactor. The concept of reaction rates is used to determine the number of neutron-water molecule interactions. Neutron energies are sampled from the prompt neutron fission spectra. Microscopic cross sections scattering angles are sampled from *Experimental Nuclear Reaction Data (EXFOR) Evaluated Nuclear Data File (ENDF)*. The concepts of vertical ionization energy and appearance energy are used to create a molecular decomposition theory based on a critical vibrational excitation energy. This was done after attempting, but eventually scrapping, a self-developed implementation of MMFF94 to model water decomposition. The resulting framework enables a simple method for modeling water radiolysis and pathways for energy absorption under neutron irradiation.

1 Background

The research of radiation interactions in nuclear reactors serve a fundamental purpose for evaluating how material properties are affected by irradiation. In solids factors such as neutron embrittlement may decrease the strength of a material over time. In liquids however, specifically water which is a very common moderator, studying the effects of radiation interactions would provide insights into the chemistry of the system. The ability to accurately model nuclear chemistry using computational models provides a theoretical model for trending chemistry which could be used in addition to physical sampling. An accurate model for simulating nuclear chemistry would allow for decreased exposure to radiation for nuclear chemists by minimizing the sampling frequency of radioactive coolant.

The following research provides framework for modeling radiolytic decomposition of water exposed to a neutron flux in a reactor core. This is done by using molecular force field concepts to partition the recoil energy from a scattered neutron into a molecular force field.

The force field chosen for this project was MMFF94 based on ease of development, widespread use, and accuracy in calculating the energy of small organic molecules (including water). Force fields utilize a system of parameterized classical physics equations to calculate energies and forces of molecules on an atom-based scale. For the calculation of energy, MMFF94 performs the following calculation: $E_{MMFF94} = \sum E_{bonds} + \sum E_{angles} + \sum E_{torsions} + \sum E_{OOP} + \sum E_{vdW} + \sum E_q$. Force

fields are able to model changes in molecular energy based on external interactions making them suitable for this assessment of decomposition given a neutron collision and associated recoil energy.

Another "force field" sort of model was attempted with the scattered neutron recoil energy only considered the vibrational energy, and it is assumed that rotational and translational components of the force field do not contribute to critical bond energies. In this context critical bond energy is considered to be the maximum O-H bond Energy in water before bond breakage.

A molecular decomposition model is created by using a combination of theories such as vertical ionization energy, appearance energy, and energy wells. By postulating a theory for molecular decomposition using these methods it is possible to perform a simple calculation to determine the rate of water molecule decomposition under neutron irradiation. This has the potential to be expanded to other molecules in order to track the concentration of several molecular species affecting nuclear chemistry.

1.1 Objectives

This report aims to calculate the rate of molecular decomposition of water exposed to a fixed neutron flux in a simulated reactor core using the following objectives:

- Calculate the neutron-water molecule reaction rate by using microscopic cross sections.

- Scale the simulation to be able to perform computations on a personal computer.

- Determine the number of neutron-water molecule interactions occurring at the atomic level. Specifically the number of neutron-hydrogen and neutron-oxygen interactions in the scaled model.

- Develop methods to sample neutron energies from the prompt neutron energy spectra.

- Calculate the energy imparted unto the incident molecule using the concept of recoil energy.

- Construct a molecular force field that can calculate energy of water in different conformations

- Develop a theory for molecular decomposition based on generally understood and accepted molecular mechanics principles.

- Use the molecular decomposition theory to calculate the rate of decomposition in the simulated reactor core by performing a simple calculation.

2 Methodology

2.1 Calculating Reaction Rates

We are going to be using the concept of reaction rates in order to estimate the number of interactions of a particular type occurring in a cubic centimeter of material in a second. From [1], the equation for reaction rates is given by:

$$R = \Phi\Sigma = \Phi N\sigma \tag{1}$$

Where:

Φ, neutron flux $\left(\frac{n}{\text{cm}^2\,\text{s}}\right)$
Σ, macroscopic cross section (cm^{-1})
N, atom density $\left(\frac{\text{atoms}}{\text{cm}^3}\right)$
σ, microscopic cross section (cm^2)

From [8] we can assume that the neutron flux in the reactor core is approximately $10^{14}(\frac{n}{\text{cm}^2\,\text{s}})$. Additionally, we can calculate the density of H2O molecules in the reactor core using the following equation from [1]:

$$N = \frac{\rho N_A}{M} \qquad (2)$$

Where:

ρ, density
N_A, Avogadro's constant
M, Molecular weight

Using the typical core parameters from [13] we can use the steam tables in [10] to obtain the density of water in our simulated reactor core model to be $\rho = 593.71617 \frac{kg}{m^3}$. Knowing the molecular weight of water is $18.016 \frac{g}{mol}$, the molecular density of water in the reactor core can be calculated using equation (2) to be $N = 1.98 \times 10^{22} \frac{molecules}{cm^3}$.

To calculate the reaction rate we must define the microscopic cross section of water. To do this we must make several assumptions:

- Microscopic cross sections are a function of neutron energy, therefore average neutron energy will be used.

- There are predominantly two "classes" of neutrons interacting with atoms. Thermal neutrons with an average energy of $\sim 0.025\ eV$, and fast neutrons with an average energy of $\sim 2\ MeV$.

- The total cross section of a molecule is the sum of its constituent atomic cross sections weighted by stoichiometry.

Using our above assumptions we can write the microscopic cross section of water as:

$$\sigma_{H2O} \approx 2\sigma_H \ + \ \sigma_O \qquad (3)$$

Where,

$$\sigma_H = (\sigma_H^{tot})_{TH} \ + \ (\sigma_H^{tot})_F$$
$$\sigma_O = (\sigma_O^{tot})_{TH} \ + \ (\sigma_O^{tot})_F$$

By using $MT = 1$, $MF = 3$ from [3] we can obtain the total microscopic cross sections for Hydrogen (^1H) and Oxygen (^{16}O) for both thermal and fast neutrons, provided in **Table A.1**. This allows us to calculate the total microscopic cross section of water to be , $\sigma_{H2O} = 71.992357\ barns$ via equation (3). And the reaction rate to be, $R = 142.54 \times 10^{12} \frac{reactions}{s}$ via equation (1).

2.2 Scaling the Simulation

Obviously, it is not feasible to simulate 10^{12} interactions, recalculating the force field properties for each molecule every iteration on a personal computer. Therefore we are going to scale the simulation in order to generalize a small sample to the entire volume of the reactor core. To do this we must determine how many water molecules are in the core. We can do this by using the molecular density, N_{H2O}, and the dimensions of the core provided above. The volume of the core approximated as a cylinder can be calculated as $37.20\ m^3$. We need to make an assumption for the metal-to-water ratio of the core, because the core volume does not entirely consist of water. Therefore, we can assume a metal-to-water ratio of 1:3. This gives the volume of water in the core to be $24.55\ m^3$. Using the above result we can calculate the number of H2O molecules in the reactor core at any moment to be $4.87 \times 10^{29}\ molecules$. An equation for the scaling factor can be written in terms of the number of water molecules in the simulation as:

$$S_f = \frac{N_{sim}}{N_{core}} \tag{4}$$

We want to pick N_{sim} such that we remove the factor of 10^{12} in the reaction rate. If we choose $N_{sim} = 10^{18}$, then by equation (4) the scaled reaction rate is, $R_{scaled} = 292.21\ \frac{reactions}{s}$.

2.3 Determining the Number of Atomic Interactions

The total microscopic cross section for neutron interactions is the sum of the microscopic cross sections for four main types of interactions, elastic scattering, inelastic scattering, fission, and capture. We are going to make the following assumptions for the total microscopic cross section in this simulation:

- ^{1}H is simply a proton. A proton has no excited states, and therefore inelastic scattering cannot occur.

- ^{16}O inelastic scattering is possible, but the threshold is $\sim 6\ MeV$, so we will ignore it for simplicity.

- ^{1}H and ^{16}O cannot undergo fission.

Therefore we will only consider the elastic scattering and capture cross sections provided by $MT = 2,\ MF = 3$ and $MT = 102,\ MF = 3$ from [3], respectively for each atom. In order to calculate the number of neutron interactions per second with either ^{1}H or ^{16}O atoms we will use the microscopic cross sections for the average energy for thermal and fast neutrons tabulated in **Table A.2**. Using equation (3) we can calculate the microscopic cross section for elastic scattering for water to be $\sigma_{H2O}^{se} = 71.326898\ barns$. We can calculate the total number of elastic scattering interactions per second, R_{se}, by using a proportion:

$$R_{se} = R_{scaled}\left(\frac{\sigma_{H2O}^{se}}{\sigma_{H2O}^{tot}}\right)$$
$$= 289.50$$

We can calculate the number of neutron captures per second, R_c, using deduction:

$$R_c = R_{scaled} - R_{se}$$
$$= 2.71$$

Moving forward we are going to assume that neutron captures are not likely to cause molecular decomposition because the energy released in this process is going to be generalized to the nucleus of the atom and not transferred to the molecular bonds. So we will neglect neutron captures.

The number of elastic scattering neutron interactions with Hydrogen per second, R_{se}^H, can be calculated using proportions:

$$R_{se}^H = \frac{2R_{se}((\sigma_H^{tot})_{TH} + (\sigma_H^{tot})_F)}{\sigma_{H2O}^{tot}}$$
$$= 267.69$$
$$\approx 268$$

We can calculate the number of elastic scattering neutron interactions per second, R_{se}^O, with Oxygen by deduction:

$$R_{se}^O = R_{se} - R_{se}^H$$
$$= 21.81$$
$$\approx 22$$

2.4   Sampling Neutron Energies

Neutrons are born fast and moderated to thermal energies. Fast neutron energies can be sampled from the prompt neutron energy spectra provided by [8], which is described by the function:

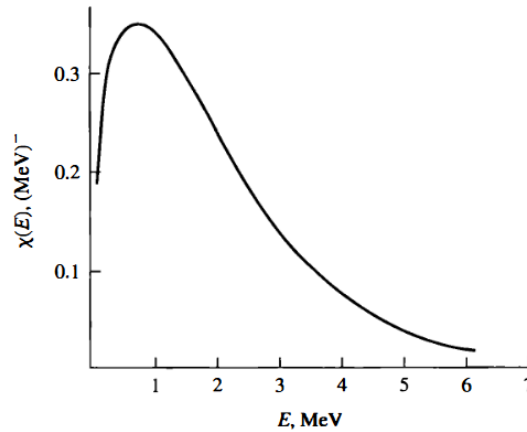$$\chi(E) = 0.453e^{-1.036E} sinh\sqrt{2.29E} \tag{5}$$

Figure 1: Prompt neutron spectrum

Where, E is the neutron energy in MeV.

To obtain neutron energies for the simulation we will perform numerical cumulative distribution function (CDF) sampling using the following method:

- Numerically integrate $\chi(E)$ to obtain the CDF.

- Normalize the CDF between 0 and 1.

- Generate a random number uniformly between zero and one.

- Interpolate the CDF at the random number to find the neutron energy.

Once the neutron energy is obtained, we can use the following equation from [8] to calculate the kinetic energy of the neutron after scattering.

$$E' = \frac{E_0}{(A+1)^2}[cos\theta + \sqrt{A^2 + sin^2\theta}]^2 \tag{6}$$

The recoil energy, E_{recoil} (energy imparted unto the target nucleus) is given by:

$$E_{recoil} = E_0 - E' \tag{7}$$

Where A is the atomic mass number and θ is the scattering angle for the neutron energy.

To obtain the scattering angle, [3] provides angular distributions of neutrons based on their energy in $MT = 2, MF = 4$. The angular distributions are expressed as a normalized probability distribution according to:

$$\int_{-1}^{1} f(\mu, E)d\mu = 1$$

Where $f(\mu, E)d\mu$ is the probability that a particle of incident energy E will be scattered into the interval $d\mu$ about an angle whose cosine is μ. The units of $f(\mu, E)$ are $(unit - cosine)^{-1}$. The distribution is represented as a Legendre polynomial series:

$$f(\mu, E) = \sum_{l=0}^{NL} \frac{2l+1}{2} a_l(E) P_l(\mu) \tag{8}$$

Where:

l order of the Legendre polynomial
a_l the lth Legendre polynomial coefficient; it is implicitly understood that $a_0 = 1$
$P_l(\mu)$ Legendre polynomial of degree l

By observing the provided Legendre coefficients, you can see that the distributions are practically flat because the higher order terms are very small. This makes $\mu = -1$ the most probable scattering angle for all neutron energies. In order to accurately sample the distribution, rejection sampling was performed using the following method:

- The maximum value of $f(\mu, E)$ is computed.

- Two sets of random numbers are generated: the first representing μ on the domain $\{-1, 1\}$, the second representing the random sample y on the domain $\{0, f_{max}\}$

- μ and y are both sampled and the value $f(\mu, E)$ is computed.

- If the sample y is less than the computed value of $f(\mu, E)$, the scattering angle is returned in radians.

2.5   MMFF94 Molecular Force Field Model

In order to model the energetics of water molecules, we self-developed a CPP implementation of the Merck Molecular Force Field 94 (MMFF94). Because we only intended to use the force field for H2O and operated under a simplified model of considering water molecules independent (no hydrogen bonding), the bond and angle parts of the energy equation are of the most interest currently. Torsions and some of the other energies (excluding OOP or out of plane bending) were also attempted to be calculated on other molecules including methane, ethane, and ethylene. The results of these are only for the purpose of constructing a robust and formalized implementation of MMFF94 and thus are left out of the report and remain only in the code base.

2.5.1   Input File

After evaluating multiple different input file formats, we chose to use 3D sdf files from the NIST Chemistry Webbook as they provided molecule connectivity and contained atomic coordinates for a computationally relaxed form of the molecule. The bond lengths and angles were corroborated by experimental equilibrium values from the CCCBDB. The input file was parsed and converted into an instance of our `Molecule` class.

2.5.2   Atom Typing

Force fields rely on assigning an integer value to (typing) each atom of a molecule, as it serves as the basis for retrieving specific parameters for bonds, angles, etc. that involve those atoms. In our implementation, we do this in a relatively hard-coded way as it is a difficult task even for commercial code-bases (RDKit, openFF, etc.) to perform. Atom typing is performed once a `Molecule` is created. Our `ForceField` class contains `maps` for storing all necessary MMFF94 force field parameters (including atom types and parameters for bond, angle, etc. such as force constants) for energy calculations. All of these parameters were found by combing through literature and other commercial implementations of MMFF94.

2.5.3   Energy Calculation

To calculate the energy of the molecules in our `ForceField`, each molecule is considered. For each molecule's found bond, angle, and torsion (based on traversing atoms connectivity) the energy is calculated depending on the atom types involved. Finally, the energy from vdW and charges is calculated. Many of these calculations require spatial vector operations that have been thoughtfully considered and written in code. All of the energies are summed up to provide us a final potential energy for molecules in our `ForceField`. Energy equations for bonds and angles are found in the appendix and can also be seen implemented in our code.

2.6 Simple Molecular Force Field Model

Once the neutron energies and scattering angles have been sampled it is possible to compute the recoil energy using equation (7). Computing the recoil energy gives values with a magnitude of $10^6 eV$. This energy is significantly larger than the equilibrium O-H bond energy in water of $5.095 eV$. Meaning every incident neutron would cause the water molecule to instantaneously decompose upon scattering. We know this is not true and therefore we must make an assumption to scale the recoil energy:

- The three primary components of a molecular force field are the rotational, translational, and vibrational energies.

- The rotational and translational energies are assumed to be classical kinetic energies related to the mass of the molecule.

- The vibrational energy is assumed to be molecular bond energy modeled using classical molecular mechanics.

- The percentage of the recoil energy imparted unto the target molecule responsible for the vibrational energy is proportional to the mass of the interacting molecules.

The final assumption is the key to scaling the recoil energy appropriately. This percentage η_n can be modeled as as fractional relation between the mass of a water molecule m_{H2O} and the mass of a neutron m_n by:

$$
\begin{aligned}
\eta_n &= \frac{m_{H2O} - \frac{m_{H2O}}{m_n}}{m_{H2O}} \\
&= \frac{m_{H2O}(1 - \frac{1}{m_n})}{m_{H2O}} \\
&= 1 - \frac{1}{m_n}
\end{aligned}
\tag{9}
$$

Recall, η_n is a percentage. Substituting the mass of a neutron into equation (10) we obtain:

$$
\begin{aligned}
\eta_n &= (1 - \frac{1}{1.0086649})(\frac{1}{100}) \\
&= 8.59 \times 10^{-5}
\end{aligned}
$$
$$
\tag{10}
$$

The percentage of recoil energy imparted unto the target molecule responsible for changing the vibrational energy is given by:

$$
\Delta(E)_{vib} = \eta_n \ E_{recoil} \tag{11}
$$

The rest of the 99.9914% of the recoil energy is transferred into rotational and translational components of the molecule. This energy is ignored because we are assuming that rotational and translational energy does not affect the chemical bonds and therefore does not contribute to molecular decomposition.

2.7 Molecular Decomposition

In order to understand what decomposition means in this context, the only concept we need to apply is that of appearance energy, which is the minimum amount of energy supplied to a molecule to produce a specific ion. **Table A.3** provides several appearance energy determinations for water. In this case the energy is supplied from the incident neutron. Molecular decomposition can be assumed to occur if the incident neutron energy is above the minimum appearance energy determination.

3 Results

3.1 MMFF94 Implementation
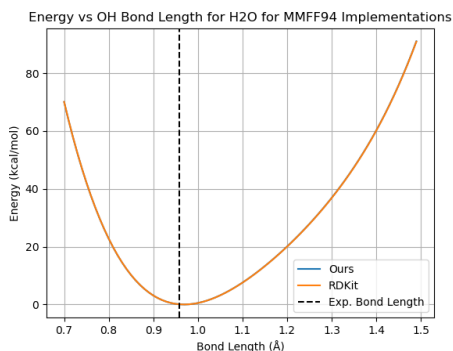
(a) H2O Energy vs OH Bond Length
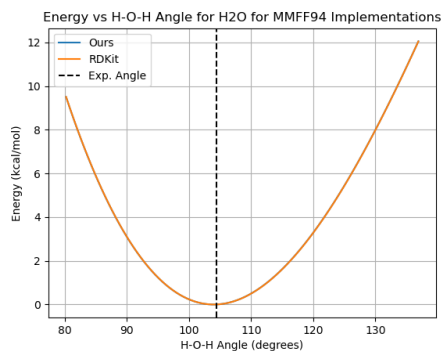
(b) H2O Energy vs HOH Angle

We compared our implementation of the MMFF94 to the RDKit one in Python to ensure correctness of our results. In the left plot above, we vary one of the OH bonds of H2O and see how the energy changes based on force field calculations. Similarly for the right plot, we vary the HOH angle of H2O and calculate the energy in the different conformations. It can be seen that our results exactly align with those of RDKit and thus are suitable for modeling purposes.

## 3.2 Scaled Decomposition Calculation

Using everything obtained so far we can calculate the number of molecular decompositions over a specific time-frame. We will assume the time period is 24 hours, or 86400 seconds. This results in approximately 25×10^6 neutron-water molecule interactions. We can take a sample of the $10,000$ interactions for neutrons incident upon either hydrogen or oxygen and generalize this to the entire sample because it is a normalized proportion. After performing this calculation and scaling the result back to the entire reactor we obtain 8.83×10^{18} decompositions, where a water molecule will decompose 72.2% of the time a neutron interaction occurs. This number of decompositions converts to 6.97×10^{-8} gallons, which is the expected result. Recall that the reaction rate was on the order of 10^{12} and the total number of water molecules in the reactor core was on the order of 10^{29}. The percentage of water molecules which experience a neutron interaction every second can be calculated to be $2.93 \times 10^{-14}\%$. This result can be represented numerically as:

$$4.87 \times 10^{29}(molecules)(2.927 \times 10^{-16}(\frac{interactions}{second}))(0.722(\frac{decompositions}{interaction}))(86400(\frac{seconds}{hour}))$$
$$= 8.89 \times 10^{18} decompositions$$

4 Discussion

During the execution of this research an interesting observation was made while attempting to create a theory for molecular decomposition. A theory for molecular composition can be created by combining the concepts of appearance energy and vertical ionization energy. Vertical ionization energy is the amount of energy a molecule in the ground state must absorb before discharging an electron, resulting in a positively charged ion, H_2O^+, without nuclear rearrangement. After ionization, the molecule is not decomposed, several things can happen after ionization:

- Recombination: The positively charged ion captures an electron and returns to a neutral state.

- Decomposition via ionization-induced proton transfer: The positively charged ion interacts with a water molecule in a proton transfer interaction:

$$H_2O^+ + H_2O \rightarrow H_3O^+ + OH$$
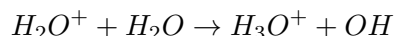
- Decomposition due to neutron irradiation: The amount of energy absorbed is so great that the molecule instantaneously decomposes into constituent ions.

Two key ideas to take away from the definition of vertical ionization energy above are "ground state" and "without nuclear rearrangement". This concept allows modeling molecular energy absorption without modifying the geometry of the atoms in the molecule.

In order to model molecular decomposition we will use the energy well theory to relate vibrational excitation to molecular decomposition. This can be described as follows:

- Vibrational excitation: The molecule climbs to a higher step in the same well (same geometry, same bonding, more internal motion).

- Electronic excitation: The system is in a new energy well with a different shape (geometry and bond stiffness change).

- Decomposition: Occurs when energy is high enough for the system to escape the well (bond breaking).

We can then make the following postulation:
The vibrational excitation energy threshold to cause molecular decomposition after ionization is equal to the difference between appearance energy and ionization energy.

An extension of this postulation is:
The appearance energy is dependent on the excitation state of the molecule.

This is written in equation form as:

$$(E_{vib})_{crit} = E_{appearance} - E_{ionization} \qquad (12)$$

This postulate is supported by comparing the excitation energies for water from research performed in [12], as shown in **Table A.4** with critical vibrational excitation energies from equation (12).The excitation energies for water are shown in **Figure 2** as potential energy curves.
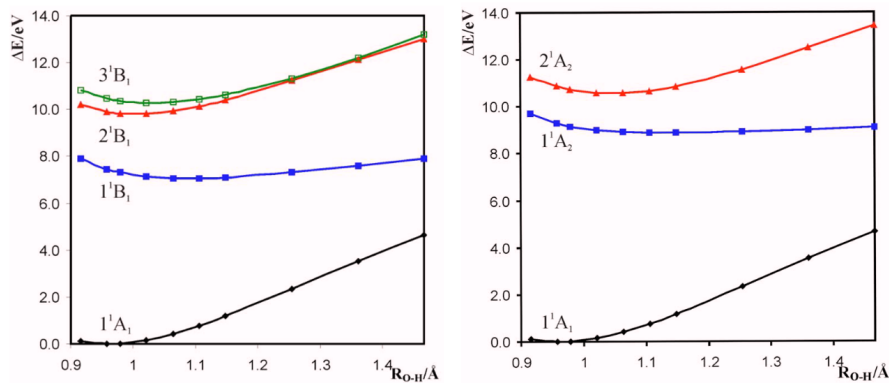

Figure 3: Potential energy curves for excited states of water

We can perform a simple classical molecular mechanics calculation to determine the O-H bond energy, for a single bond, in the ground state of water by assuming a bond strength of $k_{bond} = 19.5138\frac{eV}{\mathring{A}^2}$, an equilibrium bond length of $r_{eq} = 0.9578\mathring{A}$, and a bond length $r_{O-H} = 1.4568\mathring{A}$:

$$E_{bond} = \frac{1}{2}k_{bond}(r_{O-H} - r_{eq})^2$$
$$\approx 2.43 \ eV$$

$$(13)$$

By observing the ground state ($1 \ ^1A_1$) of water in Figure 2 compared to the calculated bond energy for a single O-H bond, you can see that at the specified bond length, the potential energy is approximately equal to twice the bond energy. This makes sense because there are two bonds in a water molecule and the H-O-H bond angle energy is negligible compared to the combined bond energy.

We can extend this observation to the rest of the excitation energies provided in **Table A.4** by halving them. Additionally, By using equation (12) and an assumed ionization of 12.6 eV, we can tabulate the critical vibrational excitation energies to form specific ions:

Excitation State	$(E_{bond})_{O-H}$ (eV)
$1\ ^1B_1$	3.95
$1\ ^1A_2$	4.555
$2\ ^1A_1$	5.605
$2\ ^1B_1$	6.5
$3\ ^1B_1$	6.595
$3\ ^1A_1$	6.61
$2\ ^1A_2$	6.715

Bond energies ($r_{O-H} = 1.4568\mathring{A}$) for a single O-H bond in water

Product Ions	$(E_{vib})_{crit}$ (eV)
$H^+ + OH^-$	3.4 ± 0.3
$H^+ + OH$	4.35 ± 0.05
$HO^+ + H$	5.48 ± 0.05
$O^+ + H_2$	6.4 ± 0.2
$O^+ + 2H$	13.9 ± 0.3

Critical vibrational excitation energies to form specific ions

By comparing the bond energies for a single O-H bond in water with the critical vibrational excitation energies, you can see that there may be a correlation between excitation states and critical vibrational excitation energies as postulated above. With the exception of the last product ion combination $O^+ + 2H$ where the energy critical excitation energy is almost double the previous value.

This is likely due to the fact that during radiolysis if two H atoms are formed within a few angstroms of eachother, they are highly likely to recombine to form H_2. It could be theorized that the difference in critical vibration excitation energy when creating diatomic hydrogen versus two hydrogen atoms is enough to overcome the bond energy of diatomic hydrogen ($4.52\ eV$) and provide them with sufficient translational energy to prevent them from interacting. However, in the context of radiolysis of water it is very highly likely that the lone hydrogen atoms will recombine with another lone hydrogen atom to form H_2, or react with some other molecule.

Our initial approach of utilizing the implementation of MMFF94 to model neutron interactions with water was put aside once we realized that the recoil energies of the neutrons were much greater than the bond dissociation energy of H2O. Because of this, we pivoted to performing a deep dive into a scaled calculation of water dissociation strictly based on theory.

5 Future Work

The result obtained above matches expectations because an insignificant amount of water decomposes in 24 hours. It would be interesting to extend these modeling assumptions to multiple chemical species responsible for affecting nuclear chemistry in a multi-physics simulation to attempt to model temporal changes in chemistry parameters. Additionally, further research related to the discussion section could show promising results for constructing a theory of molecular decomposition. The figure of potential energy curves could provide an alternative method for calculating equilibrium bond lengths, as well as bond strengths for the associated excitation states.

6 Contributions

The project was broken into two major components and the contributions from team members are outlined below.

- **Gary Patterson**: Creating a simulated nuclear reactor model, writing functions to extract data from tables for microscopic cross sections and angular distributions, sampling neutron

energies and scattering angles, modeling molecular decomposition of water and performing the final calculation to determine the percentage of water molecules which decompose from neutron interactions.

- **Suraj Rao**: Implemented entire scaffold for MMFF94 force field model. Verified the energy outputs against the RDkit implementation. Attempted MD simulation using 2D box model with neutron collisions against water molecules. Brainstormed different ways of handling water decomposition in regards to bond dissociation including final calculation performed.

7   Appendix

Typical core parameters for an 1000MWe pressurized water reactor (PWR) [13]:

$P_{avg} = 2250 \ psi$
$T_{avg} = 310.5 \ °C$
$Length = 4.17 \ m$
$Diameter = 3.37 \ m$

Calculation of equation (1):

$$R = (10^{14} \ \frac{n}{cm^2 s})(1.98 \times 10^{22} \frac{molecules}{cm^3})(71.992357 \times 10^{-24} cm^2)$$
$$= 142.54 \times 10^{12} \ \frac{reactions}{s}$$

Calculation of equation (2):

$$N_{H2O} = (593.71617 \ \frac{kg}{m^3})(\frac{1 \ m^3}{10^6 cm^3}(\frac{1000 \ g}{1 \ kg})(6.022 \times 10^{23} \ \frac{atoms}{mol})(\frac{1 \ mol}{18.016 \ g})$$
$$= \ 1.98 \times 10^{22} \ \frac{molecules}{cm^3}$$

Table A.1:

	^1H	^{16}O
Thermal	30.4009	2.90842
Fast	3.79407384	1.57964310

Table A.1: Total Microscopic Cross Sections in units of Barns

Note: $1 \ barn = 10^{-24} \ cm$

Calculation of equation (4):

$$S_f = \frac{N_{sim}}{N_{core}}$$
$$= \frac{10^{18}}{4.87 \times 10^{29}}$$
$$= 2.05 \times 10^{-12}$$

Table A.2:

		Thermal	Fast
σ_{se}	^1H	30.0683	1.57964310
	^{16}O	3.79390400	1.5796140
σ_c	^1H	3.325842×10^{-1}	3.687541×10^{-5}
	^{16}O	1.698355×10^{-4}	2.91×10^{-5}

Table A.2: Elastic Scattering and Capture Cross Sections for Oxygen and Hydrogen in units of Barns

Table A.3:

Product Ions	E_{app} (eV)
$H^+ + OH^-$	16 ± 0.3
$H^+ + OH$	16.95 ± 0.05
$HO^+ + H$	18.08 ± 0.05
$O^+ + H_2$	19.0 ± 0.2
$O^+ + 2H$	26.5 ± 0.3

Table A.3: NIST Appearance Energy Determinations for Water

Table A.4:

Excitation State	$\Delta E_{excitation}(eV)$
$1\ ^1B_1$	7.90
$1\ ^1A_2$	9.11
$2\ ^1A_1$	11.21
$2\ ^1B_1$	13.00
$3\ ^1B_1$	13.19
$3\ ^1A_1$	13.22
$2\ ^1A_2$	13.43

Table A.4: Excitation energies for excited states of water

Note: The excitation energies above are for symmetrically stretched ($r_{O-H} = 1.4568\text{Å}$) water, referred to the ground state at the experimental equilibrium geometry ($r_{O-H} = 0.9578\text{Å}$).

MM94 Bond Energy

- $E_{Bond} = 143.9325\frac{kb_{ij}}{2}(r - r_{eq})^2(1 + cs(r - r_{eq}) + \frac{7}{12}cs^2(r - r_{eq})^2)$

- Here, kb_{ij} is the force constant for the specific atom types of (i, j). r is the distance between two atoms and r_{eq} is the equilibrium distance between the two atoms.

- r is in units of Angstroms, and we get out kcal/mol for energy.

- Instead of using the pure harmonic oscillator model for the bond energy, we utilize a Morse potential as this translates to more accurate energy calculations at bond distances further from equilibrium which is important in our case of bond dissociation.

MM94 Angle Energy

- $E_{Angle} = 0.043844 \frac{ka_{ijk}}{2}(\theta - \theta_{eq})^2(1 + cb(\theta - \theta_{eq}))$

- Here, ka_{ij} is the force constant for the specific atom types of (i, j, k). θ is the angle between atoms (i, j, k) where j is the central atom and θ_{eq} is the equilibrium angle between the three atoms.

- r is in units of Angstroms, and we get out kcal/mol for energy.

- Instead of using the pure harmonic oscillator model for the bond energy, we utilize a Morse potential as this translates to more accurate energy calculations at bond distances further from equilibrium which is important in our case of bond dissociation.

Water Molecule 3D SDF File

```
water
  NIST    07301310173D 1   1.00000    -76.40895
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  3  2 0  0  0  0  0  0  0  0999 V2000
   -0.0211    -0.0020     0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
    0.8345     0.4519     0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    1.4769    -0.2730     0.0000 H   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  1  0     0  0
  2  3  1  0     0  0
M  END
> <COPYRIGHT>
Collection (C) 2016 copyright by the U.S. Secretary of Commerce on behalf of the
United States of America. All rights reserved.

> <DATE>
2013-07-30

> <CAS.NUMBER>
7732-18-5

> <SYNONYMS>
Water

> <METHOD>
B3LYP/6-31G*

> <DIPOLE.MOMENT>
2.0962 debye

> <ELECTRONIC.ENERGY>
-76.4089547246 hartree

> <IR.FREQUENCIES>
"Frequency (cm-1)"   "Intensity (km/mol)"
1713.5711  75.7263
3729.9547  1.6912
```

```
3851.5408   19.3003
```

> `<ROTATIONAL.CONSTANTS>`
```
786.82917 GHz
432.74827 GHz
279.19421 GHz
```

> `<SOFTWARE>`
```
Gaussian 09, Revision D.01
```

> `<CONTRIBUTOR>`
```
Jennifer Skerritt
```

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