CHEMICAL KINETICS VISUALIZER

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Abstract—We present an interactive educational platform designed to support both teachers and students in the teaching and learning of chemical kinetics. The platform was developed as a website hosted on GitHub Pages using Svelte and JavaScript. It provides dynamic visualizations and simulations aimed at making complex chemical concepts more accessible and engaging. Core topics include reaction order, activation energy, and potential energy surfaces, as well as catalytic processes such as catalytic hydrogenation and enzymatic catalysis. The platform also features theoretical simulators for radioactive decay, calculators for half-life computation, and a detailed simulation of the Natural Radioactive Decay Series. By integrating interactive tools and didactic animations, our solution enhances conceptual understanding and promotes active learning in chemistry education.

Index Terms—Chemical Kinetics, Educational Technology, Interactive Simulation, Catalysis, Activation Energy, Radioactive Decay, Half-Life Calculator

I. INTRODUCTION

Chemical kinetics is the branch of chemistry that studies the rates at which chemical reactions occur and the mechanisms by which they proceed. It plays a central role in understanding how reactions evolve over time, how different variables influence their speed, and how catalysts can accelerate processes without being consumed. Key concepts such as reaction order, activation energy, and catalytic pathways are essential not only in academic research but also in industrial applications and everyday phenomena.

Despite its importance, teaching chemical kinetics—especially to high school and undergraduate students—presents significant challenges. One of the primary difficulties lies in the abstract and microscopic nature of the processes involved. Many of the fundamental phenomena in kinetics occur at the atomic or molecular level, far removed from everyday sensory experience. Concepts like molecular collisions, transition states, and potential energy surfaces are inherently invisible and highly theoretical, making them difficult to grasp through traditional, static teaching methods.

To bridge this gap, educators increasingly seek dynamic and interactive tools that can help translate complex atomic-scale interactions into intuitive visual experiences. Visualization technologies and simulations provide students with the opportunity to observe and experiment with reaction mechanisms in a controlled, exploratory environment. However, there remains a lack of accessible, modern platforms that combine visual clarity, pedagogical effectiveness, and scientific rigor tailored to the context of chemistry education.

In response to this need, we developed an interactive educational website using Svelte and JavaScript, hosted on GitHub Pages. The platform covers a range of topics in chemical kinetics and radioactivity, including reaction order, catalytic mechanisms (catalytic hydrogenation and enzymatic catalysis), activation energy, and potential energy surfaces. It also features simulations of radioactive decay, half-life calculators, and visualizations of natural radioactive decay series. Our goal is to make the teaching of these abstract topics more accessible, dynamic, and engaging for both educators and students.

II. REACTION ORDERS

Reaction order is a key concept in chemical kinetics that indicates how the rate of a reaction depends on the concentration of its reactants. For a general reaction:

$$A \rightarrow \text{Products}$$

the rate law is expressed as:

$$\text{rate} = k[A]^n$$

where k is the rate constant, $[A]$ is the concentration of the reactant, and n is the reaction order. The reaction order provides information about the molecularity of the rate-determining step.

Although reactions may exhibit fractional or even negative orders, the most common orders in elementary reactions are 0, 1, and 2. This is because the probability of three or more molecules colliding simultaneously is extremely low.

A. Half-life Definition

The **half-life** $(t_{1/2})$ of a reaction is defined as the time required for the concentration of a reactant to decrease to half of its initial value. The formula for $t_{1/2}$ depends on the order of the reaction, as shown below.

B. Zero-Order Reactions ($n = 0$)

In zero-order reactions, the rate is independent of the concentration of the reactant:

$$\text{rate} = k$$

Integrated Rate Law:

$$[A](t) = [A]_0 - kt$$

Half-life:

$$t_{1/2} = \frac{[A]_0}{2k}$$

Here, the half-life depends on the initial concentration $[A]_0$ and decreases linearly over time.

C. First-Order Reactions ($n = 1$)

For first-order reactions, the rate is directly proportional to the concentration of the reactant:

$$\text{rate} = k[A]$$

Integrated Rate Law:

$$[A](t) = [A]_0 e^{-kt}$$

Half-life:

$$t_{1/2} = \frac{\ln(2)}{k}$$

In this case, the half-life is constant and independent of the initial concentration, making first-order kinetics particularly common in radioactive decay and enzymatic processes.

D. Second-Order Reactions ($n = 2$)

In second-order reactions, the rate is proportional to the square of the concentration:

$$\text{rate} = k[A]^2$$

Integrated Rate Law:

$$\frac{1}{[A](t)} = \frac{1}{[A]_0} + kt$$

Half-life:

$$t_{1/2} = \frac{1}{k[A]_0}$$

Here, the half-life is inversely proportional to the initial concentration. As the concentration decreases, the half-life increases.

Each reaction order exhibits a distinct concentration-time curve, allowing experimental determination of the order through data analysis and fitting techniques.

III. ACTIVATION ENERGY AND POTENTIAL ENERGY SURFACES

A. Activation Energy and the Arrhenius Equation

Activation energy (E_a) is the minimum amount of energy required for a chemical reaction to occur. It represents the energy barrier that reactant molecules must overcome to transform into products. This concept is central to understanding reaction rates: even highly exergonic (energetically favorable) reactions may proceed slowly if the activation energy is large.

The quantitative relationship between the rate constant k and activation energy is given by the Arrhenius equation:
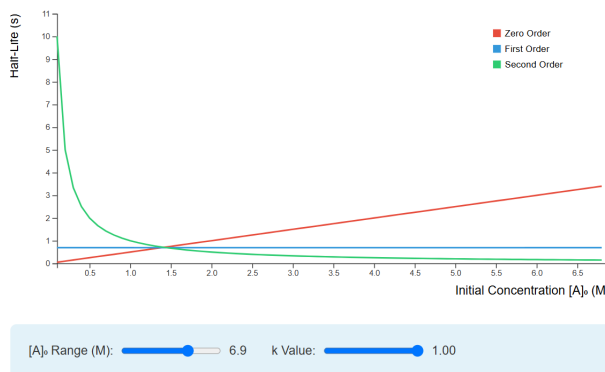
Fig. 1. Concentration vs. time curves for reactions of zero, first, and second order.

$$k = Ae^{-\frac{E_a}{RT}}$$

where:

- k is the rate constant,
- A is the pre-exponential factor (related to collision frequency and molecular orientation),
- E_a is the activation energy (in joules per mole),
- R is the universal gas constant,
- T is the absolute temperature in kelvin.

According to this equation, even a small decrease in activation energy can cause a significant increase in the rate constant, especially at moderate temperatures.

B. Relation to Brownian Motion

At the molecular scale, particles are in constant random motion due to thermal energy — a phenomenon known as **Brownian motion**. This chaotic movement results in continuous collisions among molecules. However, only a fraction of these collisions lead to reaction; specifically, only those with sufficient energy to overcome the activation barrier (i.e., $E \geq E_a$) and proper molecular orientation are effective.

Thus, activation energy acts as a filter: Brownian motion supplies the kinetic energy, but only the most energetic collisions succeed in initiating the reaction. As temperature increases, more particles have the required energy, explaining why reaction rates typically increase with temperature.

C. Potential Energy Surfaces for Different Reaction Types

Potential Energy Surfaces (PES) are graphical representations of the energy changes that occur during a chemical reaction as reactants are converted into products. They help visualize activation energy, intermediates, and the influence of catalysts. Below are three illustrative PES examples for key reaction types:
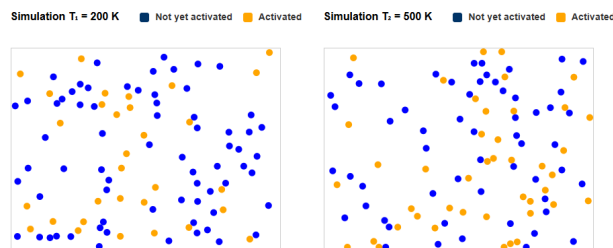
Fig. 2. Visualization of molecular activation at two temperatures (200 K and 500 K). Blue dots represent molecules that have not yet been activated, while orange dots represent activated molecules. The increased number of activated molecules at 500 K illustrates how higher temperatures enhance the probability of overcoming the activation energy barrier, as predicted by the Arrhenius equation.
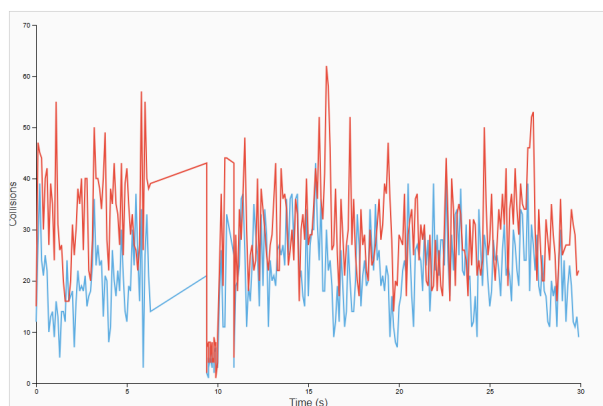

Fig. 3. Experimental simulation of concentration fluctuations over time for different reaction orders. The plot illustrates the stochastic behavior of molecular systems under kinetic processes. Despite the noisy dynamics, general trends can be extracted to determine whether the system follows zero-, first-, or second-order kinetics based on the rate at which concentrations decrease.

1) Elementary Reactions: Elementary reactions occur in a single step without intermediates. Their potential energy surface shows a direct path from reactants to products, with a single energy maximum representing the transition state:

$$\text{Reactants} \rightarrow^{\ddagger} \text{Products}$$
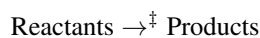
This maximum is the activation energy. Since there are no intermediates, the PES has only one energy barrier.

2) First-Order Reactions: First-order reactions often correspond to unimolecular decompositions or rearrangements. Although they may involve more complex mechanisms than elementary reactions, their overall energy profile can still be simplified as a single barrier process. The PES is similar to that of an elementary reaction, but the reaction may proceed via an internal reorganization of the molecule rather than bimolecular collision.

3) Catalyzed Reactions: Catalysts provide an alternative reaction pathway with a lower activation energy. In the PES, this appears as a modified surface with additional intermediate states and one or more lower energy transition states. Although

the overall energy difference between reactants and products remains the same, the height of the energy barrier is reduced:

$$E_{a,\text{catalyzed}} < E_{a,\text{uncatalyzed}}$$

As a result, catalyzed reactions proceed more rapidly, without altering the thermodynamics of the reaction. In biological systems, enzymes act as highly efficient catalysts by stabilizing the transition state and orienting substrates appropriately.
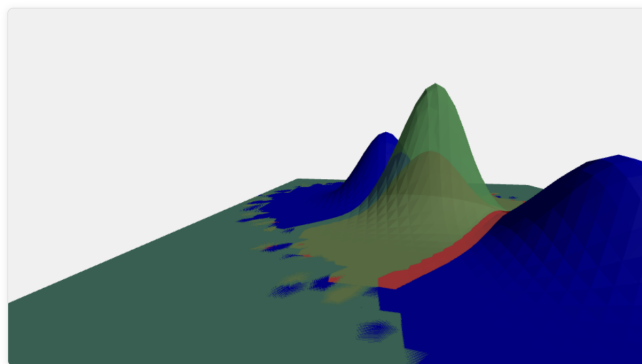

Fig. 4. Potential Energy Surfaces for (a) an elementary reaction(green), (b) a first-order reaction (blue), and (c) a catalyzed reaction (red).

The comparison of potential energy surfaces highlights the crucial role of activation energy and how catalysis enables more efficient reaction pathways.

IV. INTERACTIVE RADIOACTIVE DECAY SIMULATION AND NATURAL DECAY CHAINS

A. Interactive Radioactive Decay Simulator

Our interactive simulation tool allows users to visualize the transformation of atomic nuclei through radioactive decay. The model is built upon the classical Rutherford atomic representation, which provides an intuitive visual of the nucleus surrounded by concentric electron shells. This visualization enhances comprehension by showing electrons in well-defined orbits, although the actual quantum nature of orbitals is more complex.

Each nucleus is represented in its ground state, displaying its full complement of electrons orbiting a central nucleus. The user can observe decays in real time, with corresponding nuclear emissions such as:

- **Alpha particle:** Emission of a $^{4}_{2}\text{He}$ nucleus, decreasing the atomic number by 2 and mass number by 4.
- **Beta decay:** A neutron transforms into a proton, emitting an electron and an antineutrino; atomic number increases by 1.
- **Positron emission:** A proton is converted into a neutron, emitting a positron and a neutrino; atomic number decreases by 1.
- **Neutron emission:** The nucleus emits a free neutron, altering only the mass number.

The arrangement of electrons in orbitals reflects their energy levels. The simulator emphasizes that outer orbitals are more

diffuse and energetically closer, particularly in heavy elements, a property that has implications for nuclear and electronic interactions.
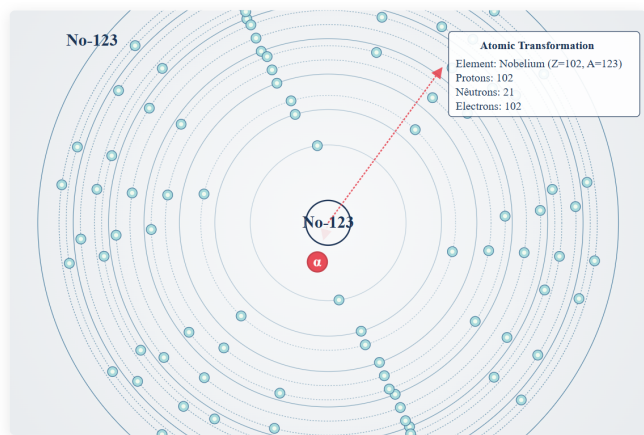

Fig. 5. Visualization of an alpha decay event for Nobelium-123 (No-123). The simulation displays the atomic structure with 102 protons, 102 electrons, and 21 neutrons. The particle (2 protons and 2 neutrons) is emitted from the nucleus, resulting in the transformation of the element. The electronic orbitals are represented following a Rutherford-like atomic model for didactic clarity.

B. Natural Radioactive Decay Series

The other component of our platform focuses on naturally occurring radioactive decay chains. These are sequences of nuclear transformations by which unstable heavy isotopes decay into stable lead (Pb) isotopes. Each decay proceeds via a combination of alpha and beta decays, and is governed by the half-lives of the isotopes involved.

Our system includes the three well-known natural decay series:

1) **Thorium series:**

$$^{232}\text{Th} \rightarrow \cdots \rightarrow {}^{208}\text{Pb}$$

2) **Uranium series:**

$$^{238}\text{U} \rightarrow \cdots \rightarrow {}^{206}\text{Pb}$$

3) **Actinium series:**

$$^{235}\text{U} \rightarrow \cdots \rightarrow {}^{207}\text{Pb}$$

Each decay chain is visualized dynamically: selecting a series from the dropdown menu reveals its full sequence, isotopic transformations, and half-lives. The system provides users with insight into nuclear stability, the longevity of radioactive isotopes, and the origin of naturally occurring lead.

V. CATALYSIS

Catalysis is the acceleration of a chemical reaction by a substance called a **catalyst**, which lowers the activation energy required for the reaction to occur. Catalysts participate in the reaction mechanism but are regenerated at the end of the process, allowing them to catalyze multiple reaction cycles.
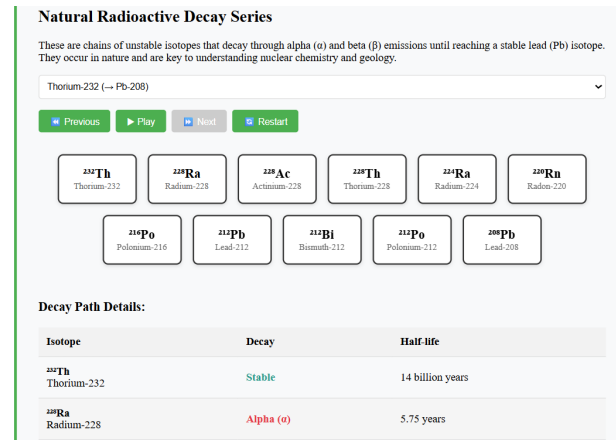

Fig. 6. Interactive interface of the natural radioactive decay simulator displaying the Thorium-232 decay series. The sequence shows unstable isotopes undergoing alpha and beta emissions until reaching the stable lead isotope. The table below details the type of decay and the half-life of each isotope in the path.

A. Energy Profile with and without Catalyst

In an uncatalyzed reaction, reactants must overcome a significant energy barrier (activation energy) to form products. A catalyst introduces an alternative reaction pathway with a lower activation energy, thereby increasing the rate of reaction without altering the thermodynamic properties such as the enthalpy change (ΔH). This effect is commonly illustrated by an energy diagram comparing the catalyzed and uncatalyzed reactions.
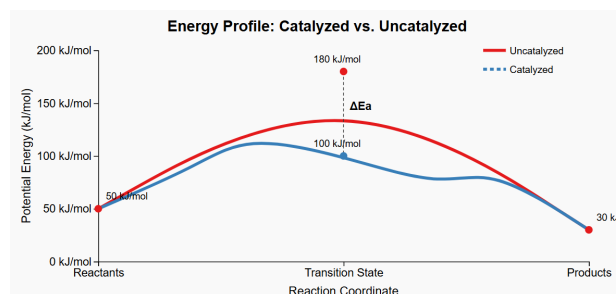

Fig. 7. Reaction energy profile with and without catalyst. The catalyst lowers the activation energy, allowing the reaction to proceed more quickly.

B. Catalysis via Adsorption Mechanism

In **heterogeneous catalysis**, especially on solid surfaces, the mechanism often involves:

- **Adsorption**: Reactants are adsorbed onto the catalyst's surface.
- **Activation**: Bonds are weakened or broken upon adsorption.
- **Reaction**: New bonds form between fragments.
- **Desorption**: Products leave the surface, freeing active sites.

This is especially effective in surface reactions such as hydrogenation over metal catalysts.
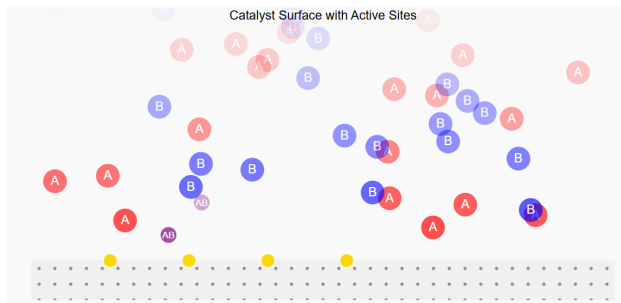
Fig. 8. Illustration of a heterogeneous catalytic mechanism on a solid surface. Reactant molecules A (red) and B (blue) interact with the catalyst's active sites (yellow dots) where they adsorb, react to form product AB (purple), and desorb, freeing the site for a new cycle.

C. Types of Catalysis

- **Homogeneous Catalysis**: Catalyst is in the same phase as the reactants. Example: acid-catalyzed esterification in liquid phase.
- **Heterogeneous Catalysis**: Catalyst is in a different phase, typically a solid in contact with gaseous or liquid reactants. Example: catalytic hydrogenation on platinum.
- **Enzymatic Catalysis**: Specialized biological catalysis where enzymes (protein molecules) act as highly specific and efficient catalysts under mild conditions.

VI. CONCLUSION

This project successfully achieved its goal of creating a didactic and interactive platform to support the teaching and learning of key concepts in chemical kinetics, radioactive decay, and catalysis. By combining scientific accuracy with clear visual representations, we developed a resource that helps students and educators explore complex chemical phenomena in an accessible and engaging way.

Through dynamic diagrams, mechanistic animations, and explanatory content, the platform illustrates the step-by-step processes underlying nuclear transformations and catalytic mechanisms. These tools foster a deeper conceptual understanding, bridging the gap between abstract theory and observable behavior.

The integration of energy profiles, reaction pathways, and molecular-level interactions demonstrates how chemical transformations occur both in natural and technological contexts. This educational tool not only reinforces classroom content but also serves as a foundation for further inquiry in physical chemistry and related fields.

Overall, the platform stands as a meaningful contribution to science education, using modern digital tools to bring invisible processes to life and promote more effective learning.

VII. REFERENCES

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