Water Pollutant Behavior under Different Reaction Kinetics and Flow Regimes

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Introduction

This research project will study how dissolved water pollutants, such as nanomaterials, behave in water under different reaction kinetics and flow regimes within model reactor vessels constructed.

A safe and nontoxic version of a pollutant was used, known as crystal violet, a purple dye that behaves similarly to common water pollutants.

Crystal violet readily reacts with hydroxide ions to produce a compound that is no longer purple, but colorless. Thus, in a basic solution of crystal violet, the purple color will gradually fade to clear. The picture below demonstrates the reaction.

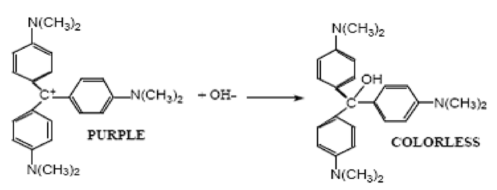
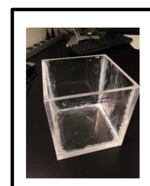


Image courtesy of Chem-ist-ry.us

Design for the flow regimes constructed in this laboratory were based on prior research in studies in both environmental textbooks and journals. [1] [2] In a real world setting, the batch reactor is commonly used in water treatment plants to treat groundwater and wastewater. Completely stirred reaction chambers are used to soften drinking water, which helps to prevent the clogging and deterioration of pipes. Plug-flow reactors help to manage acidity levels in a well controlled environment. The meandering river model represents a sinuous body of water like a river. Finally, the dispersion plates help to mimic the natural barriers in waterways, such as rocks.

Models



Batch Reactor: Closed container to react two products completely together until the reaction is complete or an equilibrium is reached.

Completely Stirred Reaction Chamber: Balanced inflow and outflow of products and reactants help to establish an equilibrium for any reaction.

Plug-Flow Reactor: Helps to demonstrate the reaction as it progresses through time and travels through the reactor. In our experiments, the tubes gradient from purple to clear.

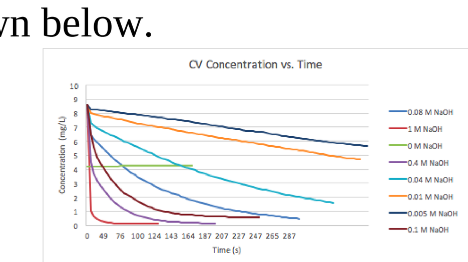
Meandering River: Demonstrates the kinetics of a real world waterway with curvature.

Dispersion Plates: Demonstrate the kinetics of a real world waterway with rocks, debris, or other obstacles that prevent an evenly distributed flow of water.

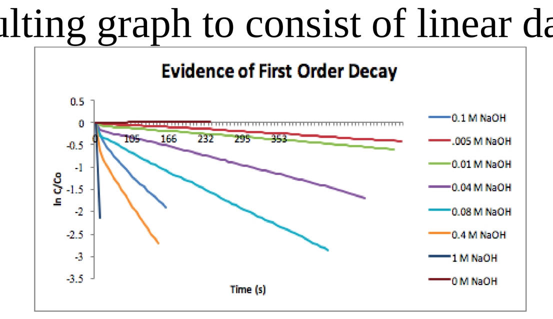
Experimentation, Data, and Graphs

Batch Reactor

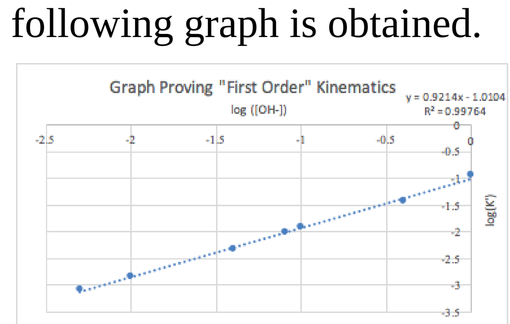
Several experiments were conducted in which NaOH of known concentration was mixed into crystal violet. The absorbance of the solution over time was recorded, and graphed a curve, as shown below.



In order to conclude that the reaction followed first order kinetics to make future mathematics simpler, $\ln[Cv_t]$ versus $\ln[Cv_t]/\ln[Cv_0]$ at various times t was graphed. If the reaction was first order we would expect the resulting graph to consist of linear data



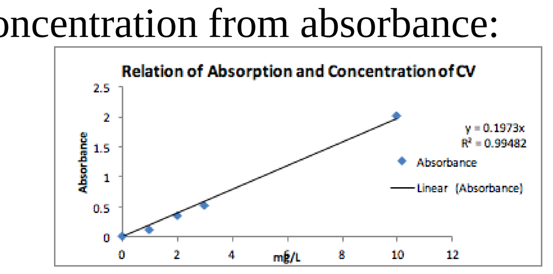
Since the reaction was determined to be first order, it can be modeled by the equation $(d_{CV})/(d_t) = -k[CV]^1[OH^-]^\beta$, where $-k[CV]^1$ is simplified as k'. When the $\log[OH^-]$ versus $\log[k']$ is recorded, the following graph is obtained.



From this graph, valuable information can be obtained regarding the reaction between crystal violet and hydroxide. The slope tells us that the reaction is to the .92nd order with respect to hydroxide (close to the theoretical 1st order), the y intercept is the logarithm of the rate constant, k, for the reaction.

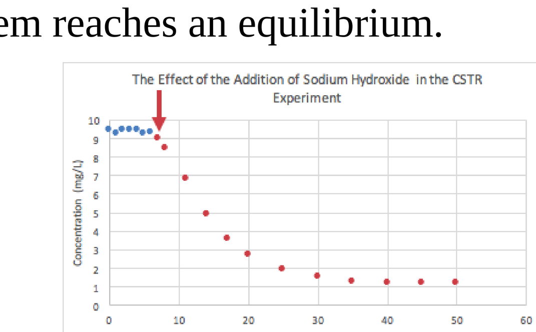
Absorbance and Concentration

Experimental data were obtained from the absorbance of the solution, which was then converted to [Cv] in mg/L. Prior to beginning experimentation, a standard model was constructed by measuring the absorbance of different concentrations of crystal violet to obtain an equation for solving for concentration from absorbance:



Completely Stirred Reaction Chamber (CSTR)

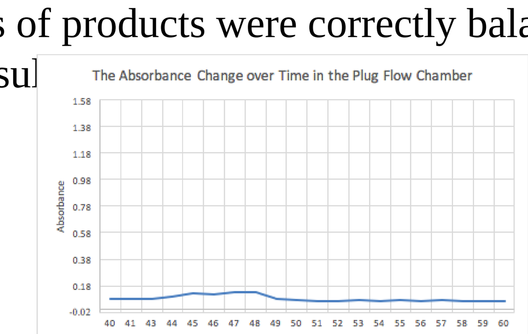
The next phase of experimentation was performed in a completely stirred reaction chamber, or CSTR. To illustrate the reaction of crystal violet and sodium hydroxide from the absorbance of the solution, the following graph was obtained, showing the absorbance of the solution in the CSTR over time. The red arrow indicates the time at which hydroxide was introduced. The rate of the reaction levels off eventually due to the reaction reaching what is known as the stable state, where the rate corresponds to the flow rate of the system, and thus the system reaches an equilibrium.



Plug-Flow Reaction Chamber

The plug flow reactor demonstrates a reaction at various stages in time. The reaction progresses as it moves through the reactor, producing a gradient from purple to clear color.

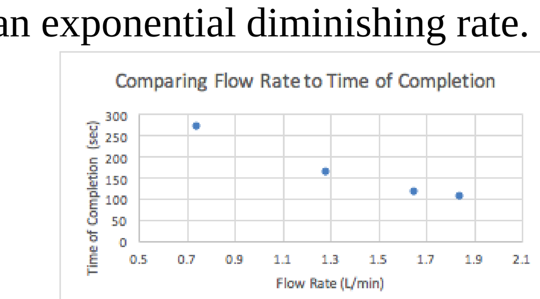
The end concentration of the plug flow, if the calculations were performed correctly, should hold at a stable state rate. The constant line shown below verifies that the reaction progressed at the predicted rate and that the concentrations and flow rates of products were correctly balanced produced the desired resul



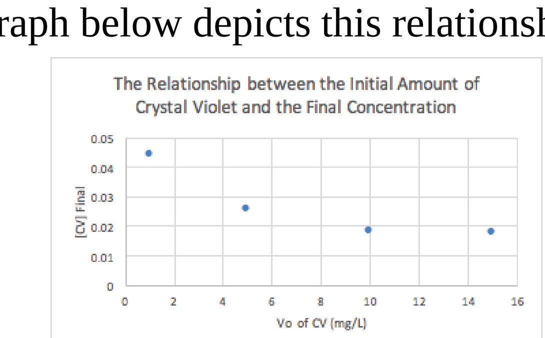
Meandering River System

With the meandering river, it was possible to demonstrate the effects of a sinuous waterway. For example, near the edges of such a path the water moves more slowly than in the middle, forming eddies.

The experiments showed that the slower the water moves, the more time it takes for the pollutant to be flushed. The graph below shows flow rate versus time to flush pollutant, and it is visible that this phenomenon occurs at an exponential diminishing rate.

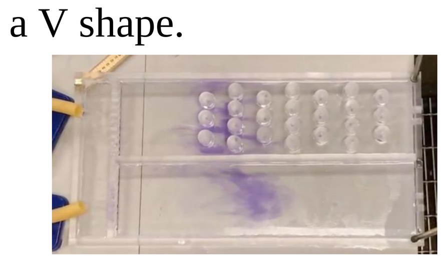


The experiments also compared the initial volume of crystal violet added to its final concentration and demonstrated that when the initial amount of crystal violet increases, the final concentration decreases. The graph below depicts this relationship.



Dispersion Plates

The final chamber was a two-sided tray that allowed water to flow down one side uninterrupted, and down the other through interchangeable plates with pegs on them. This mocked pollutant interference with obstacles. On the pegboard, it was found that the crystal violet dispersed in a normal distribution curve. On the obstacle-free plate, the crystal violet dispersed into a V shape.



Conclusions

From our experiments with the batch reactor, we are able to conclude that the reaction of crystal violet with hydroxide follows first order kinetics with respect to crystal violet, and to the .92nd order with respect to hydroxide. The CSTR chamber helped to confirm our mathematics by matching our predicted stable state for the system. The plug flow reactor helped to demonstrate the progression of the reaction over time. The meandering river and dispersion plates helped to demonstrate pollutant kinetics in natural waterway settings.

Through all of these flow regimes, the kinetics of pollutants can be thoroughly analyzed. By understanding how pollutants travel, scientists can be able to prevent, reduce, and remove chemicals that are harmful to the environment. Water sanitation plants use these models to eliminate dangerous minerals such as lead, and diseases from our drinking water.

There are innumerable ways to expand the studies into water pollutants. There are tens of thousands of miscellaneous chemicals that impact the environment and only a minuscule fraction of them have been fully understood. By creating general models that can apply to most of them, scientists are able to react sooner and prevent environmental devastation.

Acknowledgements

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