Dye Fading Kinetics Experiment

Obtain Kinetic Parameters from Dynamic Data
Introduction & Objectives

- Phenolphthalein desired to be used to find residence time of Industrial CSTR’s

- Temperature Range: 60 – 120 °F

- Find:
  - Order
  - Arrhenius constants
  - Activation Energy
  - Heat of Reaction
  - Equilibrium constant

\[ Ph + 2OH^- \rightarrow Ph^{2-} \] \hspace{1cm} \text{fast}
\[ Ph^{2-} + OH^- \leftrightarrow PhOH^{3-} \] \hspace{1cm} \text{slow}
Experimental Methods

- Experimental Apparatus

![Experimental Apparatus Diagram]

- Experimental Design
  - Isothermal Runs
  - Dynamic Temperature Runs
Theory

- **Reaction**
  \[ Ph^2^- + OH^- \leftrightarrow PhOH^3^- \]

- **Elementary reactions rates**
  \[ -\frac{d[Ph^2^-]}{dt} = -r = k_1[Ph^2^-][OH^-] - k_2[PhOH^{-3}] \]

- **Beer-Lambert’s Law**: relates the absorption of light to the properties of the material through which the light is travelling

---

Chen & Laidler, 1959

---

![Chemical structures](image-url)
The Traditional Approach

- Arrhenius Equation to find $E_a$ and $A$
  - $k = A \exp \frac{-E_a}{RT}$ or rearranged...
  - $\ln(k) = \frac{-E_a}{R} \frac{1}{T} + \ln(A)$
Calculate the Heat of Reaction

- Van’t Hoff Equation to find $\Delta H^o$
  \[ \ln \left( \frac{K_2}{K_1} \right) = \frac{-\Delta H^o}{R} \left( \frac{1}{T_2} - \frac{1}{T_1} \right) \]

- $\Delta H^o$ from $E_a$
  \[ \Delta H^o = E_{a(fwd)} - E_{a(rev)} \]
  - Exothermic: $-\Delta H^o$

http://image.tutorvista.com/cms/images/44/Acitvation%20enthalpy.JPG
Simulate Dynamics

- Graph 1: Temperature (K) vs. Time (min)
- Graph 2: Absorbance vs. Time (min)

- Temperature increases linearly with time.
- Absorbance decreases over time for both PhOH$_3^-$ and Ph$_2^-$.
Noise

T = 60°F

± ??
± 0.008
± 0.003
Results – Data Summary

- Isothermal runs
  - Equilibrium

For temperatures of 60°F and 110°F, absorbance over time is shown in the graphs.
Non-isothermal Runs

- No clear equilibrium
Estimate with Dynamic Data

- Solver required 34 Iterations
- Bounds on $E_a$ and exponents
- Solution Time: $< 1.0$ Second