ACS Spring National Meeting & Expo, 2020

Adsorption of Catechol/Hydroquinone on TiO_2 and Iron(III) Oxide

Kotaiba Abugazleh
Environmental Science Program

Motivation of Research

- The problem of environmental pollution is increasing and its impacts are touching down everywhere.
- Organic pollutants such as PCPs have many applications in human and industrial activities.

Impact of Environmental Pollution

Warmer, Warmer Everywhere

Nearly every region of the globe saw warmer than average temperatures last year.

LAND AND OCEAN TEMPERATURE PERCENTILES

Jan.-Dec. 2017

SOURCES: NOAA

InsideClimate News

Global water distribution

Source: U.S. Geological Survey Department of the Interior/USGS

Environmental Pollution

- Any undesirable change in physical, chemical, or biological characteristics of any component of the environment.
 - Water Pollution
 - Air Pollution

Objectives of Research

- Investigate adsorption characteristics of organic pollutants (Catechol, Hydroquinone) on the surface of adsorbents (Titanium dioxide, Iron oxides) in aqueous solutions.
- Test the effectiveness of Titanium dioxide (TiO_2) and Iron oxide (Fe_2O_3) as adsorbents for the Hydroquinone and Catechol as pollutants in aqueous solutions.

Spectroscopy Techniques used in this research

Thermo Scientific Nicolet 8700 FT-IR spectrometer

- Volatile chemicals.
- Separate complex mixtures.

Tested Pollutants

- **Catechol $C_6H_6O_2$**

- ☐ **Uses:**

- Photographic developer and fur/hair dyes.
- Pharmaceuticals and PCPs
- Antioxidant in perfumes.

- ☐ **Harmful effects**

- Severe skin burns.
- Hypertension.
- Animal carcinogen if swallowed.

- **Hydroquinone $C_6H_6O_2$**

- ☐ **Uses:**

- Skin bleaching agent, resin coating in cans.
- Intermediate to produce antioxidants for rubber and food.

- ☐ **Harmful effects**

- Enhance carcinogenic risk by generating DNA damage.
- Compromise immune system.

Tested Oxides

➤ Titanium Dioxide (TiO_2)

❑ Properties:

- High melting and boiling points.
- Insoluble in water.
- UV light resistance.
- Large Surface area.

Source: Huang et al.(2016) Promotional effect of the TiO_2 (001)

➤ Iron (III) oxide (Fe_2O_3)

❑ Properties:

- High melting and boiling points.
- Magnetic properties.
- Hardness and elastic.
- Large Surface area.

Source: www.webelements.com/

Equipment and Materials

- Thermo Nicolet 8700 Fourier-Transform Infrared Spectrometer (FT-IR) equipped with:
- ZnSe Attenuated Total-Reflection (ATR) crystal.
- HgCdTe (MCT) detector cooled by liquid nitrogen.

Calibration Data

Adsorption Equilibrium

- **Adsorption vs. Absorption**
- Adsorption is accumulation of molecules on a surface (a surface layer of molecules) in contact with a gas or water phase.
- Absorption is dissolution of molecules within a phase, e.g., within an organic phase in contact with an air or water phase.
- An adsorption isotherm is a curve explained by a q_e vs. C_e relationship at equilibrium.
- Adsorption isotherm can take multiple forms.

Adsorption Capacity

- To identify the maximum adsorption capacity of the oxide(TiO_2 , Fe_2O_3), the two most common adsorption isotherms, Freundlich and Langmuir isotherms, were fitted to data for both HQ and CAT.
- The isotherm with the highest combined R^2 was used as the isotherm that best represents the adsorption characteristics.

A) Freundlich

$$q_e = K_f C_e^{1/n}$$

- Heterogeneous surface.
- Assumes non-equivalent sites
- Very empirical
- Provides probability of adsorption

Freundlich linear form :

$$\log(q_e) = \log(K_f) + \frac{1}{n} \log(C_e)$$

B) Langmuir

$$q_e = \frac{b \cdot C_e \cdot Q_o}{1 + b C_e}$$

- Homogeneous surface.
- Assumes limited equivalent sites.
- Assumes monolayer coverage.
- Has a rational basis.

Langmuir linear form:

$$\frac{1}{q_e} = \frac{1}{Q_o} + \frac{1}{b Q_o C_e}$$

Adsorption Isotherm

R^2 Value				
	TiO ₂		Fe ₂ O ₃	
	Catechol	Hydroquinone	Catechol	Hydroquinone
Langmuir	0.94	0.91	0.68	0.06
Freundlich	0.47	0.92	0.98	0.95

Adsorption kinetics

	R^2 Value			
	TiO ₂		Fe ₂ O ₃	
	Catechol	Hydroquinone	Catechol	Hydroquinone
Pseudo first order	0.007	0.479	0.592	0.517
Pseudo second order	0.989	0.985	0.900	0.999
Elovich	0.334	0.365	0.6	0.517
Intra-particle	0.295	0.326	0.621	0.556

Adsorption pH

- Point of zero charge (pzc): The pH where the net total particle charge is zero is called the point of zero charge.

- Positive or negative charged surface of TiO₂ / Fe₂O₃ which determined by the solutions pH and their pH_{pzc}.

Conclusion

- Using Fe_2O_3 , CAT and HQ follow Freundlich isotherm, while using TiO_2 the Langmuir model was the best fit for CAT and HQ .
- This may be due to:
 - Position of OH and nature of ring influence binding mode on solid surface (geometry of CAT and HQ).
- TiO_2 is seen as a good adsorbent for Catechol and Hydroquinone (Langmuir adsorption isotherm), indicating a strong chemical binding to the surface, lending Cat /HQ ideal to be removed by TiO_2 from wastewater