



Selective Isolation of Toxins in Runoff Water Via Absorbent Cellulose Matrix Doped with Activated Carbon Black

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Purpose and Motivation

The motivation for our project stems from the problem of overflow of harmful nutrients into aquatic ecosystems. Runoff water from farms or large gardening facilities contains heavy amounts of nitrates. In excess, nitrates, combined with other nutrients, can cause nearby water sources such as lakes, ponds, and even segments of rivers to experience eutrophication, which hinders the sustenance of life. The proposed solution is to design a material that can selectively remove the nitrates from runoff before the contaminated water reaches a water source. The impact of this project is a potential increase in runoff cleanliness and environmental sustainability from farm areas.

Methodology

Our tasks separated into several parts:

- Define project purpose and scope
- Literature research of activated carbon black (ACB) and cellulose matrix
- Model ACB interaction with cellulose matrix
- Calculate and simulate various cellulose and ACB configurations
- Purchase supplies
- Synthesize prototype for testing
- Analyze data to determine design effectiveness

Why activated carbon black?

ACB has the ability to improve the surface mobility of natural organic matter that is found in runoff (1). It is used in water treatment and is specially suited to selectively remove nitrates and heavy metal ions from solution. Activity can be separated into three categories: adsorption, mechanical filtration, and ion exchange. Physical adsorption between the adsorbent and the adsorbate involves attraction via electrical charge differences, while chemical adsorption is the product of a reaction between them. Mechanical filtration involves the physical separation of suspended liquids from a liquid passing through carbon arrayed as a porous medium. Ion exchange is defined as a reversible chemical reaction between a solid and an aqueous solution that allows the interchange of ions.



Figure 1: Specifications from purchased Fisherbrand ACB

Modeling

Langmuir Isotherm

We used the Langmuir isotherm to predict the adsorbance of nitrates onto our ACB particles (equation 1). Q_m is the maximum sorbance limit of our ACB particles, K_L is the ACB constant of surface energy, C_e is the equilibrium concentration, and q is the equilibrium capacity of adsorption.

$$q = \frac{Q_m K_L C_e}{1 + K_L C_e} \quad (1)$$

The Langmuir isotherm is a scientific tool used to understand adsorption trends, and was a critical component of our calculations and analysis (figure 2).

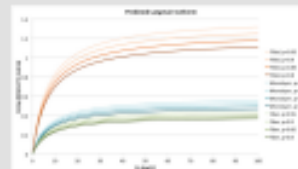


Figure 2: Predictions of the maximum adsorbance of nitrates onto our carbon black surface. Several different possible porosities are examined.

Calculations

The size of our carbon black particles was selected based on the sizes available for purchase and the size of our pores. Several scenarios were investigated for the possible adhesion of the carbon black molecules into the cellulose matrix. We focused on three scenarios:

- A perfect cube or a perfect sphere with a diameter of $300\mu\text{m}$ (figure 3). The ACB particles were assumed to fill the entire volume of the cellulose pore with maximum packing fraction.
- A perfect sphere with a diameter of $300\mu\text{m}$. The cubic pore shape was not considered for this scenario. Instead of filling the entire volume, the ACB particles were designed to create a monolayer on the internal surface of the cellulose pore, with a layer thickness of $50\mu\text{m}$.
- A wire frame cube with a side length of $300\mu\text{m}$ and an average fiber width of $40\mu\text{m}$ (figure 4). The ACB particles were designed to linearly fit on top of the inner surface of the fibers.

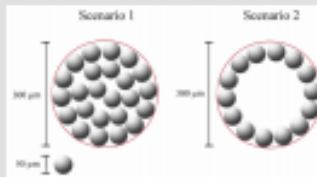


Figure 3: A perfect sphere filled with ACB (left) and a spherical monolayer of ACB (right)

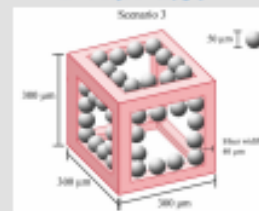


Figure 4: A wire frame cube with lined fibers

Table 1 - Comparison of Predicted Sorbance Parameters

	Scenario 1	Scenario 2	Scenario 3
P_1 (particle density)	20	90	70
R_p (pore diameter)	2.94×10^{-4}	9.67×10^{-4}	9.67×10^{-4}
Sub-volume ¹	1.13×10^{-23}	4.87×10^{-24}	3.83×10^{-24}
Max adsorbed nitrate for 1 liter of water ²	2.08E-11	1.89E-10	8.79E-10
Q_m (mg/g)	11.94E-19	8.58E-14	8.58E-12

Table 1: Comparison of our predictions for different adsorbance scenarios

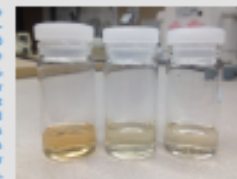
Final Results

The maximum number of ACB particles that can be adsorbed onto the internal surface of a single pore was calculated for the three scenarios (Table 1). The maximum adsorbance limit, Q_m , was calculated.

Results

Synthesis and Testing

The polymer matrix was created by mixing sawdust with poly(ethylene glycol) in acidic conditions, and baking the resulting mixture for 7 minutes at 130°C . Carbon black was mixed with CaCl_2 in order to positively charge the carbon black additive, so that when we add it to the polymer matrix for our final product, negative nitrate ions will be electronically attracted to the resulting mesh. The nitrate testing kit results (figure 5) show the amount of nitrate in the solution. A darker yellow color indicates the presence of nitrates in the solution.



In application, a $1\text{ m} \times 1\text{ m} \times 10\text{ cm}$ mat of our matrix could theoretically absorb all 2.125 g of the expected nitrates from runoff into the Potomac after a moderate rainstorm. To maintain ecosystem health, local nitrate conditions should be considered.

Conclusions

Our main design goals were to fabricate a novel filtration mat that is harmless to the environment and can filter out harmful pollutants such as phosphates, nitrates, and heavy metal ions. Due to feasibility considerations, our project scope narrowed to selective removal of nitrates. Extensive literature research suggests that ACB particles have not yet been used in conjunction with a cellulose matrix. There is still theoretical and experimental work to be done to verify the accuracy of our modeling assumptions; however, these assumptions allowed us to design a device that can filter out significant amounts of nitrate from runoff water (figure 6). Overall, we were successful in selecting appropriate materials for an environmentally friendly device, developing models for the adsorption mechanism of our device, and in determining predictive theories for the molecular interactions occurring between the cellulose and the ACB and between the nitrates and the ACB.

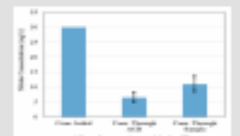


Figure 6: Graphical representation of nitrate testing results