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Abstract

This study investigates the adsorption of acetylsalicylic acid (ASA) using activated carbon, integrating Monte Carlo Bayesian modeling. Batch adsorption experiments examined the influence of adsorbent mass, contact time, and pH. Fixed-bed column studies evaluated feed-flow rate, adsorbent bed, and initial ASA concentration. The Monte Carlo Bayesian method was employed for parameter estimation and to enhance the understanding of adsorption mechanisms.

1 Introduction

The presence of pharmaceutical compounds, including acetylsalicylic acid (ASA), in water bodies is an environmental concern. Adsorption is a promising technique for removing these pollutants. This research combines batch adsorption experiments and fixed-bed column studies with Monte Carlo Bayesian modeling to evaluate and optimize ASA mitigation.

2 Materials and Methods

2.1 Batch Adsorption Experiments

Batch experiments were conducted using a design of experiments (DOE) to study the effects of pH, adsorbent mass, and contact time on ASA adsorption. The equilibrium adsorption quantity (q_e) was the response function.

2.2 Fixed-Bed Column Experiments

Fixed-bed column studies simulated continuous-flow conditions to assess the impact of feed-flow rate, adsorbent bed, and initial ASA concentration on adsorption performance.

2.3 Monte Carlo Bayesian Modeling

The Monte Carlo Bayesian method was used for parameter estimation and uncertainty analysis to improve the predictive capabilities of the adsorption process model.

3 Results and Discussion

3.1 Batch Adsorption

The batch adsorption experiments revealed the influence of pH, adsorbent mass, and contact time on ASA removal efficiency. The maximum ASA removal was observed around pH 7.

3.2 Fixed-Bed Column Studies

Fixed-bed column studies provided insights into the dynamic behavior of the adsorption process, including breakthrough curves and adsorption capacity.

3.3 Modeling Results

The efficiency of ASA adsorption achieved was 2.5 mg g^{-1}. The pseudo-first-order (PFO) kinetic model showed a lower Bayesian information criterion (BIC) value (113.72). The diffusion of the column bed (D_z) and the Langmuir constant (K_L) presented significant variation. The model effectively simulates breakthrough curves.

4 Conclusion

This study demonstrates the effectiveness of activated carbon for ASA removal and the utility of Monte Carlo Bayesian modeling for optimizing the adsorption process. The findings contribute to the development of efficient pharmaceutical removal methods and sustainable water resource management.

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