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**Multi-Scale Simulation for Contaminants Transport in Organic Enriched Water
Infiltration Process**

Thesis Booklet

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1. Introduction

Soil aquifer treatment (SAT) systems are emerging as effective solutions for wastewater treatment. They offer environmentally sustainable and cost-effective approaches to reduce pollutant levels in water resources. This study compares different soil types in SAT systems, examines infiltration rates, wetting and drying cycles, and pollutant interactions. It sheds light on how pollutants move through SAT systems. By using experiments, models, and statistics, it can provide new insights to improve SAT system design and operation for better pollutant removal.

2. Material and methods

Comprehensive investigations used to explore contaminants behavior in SAT systems under different aspects from filtrate media of soils, infiltration rate and operating conditions. Synthetic wastewater designed and prepared in the lab mirroring the real wastewater pollutant compositions as shown in table 1, also lab-scale columns were used to simulate real-world conditions and maintain controlled experiments.

Table 1 The chemical composition for the synthetic wastewater effluents

Chemicals	Mass (mg/1L)	Chemicals	Mass (mg/1L)
CH ₃ COONa.3H ₂ O	130	H ₃ BO ₃	2.65
NH ₄ Cl	100	CuSO ₄ .5H ₂ O	15
KH ₂ PO ₄	175	KI	15
MgSO ₄ .7H ₂ O	100	MnSO ₄ .4H ₂ O	15
CaCl ₂ .2H ₂ O	15	(NH ₄) ₆ Mo ₇ O ₂₄ .4H ₂ O	5
NaHCO ₃	200	ZnSO ₄ .7H ₂ O	15
KCl	35	CoCl ₂ .6 H ₂ O	15
EDTA	500	Yeast extract	200
FeCl ₃ .6H ₂ O	15	Peptone	200

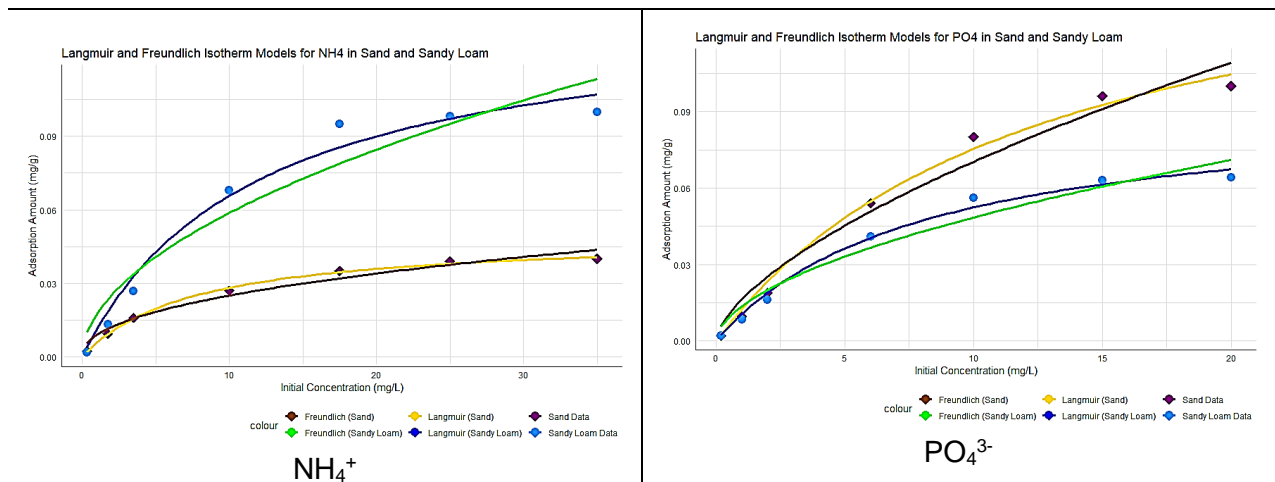
The methodology included selecting parameters such as filtrate media (Sand and Sandy loam) soils, infiltration rates (0.50 mL/min, and 10 mL/min), and operational conditions (wet and dry conditions) to provide a comprehensive and detailed understanding of how varying these conditions impact contaminants removal and transport processes from synthetic wastewater effluents through soil aquifer treatment system.

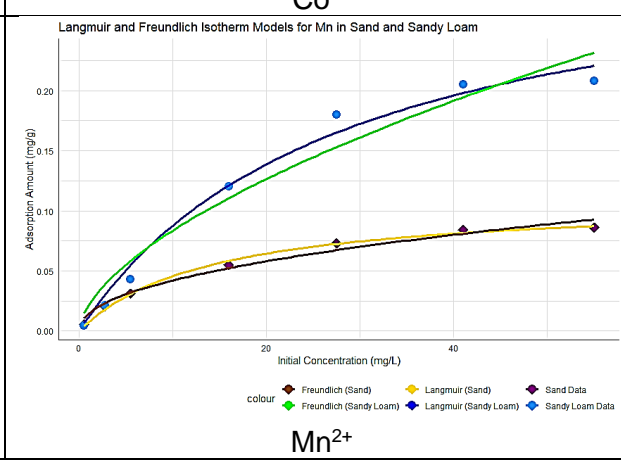
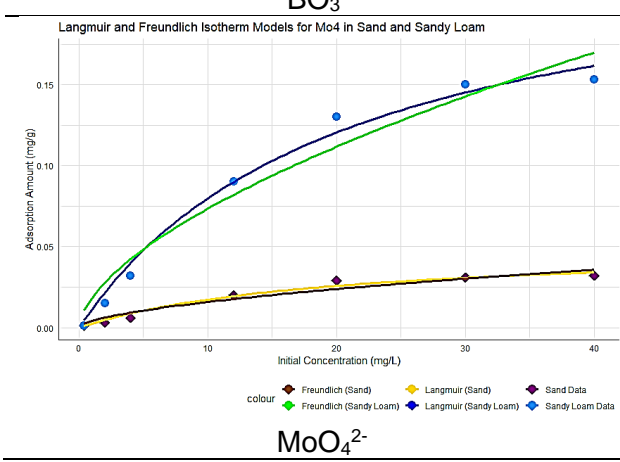
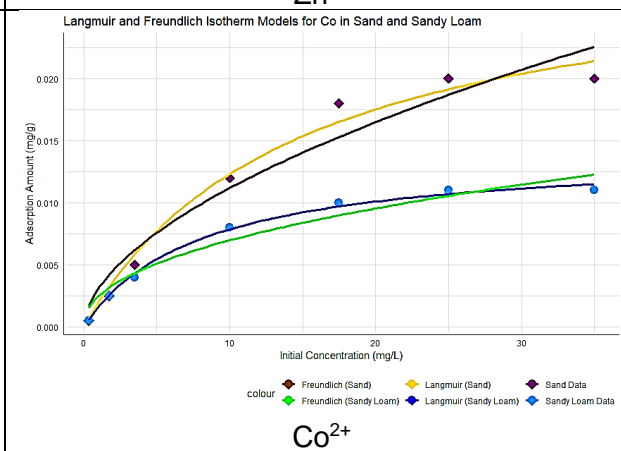
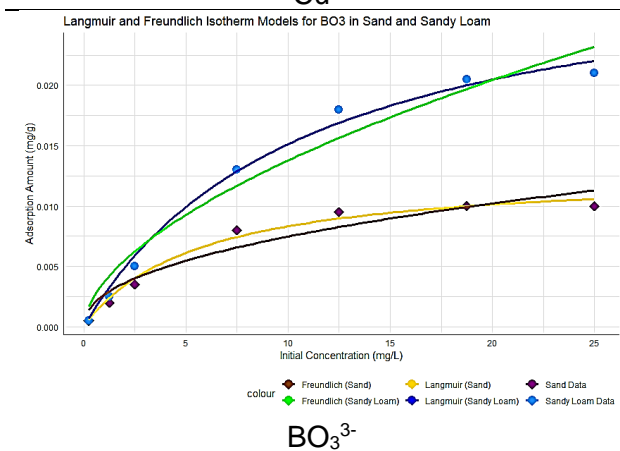
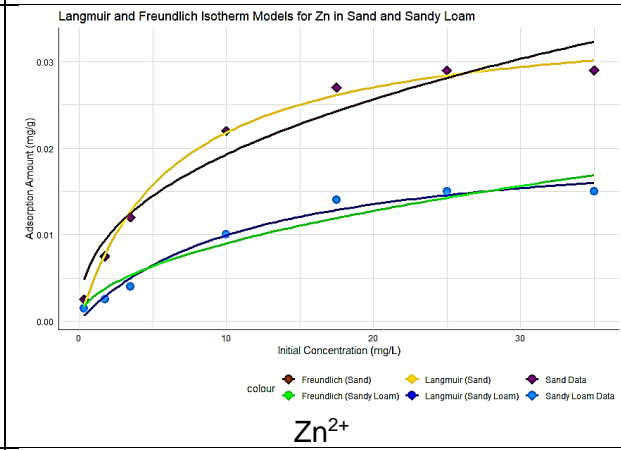
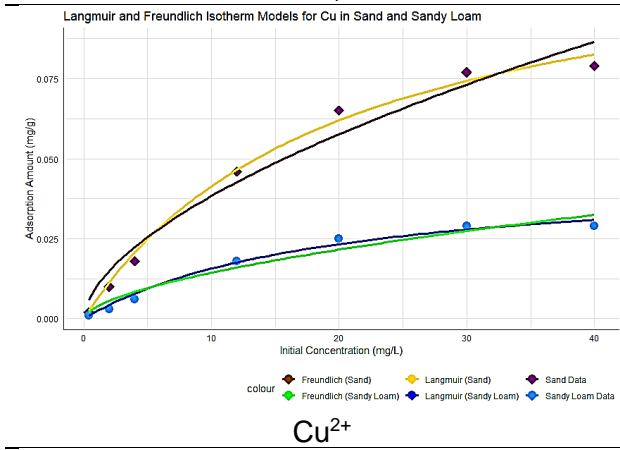
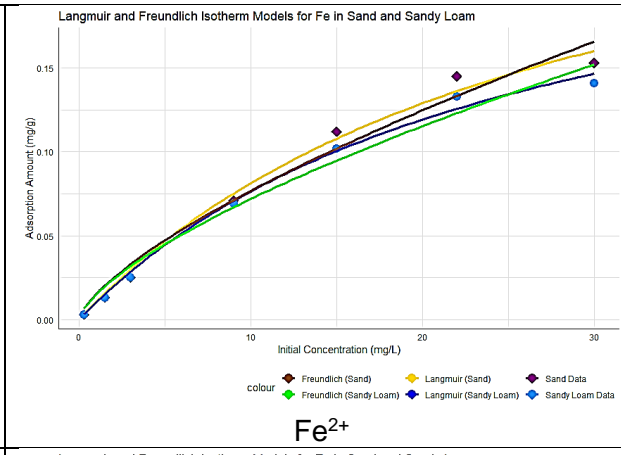
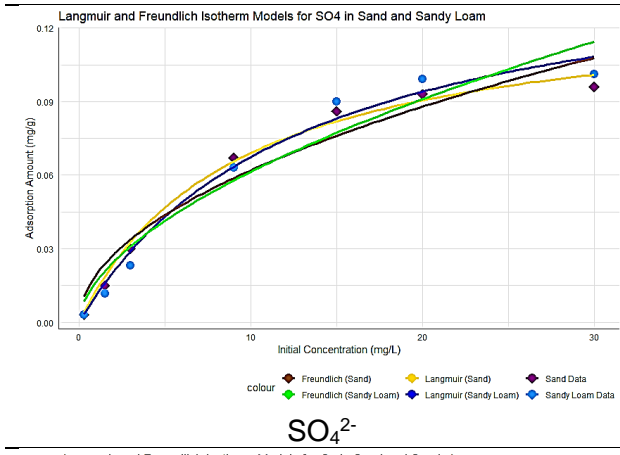
3. Comparative Investigation and Performance Evaluation of Different Soil Types in Enhancing Pollutants Removal from Synthetic Wastewater in Soil Aquifer Treatment System

This chapter presents a comprehensive analysis, combining static adsorption studies and dynamic column experiments, to offer a novel and detailed understanding of the performance of SAT systems using sand and sandy loam soils. This study significantly contributes to the understanding of how different soil types perform in SAT systems and offers practical insights for optimizing the design and operation of these systems based on specific environmental conditions and pollutant profiles. The ability to correlate the adsorption capacity with real-world pollutant retention and removal efficiency provides a robust framework for designing and improving SAT systems to achieve more effective wastewater treatment.

The comparative use of Freundlich and Langmuir isothermal models provided new insights into the adsorption characteristics of sand and sandy loam soils, as shown in Figure 1. The findings revealed that sandy loam generally has a higher adsorption capacity for certain pollutants, while sand excels in others. The preferential fit of the Langmuir model for sandy loam pollutants further emphasizes its effectiveness in characterizing adsorption behavior, contributing to the optimization of SAT systems based on soil type.

Figure 1 Freundlich and Langmuir isothermal models for synthetic wastewater pollutants in sand and sandy loam soils





The dynamic column experiments revealed significant differences in the removal efficiencies of various pollutants between sand and sandy loam soils. Sandy loam demonstrated superior removal capabilities for pollutants such as NH_4^+ , PO_4^{3-} , Cu^{2+} , Mn^{2+} , MoO_4^{2-} , Zn^{2+} , Co^{2+} , and BO_3^{3-} , with removal rates substantially higher than those observed in sand. Conversely, sand exhibited greater efficiency in removing NO_2^- , NO_3^- , SO_4^{2-} , and Fe^{2+} . This differential behavior underscores the need for a tailored approach in selecting soil media based on the specific pollutants present in SAT systems. Moreover, the application of breakthrough curve analysis to quantify the area under the curve (AUC) provided a comprehensive measure of the total pollutant removal. This approach allowed for the detailed assessment of the retention capacities and adsorption behaviors of the soils, revealing the intricate processes governing pollutant removal in SAT systems. The AUC calculations highlighted the dynamic performance of sand and sandy loam soils in real-world scenarios, demonstrating the utility of this method in evaluating and optimizing SAT system designs.

4. Understanding the Role of Infiltration Rate on Contaminants Fate and Transport in Soil Aquifer Treatment System: Experimental, Modeling, and Statistical Analysis Approaches

This chapter elucidates the role of infiltration rate in pollutant removal within SAT systems. It combines experimental data, modeling insights, and statistical analysis to present a comprehensive understanding of how varying infiltration rates impact pollutant behavior and removal efficiency.

Infiltration rate significantly affects the transport and removal of various pollutants. A lower infiltration rate (0.5 mL/min) enhances pollutant removal through increased contact time with the sand media, leading to higher adsorption and more efficient biogeochemical reactions. In contrast, a higher infiltration rate (10 mL/min) reduces contact time, resulting in less effective pollutant removal and higher effluent concentrations. By identifying how different pollutants respond to changes in infiltration rate, NH_4^+ , PO_4^{3-} , SO_4^{2-} , Fe^{2+} , Mn^{2+} , MoO_4^{2-} , Zn^{2+} , and Co^{2+} these pollutants show significantly better removal at the lower infiltration rate. However, NO_3^- , NO_2^- , Cu^{2+} , and BO_3^{3-} these pollutants exhibit higher removal at the higher infiltration rate, suggesting that specific conditions may benefit their removal.

The detailed experimental breakthrough curves demonstrate clear trends in pollutant removal efficiency under different infiltration rates. The findings confirm that a slower infiltration rate generally leads to better removal due to extended contact time.

The 2-D spatial concentration distributions and breakthrough curve modeling support the experimental observations. Models effectively capture pollutant behavior over time and depth, reinforcing the experimental results and providing a visual representation of pollutant transport dynamics.

The statistical analysis using t-tests provides quantitative evidence of the impact of infiltration rate on pollutant removal. The p-values reveal statistically significant differences in pollutant concentrations between the two infiltration rates, validating the experimental and modeling results.

The chapter findings highlight the importance of customizing infiltration rates based on specific pollutants to optimize removal efficiency. This approach allows for tailored SAT system operation, potentially improving treatment performance for diverse wastewater compositions.

5. Quantifying the influence of dynamic pulsed of wetting and drying on the transformation and fate of synthetic wastewater pollutants in soil aquifer treatment system

This chapter explains the complex interactions between wetting and drying cycles and pollutant dynamics in SAT systems. The findings contribute to a deeper understanding of pollutant removal processes and offer valuable insights for optimizing system design and operation.

The impact of wetting and drying cycles on the overall performance of the SAT system as a nature cyclic based on seasonal variation, these conditions leads to fluctuations in pollutant removal efficiency, affecting treatment performance and the physical properties of the sand column.

The use of robust statistical analysis, including logistic regression models, correlation studies and factorial interaction trends, provides a detailed understanding of the relationships between pollutants and environmental factors. This approach offers new perspectives on how these factors collectively impact pollutant behavior and treatment efficacy.

pH, Dissolved Oxygen (DO), and Oxidation-Reduction Potential (ORP) factors interact with wetting and drying cycles to influence pollutant removal. Strong correlations and interactions between these factors and pollutant concentrations highlight their pivotal role in the treatment process.

NH_4^+ concentrations increase during wet periods due to enhanced leaching but are more effectively removed during dry periods through adsorption and potential microbial

processes. This highlights the critical role of drying phases in improving NH_4^+ removal efficiency.

NO_2^- concentrations are lower during wet periods due to limited nitrification, whereas NO_3^- concentrations show varied responses influenced by DO, pH, and ORP. This underscores the differential behavior of nitrogen species under varying wetting conditions.

Variability in SO_4^{2-} concentrations with respect to wet and dry cycles and their association with environmental factors such as pH and ORP provides new insights into the complexities of sulfate dynamics in SAT systems.

Increased PO_4^{3-} concentrations with higher DO, pH, and ORP, and more effective removal during dry periods, illustrate the importance of environmental conditions in phosphate management.

Fe^{2+} , Cu^{2+} , Mn^{2+} , MoO_4^{2-} , Zn^{2+} , and Co^{2+} specific patterns in the transport and removal of these metal ions, with wet conditions generally favoring lower concentrations. Each metal ion exhibits distinct correlations with DO, ORP, and pH, indicating their unique responses to environmental conditions.

A unique flocculation pattern in BO_3^{3-} concentrations, with higher levels during wet periods due to leaching and dissolution. This finding suggests complex interactions between BO_3^{3-} adsorption, precipitation, and desorption processes.

In summary, wetting and drying cycles emerge as critical determinants in the fate, transport, and treatment of infiltrated wastewater pollutants in the sand column. Recognizing and incorporating these cycles into system design and operation protocols is paramount for achieving and maintaining optimal system efficiency.

6. Conclusion

This thesis has advanced our understanding of soil aquifer treatment (SAT) systems and their efficacy in removing pollutants from wastewater. Through comprehensive investigations into the static adsorption behavior, dynamic breakthrough curve analysis, influence of infiltration rates, wetting and drying cycles, and synergistic and competitive pollutant interactions, key insights have been gleaned to inform system optimization strategies. The integration of experimental, modeling, and statistical approaches has facilitated a comprehensive assessment of pollutant behavior in SAT systems, highlighting the importance of tailored design considerations and management practices. Moving forward, these findings will contribute to the development of sustainable wastewater treatment solutions, safeguarding sustainable water resources.

7. New Scientific Results

This study presents insights into the performance of soil aquifer treatment systems by comparing the adsorption, affinities and pollutant removal capabilities of sand and sandy loam soils. Through a combination of static adsorption studies and dynamic column experiments, it was found that sandy loam generally exhibited higher adsorption capacities for pollutants like NH_4^+ , PO_4^{3-} , and heavy metals, while sand was more efficient in removing NO_2^- , NO_3^- , SO_4^{2-} , and Fe^{2+} . The research utilized Freundlich and Langmuir isotherms to characterize the adsorption and affinities behaviour for soils, with the Langmuir model showing a better fit for sandy loam. Breakthrough curve analysis provided a quantitative measure of pollutant retention, offering practical guidance for optimizing SAT system designs based on specific soil types and pollutant profiles.

The infiltration flow rate plays a critical role in pollutant removal efficiency within SAT systems. A lower infiltration rate (0.5 mL/min) significantly enhances the removal of pollutants like NH_4^+ , PO_4^{3-} , and heavy metals due to increased contact time leading to higher adsorption and more efficient biogeochemical reactions, while a higher rate (10 mL/min) improves the removal of pollutants like NO_3^- and NO_2^- . Experimental data, breakthrough curve modeling, and statistical analysis confirm these patterns, providing a clear understanding that optimizing infiltration rates based on specific pollutants can enhance SAT system performance.

The significant impact of wetting and drying cycles on pollutant behavior in SAT systems. Wet periods increase NH_4^+ leaching, while dry periods enhance NH_4^+ removal through adsorption and microbial processes. Nitrogen species (NO_2^- and NO_3^-) respond differently to wet and dry conditions, influenced by pH, DO, and ORP. Metal ions like Fe^{2+} , Cu^{2+} , and Zn^{2+} show lower concentrations during wet periods due to varied interactions with environmental factors, while PO_4^{3-} removal is more effective during dry phases. The study highlights the importance of accounting for these cycles in system design to optimize wastewater treatment.