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

Thesis Booklet

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Contents

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 1The chemical composition for the synthetic wastewater effluents

Chemicals	Mass (mg/1L)	Chemicals	Mass (mg/1L)
$CH_3COONa.3H_2O$	130	H_3BO_3	2.65
NH_4Cl	100	$CuSO_4.5H_2O$	15
KH_2PO_4	175	KI	15
$MgSO_4 \cdot 7H_2O$	100	$MnSO_4.4H_2O$	15
$CaCl_2 \cdot 2H_2O$	15	$(NH_4)6Mo_7O_{24}.4H_2O$	5
$NaHCO_3$	200	$ZnSO_4.7H_2O$	15
KCl	35	$CoCl_2.6\ H_2O$	15
EDTA	500	Yeast extract	200
$FeCl_3.6H_2O$	15	Peptone	200

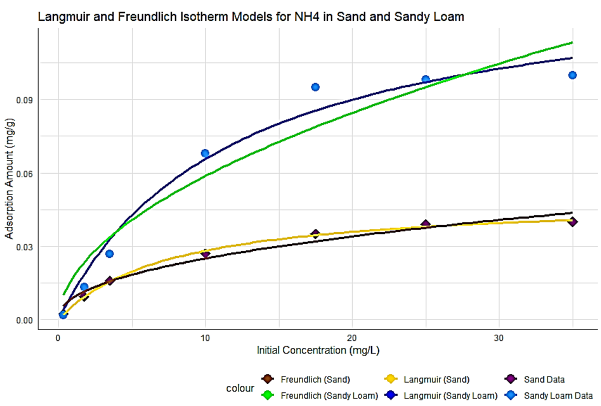
The methodology included selecting parameters such as filtrate media (Sand and Sandy loam) soils, infiltration rates (0.50 mL/min, and 10 mL/min), and operational conditions (wet and dry conditions) to provide a comprehensive and detailed understanding of how varying these conditions impact contaminants 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**

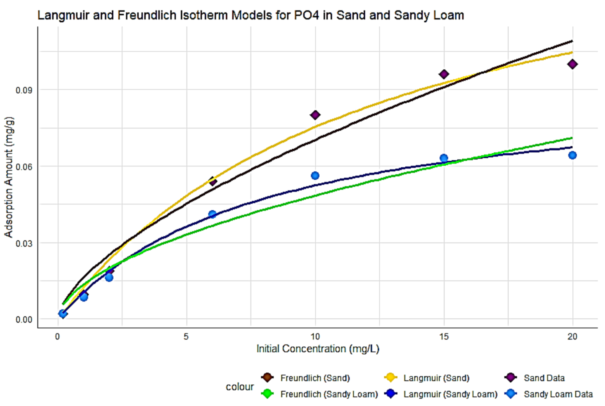
This chapter present comprehensive analysis, combining static adsorption studies and dynamic column experiments, offers a novel and detailed understanding of the performance of SAT systems using sand and sandy loam soils for significantly contribute to the understanding of how different soil types perform in SAT systems and offer 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.

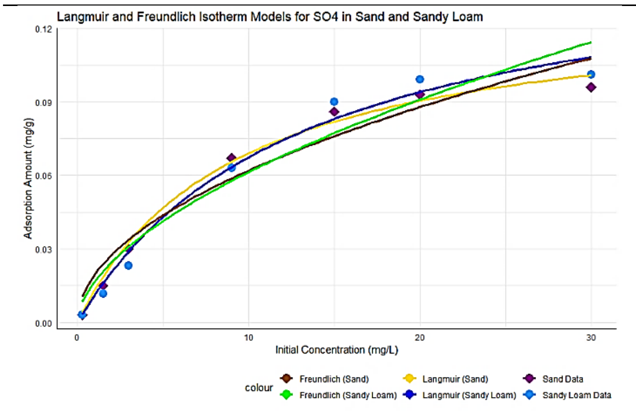
Figure 1Freundlich and Langmuir isothermal models for synthetic wastewater pollutants in sand and sandy loam soils



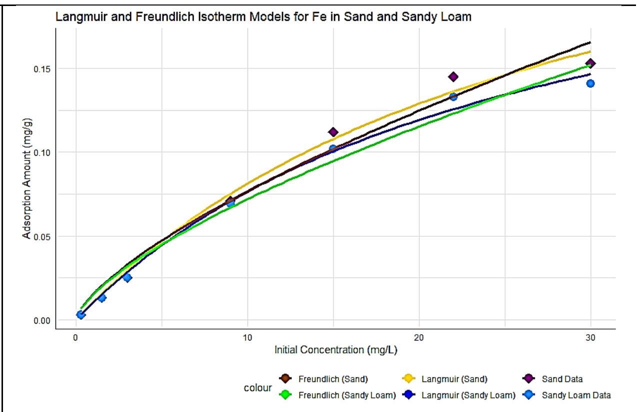
NH_4^+



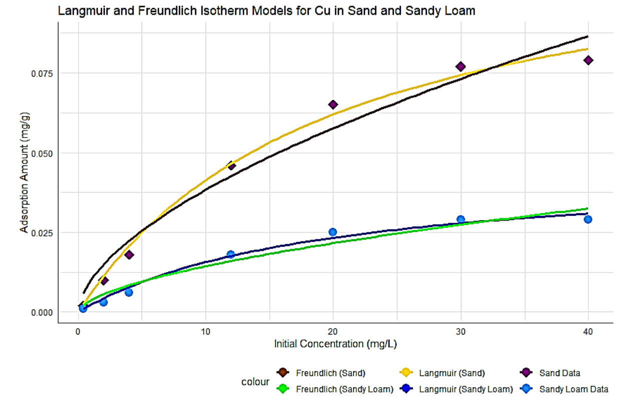
PO_4^{3-}



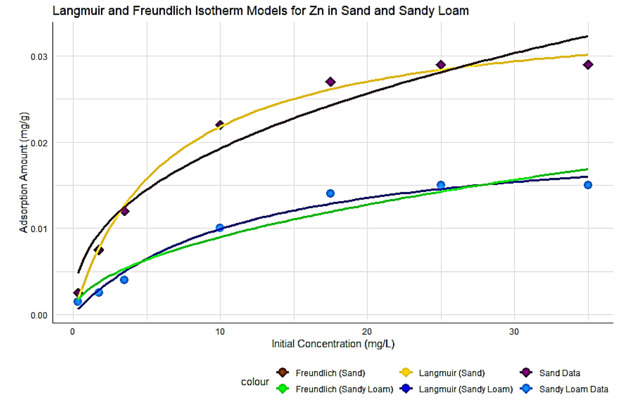
SO_4^{2-}



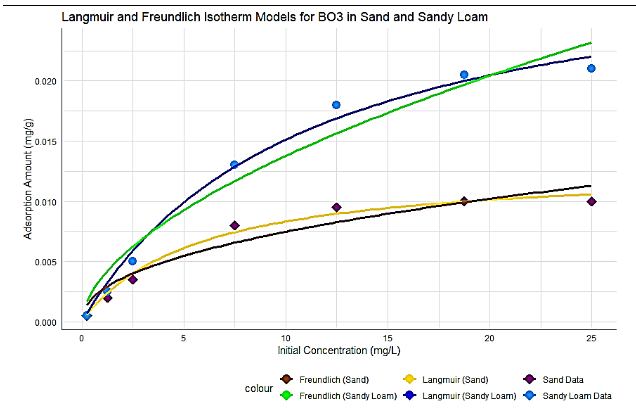
Fe^{2+}



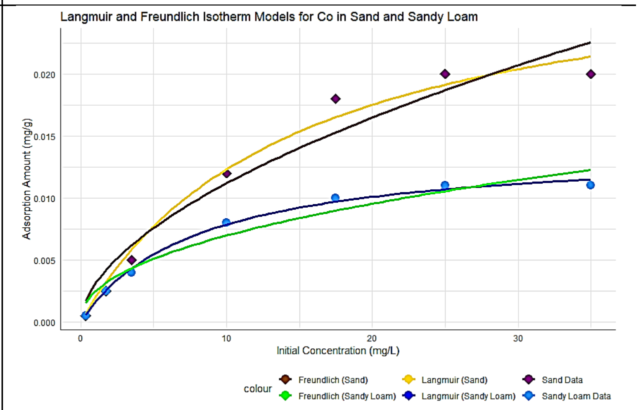
Cu^{2+}



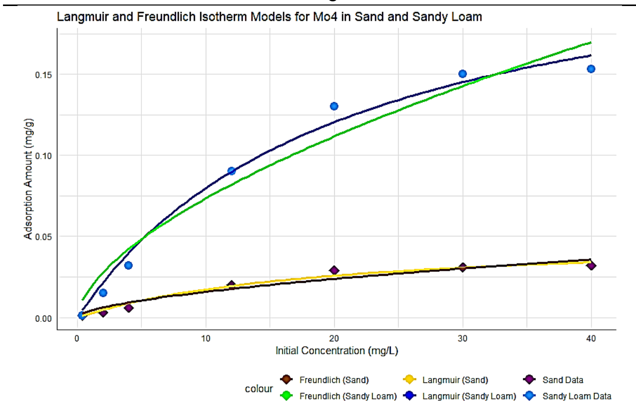
Zn^{2+}



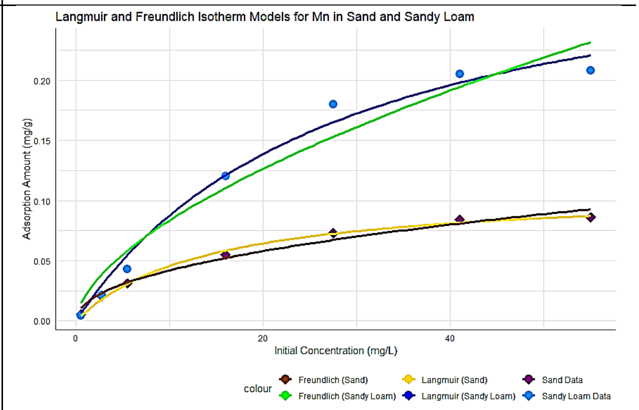
BO_3^{3-}



Co^{2+}



MoO_4^{2-}



Mn^{2+}

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

Thesis 1. Comparative soil types in pollutant removal for SAT systems

I used two methods in comparing the performance of sand and sandy loam soils in removing pollutants, while also assessing the scalability of the results based on SAT system considerations. The first method involved the isothermal adsorption technique, which was used to study the static and equilibrium conditions between infiltrated pollutants and the soil particle matrix. The second method simulated real-world SAT systems through dynamic column investigations. All laboratory investigations aimed to quantify the effect of the infiltrate media and soil selection on SAT system performance.

The comparative analysis of soil adsorption performance using Freundlich and Langmuir isothermal models provided new insights in to the adsorption processes relevant to SAT systems, particularly regarding the adsorption characteristics and pollutant affinities of sand and sandy loam soils. Freundlich accommodates heterogeneous surfaces, while Langmuir provides insights into monolayer adsorption, covering a broad spectrum of adsorption behaviors. The findings revealed that sandy loam generally has a higher adsorption capacity for pollutants due to its higher organic matter content and greater pollutant affinity intensity.

Dynamic column experiments simulating real-world scenarios of partially treated wastewater infiltration revealed significant differences in the removal efficiencies of various pollutants between sand and sandy loam soils. These differences are attributed to variations in soil characteristics such as texture, structure, porosity, pH, and organic matter content. 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. However, sand exhibited greater efficiency in removing NO_2^-, NO_3^-, SO_4^{2-}, and Fe^{2+}.

The area under breakthrough curve (AUC) calculations highlighted the dynamic pollutant removal performance of sand and sandy loam soils in real-world scenarios. This method demonstrates its utility in evaluating the performance of SAT systems, providing a practical measurable index for assessing SAT performance based on specific soil types and pollutant profiles.

Thesis 2. Infiltration rate impact on pollutants transport in SAT systems

The infiltration rate significantly influences the transport, retention and removal of various pollutants. A lower infiltration rate (0.5 mL/min) enhances pollutant removal by increasing contact time with the sand medium particles matrix, facilitating higher adsorption and more efficient biogeochemical reactions due to prolonged interaction between pollutants and the microbial community within the system. In contrast, a higher infiltration rate (10 mL/min) reduces contact time, resulting in less effective pollutant removal and higher effluent concentrations.

Understanding how different pollutants respond to changes in infiltration rate reveals significant variations in their removal efficiencies. Pollutants such as NH_4^+, PO_4^{3-}, SO_4^{2-}, Fe^{2+}, Mn^{2+}, MoO_4^{2-}, Zn^{2+}, Cu^{2+} and Co^{2+} exhibit significantly better removal at the slower infiltration rate due to enhanced adsorption and microbial degradation interactions. However, pollutants such as NO_3^-, NO_2^-, and BO_3^{3-} show higher removal at the higher infiltration rate likely due to reduced production rates, particularly for nitrogen species. These findings suggest that specific conditions tailored to the pollutant profile may optimize removal processes.

The two-dimensional spatial concentration distributions and breakthrough curve modeling, developed using random walk technique, represent an innovative approach that effectively simulates particle dispersion and advection in porous media. This method demonstrates high efficiency and accuracy, particularly under conditions with steep pollutant gradients, making it a valuable tool for modeling dynamic contaminant transport plumes in SAT systems. The developed models calibrated with experimental observations by accurately capturing pollutant behavior over time and depth. These models reinforce experimental results and provide a visual representation of pollutant transport dynamics while characterizing key transport parameters. Capillary diffusivity, which drives solute movement in unsaturated soils, surpasses molecular diffusion and dispersion in dominance, especially under low infiltration rates where it enhances adsorption and retention.

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.

Thesis 3. Impact of pulsed wetting and drying on pollutant fate in SAT systems

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

The use of robust statistical analysis, including logistic regression models, correlation trends and factorial interaction analysis as an innovation framework to validate and track the geochemical interactions, provides a detailed understanding of the relationships between pollutants and climatical and operational 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.

Nitrogen species (NH_4^+, NO_2^-, and NO_3^-) exhibit dynamic behaviors during wet and dry periods in the SAT system. NH_4^+ concentrations increase during wet periods due to enhanced leaching but are more effectively removed during dry phases through adsorption and nitrification potential microbial processes, highlighting the critical role of drying in improving NH_4^+ removal efficiency. In contrast, NO_2^- concentrations are lower during wet periods due to limited nitrification, while NO_3^- concentrations show varied responses influenced by DO, pH, and ORP, underscoring the differential behavior of nitrogen species under fluctuating wetting conditions.

Increased PO_4^{3-} concentrations during wet periods, associated with higher DO, pH, and ORP interactions, and more effective removal during dry periods due to immobilization and geochemical reactions, highlight the importance of wet/dry conditions in phosphate management. Meanwhile, The variability in SO_4^{2-} concentrations during wetting and drying cycles, influenced by wet/dry factors such as pH and ORP, provides new insights into the complexities of sulfate dynamics in SAT systems.

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 influencing the oxidation or precipitation of these metals, indicating their unique responses to wet/dry conditions. In contrast, BO_3^{3-} concentrations display a distinct fluctuation pattern, 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.

8. Author Individual Scientific Works

Journal papers

Gharbia, A.S., Zákányi, B. & Tóth, M. Impact of sand media continuous drying and rewetting cyclic on nutrients transformation performance from reclaimed wastewater

effluent at soil aquifer treatment. Sci Rep 14, 8065 (2024). https://doi.org/10.1038/s41598-024-58787-0

Gharbia, A. S., Zákányi, B., & Tóth, M. (2022). Experimental and numerical study for the adsorption behavior of Cu (II) and Mn (II) in quartz sand. Sustainable Water Resources Management, 8(5), 1-9. https://doi.org/10.1007/s40899-022-00725-x

Abdalkarim S. Gharbia, Salem S. Gharbia, Hassan Tamous, Thaer Abushbak, Balázs Zákányi, Márton Tóth,. (2021). Optimization modeling for the use of antiscalants in the brackish RO desalination plants. Desalination and Water Treatment, 224 (2021) 12–20. doi: 10.5004/dwt.2021.27176

Conferences papers

Gharbia, A. S., Zákányi, B., & Tóth, M. (2023). Manganese and Cobalt Metals Interrelations With Ammonium Performance In Soil Aquifer Treatment. Young Scientist 2023 Slovakia conference. Web of Conferences. http://dx.doi.org/10.1051/matecconf/202338501008

Abdalkarim S. Gharbia, Viktória Mikita, Balázs Zákányi, Márton Tóth (2023). IMPACTS OF SHORT-TERM CONTINUOUS DRYING AND REWETTING CYCLES ON NITRATE (NO3-) AND PHOSPHATE (PO43-) BEHAVIOR IN SOIL AQUIFER TREATMENT OF INFILTRATED WASTEWATER. URBAN WATER 2023 conference, VELKÉ BÍLOVICE, Czech Republic. (Book ISBN: 978-80-86020-97-6) pages 256-263.

Abdalkarim S. Gharbia, Balázs Zákányi, Márton Tóth (2023). OPTIMIZING PHOSPHATE REMOVAL BY MANIPULATING MANGANESE AND COBALT LEVELS IN SOIL AQUIFER TREATMENT SYSTEM. MultiScience - XXXVI. microCAD International Multidisciplinary 2023 conference, University of Miskolc, Hungary.

Abdalkarim S. Gharbia, Balázs Zákányi, Márton Tóth. EQUILIBRIUM ADSORPTION MODELING FOR TERNARY MULTI-METALS IN THE CLAY SOIL. Műszaki Földtudományi Kar MFK conference volume titled the New results in earth and environmental science, University of Miskolc (2022) pp. 291-298.

Abdalkarim S. Gharbia, Balázs Zákányi, Márton Tóth. EXPERIMENTAL AND NUMERICAL STUDIES FOR THE ADSORPTION BEHAVIOR Cu(II) AND Zn(II) IONS ON A FIXED CLAY BED. In: Szigyártó, Irma-Lídia; Szikszai, Attila (eds.) XVII. Kárpát-medencei Környezettudományi Konferencia = 17th Carpathian Basin Conference for Environmental Sciences, konferenciakötet = conference proceedings, Cluj-Napoca, Romania: Ábel Kiadó (2022) pp. 220-226. , 7 p. Scientific

Márton Tóth, Balázs Kovács, Imre Czinkota, Abdalkarim S. Gharbia, Noémi Szász, István Székely. INVESTIGATION OF SELECTIVE DYNAMIC ADSORPTION OF SCANDIUM ON CH COLLECTOR. Műszaki Földtudományi Kar MFK conference volume titled the New results in earth and environmental science, University of Miskolc (2022) pp. 299-304

Conferences presentations

Optimizing Phosphate Removal By Manipulating Manganese and Cobalt Levels in Soil Aquifer Treatment System, MultiScience - XXXVI. microCAD International Multidisciplinary 2023 conference, University of Miskolc, Hungary. 12th – 13th October, 2023.

Impacts of Short-Term Continuous Drying and Rewetting Cycles on Nitrate (NO3-) and Phosphate (PO43-) Behavior in Soil Aquifer Treatment of Infiltrated Wastewater, URBAN WATER 2023 conference, VELKÉ BÍLOVICE, Czech Republic. 4th – 6th October, 2023.

Manganese and Cobalt Metals Interrelations with Ammonium Performance in Soil Aquifer Treatment, 1st V4 Meeting of Circular Wastewater Management in conditions of 4 countries: concepts, approaches and technologies, Slovakia, 28th – 31th March 2023.

pH Impact on The Cu (II) Adsorption Behavior in The Quartz Sand, 5th SADC Groundwater Conference. GROUNDWATER: MAKING THE INVISIBLE VISIBLE FOR SOCIO-ECONOMIC DEVELOPMENT, Hybrid conference, 16th - 18th of November 2022.

Adsorption and Desorption Competitive Mechanism for Binary Heavy Metals in Quartz Sand, MultiScience - XXXV. microCAD International Multidisciplinary Scientific Conference, theme: Modern Materials Science and Engineering, conference, 13th – 14th of October 2022.

Simulation of Heavy Metals Fate in Quartz Sand Bed Column, 49th IAH Congress (The International Association of Hydrogeologists). Groundwater Sustainability and Poverty Reduction, theme: Managed aquifer Recharge, online conference, 19th - 22nd of September 2022.

Experimental and Numerical Study for the Adsorption Behavior of Cu (II) and Mn (II) in Quartz Sand, 4th SADC Groundwater Conference. THEME: Towards a Water Resilient SADC-Groundwater Systems Thinking, Virtual conference, 10th - 12th of November 2021.

Adsorption and mobility fate of copper Cu (II) in the quartz sand, Faculty of Earth Science and Engineering PhD Forum, University of Miskolc, 18th of November 2021.