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COMPUTATIONAL MODELLING AND DIGITAL TWINS

Exploring the Circular Economy Potential of the ASPIRE Method: A Numerical Study on Copper Ion Trapping

This study explores the Accelerated Supergene Processes in Repository Engineering (ASPIRE) concept for long-term trapping of copper ions from contaminated water using numerical simulations. The ASPIRE method offers a sustainable approach to water remediation and resource recovery through permeable reactive barriers. A numerical framework, based on unsaturated soil mechanics and reactive transport, is presented, considering water flow, copper ion transport, adsorption, and precipitation. A case study evaluates the ASPIRE concept's performance over a 5-year period, demonstrating the system's effectiveness in capturing approximately 45,000 kg of copper. Adsorption and precipitation mechanisms contribute to the enrichment process. The study highlights the importance of monitoring and maintenance to address potential challenges like clogging. The findings support the feasibility of the ASPIRE concept as a promising approach for simultaneous water remediation and resource recovery, aligning with circular economy principles.

Keywords:

ASPIRE concept, copper ion trapping, permeable reactive barriers, numerical simulation, circular economy.

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INTRODUCTION

The treatment of contaminated wastewater is a critical environmental challenge that requires effective remediation methods. While numerous techniques have been developed to address this issue, the focus has primarily been on purifying wastewater sources by removing contaminants. However, a novel approach known as the accelerated supergene processes in repository Engineering (ASPIRE) method [1–3] at the same time, they must sustainably manage continued multimillion tonne annual arisings of mineral-dominated wastes from mining and industry. In an antithesis of circular economy principles, these wastes continue to be landfilled despite often comprising valuable components, such as critical metals, soil macronutrients and mineral components which sequester atmospheric carbon dioxide (CO₂), shifts the paradigm by emphasizing the enrichment of valuable metal materials in contaminated water for potential future utilization.

In contrast to conventional methods like “Pump and Treat,” which can be energy-intensive and limited in scale, the ASPIRE method offers a more sustainable and passive approach through the use of permeable reactive barriers (PRBs). PRBs have been extensively studied for their efficacy in removing specific contaminants from groundwater, mine drainage, etc., showcasing their potential in environmental remediation. The unique advantage of the ASPIRE method lies in its dual functionality of purifying wastewater and concentrating valuable metals, aligning with the principles of a circular economy by promoting resource recovery.

Before real-world implementation, it is crucial to evaluate the ASPIRE concept's feasibility and potential outcomes through numerical simulations. This study aims to investigate the ASPIRE concept's capabilities, providing valuable insights for further development and decision-making.

THE NUMERICAL FRAMEWORK

In this section, the governing equations of the numerical framework that describe the transport of liquid and ionic species within the trapping area are presented.

Wastewater flow

In practical implementations, the ASPIRE concept's capture zone may experience unsaturated conditions due to its interaction with the surrounding environment. To properly describe wastewater flow in this context, we employed the theory of unsaturated soil mechanics [4] in our numerical simulations.

$$S_r \rho_w \frac{\partial n}{\partial t} - \frac{n C_m}{g} \frac{\partial s}{\partial t} + n S_r \frac{\partial \rho_w}{\partial t} - \nabla \cdot (n S_r D_w) \nabla \rho_w + \nabla \cdot (\rho_w v_w) = 0 \quad (1)$$

where S_r (-) is the saturation, ρ_w (kg·m⁻³) is the wastewater density, n (-) is the porosity, t (s) is the time, C_m (m⁻¹) is the specific liquid wastewater capacity, g (m·s⁻²) is the gravity acceleration, s (Pa) is the total suction, D_w (m²·s⁻¹) is the wastewater diffusivity.

The Darcy type flow is used for the description of solution flow in the unsaturated trap porous material by considering the driving forces of suction and gravity:

$$v_w = \frac{\kappa \cdot \kappa_{rw}}{\mu_w} \nabla (s + \rho_w g D) \quad (2)$$

where v_w (m·s⁻¹) is the liquid wastewater velocity, κ (m²) is the intrinsic saturated wastewater permeability, κ_{rw} (-) is the relative wastewater permeability, μ_w (Pa·s) is the dynamic viscosity of wastewater, D (m) is the wastewater head.

Besides, the intrinsic saturated wastewater permeability is obtained through the original Kozeny-Carman equation:

$$\kappa = \frac{\kappa_0 (1 - n_0)^2}{n_0^3} \cdot \frac{n^3}{(1 - n)^2} \quad (3)$$

where κ_0 (m²) is the initial intrinsic saturated wastewater permeability, n (-) is the initial porosity.

Copper ion transportation and precipitation

The copper ions are considered a dilute species and are transported along with the wastewater flow in unsaturated media. During the transport process, the effects of dispersion, diffusion, chemical reactions, and precipitation are taken into account.

$$\frac{\partial (n S_r c_i)}{\partial t} + r_{ads,i} = n S_r \cdot (r_{eq,i} + r_{kin,i}) - \nabla \cdot (\rho_w v_w c_i - (D_{d,i} + D_{e,i}) \nabla c_i) \quad (4)$$

where c_i (mol·m⁻³) is the concentration of aqueous species, $D_{d,i}$ (m²·s⁻¹) and $D_{e,i}$ (m²·s⁻¹) are the effective dispersion and diffusion tensor of aqueous species, respectively. r_{ads} (mol·m⁻³·s⁻¹), $r_{eq,i}$ (mol·m⁻³·s⁻¹) and $r_{kin,i}$ (mol·m⁻³·s⁻¹) are the reaction rates caused by adsorption, equilibrium chemical reaction and kinetic chemical reaction, respectively.

The Langmuir type of adsorption is adopted for illustrating the adsorption process:

$$r_{ads,i} = \rho_s (1 - n) \cdot \frac{\partial \left(\frac{K_{L,i} C_{ads,max,i} c_i}{1 + K_{L,i} c_i} \right)}{\partial c_i} - \frac{K_{L,i} C_{ads,max,i} c_i}{1 + K_{L,i} c_i} \cdot \rho_s \frac{\partial n}{\partial t} \quad (5)$$

where ρ_s (kg·m⁻³) is the density of solid particles, $K_{L,i}$ (m³·mol⁻¹) is the Langmuir constant, $C_{ads,max,i}$ (mol·kg⁻¹) is the constant for the maximum adsorption.

The effective dispersion tensor is built from the dispersivities through the following form:

$$D_{dxx} = \alpha_l \frac{v_x^2}{|v_w|} + \alpha_t \frac{(v_y^2 + v_z^2)}{|v_w|}, D_{dxy} = D_{dyx} = (\alpha_l - \alpha_t) \frac{v_x v_y}{|v_w|} \\ D_{dxx} = \alpha_l \frac{v_x^2}{|v_w|} + \alpha_t \frac{(v_y^2 + v_z^2)}{|v_w|}, D_{dxy} = D_{dyx} = (\alpha_l - \alpha_t) \frac{v_x v_y}{|v_w|} \\ D_{dyy} = \alpha_l \frac{v_y^2}{|v_w|} + \alpha_t \frac{(v_x^2 + v_z^2)}{|v_w|}, D_{dzz} = D_{dzz} = (\alpha_l - \alpha_t) \frac{v_x v_z}{|v_w|} \quad (6)$$

The components of the velocity field v_w (m·s⁻¹) in the x , y , and z directions correspond to the fluid velocities v_x (m·s⁻¹), v_y (m·s⁻¹), and v_z (m·s⁻¹), respectively. The longitudinal and transverse dispersivities are represented by α_l (m) and α_t (m), respectively.

In the trapping area, the copper ions are assumed to be collected as a solid and adhere to the surface of the porous media. And the Monod type equation is applied to describe the global precipitation process. The accumulation of precipitates containing copper elements occupies the void space of the porous material, thereby changing the porosity of the trapping area. The change of porosity due to precipitation is calculated in the following formula:

$$\frac{\partial n_p}{\partial t} = (r_{eq,i} + r_{kin,i}) \cdot V_{m,i} = c_o \frac{c_i}{K_M + c_i} \cdot V_{m,i} \quad (7)$$

In addition, the change of porosity due to adsorption is calculated through:

$$\frac{\partial n_{ads}}{\partial t} = r_{ads,i} \cdot V_{m,i} \quad (8)$$

And therefore, the total porosity n is obtained from the equation:

$$n = n_0 - n_p - n_{ads} \quad (9)$$

where n_p (-) and n_{ads} (-) are the porosity occupied by the precipitation and adsorption, respectively. $V_{m,i}$ ($\text{m}^3 \cdot \text{mol}^{-1}$) is the molar volume, K_M (mol/m^3) is the constant parameter in Monod equation, c_o ($\text{mol} \cdot \text{m}^{-3}$) is the inflow concentration.

CASE STUDY ON THE ASPIRE CONCEPT

A numerical case study is provided in this section to preliminary test the long-term application capacity of the ASPIRE concept in trapping copper ions from contaminated water under a real condition. In addition, the model is discretized and solved by COMSOL Multiphysics 6.2 through the PDE interfaces.

Geometry size and mesh

A $10 \text{ m} \times 10 \text{ m} \times 5 \text{ m}$ porous trapping area (eg. permeable reactive barrier, reactive soil) is used for the simulation. Copper ion-rich contaminated water is injected from the top surface at a constant velocity of $5 \text{ E-6 m} \cdot \text{s}^{-1}$ and flows out through 0.2 m diameter pipes installed at 1 m intervals at the bottom. All other parts of the geometry are sealed. The geometry size and its related mesh are illustrated in Fig 1.

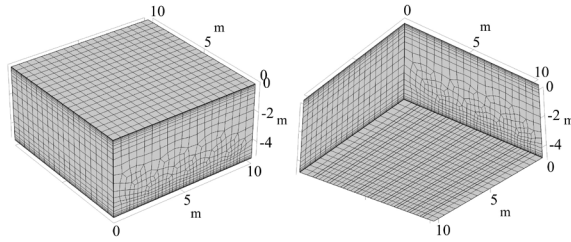


Fig 1. Geometry and mesh of the trapping area from different viewing angles.

Boundary conditions and constant parameters

The inflow wastewater at the top of the trapping area is characterized as follows:

$$-\vec{n} \cdot \rho_w v_w = \rho_w v_0 \quad (10)$$

The wastewater flowing out through the pipes is represented by setting the suction at the boundary to zero, as the pipes are in direct contact with the atmospheric air:

$$s = 0 \quad (11)$$

The copper ions flow along with the wastewater through the top surface, as described by the following expression:

$$\vec{n} \cdot (v_w c_i - (D_{d,i} + D_{e,i}) \nabla c_i) = \vec{n} \cdot v_w c_0 \quad (12)$$

The copper ion is forbidden to diffuse and disperse on the sealed boundary:

$$-\vec{n} \cdot (-(D_{d,i} + D_{e,i}) \nabla c_i) = 0 \quad (13)$$

where v_0 ($\text{m} \cdot \text{s}^{-1}$) is the inflow velocity of the contaminated water.

Furthermore, the constant parameters employed in this numerical study are summarized and presented in Table 1.

ρ_s	κ	n_c	K_m
2620[5] kg/m^3	1E-12[6] m^2	0.389	0.012 mol/m^3
$V_{m,i}$	c_0	v_0	μ_w
1E-4 m^3/mol	3.1476 mol/m^3	5E-6 m/s	1E-3 $\text{Pa} \cdot \text{s}$

Table 1. Constant parameters for numerical simulation

Simulation results

As the copper precipitates continuously accumulate in the trapping area, the occupied pore space may hinder wastewater flow and subsequently lead to clogging. Consequently, the simulation is terminated when the porosity of the porous media falls below 0.1. This section illustrates the geochemical characteristics of the trapping area at 365 days.

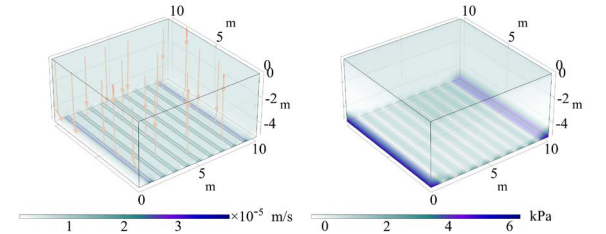


Fig 2. Velocity (left) and pressure (right) distributions in trapping area at 365 days.

Fig. 2 shows the velocity and pressure distributions in the trapping area after 365 days. The wastewater flows from the top surface of the trapping system with a velocity close to the injected velocity of $5 \times 10^{-6} \text{ m/s}$ (as shown by the orange lines). The outflow velocity from the pipes installed at the bottom is higher than that inside the trapping area due to the pressure difference between the trapping area and the surrounding atmosphere. Moreover, the outflow wastewater near the vertical surrounding walls exhibits the highest velocity, which is caused by higher wastewater pressure resulting from the effects of gravity and the sealed boundary condition. Additionally, since higher wastewater pressure may lead to mechanical damage and fractures, attention should be paid to the interval areas of the installed pipes and the regions near the sealed walls that experience higher wastewater pressure, as these areas require stronger structural integrity to maintain the normal and safe operation of the system.

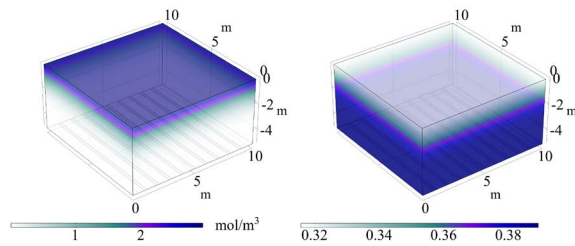


Fig 3. Copper ion concentration (left) and porosity (right) distributions in trapping area at 365 days.

Fig. 3 illustrates the concentration distributions of the copper ions in the trapping area as well as the potential clogging due to copper particulate precipitation. The figure shows that the copper ion concentration decreases with increasing depth. Furthermore, after 365 days of operation, the copper ions initially injected from the top surface have reached an area with a depth of approximately 2 m. As physical adsorption and chemical reactions continuously occur along with the flow of copper ions, the void pore volume is occupied by the precipitated copper particulates, leading to a decrease in the porosity of the trapping system as the depth increases. Specifically, the porosity at the top decreases by 17% from the initial value of 0.389 to around 0.32, indicating that after one year of operation, the system is not seriously affected by clogging problems. However, clogging issues should be monitored over time to ensure proper system operation.

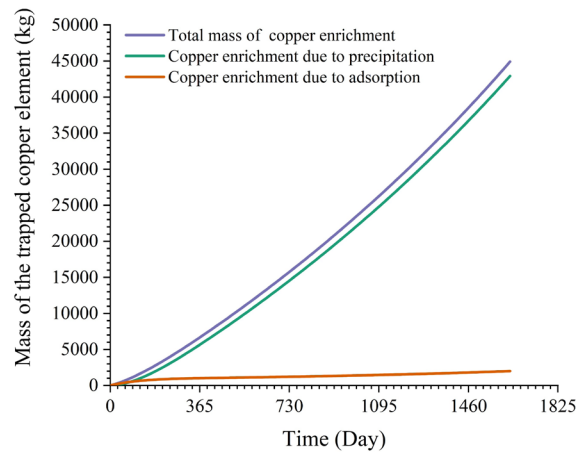


Fig 4. Mass of the trapped copper element according to time.

Fig. 4 demonstrates that both adsorption and precipitation contribute to the total copper enrichment, with adsorption initially being the dominant mechanism. However, as time progresses, precipitation becomes increasingly significant. The total mass of copper enrichment reaches approximately 45,000 kg by the end of the nearly 5-year period, highlighting the system's effectiveness in capturing and accumulating copper elements from contaminated water.

CONCLUSIONS

The numerical case study presented in this paper demonstrates the potential of the ASPIRE concept for the long-term trapping of copper ions from contaminated water under realistic conditions. The simulation results highlight the effectiveness of the system in capturing and accumulating copper elements over a nearly 5-year period, with a total mass of copper enrichment reaching approximately 45,000 kg for a trapping zone with the dimension of 10 m in length, 10 m in width, and 5 m in depth. The study also reveals the interplay between adsorption and precipitation mechanisms, with adsorption initially dominating and precipitation becoming increasingly significant over time. Furthermore, the analysis of velocity, pressure, copper ion concentration, and porosity distributions provides valuable insights into the system's performance and potential challenges, such as clogging and structural integrity requirements. These findings underscore the importance of monitoring and maintenance to ensure the proper operation of the ASPIRE system. Overall, this numerical investigation supports the feasibility of the ASPIRE concept as a promising approach for the simultaneous remediation of contaminated water and the recovery of valuable resources, aligning with the principles of a circular economy.

It is important to note that the results of this study are based on numerical simulations, and the constant parameters and boundary conditions employed in this investigation require further experimental validation. Moreover, additional research and field-scale implementations are necessary to confirm the effectiveness of the ASPIRE concept and optimize its design for a wide range of environmental conditions and contaminants.

Conflicts of Interest

The authors declare no conflict of interest.

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