Simulation of Acid Mine Drainage Processing Using 3-Stage Membrane Filtration in Aspen Plus

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Abstract. Acid mine drainage (AMD) is a mining-related problem that is causing harm to the natural ecosystem. The AMD originates from oxidized and sulfide ore stockpiles and contains high concentrations of dissolved copper and other contaminants. Therefore, many applications have been taken account into to process this highly acidic stream. In this research, Aspen Plus software is employed to simulate and analyze copper and water recovery efficiency of AMD generated from the stockpile of the Erdenetiin Ovoo deposit in at Gal Sentii LLC, Mongolia. The simulation incorporates a membrane filtration train consisting of ultrafiltration (UF) followed by two stages of nanofiltration (NF1 and NF2), modeled under steady-state conditions using the ELECNRTL thermodynamic method. Results show that the integrated system achieves high copper removal efficiency, with NF1 and NF2 reaching 98.99% and 100% separation, respectively. Water recovery remained effective throughout the process, reaching 90.08% in UF, 83.14% in NF1, and 99.90% in NF2. Total water hardness was reduced from 5918.81 mg/L to 0 mg/L, meeting the Mongolian MNS 4943:2015 standard for clean water. Although the permeate remained slightly acidic (pH ~3.67-3.93), the simulation confirms that membrane-based treatment is a viable strategy for both copper recovery and AMD remediation in cold-climate mining environments such as Mongolia.

Keywords: Acid mine drainage, Aspen Plus simulation, membrane filtration, environmental remediation.

1 Introduction

Mongolia hosts significant copper mineral deposits, including the Erdenetiin Ovoo deposit in Erdenet, which contains various oxidized and sulfide copper minerals such as malachite, azurite, chalcopyrite, and bornite. These minerals, upon exposure to atmospheric and mining conditions, undergo weathering and oxidation processes that generate AMD - a highly acidic aqueous effluent rich in dissolved metals and sulfate ions [1]. AMD is a form of leachate characterized by a pH value below 3 and high concentrations of heavy metals such as calcium (Ca), copper (Cu), and iron (Fe). The

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phenomenon of AMD formation is explained through Academician A.E. Fersman's theory of hypergenesis. He was the first to describe hypergenesis as the process by which the types and quantities of minerals undergo transformations on the Earth’s surface within the biosphere.

Over time, complex chemical and physical interactions occur across the atmosphere, hydrosphere, and the Earth's surface (lithosphere/metosphere). These processes exert both endogenic and exogenic influences on the environment and living organisms. When hypergenesis occurs in mine waste dumps, acid-generating reactions are triggered within ore bodies, resulting in physicochemical transformations that lead to the formation of new compounds and substances. Oxidation of sulfur-bearing metallic ores within mine dumps—through interaction with atmospheric oxygen and rainwater—produces sulfates of iron and other metals, along with sulfuric acid. This newly formed sulfuric acid is then washed down through the waste pile by rainfall, leaching out through the base and forming AMD [2-3].

The formation of AMD is influenced by several factors, including the local geological and hydrological conditions, climatic conditions, the morphology of the main waste dump, and the elevation of the pile itself. These factors directly affect the oxidation of sulfide minerals present within the dump structure. Climatic conditions such as precipitation, humidity, and temperature play a significant role in accelerating or moderating AMD generation processes. In addition to these abiotic factors, certain types of bacteria also contribute to the process by enhancing the rate of sulfide mineral oxidation [4].

AMD poses serious environmental challenges due to its acidity and heavy metal content, which can contaminate local water bodies and ecosystems if untreated [5]. Recovering valuable metals like copper from AMD not only mitigates environmental damage but also enhances resource efficiency and economic viability [6]. Among various treatment methods, membrane filtration technologies such as microfiltration (MF), ultrafiltration UF, nanofiltration NF, and reverse osmosis have gained prominence for their ability to selectively separate metals and purify water streams [7].

Process simulation software, notably Aspen Plus, provides a powerful platform to model complex hydrometallurgical and water treatment processes under varying operational conditions. Using thermodynamic methods like ELECNRTL, Aspen Plus can accurately simulate electrolyte behavior and ion interactions in multi-phase systems, enabling prediction of process performance, energy consumption, and water recovery efficiency [8].

This study focuses on model-based predictions for treatment of AMD generated from the Erdenetiin Ovoo copper ore stockpile using an integrated membrane filtration train simulated in Aspen Plus. The primary objectives are to evaluate copper recovery potential and water purification efficiency in a steady-state system incorporating microfiltration, ultrafiltration, and dual-stage nanofiltration/reverse osmosis units. The model aims to provide insights into process optimization and environmental remediation strategies suitable for mining operations in cold-climate regions like Mongolia.

2 Materials and Methods

Ore Stockpile

The ore stockpiles from the Erdenetiin Ovoo deposit in Erdenet, Mongolia consist of oxidized and sulfide copper-bearing minerals. These include malachite, azurite, delafossite, cuprite, chalcocite, covelline, chalcopyrite, bornite, and pyrite. These ores are major sources of copper ions when subjected to leaching under acidic conditions, generating AMD. From there are 12 different stockpiles originated from the Erdenetiin Ovoo, the “8a” off-balance stockpile design is used in this research.

AMD process

Acid mine drainage is produced from the weathering of these ores under natural or mining-exposed environments. The AMD is collected and subjected to a multi-stage treatment process aimed at copper recovery and water purification. The main contaminants include Cu^{2+}, Fe^{2+}, SO_4^{2-}, H_3O^+, and residual acidic components.

Filtration process

The filters used in purifying AMD in Galsentii LLC is 3-stage membrane filters which are Ultra-filtration (UF), Nanofiltration (NF1), and Nanofiltration with Reverse osmosis design (NF2).

Ultrafiltration membranes operate on a similar principle to reverse osmosis but have larger pore sizes, typically ranging from 0.002 to 0.03 micrometers, and function under low pressure. Ultrafiltration membranes do not allow organic molecules with molecular weights over 800 Daltons to pass through and generally operate under pressures less than 5 bar.

Nanofiltration uses membranes that combine properties of UV membranes and reverse osmosis. Nanofiltration allows monovalent ions such as sodium and potassium to pass through, but blocks divalent ions like calcium and magnesium, as well as organic molecules with molecular weights over 200 Daltons. Nanofiltration is especially effective at removing color and organic compounds, typically operating at around 5 bar pressure.

Aspen Plus modeling

The simulation of the treatment process was carried out using Aspen Plus software. A steady-state model was developed using the ELECNRTL method with a maximum of 30 iterations and 0.0001 error tolerance. The feed is based on the important minerals in the stockpile as given in Table 1. In addition, other important ions during the weathering process and their chemical reactions have been considered.

Table 1. The minerals of the “8” off-balance stockpile at the Erdenetiin Ovoo deposit

№	Component	Type	Formula

1	Water	solid	H_2O
2	Malachite	solid	$Cu_2(OH)_2CO_3$
3	Azurite	solid	$Cu_3(OH)_2(CO_3)_2$
4	Dela-fossite	solid	$CuFeO_2$
5	Cuprite	solid	Cu_2O
6	Chalcocite	solid	Cu_2S
7	Covelline	solid	CuS
8	Chalcopyrite	solid	$CuFeS_2$
9	Bornite	solid	Cu_5FeS_4
10	Pyrite	solid	FeS_2
11	Sodium hydroxide	conventional	$NaOH$

During the oxidation and weathering processes taking place in the stockpile and the formation of AMD, the Al^{3+}, Fe^{2+}, Cu^{2+}, Ca^{2+}, Mg^{2+}, SO_4^{2-}, H_3O^+ ions are considered to be the most important and the most frequent ones which are highlighted to this study.

One of the models used was the ELECNRTL model, which was combined with the RK equation of state. This model in Aspen Plus is used to determine concentrations in both aqueous and solvent mixtures. It is useful for simulating the vapor-liquid equilibrium in electrolytic systems and calculating the excess Gibbs free energy of electrolytes. This model is appropriate for systems involving electrolytes where correct description of ion interactions is required.

3 Results and Discussion

Acid mine drainage is considered one of the main hydrological and geochemical issues resulting from anthropogenic (human-induced) impacts on the geosphere, and it occurs consistently in all regions where intensive mining operations are conducted**.**

Among the many methods of neutralizing AMD (Figure 1) to make it eco-friendly, which can be categorized into active and passive methods, establishing infrastructure is an important step to ensure maintenance and sustainability. The hybrid method of processing AMD to produce pure water using filtration and pure copper using SX-EW method is a unique and viable green technology. On top of that, applying modeling and simulation techniques for the technicality can have numerous benefits of maintaining efficiency even during harsh weather conditions and other force majeure.

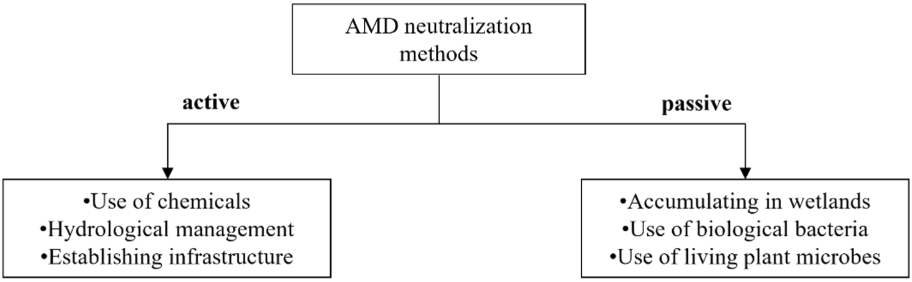

Figure 1. Methods of neutralizing AMD [9-10]

The general scheme of processing AMD from the stockpile is shown in Figure 2, where both the retentate and the permeate of the filters are being processed into high purity copper plates and pure water. In this research, we focused on modeling the 3-stage filtration part of the general process and analyzing the recovery of copper ions and water.

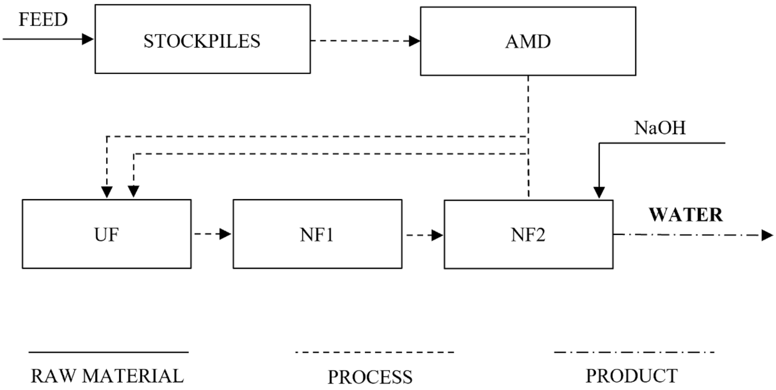

Figure 2. The main process scheme

NF1 stream go through SX-EW process for copper recovery since it is rich in copper ions.

3.1 Process Modeling and Simulation

Figure 3 illustrates the main Aspen Plus flowsheet. The filtration train includes UF, and two stages of nanofiltration NF1 and NF2. Streams were color-coded for clarity: red for AMD, purple for retentates, and green for permeates.

Table 1 presents calculated performance indicators based on each filter unit's inlet, permeate, and retentate compositions.

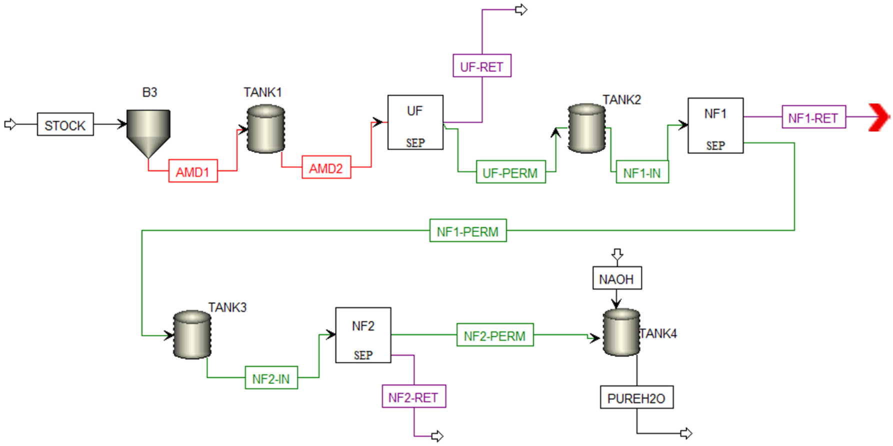

Figure 3. The AMD formation and 3-stage filtration process scheme on Aspen Plus

Figure 3 illustrates the main Aspen Plus flowsheet used for the simulation of copper recovery and water purification from AMD. The diagram includes all key blocks and process streams, labeled to reflect the actual simulation setup (Table 2).

The NF1-RET (the retentate of the NF1) will be going into further process of copper recovery since it has copper rich stream, given in Figure 3 with a red arrow.

Table 2. The streams, blocks and their descriptions which are used to model the AMD formation and 3-stage filtration processes.

Streams	**Blocks**
○ STOCK: Initial ore feed into the system ○ AMD1: First acidic drainage stream generated from the ore ○ AMD2: Pre-treated AMD stream after neutralization and tank storage ○ UF-PERM / UF-RET: Permeate and retentate from the UF (Ultrafiltration) unit ○ NF1-IN: Feed into the first nanofiltration unit ○ NF1-PERM / NF1-RET: Permeate and retentate from the NF1 unit ○ NF2-IN: Feed into the second nanofiltration/reverse osmosis unit	○ B3 (MIXER): Initial mixer to generate AMD from ore and water ○ TANK1: Buffer tank after AMD generation ○ UF: Ultrafiltration unit to remove larger particles ○ TANK2: Collection tank post-UF for NF1 feed preparation ○ NF1: First-stage nanofiltration to reject metals and recover water ○ TANK3: Holding tank before the final NF2 purification stage ○ NF2: Nanofiltration stage for final water polishing

○ NF2-PERM / NF2-RET: Permeate and retentate from the NF2 unit ○ PUREH2O: Final treated water stream collected after TANK4 ○ NAOH: Sodium hydroxide reagent for pH adjustment	○ TANK4: Final storage tank for clean water (PUREH2O)

From the stockpile, in B3 mixer, AMD stream is being formed (AMD1) imitating the natural weathering process with the feed given in Table 1. AMD2 stream differs from AMD1 stream by having accumulated in a pond/TANK1. Then, 3-stage membrane filtrations UF, NF1, NF2 (with reverse osmosis setting) come in place with each having TANK2, TANK3, and TANK4, which each having inlet, retentate, and permeate streams.

Each unit operation and stream were modeled in steady-state, and the ELECNRTL thermodynamic method was used for accurate ion and electrolyte behavior prediction. This flowsheet allows sequential treatment of AMD, enabling both copper recovery and environmental remediation.

Table 3. Some ion concentrations (g/l) in feed, each filtration, and final product

Ions	FEED	UF	NF1	NF2	WATER
H_2O	1003.869	1004.606	1002.276	1001.267	999.801
Cu^{2+}	5.951	6.484	0.078	0.000	0.000
Al^{3+}	2.077	2.263	0.027	0.000	0.000
Mg^{2+}	1.158	1.262	0.015	0.000	0.000
Ca^{2+}	0.266	0.289	0.003	0.000	0.000
HSO_4^{2-}	0.106	0.041	0.003	0.000	0.000
Fe^{2+}	0.063	0.068	0.001	0.000	0.000
H_3O^+	0.011	0.004	0.004	0.004	0.004

Given in Table 3, the ion concentrations were calculated regarding the flow ratio and following parameters were calculated with Equations 1-5.

In Table 5, the following parameters have been calculated from the Aspen simulation based on each filter's inlet stream, permeate, and retentate.

Equations list:

$$pH =- log_{10}([H_3O^+]) \tag{1}$$

$$Total\ hardness\ (mgCaCO_3/L) = \frac{100.0869}{40.078} Ca^{2+}(mg/L) + \frac{100.0869}{24.305} Mg^{2+}(mg/L) \tag{2}$$

$$\text{Separation efficiency} = \left(1 - \frac{C_{out} \cdot V_{out}}{C_{in} \cdot V_{in}}\right) \cdot 100 \tag{3}$$

$$Water\ recovery = \left(\frac{[H_2O] \cdot V_{out}}{[H_2O] \cdot V_{in}}\right) \cdot 100 \tag{4}$$

$$Cu\,Recovery = \left(\frac{C_{out}\cdot V_{out}}{C_{in}\cdot V_{in}}\right)\cdot 100 \qquad (5)$$

From the equations above, we can determine the efficiency of each filter in removing ions (e.g., Cu^{2+}), the recovery rates of both water and Cu^{2+}, and assess whether the system supports the sustainable use of the main products. Additionally, we can evaluate whether the filtered water meets the Mongolian wastewater standard (MNS4943:2015) [11], as summarized in Table 4 and 5. The purpose of the Mongolian National Standard MNS 4943:2015 is to establish the maximum allowable concentrations of pollutants in wastewater discharged into the environment from household use, as well as from industrial and service activities.

The initial pressure and temperature are 1.00 bar and 10.00°C, and the following parameters given for each filtration system are dependent on the flow ratio of each inlet stream. The moderately constant temperature is maintained throughout the whole process regardless of the pressure changes.

Table 4. Simulation temperature, pressure, and pH conditions of the feed, permeate stream of each filter, and the final product.

Parameter	FEED	UF-PERM	NF1-PERM	NF2-PERM
Temperature, °C	10.00	10.16	11.14	11.37
Pressure, bar	1.00	8.00	55.00	35.00
pH	3.50	3.93	3.73	3.67
Water hardness, g/l	5.43	5.92	0.07	0.00
Volume flow, cum/hr	20.00	18.00	15.00	15.00

Table 4 presents the simulated temperature, pressure, pH, water hardness, and volumetric flow rate for each stream in the membrane filtration process treating AMD. The feed stream enters the system at 10 °C, 1 bar, and a strongly acidic pH of 3.50, with a high water hardness of 5.43 g/L. As the stream progresses through the filtration stages (UF, NF1, and NF2), pressure increases according to drive membrane separation, reaching up to 55 bar in NF1. The pH gradually increases but remains acidic, while water hardness significantly decreases - dropping to 0.07 g/L after NF1 and approaching negligible levels (<0.001 g/L as $CaCO_3$ equivalent) after NF2. This result indicates effective removal of hardness-forming ions, consistent with the high selectivity of nanofiltration membranes toward multivalent cations. Volume flow also decreases slightly across stages, with a final water stream flow of 15.10 m^3/h, confirming high water recovery through the process. The NF2-PERM then undergoes NaOH treatment for pH adjustment.

Table 5. Calculated parameters of each filtration using the Equations 1-5.

Filter	Separation Efficiency, %	Water Recovery, %	Copper Recovery, %
UF-PERM	1.94	90.08	98.06
NF1-PERM	98.99	83.14	1.00
NF2-PERM	100.00	99.90	0.00

Table 5 summarizes the performance of each membrane stage in the AMD treatment process. The UF stage achieved a modest 1.94% copper separation efficiency, but allowed high water (90.08%) and copper (98.06%) recovery, making it suitable for pre-treatment. In NF1 stage, copper separation drastically improved to 98.99%, though copper recovery dropped to 1.00%, indicating effective rejection of copper ions. NF2 stage completed the purification process, reaching 100% copper separation efficiency and 99.90% water recovery, confirming its role as the final polishing step in achieving ultra-pure permeate.

3.2 Simulation Observations

1. Separation Efficiency: The separation efficiency increased significantly through the filtration stages. The UF stage showed a modest copper separation efficiency of 1.94%, likely due to concentration polarization effects at the membrane surface. NF1 stage demonstrated a high copper removal efficiency of 98.99%, while NF2 stage achieved complete Cu^{2+} removal (100%), indicating effective multi-stage retention.
2. Water Recovery: Water recovery was highest in NF2 (99.90%) and lowest in NF1 (83.14%), with the UF stage yielding 90.08% recovery. These results reflect the membrane types and driving pressures used in each stage—UF operated at a moderate pressure (8 bar), while NF1 (55 bar) and NF2 (35 bar) provided higher driving forces for permeate flow. Slight water mass losses across stages may also point to minor numerical or setup losses in the simulation.
3. Copper Recovery: The UF stage allowed 98.06% of copper to pass through into the permeate, whereas NF1 retained nearly all Cu^{2+}, with only 1.00% reaching its permeate. In NF2, no copper was detected in the permeate, confirming full retention. This highlights the role of the NF1 membrane as the primary copper separation barrier, supported by polishing in NF2.
4. pH Values: The pH of each stage remained slightly acidic due to the high concentration of hydronium ions across all stages. The UF permeate pH was 3.93, slightly higher than the feed (3.50), while NF1 and NF2 permeates remained consistently acidic at 3.73 and 3.67, respectively. This suggests partial retention of H^+ ions but insufficient to neutralize acidity, even after multi-stage treatment. Hardness Removal: Water hardness decreased significantly across the filtration train - from 5.43 g/L in the feed to 0.07 g/L after NF1, and 0.00 g/L after NF2. Using the $CaCO_3$-based conversion, this corresponds to a reduction from approximately 5918.81 mg/L to 0 mg/L, which meets the MNS 4943:2015 standard for drinking water in Mongolia. The NF2 membrane effectively removed residual Ca^{2+} and Mg^{2+} ions, confirming its critical role in final water polishing.
5. Process Performance Summary: The multi-stage membrane process demonstrated excellent removal efficiency for copper and hardness, with high water recovery, especially in the final NF2 stage. The pH remained low, suggesting the need for a final neutralization step if intended for potable use. Overall, the system's performance is well-aligned with industrial requirements for advanced water purification and metal ion removal.

4 Conclusion

This study covers model-based predictions for treatment of AMD from the Erdenetiin Ovoo copper stockpile using a membrane filtration train in Aspen Plus. The process, consisting of ultrafiltration and two nanofiltration stages NF1 and NF2, demonstrated high performance in both metal removal and water recovery. Copper was almost completely removed, with NF1 and NF2 achieving separation efficiencies of 98.99% and 100%, respectively. The UF stage allowed 98.06% copper recovery, supporting downstream purification.

Water recovery was also efficient across the system: 90.08% in UF, 83.14% in NF1, and 99.90% in NF2. Total water hardness was reduced from 5918.81 mg/L (as $CaCO_3$) in the feed to 0 mg/L (negligible levels of <0.001 g/L as $CaCO_3$ equivalent) after NF2, fully meeting Mongolia's MNS 4943:2015 clean water standard. While permeate pH remained acidic (~3.67–3.93), the simulation confirmed that membrane filtration is an effective approach for AMD treatment, enabling both environmental protection and copper recovery in mining operations.

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Disclosure of Interests. It is now necessary to declare any competing interests or to specifically state that the authors have no competing interests. Please place the statement with a third level heading in 9-point font size beneath the (optional) acknowledgments[1], for example: The authors have no competing interests to declare that are relevant to the content of this article. Or: Author A has received research grants from Company W. Author B has received a speaker honorarium from Company X and owns stock in Company Y. Author C is a member of committee Z.

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