Artificial Intelligence-Driven Oxidation Technologies for Sustainable Mining Wastewater Treatment: Process Optimization, Pollutant Degradation, and Future Perspectives

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Abstract

Mining and mineral-processing operations produce waste water containing flotation reagents, cyanide species, residual organics, dissolved metals and oxyanions in large quantity that are not easily treated by traditional biological and physicochemical treatment methods. Advanced oxidation processes (AOPs) utilize highly active species like hydroxyl (•OH) and sulfate ($SO_4^{\bullet-}$) radicals to mineralize refractory organics and to transform redox-active inorganic species, but their efficiency is not linear with oxidant dose, pH, catalyst characteristics, light or current input, and water-matrix composition. Artificial Intelligence (AI) and Machine Learning (ML) are the most practical ways that these interacting variables can be modeled, optimized and controlled. This review summarizes 97 sources on the chemistry of the Fenton, ozone, photocatalytic, electrochemical and sulfate-radical AOPs, the primary ML families (artificial neural networks, tree ensembles, metaheuristic optimizers, deep learning, quantitative structure–activity relationships and explainable AI), AI-assisted catalyst discovery and generative inverse design, AI for process optimization and pollutant degradation, and the energy, life cycle and techno-economic aspects for sustainable mine-water management. Kinetic and equilibrium analysis demonstrate that the range of rate constants for ozone is about ten orders of magnitude, the photoactive species $FeOH^{2+}$ has an optimum pH of 2.8, and at

pH 10, carbonate can remove most of the •OH from target contaminants; AI models must reflect these trends if they are to be transferred from the lab to real mine water. Of the 96 dated references in the cited literature, 69 (72%) appeared since 2020 and AI oriented works surpassed purely chemical and process works in 2024. However, key gaps are the lack of real datasets for mining-effluent, low transferability of models, low mechanistic and data-driven model integration, and the lack of interpretable digital twins with energy awareness.

Keywords: advanced oxidation processes; artificial intelligence; machine learning; mining wastewater; hydroxyl radical; sulfate radical; process optimization; catalyst design; sustainability

1. Introduction

Water scarcity is growing globally due to population growth, climate variability and increasing demand from industry, and recovery and use of process water has become a strategic priority for water, rather than just an option [1]. Industrialization and urbanization have worsened water quality and air quality while also increasing climate pressures, and extractive industries are one of the sectors that uses the most water and is most polluting [2]. Mining wastewater, process water from flotation and leaching circuits, tailings seepage and/or mine drainage contain high ionic strength, extreme pH, dissolved metals and persistent organic reagents. These matrices are often too recalcitrant to be treated by conventional treatment trains that involve coagulation, sedimentation, adsorption and biological oxidation, that either transfer pollutants to another phase or are toxic to the biological component [3].

The Advanced oxidation processes have been developed to overcome this limitation because strong and mostly non-selective oxidants are formed in situ, among them the hydroxyl radical which reacts with organic molecules with near diffusion-controlled rates and can convert them to CO2, water and mineral acids [4]. All of the •OH based AOP's are based on the environmental chemistry of •OH, including how it forms and how it is scavenged by constituents of natural waters [5]. Recent reviews have been published that report on the rapidly expanding field of hybrid and catalytic AOPs and the continuing problems of cost, energy usage and scavenging by background ions and scaling up [6]. Other comparative analyses of costs for priority hazardous chemicals also reveal that AOPs are economically viable to a great extent depending on the targeted compound and the selected oxidant system [7].

AI first steps into environmental engineering as a means to predict the behavior of a nonlinear system which is not amenable to description by first principles [8]. In the AOP field, there are new advances on the catalytic active-site engineering, oxidation-pathway regulation and optimizing reaction conditions [9]. Due to the various coupled variables affecting the performance of AOP, such as oxidant and catalyst dose, pH, temperature, irradiance, current density and water matrix [10] data-driven models are complementary to kinetic theory. AI has been woven into the fabric of many sophisticated treatment systems [11] and "explainable" AI approaches are starting to uncover what operating parameters are truly influencing AOP performance [12]. New developments suggest the integrated, intelligent oxidation platforms which combine sensing, prediction and control [13].

Fortunately, this is not enough; although there has been significant progress, there is still no review that has explicitly addressed the particular requirements of the mining wastewater problem: high salinity and metal concentrations that scavenge radicals, ore-specific and variable chemistry, remote sites with limited energy supply, and strict discharge/reuse constraints. There is no study specifically related to mining effluents in the literature compiled for this review, and this evidence is therefore transferred from industrial, textile, pharmaceutical, petroleum and municipal applications and the uncertainty of transfer is indicated where appropriate. The 97 references were coded by title and scope into the two groups for AI (61) and the chemistry, process and context (36), and the year of publication was noted.

The goals of this review are to (i) summarize the oxidation chemistries relevant to mine water and the kinetic and equilibrium regimes that govern them (Section 2); (ii) classify the AI and ML methods used in oxidation systems (Section 3); (iii) review AI-guided catalyst discovery (Section 4) and AI driven process optimization and pollutant degradation (Section 5); (iv) discuss sustainability, energy and life-cycle implications and propose a closed-loop framework (Section 6); and (v) define a research agenda (Section 7).

2. Fundamentals of Oxidation Technologies for Mining Wastewater

The common theme of all AOPs is that they produce a short-lived highly reactive oxidant that is generated at a rate that exceeds the rate of consumption by the water matrix, thereby exposing the target pollutants to attack prior to scavenging of the oxidant. They are attractive because of the targets they can oxidize, such as refractory organic reagents, cyanide species and reduced inorganic ions, and metal ions can be changed to less mobile oxidation states.

2.1 Reactive species, thermodynamics and kinetics

Second-order rate constants for the reaction of the hydroxyl radical with most organic compounds range about 108–1010 M−1 s−1; this rate constant was first measured in atmospheric chemistry using structure–reactivity relationships for H-abstraction and addition reactions [14]. In water treatment, oxidants are classified as selective oxidants (chlorine, chlorine dioxide, ferrate(VI) and ozone), which have rate constants that vary by many orders of magnitude depending on the presence of electron rich moieties, and non-selective oxidants, •OH [15]. This is important for the mining effluents because bicarbonate, carbonate, chloride and natural organic matter compete for radicals and can absorb a large portion of the oxidant dose [5]. The thermodynamic driving force of the main oxidants are compared in Figure 1 and the kinetic selectivity in Figure 2.

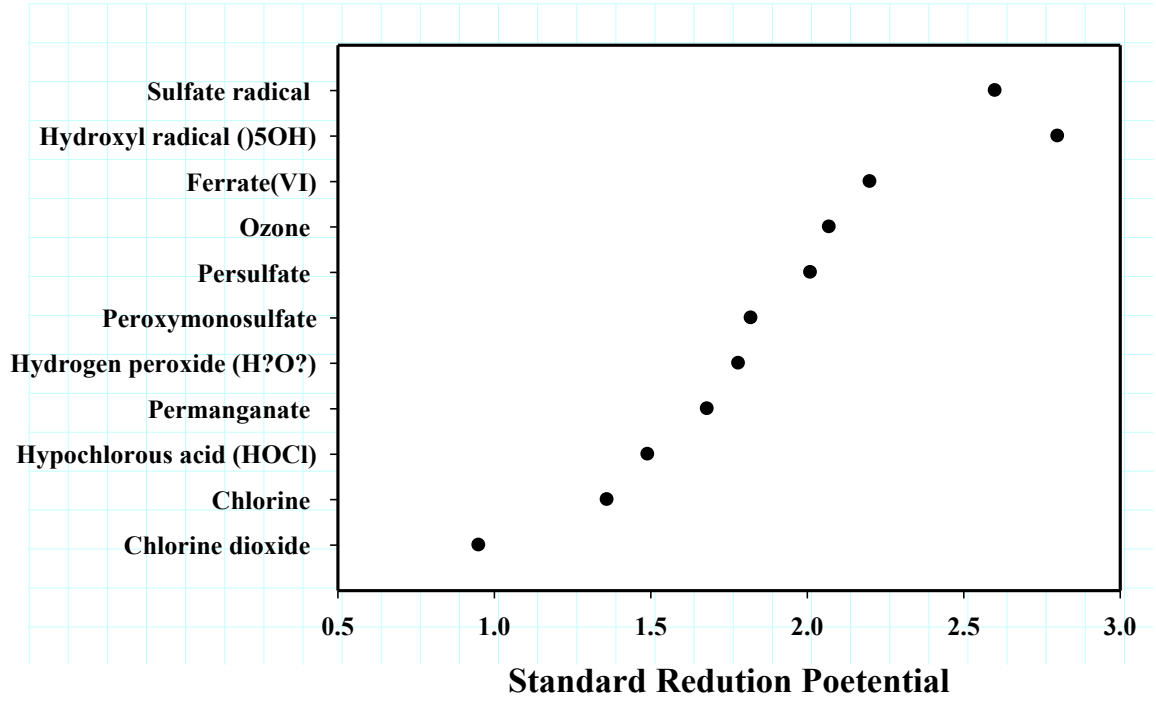


Figure 1. Standard reduction potentials (E°, V vs SHE) of oxidants used in water treatment [4], [5], [15].

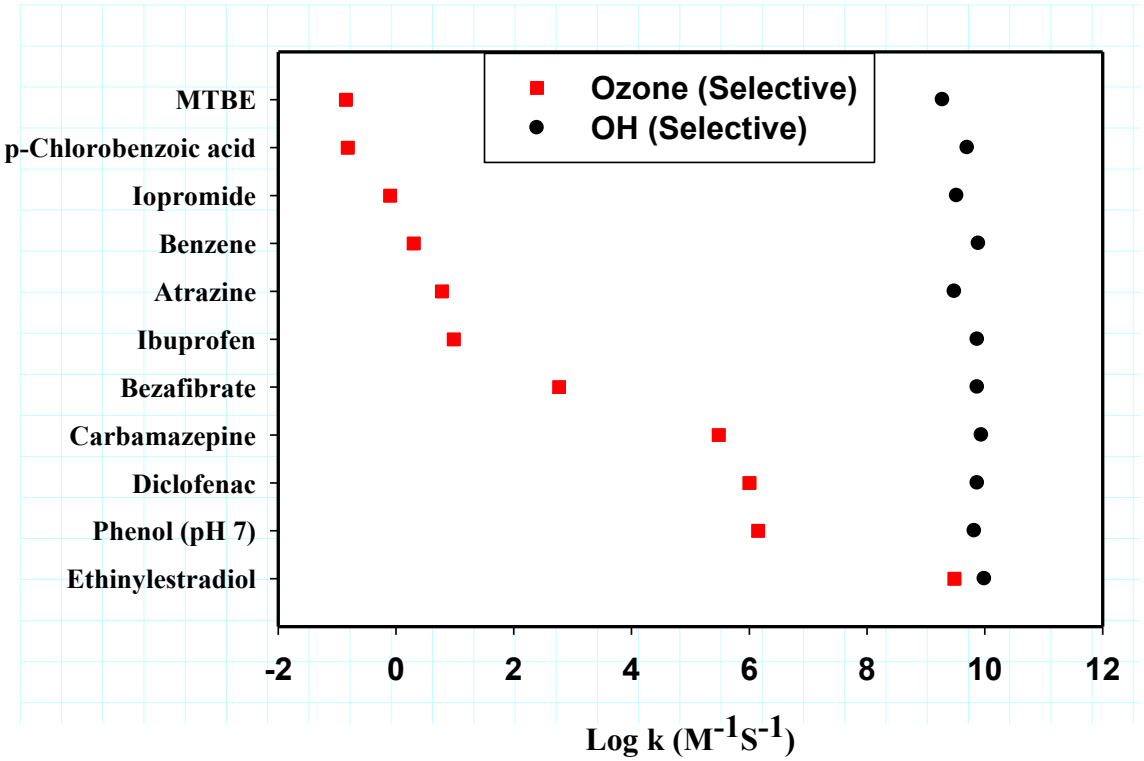


Figure 2. Second-order rate constants of ozone (black) and •OH (red) with eleven representative organic micropollutants at pH 7 [15].

This contrast gives rise to a key modelling decision. In the ozone case, removal relies on molecular structure, therefore the molecular structure needs to be described by AI models (Section 3.3). Rate constants are almost constant with •OH and are dependent on the exposure of the radicals and the scavenging of the matrix (Section 2.8) which is generally in favour of removal; process-level input features, therefore, govern removal.

2.2 Families of advanced oxidation processes

There are five families of AOPs that are relevant to mine water. The Fenton-based processes are well studied and have been extensively optimized for organic wastewater [16] and variants of the Fenton process, such as the Fenton-like and photo-Fenton processes have been found to yield faster iron cycling and higher mineralization [17]. The decomposition of ozone generates •OH, which is highly reactive and reacts with electron rich sites, as well as ozone itself. The generation of ozone, mass transfer and applications are discussed in [18]. Photochemical processes involve breaking apart the oxidants or exciting the chromophores or semiconductors using UV or visible light [19]. The electrochemical methods produce oxidants at the electrode and have been extensively used for synthetic dye wastewaters [20]. Sulfate-radical AOPs (SR-AOPs) consist of persulfate or peroxymonosulfate activators which have been examined for

domestic and industrial wastewater on degradation efficiency and the mechanism [21]. These families, and their fit with mining wastewater are summarized in Table 1 below, at the end of Section 2.7.

2.3 Fenton and photo-Fenton processes

The iron-promoted oxidation of tartaric acid, reported in 1894 [22] was the birth of fenton chemistry. The catalytic decomposition of H2O2 using ferrous iron (Eq. 1) is its main step:

$$Fe^{2+} + H_2O_2 \rightarrow Fe^{3+} + \bullet OH + OH^- \quad (1)$$

The related chemistry, including Fe(III) reduction, ferryl intermediates and photo-assisted cycles, has been reviewed in depth [23]. Iron-mediated photodegradation of a chlorinated herbicide confirms the benefit of UV-assisted iron cycling [24]. Under irradiation, Fe(III) hydroxo complexes are photoreduced to Fe(II) with release of •OH (Eq. 2), so the distribution of Fe(III) species controls the photo-Fenton rate (Figure 3).

$$FeOH^{2+} + h\nu \rightarrow Fe^{2+} + \bullet OH \quad (2)$$

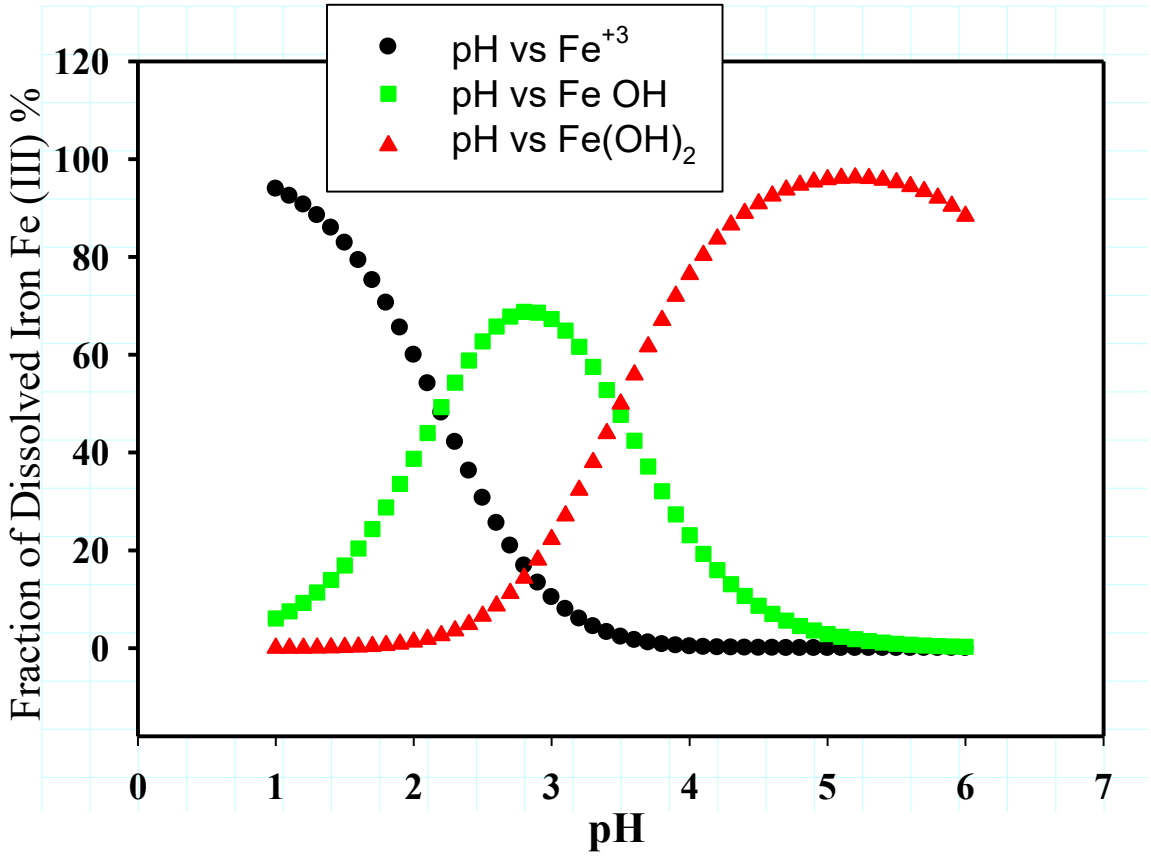


Figure 3. Equilibrium distribution of dissolved monomeric Fe(III) species between pH 1 and 6 [22-24].

The different distribution of Fe species in water is responsible for the narrow pH optimum of the experimental results, which corresponds to a pH near 3, due to the high photoactivity of $FeOH_2^+$ and its importance as a source of •OH in photo-Fenton systems [23]. The pH range of acid mine drainage (2.5–3.5) is naturally within this range and the dissolved iron can serve as an in situ catalyst. To use neutral or alkaline mine water, it would have to be acidified, which an optimizer would need to take into account, while the heterogeneous Fenton-like catalyst (Section 4) would work better at a higher Ph.

2.4 Heterogeneous photocatalysis

The electron–hole pair generated by the absorption of photons with energy greater than the band gap of the semiconductor, in this case TiO_2, by heterogeneous photocatalysis can lead to the formation of •OH at the surface (Eq. 3):

$$TiO_2 + h\nu \rightarrow e^-(cb) + h^+(vb); \quad h^+(vb) + H_2O \rightarrow \bullet OH + H^+ \tag{3}$$

The classic mechanistic analysis showed that photocatalytic degradation kinetics of organic water contaminants are consistent with •OH attack [25]. Turbidity and coloured species in mine water attenuate light, and dissolved metals can foul catalyst surfaces; both are key limitations at mine sites.

2.5 Electrochemical advanced oxidation processes

Electrochemical AOPs can be developed to produce oxidants at the anode or H_2O_2 at the cathode without the use of bulk chemicals and recent studies have focused on the detection of reactive species and understanding of the mechanisms [26]. Electro-Fenton technology is a combination of cathodic generation of H_2O_2 and iron catalysis [27]. The conductivity of many mine waters is high, which is advantageous as it reduces cell voltage, but helps to create active chlorine and chlorinated by-products from chloride.

2.6 Hybrid processes and early data-driven examples

It is common practice to combine oxidation with other unit operations. A surrogate-based control strategy is employed for management of operating cost in landfill leachate through an O_3/H_2O_2 stage followed by Anammox-based biotreatment and activated carbon adsorption, which is an operating strategy transferable to variable streams of mine water. Data-driven tools have also been introduced to oxidation chemistry: the exposure of •OH during ozonation was predicted from kinetic parameters from ozonation, and adsorptive and photocatalytic removal of a phenolic was predicted by artificial neural networks [29, 30]. Life-cycle analysis of

electrochemical AOP indicates that the environmental performance is mainly influenced by the choice of electricity source and the electrode materials [31] and a predictive emission model of ozone was developed using XGBoost (eXtreme Gradient Boosting) [32].

2.7 Catalytic materials

The maximum photocatalytic and Fenton-like efficiency are determined by the catalyst properties. While the structural variation of TiO_2 has been correlated with its band gap [33], the use of nanowire morphology for the removal of dyes using a simple synthesis was shown for phosphorus-doped graphitic carbon nitride [34] and the application of nanowire morphology for charge transport within semiconductor devices to control charge transport within ZnO-based devices was demonstrated, which is relevant for the design of photocatalysts [35]. Another application of interest to the mining industry, where Se is a common component of coal and metal-mine effluents, is the photocatalytic reduction of Se(IV) over a recyclable TiO_2/BiOBr/cloth catalyst [36] combined with the use of ML modelling and analysis of the mechanism. Synthesis route also induces significant changes in magnetite modified metal–organic framework particles properties, impacting magnetically recoverable catalysts [37].

Table 1. Principal oxidation technologies and their relevance to mining wastewater.

Technology	Main oxidant(s)	Typical operating window	Strengths for mine water	Limitations for mine water	Refs.
Fenton / Fenton-like	•OH from Fe^{2+}/H_2O_2	pH 2.5–4; ambient temperature	Uses dissolved Fe in acidic drainage; simple reactors	Iron sludge; narrow pH window; Cl^- and SO_4^{2-} complex Fe	[16], [22], [23]
Photo-Fenton	•OH; Fe(III)/Fe(II) photocycling	pH 2.5–4; UV or solar	Faster Fe regeneration; lower reagent dose	Light attenuation in turbid water	[17], [24]
Ozonation / peroxone	O_3, •OH	pH 7–11 for the •OH route	Effective on cyanide and electron-rich organics; no sludge	Gas–liquid mass transfer; carbonate scavenging	[18], [28], [29]
Heterogeneous photocatalysis	•OH, h^+, $O_2•^-$	Near-neutral pH; UV or visible light	Catalyst reuse; potential solar operation	Metal fouling; turbidity; catalyst recovery	[25], [30], [33], [36]
Electrochemical AOPs / electro-Fenton	M(•OH), active chlorine, H_2O_2	Wide pH; current-controlled	High conductivity lowers energy demand	Electrode cost; chlorinated by-products	[20], [26], [27], [31]
Sulfate-radical AOPs	$SO_4•^-$, •OH	pH 3–9; heat, UV, metal or carbon activation	Longer radical lifetime; broad pH range	Adds sulfate; activator leaching	[21]

2.8 Matrix effects in mining wastewater

The composition of mine-waters is very different to the synthetic media that are typically used in most tests of AOP. Table 2 shows the principal factors in the matrix, with their possible implications for modelling, and Figure 4 quantifies the principal factors, carbonate scavenging.

Table 2. Mining-wastewater matrix factors that affect oxidation performance, and their implications for AI modelling.

Matrix factor	Effect on oxidation	Implication for AI models	Refs.
pH (acidic drainage to alkaline cyanidation water)	Governs Fe solubility, O_3 decomposition and the •OH potential	Essential input feature with strong interaction terms	[4], [16], [18]
Carbonate and bicarbonate alkalinity	Scavenges •OH, forming the weaker CO_3•$^-$	Alkalinity as an input; scavenger-aware features	[5], [15]
Chloride and high salinity	Converts •OH and SO_4•$^-$ to chlorine radicals; possible chlorinated by-products	Track Cl^-; flag by-product risk as an output	[5], [21], [26]
Dissolved metals (Fe, Mn, Cu)	Catalyse Fenton-like reactions or consume oxidant	Metal speciation features; regime classification	[23], [27]
Sulfate	Complexes Fe(III); limits SR-AOP discharge	Constraint in multi-objective optimization	[21]
Suspended solids and colour	Attenuate UV and visible light	Turbidity or optical sensors as model inputs	[19], [25]
Variable flow and composition	Time-varying load from ore changes and rainfall	Time-series models; surrogate-based adaptive control	[28], [29]

Carbonate scavenging can be evaluated with competition kinetics: the share of •OH that reacts with a target pollutant T equals the target's share of the total •OH sink (Eq. 4):

$$f(T) = k(T)[T] / (k(T)[T] + k(HCO_3^-)[HCO_3^-] + k(CO_3^{2-})[CO_3^{2-}] + k(DOM)[DOC]) \quad (4)$$

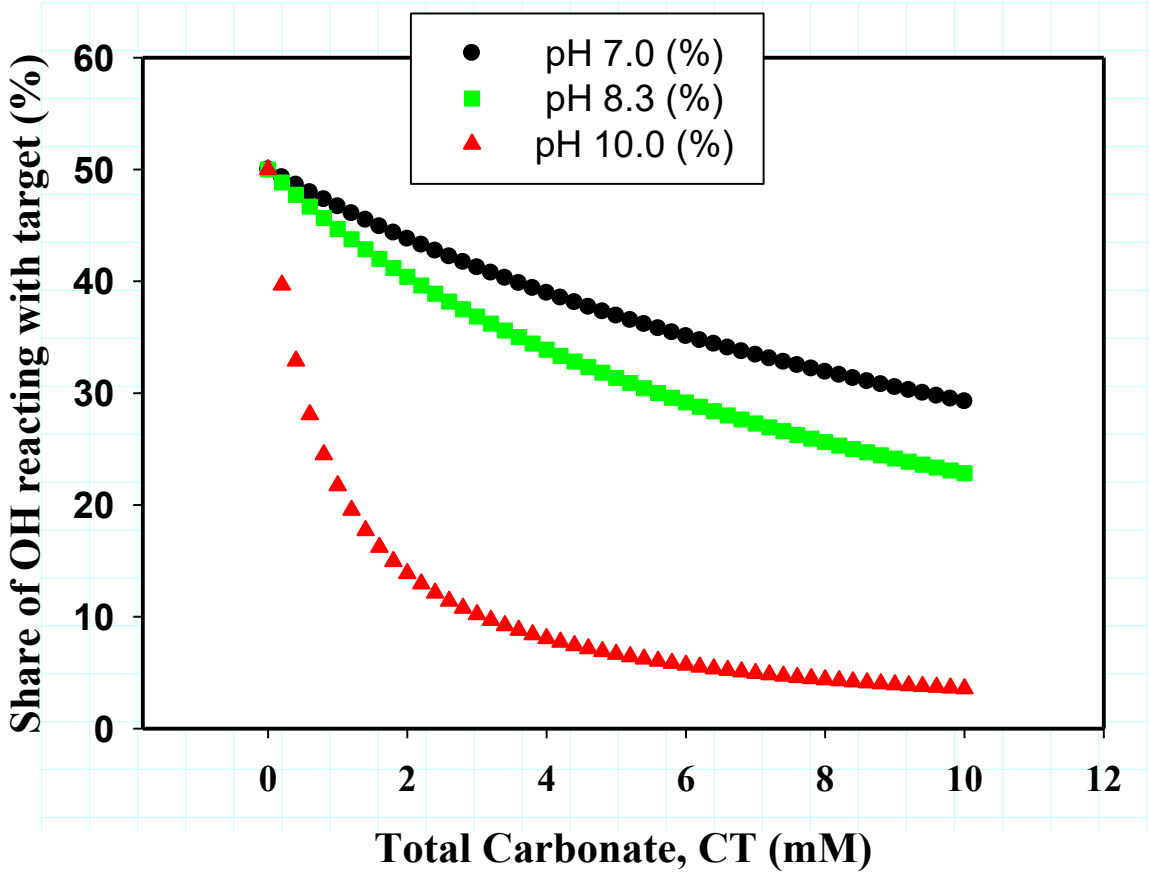


Figure 4. Computed share of •OH reacting with a target pollutant in water [5,15].

This is a strongly non-linear response to pH. When the total amount of carbonate is 10 mM, at pH 7, the target is reduced to 29%. With the pH of cyanidation circuits being typical of 10, 2 mM already reduces it to 14%, as carbonate reacts with •OH approximately 46 times faster than bicarbonate [5, 15] A model calibrated with carbonate-free laboratory water then would predict too much use of •OH in alkaline mine water by approximately 3.6 times at 2 mM •OH.A model trained with carbonate-free laboratory water would then overpredict the use of •OH in alkaline mine water by about 3.6 times at 2 mM •OH, thus introducing another transferability issue (revisited in Section 7).

3. Artificial Intelligence and Machine Learning Methods for Oxidation Processes

AI can be used in oxidation systems in three ways: predicting the output of the process from the operating inputs, searching the input space for an optimal set of operating conditions, and explaining and/or designing the chemistry itself. One of the key concepts in modern AI is representation learning, where deep learning is most well-known [38]. In water applications, the use of ML has been employed to assess water quality for more than 10 years [39]. A trained

surrogate model is then usually used in conjunction with an optimizer such as a genetic algorithm [40] that evolves candidate solutions using selection, crossover and mutation and a particle swarm optimiser [41] that moves the candidate solutions to the best individual and swarm positions. The use of AI in wastewater treatment has been reviewed, with the use of AI for predicting wastewater flow and waste water parameters steadily expanding from plant level to process level [42, 43].

3.1 Mechanistic, hybrid and system-specific models

Data-driven models are used in addition to, and not in place of, mechanistic models. Intrinsic rate data has been transferred from microreactor to larger reactors using modelling of the reactors, as shown by modelling [44]; simulation has also been used in combination with optimization for pharmaceutical removal by SR-AOPs [45]. There are now book-length treatments that cover all aspects of the use of AI in treatment systems [46]. In each oxidation system, ML has been used to design Fe–Ni bimetallic catalysts for the photo-Fenton degradation of ciprofloxacin [47], to accurately predict and intelligently control the COD removal in the electrocoagulation system combined with catalytic ozonation [48] and to develop interpretable predictive models for the metal-, UV- and heat-activated persulfate systems [49].

3.2 Artificial neural networks and explainable AI

The most popular model in the environmental engineering is the artificial neural networks model (ANNs) which is used to model nonlinear and multivariable responses without an explicit model [8]. Early black-box ANN models have been used to forecast performance of the treatment plant using the routine data from the plant influent [50]. Now, their opacity is overcome by explainable AI (XAI) techniques, which have shed light on the sludge predictions made with ML models in treatment plants [51] and explained the principles, operations and performance of advanced oxidation systems [12].

3.3 QSAR and structure based models

Molecular descriptors, which are used to describe the structure of a molecule, are related to its reactivity or toxicity in quantitative structure–activity relationships (QSAR). The •OH rate constant for VOCs have been predicted by QSAR models [52] as well as acute aquatic toxicity [53]. QSAR can provide a pathway that allows for the prediction of the reactivity of reagents in flotation processes, as well as their transformation products, for which the rate constant is known to depend strongly on structure (Figure 2) for ozone-based processes.

3.4 Comparative use of machine-learning families

AI based wastewater optimization has been reviewed as moving from prediction to multi-objective control [54] and ML techniques have been compared for the prediction of treatment-plant performance [55]. In AOPs in particular, ANNs have been used to model, simulate and predict the performance of the treatment process in recalcitrant wastewater treatment [56]. Tree ensembles are good at processing tabular process data, and they also provide feature importance that is built in, such as random forest for photocatalytic treatment over Mn-doped BiFeO3 [57] and XGBoost for ozone prediction [32].

3.5 Energy and process-wide modelling

Energy savings in sewage sludge incineration in treatment plants have been optimised by monitoring incineration processes [58] and energy optimisation has been comprehensively reviewed based on modelling of treatment processes, either mechanistic or data-driven [59]. The main method families and their role in AOPs are summarized in Table 3.

Table 3. Main AI and ML method families applied to oxidation-based treatment.

Method family	Principle	Strengths	Limitations	Typical role in AOPs	Refs.
Artificial neural networks (MLP, RBF)	Layered nonlinear function approximation	Captures interactions; mature tools	Data-hungry; opaque; overfits small designs	Predict removal, COD or TOC from operating variables	[8], [30], [50], [56]
Tree ensembles (RF, GBM, XGBoost)	Aggregated decision trees	Robust on tabular data; feature importance	Poor extrapolation beyond the training range	Performance prediction; variable ranking	[32], [57]
Kernel methods (SVM, SVR)	Margin-based classification and regression	Good on small datasets	Kernel tuning; limited scalability	Small-sample degradation modelling	[39], [55]
Metaheuristics (GA, PSO)	Population-based global search	Finds optima of black-box surrogates	Computational cost; no uncertainty estimate	Optimize dose, pH, time and current	[40], [41]
Deep learning	Multi-layer representation learning	Handles spectra, images and molecular graphs	Large data needs; limited interpretability	Contaminant screening; catalyst representation	[38]
QSAR	Descriptor–activity regression	Predicts for untested compounds	Applicability-domain limits	•OH rate constants; toxicity of products	[52], [53]
Explainable AI (SHAP, partial dependence)	Post hoc attribution of model outputs	Builds trust; reveals governing variables	Explanations only as good as the model	Identify key operating variables	[12], [49], [51]
Hybrid kinetic–ML models	Mechanistic model with data-driven terms	Physically consistent; better extrapolation	Requires kinetic knowledge	Scale-up and reactor design	[44], [45], [59]

4. AI-Guided Catalyst Discovery and Inverse Design

Catalysts are the ceiling for efficiency of AOP, and AI is changing the catalyst development process from trial-and-error synthesis to prediction and generation. The application of AI to heterogeneous catalysis in AOP has been described as a pathway to speed-up screening, mechanistic elucidation and rational design [60].

4.1 High-throughput screening and descriptor models

Combined with high throughput experiments, ML can reduce the discovery loop by suggesting the next experiments to run [61]. The electronic-structure descriptors have been used to screen bimetallic catalysts [62] and comprehensive strategies on the selection of descriptors and ML-based model validation have been provided, which can be translated to other cases [63]. Experimental and computational data are now known to be necessary for successful ML for heterogeneous catalysis [64].

4.2 Generative and inverse design

In generative models, the direction of the model is reversed and it suggests structures that satisfy a target property. Stable crystals, with desired chemistry and properties, have been designed using a generative model of inorganic materials [65], a generative pretrained transformer has been developed for heterogeneous catalysts [66] and a generative adversarial network has been used in combination with the microkinetics derived from first principles to design heterogeneous catalysts [67]. The prediction of transition-metal complexes has moved from high-throughput screening to the use of ML surrogates [68]; the activity and selectivity of bimetallic catalysts to ethanol reforming have been predicted using ML [69]; and computer-driven workflows have predicted catalysts with higher selectivity [70]. The field is evolving beyond a mere description of an oxidation to inverse design for advanced oxidation [71]. None of these generative methods have been used to develop the catalysts for AOP of mine-water, which has to be both salt tolerant and sulfate and metal fouling tolerant.

4.3 Learning from scarce and structured data

There are very few data available for mine-water conditions, making it difficult to train with much data. GNNs have the ability to learn relations between entities and excel in few-shot scenarios, which is desirable for molecular and crystal graphs, as demonstrated in SAR image classification [72]. Another trend being accelerated by deep learning is the screening of emerging contaminants [73] that may prioritize the transformation products that oxidation catalysts need to be able to destroy. Similar to the waste-derived carbon, the mine sludges and

tailings could be considered as potential catalysts and catalyst supports because of their high iron content, but this is not yet demonstrated using AI-accelerated workflows. The strategies are summarized in Table 4.

Table 4. AI strategies for designing oxidation catalysts and their potential for mining-wastewater AOPs.

Strategy	Data source	Output	Demonstrated in	Potential use for mine-water AOPs	Refs.
Descriptor-based ML screening	DFT descriptors; literature data	Ranked candidate catalysts	Bimetallic catalysts	Screen Fe-, Mn- and Cu-based Fenton-like catalysts	[62], [63], [69]
ML with high-throughput experimentation	Automated synthesis and testing	Active-learning experiment plans	Heterogeneous catalysis	Rapid testing in real mine-water matrices	[61], [64]
ML for transition-metal complexes	Computed properties of complexes	Property surrogates	Transition-metal chemistry	Homogeneous activators for persulfate	[68]
Selectivity-prediction workflows	Experimental selectivity data	Higher-selectivity catalysts	Catalyst selectivity	Favour target oxidation over scavenging	[70]
Generative models (diffusion, GPT, GAN)	Crystal databases; microkinetics	New candidate structures	Inorganic materials; heterogeneous catalysts	Inverse design of salt- and fouling-tolerant catalysts	[65], [66], [67]
Graph and deep learning	Molecular and crystal graphs	Structure–property models from few data	Few-shot learning; contaminant screening	Learning from small mine-water datasets	[72], [73]
ML-guided AOP catalyst design	AOP degradation experiments	Optimized composition and support	Fe–Ni/sludge-carbon photo-Fenton; TiO_2 band gap	Waste-derived catalysts from mine sludge	[33], [47], [60], [71]

5. AI-Driven Process Optimization and Pollutant Degradation

Optimization of AOP-based water treatment has been performed for many decades, with either one-factor-at-a-time experiments or response-surface designs. AI does away with these and uses a surrogate model that learns the response surface and an optimizer that searches it.

5.1 Pharmaceuticals and research trends

Pharmaceuticals are one of the most studied target classes: the removal of pharmaceuticals in water by AOPs has been comprehensively reviewed [75] and the optimization of AOPs for water contaminated with pharmaceuticals has been attempted using AI [76]. The number of publications reporting on the use of AIOPs for water decontamination shows a strong increase, which is reflected in the emerging literature that has been cited in this review, shown in Figure 5 [77] also reveals this emergence of AI-integrated AOPs.

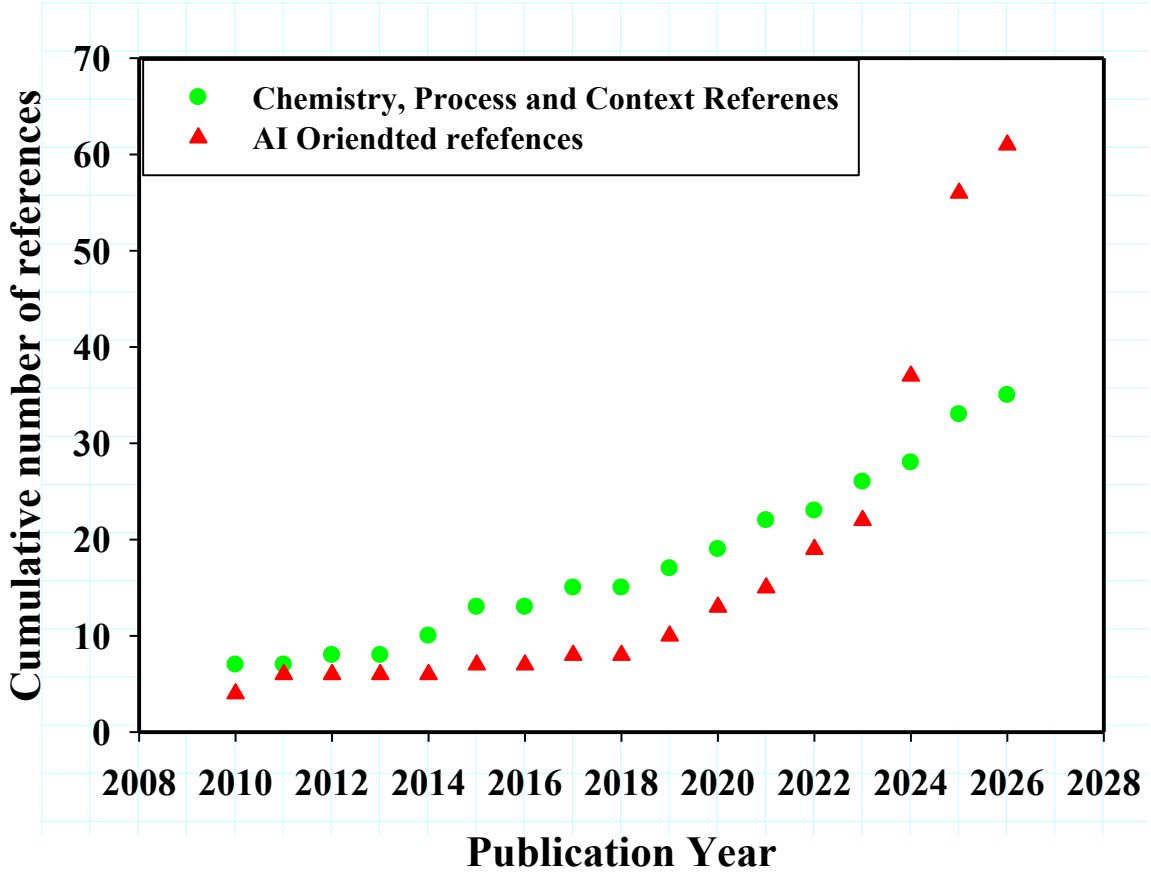


Figure 5. Cumulative growth of AI-oriented references (red) versus chemistry, process and context references (green) cited in this review, 2010-2026.

Of the 96 dated references, 69 (72%) were published from 2020 onward and 41 (43%) in 2024-2025 alone, whereas most of the underlying oxidation chemistry was established before 2010.

5.2 Chemical dosing, dyes and full-scale plants

In wastewater purification and treatment, AI is starting to be used in dosing control for chemicals [78]. Dye removal from the textile wastewater by the sulfate-radical AOP has been modelled using the artificial intelligence optimization method [79] and an artificial neural network – PSO Hybrid model has been adopted for describing dye removal by Fe(II)/chlorine and H_2O_2/periodate oxidation [80]. On a larger scale, a combination of advanced-oxidation dye-wastewater treatment plant was designed and developed using data-driven predictive performance modelling [81].

5.3 Catalytic and photocatalytic systems

There has been a review of the use of ML-aided AOPs in water-treatment applications [82]. It has been predicted the catalytic performance of the removal of hazardous nitrophenols and azo dyes [83] and now supervised learning models are used to guide photocatalysis for wastewater

treatment [84]. Table 5 summarizes representative applications and judges their transferability to mining wastewater.

Table 5. Representative AI and ML applications to oxidation processes, with their transferability to mining wastewater.

Ref.	Oxidation process	Target pollutant or matrix	AI/ML approach	Objective	Transferability to mine water
[29]	Ozonation	•OH exposure in water	Several ML regressors on ozone-decay kinetics	Predict •OH exposure	High: cyanide and reagent oxidation
[36]	Photocatalytic reduction (TiO_2/BiOBr/cloth)	Se(IV)	ML modelling with mechanism study	Predict removal; recyclable catalyst	High: selenium in mine effluents
[47]	Photo-Fenton (Fe–Ni on sludge-derived carbon)	Ciprofloxacin	ML-guided catalyst design	Maximize degradation	Medium: catalyst concept for acidic drainage
[48]	Electrocoagulation + catalytic ozonation	Pharmaceutical wastewater (COD)	ML prediction and intelligent control	Predict and control COD removal	High: combined metal and organic removal
[49]	Persulfate (metal, UV and thermal activation)	Organic pollutants	Interpretable ML	Predict and explain degradation	Medium: sulfate burden must be managed
[57]	Photocatalysis (Mn-doped $BiFeO_3$)	Wastewater pollutants	Random forest; XGBoost	Predict removal efficiency	Medium: turbidity limits light
[76]	Several AOPs	Pharmaceutical compounds	AI-based optimization	Optimize operating conditions	Medium: analogues of organic reagents
[79]	Sulfate-radical AOP	Textile dye	AI-based optimization	Model and optimize removal	Medium: analogues of flotation reagents
[80]	Fe(II)/chlorine; H_2O_2/periodate	Textile dye	ANN–PSO hybrid	Model and optimize removal	Medium: alternative oxidants
[81]	Combined AOP plant	Dye wastewater	Data-driven predictive modelling	Plant design and performance	High: plant-scale approach

6. Sustainability, Energy, Life Cycle and Techno-Economic Considerations

The sustainability case for AI-driven oxidation rests on doing less: lower oxidant and energy input per unit of pollutant removed, fewer by-products and less over-treatment.

6.1 Techno-economics and electrochemical integration

The cost benefits of AI integration with conventional treatment appear to be limited to the savings from chemical and energy savings, with the expenses of sensor and data-infrastructure outweighed by those gains [85]. It has been concluded that AI is crucial in optimizing electrochemical processes for water and wastewater remediation [86] and electrocoagulation [87]. Fenton photo systems included complex neural networks, as an example, to model the degradation of petroleum hydrocarbons [88] applicable to fuel and oil spills to mine sites.

Across the AI for-oxidation studies mentioned here, the most popular are Fenton/photo-Fenton with two studies (47, 88) and ozonation with two studies (29, 48) while combined or unspecified AOPs and photocatalysis studies are the most numerous.

6.2 Energy, toxicity and adoption

The most economical AOP varies with target compound [7] with energy being the dominant operating cost of most AOPs. Energy optimization along with AI-based adsorption is used for sustainable water treatment [89] and a fifteen year timeline of the progress and research of AOP effects has been presented to aid in determining which processes are worth investing in with AI [90]. However, optimizing removal is not enough, there are algorithms that have been developed which predict the ecotoxicity of industrial effluents that can be used to aid in the control strategies, and reviews of AOPs for industrial wastewater have identified "matrix complexity" and "cost" as principal barriers to the adoption of such technologies [91, 92]. AI is being used to manage energy in treatment plants increasingly and can move the energy-heavy oxidation to times when renewable energy is abundant, particularly at remote sites where there is limited power from the grid or diesel.

6.3 Life-cycle assessment and residuals

The wastewater is not a disposal issue anymore but a sustainability resource with the development of integrated solutions that include emerging treatment technologies and IoT monitoring [94]. To address gaps in the inventory and speed up the prediction of impacts, ML is being incorporated into life-cycle assessment [95] [96]. The use of feature-selection techniques in conjunction with ML has also been helpful in the prediction of sludge production in an actual advanced biological treatment plant [97] whose management is crucial to the footprint of Fenton-based processes.

6.4 A closed-loop framework for mine water

The elements of Figure 6 are found in various publications in isolation, for example, real time predictive exposure to •OH [29], intelligent control of COD [48], AI chemical dosing [78], kinetic scale-up models [44], smart energy management [93] and ML-based life-cycle assessment [95, 96]. It is novel for mining because it uses sustainability indicators as live optimization constraints, instead of merely an audit afterwards.

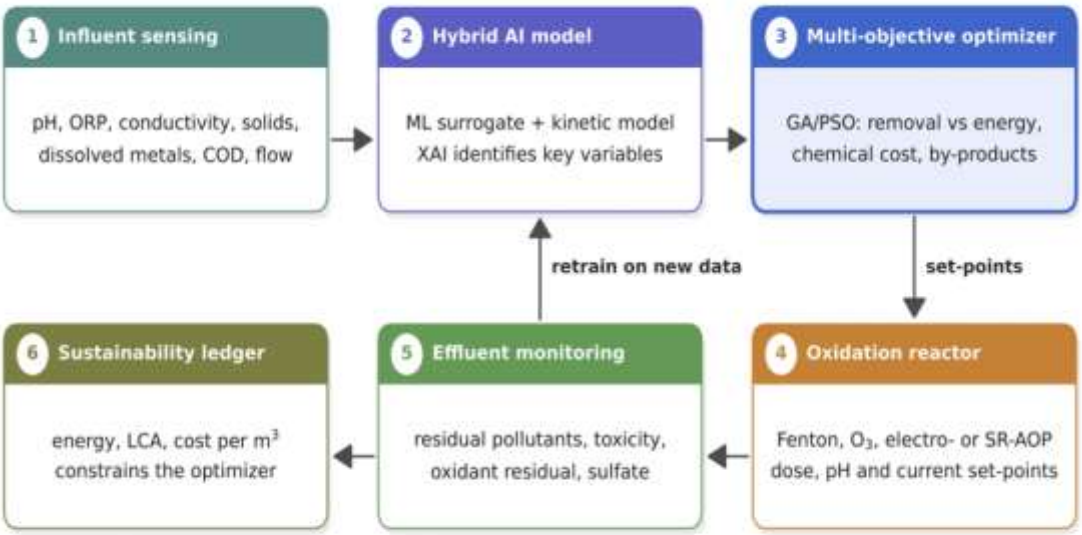


Figure 6. Proposed closed-loop framework for AI driven oxidation of mining wastewater [29,44,48,78,93,95.96].

7. Challenges, Research Gaps and Future Perspectives

The largest barrier to AI-driven oxidation of mining wastewater is empirical rather than algorithmic: almost no published model has been trained on real mine-water data.

7.1 Data scarcity and transferability

For the most part, an AI-AOP model is put together with 10–100 or a couple hundred laboratory tests using synthetic single-pollutant solutions. However, as can be seen in Figure 4, such models cannot be extrapolated to effluents containing high levels of carbonate, chloride or metals that scavenge radicals [5]. There is a need for shared and standardized mine-water data sets, transfer learning methods across different ore types and few-shot methods like graph neural networks [72].

7.2 Interpretability and mechanistic consistency

Black-box predictions are not easy to certify for discharge compliance. Interpretable AI [12] and hybrid kinetic–ML models [44] should be adopted as a standard practice and model output should be validated with known radical chemistry [14] and [15].

7.3 By-products and toxicity

Partial oxidation may result in the formation of products that are more toxic than the parent compound, and chloride-rich waters from mines may increase the likelihood of the formation of halogenated by-products. Boosting algorithms for toxicity prediction [91] and aquatic toxicity QSAR [53] should be incorporated into optimization objectives, not evaluated at the end. Boosting algorithms for toxicity prediction [91] and aquatic toxicity QSAR [53] should be part of the optimization objectives, not post optimization evaluation.

7.4 Scale-up, sensing and deployment

Optima in the lab rarely make the transition to scale up as mass transfer and light and current distribution change. There are bridges, such as microreactor kinetics [44] and plant-scale data-driven design [81] but comprehensive online sensors for oxidant residuals, metals, and toxicity are not widely available. Little attention has been given to deployment of edge computing and cyber security for remote mine sites.

7.5 Sustainability metrics

Here only two of the references refer to life-cycle assessment (LCA) with ML [95] and [96]. Energy per order of pollutant removal, carbon footprint and cost per cubic meter should also be reported with removal efficiency to enable AI to optimize for both sustainability and removal. These challenges and research priorities are summarized in Table 6.

Table 6. Key challenges and research priorities for AI-driven oxidation of mining wastewater.

Challenge	Current status	Research priority	Refs.
Lack of mining-specific datasets	Models trained on synthetic, single-pollutant laboratory data	Open, standardized mine-water datasets with matrix metadata	[77], [90], [92]
Matrix effects (Cl^-, SO_4^{2-}, HCO_3^-, metals)	Scavenging rarely represented as a model input	Scavenger-aware features and kinetic priors	[5], [15], [21]
Limited transferability	Models validated only within the training range	Transfer learning, few-shot learning and applicability-domain checks	[63], [72]
Interpretability	Many black-box ANN and ensemble models	XAI and hybrid mechanistic–ML models as standard practice	[12], [44], [51], [59]
By-product toxicity	Removal optimized; toxicity assessed afterwards	Toxicity-constrained multi-objective optimization	[53], [73], [91]
Catalyst stability in saline, metal-rich water	Catalysts tested in clean matrices	Generative inverse design of fouling-tolerant catalysts	[65], [66], [67], [71]
Scale-up and real-time control	Few pilot- or plant-scale AI deployments	Digital twins with online sensing and adaptive retraining	[28], [48], [81]
Sustainability accounting	Energy and life-cycle indicators rarely reported	ML-assisted LCA and energy-aware optimization	[85], [93], [95], [96]

8. Conclusions

Technically, oxidation with the help of AI can be applied to the treatment of wastewater generated during mining activities, but the evidence base is largely from other sectors. The following is a summary of the main findings of this review.

1. Oxidation chemistry is well developed. There are oxidation methods that can target pollutants in mine water, such as AOPs (based on OH• and SO_4•−), Fenton, ozonation, photocatalysis, and electrochemical oxidation, which are all sensitive to the presence of carbonate, chloride, sulfate and metals, at pH 10, 2 mM carbonate decreases the percentage of the target molecules that can be treated by •OH from 50% to 14%.

2. Kinetic selectivity determines the model design. The ozone rate constants vary by several orders of magnitude and require structure-based descriptors, while the near uniform rate constants for •OH require process-based descriptors, such as radical exposure and scavenger load.

3. Laboratory-based AOPs can be reliably modeled and optimized by ANNs, tree ensembles and GA/PSO optimizers, with mechanistic insights and transferability provided by QSAR, explainable AI and hybrid kinetic ML models.

4. The effort invested in the research is not uniform, with the mineral processing routes (fenton/photo, Fenton and ozonation) being the routes with the least AI studies, whereas photocatalysis and combined AOPs dominate. In the referenced literature, works related to AI surpassed chemistry and process works in 2024.

5. AI Catalyst Design is progressing rapidly but hasn't focused on salt and fouling resistant catalysts for mine water.

6. The best way for achieving sustainable, compliant mine-water oxidation is to implement Closed-loop digital twins that consider energy, life-cycle and toxicity indicators as live constraints.

Open mine water datasets, pilot scale AI-driven AOPs at operating mines, and toxicity and energy constrained optimization are priority next steps.

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