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Mine Water Treatment and the Use of Artificial Intelligence in Acid Mine Drainage Prediction

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Abstract
Acid Mine Drainage (AMD) emanating from coal, gold and copper mining has been widely reported with various negative environmental effects. Challenges associated with mine water can be experienced at a local and a regional scale. Such challenges include contamination of potable water and agricultural lands, and disrupted growth and reproduction of aquatic plants and animals. Therefore, it is critical to implement long term mine water management solutions including treatment of AMD. Treatment options can be broadly classified into passive and active treatment technologies. Both active and passive treatment technologies have their own advantages and disadvantages.

Prediction of AMD quality bears important consequences for long term management of water resources and therefore it is critical to improve the predictive capability of mine water using reliable and modern techniques. Artificial Intelligence (AI) is currently seeing a major interest in all spheres of life and interest from society in general. In this chapter, the authors highlight certain important aspects regarding AMD: generation, remediation, quality prediction using conventional and AI techniques and their limitations. A case study using a hybrid AI system to predict mine water quality is presented and discussed.

Keywords: Acid mine drainage, passive treatment, active treatment, artificial intelligence, long short-term memory, artificial neural networks

List of Abbreviations

AI	Artificial Intelligence
ALD	Anoxic Limestone Drain
AMD	Acid Mine Drainage
ANFIS	Adaptive Fuzzy Interference System
ANN	Artificial Neural Network
BPNN	Back-Propagation Neural Network

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BWPCW	Brugspruit Water Pollution Control Works
DAS	Dispersed Alkaline System
DO	Dissolved Oxygen
DWAF	Department of Water Affairs and Forestry
ECL	Environmental Critical Level
EWRP	eMalahleni Water Reclamation Plant
GARD	Global Acid Rock Drainage
HDS	High Density Sludge
HiPRO	High Recovery Precipitating Reverse Osmosis
LDS	Low Density Sludge
LSTM	Long Short-Term Memory
MEND	Mine Environment Neutral Drainage
OCWRP	Optimum Coal Water Reclamation Plant
OLC	Open Limestone Channel
PCR	Pulsed Carbonate Reactor
PL	Predictive Learning
RAPS	Reducing and Alkalinity Producing System
RBF	Radial Base Function
REE	Rare Earth Element
RF	Random Forest
RGA	Real-Value Genetic Algorithm
RNN	Recurrent Neural Network
RO	Reverse Osmosis
SAPS	Successive Alkalinity Producing System
SRB	Sulfate Reducing Bacteria
SVM	Support Vector Machine
TDS	Total Dissolved Solids
WNN	Wavelength Neural Network

2.1 Acid Mine Drainage (AMD)

2.1.1 AMD Generation

While mining contributes largely to economic and social development in South Africa, its negative environmental impacts are a challenge not only at a local but also at a regional scale [1]. Environmental impacts include the contamination of streams, groundwater, and agricultural land [2, 3]. Ample studies have been conducted, and there is a large volume of literature available about acid mine drainage (AMD) production and its negative effects on the environment worldwide [4–10]. AMD is characterized by a low pH (<5.6) and high acidity, high concentrations of sulfate (SO_4^{2-}), metals and metalloids [1, 11–16]. Most of these constituents, at high concentrations, qualified as toxic in different environmental media, might be harmful to human life and result in negative effects on the ecosystem [17–24].

AMD is primarily engendered from the exploitation of commodities such as coal, gold, copper, and nickel. Minerals containing these elements usually occur in ore bodies that have acid-forming di-sulfide-bearing minerals which are mainly pyrite and marcasite (FeS_2)

[25]. AMD is generated as a result of the oxidation of di-sulfide minerals in the presence of water and oxygen [3, 26–30]. Research on AMD from other sulfide minerals such as pyrrhotite (FeS), chalcocite (Cu_2S), galena (PbS), sphalerite (ZnS), chalcopyrite ($CuFeS_2$), millerite (NiS), and mackinawite [(Fe,Ni)S] is limited [28]. Many authors illustrate examples of chemical reactions during AMD production using pyrite as a common sulfide mineral [28–36]. The foremost reaction is the oxidation of pyrite into (SO_4^{2-}), ferrous iron (Fe^{2+}), and protons (H^+, Eq. 2.1)

$$FeS_2(s) + 3.5\,O_2(g) + H_2O\,(l) \rightarrow Fe^{2+}(aq) + 2\,SO_4^{2-}(aq) + 2\,H^+(aq) \tag{2.1}$$

Fe^{2+} is then oxidized to ferric iron (Fe^{3+}) (Eq. 2.2):

$$4\,Fe^{2+}(aq) + O_2(g) + 4H^+(aq) \rightarrow 4Fe^{3+}(aq) + 2\,H_2O\,(l) \tag{2.2}$$

Oxidation of the ferric ion can produce soluble ferrous ion (Fe^{2+}), SO_4^{2-}, and more protons (Eq. 2.3):

$$FeS_2(s) + 14\,Fe^{3+}(aq) + 8\,H_2O\,(l) \rightarrow 15\,Fe^{2+}(aq) + 2\,SO_4^{2-}(aq) + 16\,H^+(aq) \tag{2.3}$$

2.1.2 Factors Controlling AMD Generation

The occurrence and rate of AMD generation are dependent on many factors and are site-specific [27]. The primary factors include the geological and hydrological characteristics of the site, type of sulfide mineral(s) present and their surface area, availability of oxygen, pH and temperature of the interacting water, heat that is being generated as a result of chemical reactions, chemical reactivity of Fe^{3+} in the system, and the availability of bacteria to catalyze the oxidation reaction, among others [27, 38]. For example, easily oxidized sulfide minerals (e.g., framboidal pyrite, marcasite, and pyrrhotite) result in a faster generation of acid. Sulfate compounds also add to the generation of AMD by contributing to the release of constituents such as Fe, Ni, and U in solution [27, 38]. Climate is also an important factor influencing the rate and effects of AMD. The generic process for the generation of AMD incorporates sulfide sources, water sources, and mixing zones where sulfide minerals are exposed to water in an oxidizing environment (Figure 2.1) [23]. South Africa has a prominent east to west climatic slope where annual rainfall ranges between 100 mm and 1,000 mm in the west and east respectively. Annual evapotranspiration potentially increasing from about 1,500 mm in the east to 3,000 mm in the west. Such climatic conditions result in most parts of the country to experience a negative water balance where rainfall is lesser than evapotranspiration. During dry periods, solid efflorescent salts are generated and the solutes that are formed, such as Fe, H^+, and SO_4^{2-}, are released when dissolved during the rainy seasons [39–41].

Younger [43] has described the process of mine flooding and its influence on acid generation, based on experience in British coal mines. During the period of active operation of an underground mine, the open mine workings allow the reaction between oxygen in the

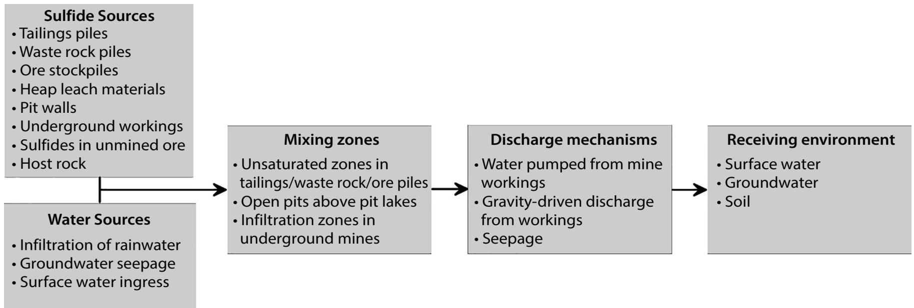

Figure 2.1 Generic process for the generation of AMD incorporating sulfide sources, water sources, and mixing zones where sulfides are exposed to water in an oxidizing environment (modified after the Global Acid Rock Drainage Guide [42]).

air-filled voids, water seeping through the mine and the surrounding rock mass, and sulfide in the mine and rock mass to interact. This oxidizes pyrite, generating AMD as well as solid weathering products in the form of acidic sulfate-bearing minerals. On the cessation of underground operations, as the underground mine workings flood, these minerals are dissolved, resulting in the first flush of acidic water. The flooding of the workings reduces the availability of oxygen, substantially reducing the oxidation of pyrite and the generation of new acidity. Younger [43] describes the two types of acidity generated within a mine void as juvenile acidity—the acid generated by the oxidation of fresh sulfide minerals—and vestigial acidity—the acidity generated by the dissolution of secondary minerals which accumulated during active mining. Mine flooding largely excludes oxygen from the flooded workings, reducing the generation of new juvenile acidity, often leading to substantial improvements in water quality once the first flush, which liberates vestigial acidity from secondary minerals, has dissipated. Where mine workings remain air-filled after mine flooding, juvenile acidity may still be generated for many years following partial mine flooding.

A permanent infiltration zone may develop where the discharge point from a mine void is located at a topographic level below the level of the highest lying shallow mine workings. This will result in a water level in the underground mine workings which is below

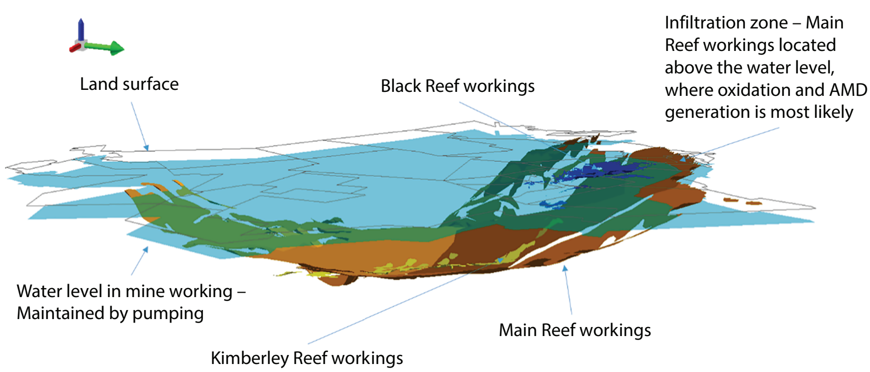

Figure 2.2 Three-dimensional model of South Africa's East Rand Goldfield, showing the presence of unflooded workings above the water level within the voids, as currently maintained by pumping.

the shallow workings in the high-lying areas of the mine or complex of mines which will continue to contribute acidity. The water level may be maintained by pumping, as is currently the case in South Africa's Witwatersrand Goldfields (Figure 2.2), or by gravity-driven discharge via a low-lying shaft or adit.

The Transvaal and Delagoa Bay Colliery in South Africa's Mpumalanga Coalfield is another example of a mine where acid generation continued for many years after flooding [7]. Located on a hillside, the mine workings were allowed to flood. Water entering the mine tended to flow through the workings, leaving a partially air-filled void with the continued generation of acidity. When the effect of this mine was investigated in the early 2000s, low pH values and extremely high sulfate concentrations were still recorded in the discharged water more than half a century after the cessation of mining.

2.2 Remediation of AMD

2.2.1 Introduction

Different AMD control technologies have been investigated, demonstrated, and implemented in different countries such as the United State of America (USA), China, Canada, Australia, Germany, Spain, and South Africa. There are numerous studies and a large volume of literature about AMD treatment techniques available for remediation worldwide. Chemistry and flow rate of the discharge, designated use, space availability, and seasonal fluctuations of the receiving stream are important factors when selecting an appropriate treatment technology [44–47]. There are two broad classes of technologies to treat AMD: passive and active treatment technologies [47–49].

2.2.2 Passive Treatment of AMD

Passive treatment is considered a long-term solution for the management of polluted mine water in many parts of the world [50, 51]. This treatment technique is usually associated with low costs of operation, monitoring, and maintenance [51–53] since it relies on natural ameliorative processes and accessible energy sources to remove contaminants in the water [55]. PIRAMID Consortium [45] defines passive treatment as "the improvement of water quality using only natural available energy sources in gravity-flow treatment systems which are designed to require only infrequent maintenance to operate successfully over their design life".

Different types of passive treatment technologies are available. Examples of passive treatment technologies include anoxic limestone drains (ALDs), aerobic and compost wetlands, reducing and alkalinity producing systems (RAPS, initially called SAPS) and dispersed alkaline systems (DASs). Passive treatment systems range from technologies that were successfully implemented at a full scale, to technologies that are currently being tested at a laboratory scale. The chemistry of AMD discharge (pH, acidity, Fe^{2+}/Fe^{3+}, Al, Mn, SO_4^{2-}), dissolved oxygen (DO), flow rate, and the topography are factors taken into consideration when evaluating and selecting the appropriate passive treatment type [51, 54–57].

Selecting a suitable passive treatment system depends on the chemistry and flow rate of the water to be treated (Figure 2.3) [53–58]. When the pH of water is net alkaline, a settling

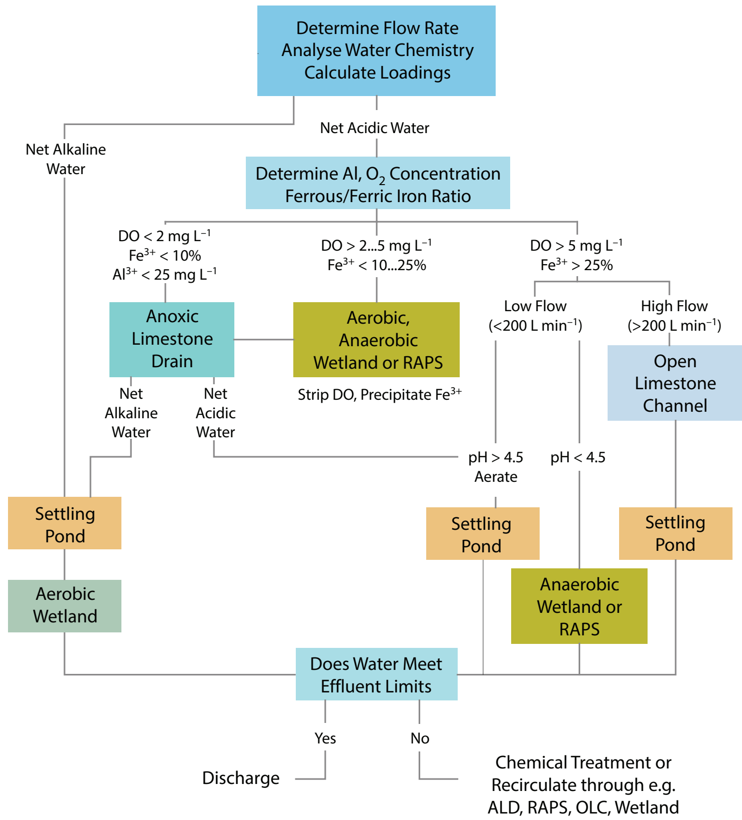

Figure 2.3 Flowchart assisting in the selection of a suitable passive treatment technology for polluted mine water (modified after [53]); image courtesy Christian Wolkersdorfer.

pond may be used to settle most of the suspended solids, followed by an aerobic wetland to oxidise and precipitate metals present in high concentrations (Figure 2.3). In the case of net acidic water, the chemistry of the water should be studied thoroughly to determine the DO concentration, Fe^{2+}/Fe^{3+} ratio, and Al concentrations. If the DO concentration is less than 2 mg/L, the Fe^{3+} concentration is less than 10% of total Fe, and the Al concentration is less than 25 mg/L, ALD will be the best suitable treatment system to use.

For further selection, when AMD has a DO concentration between 2 and 5 mg/L and the Fe^{3+} concentration ranges between 10 and 25% of the total Fe, a SAPS/RAPS can be used. These systems include a combination of an anaerobic or aerobic wetland and ALD. When acidic water (pH less than 4.5 in this case) has a DO concentration of more than 5 mg/L, the Fe^{3+} concentration is more than 25% of the total Fe and a low flow rate (less than 200 mg/L), an anaerobic wetland or SAPS may be used to treat the mine water. However, if the water has a pH of more than 4.5 with the same DO concentration, Fe^{3+} concentration and low flow rate mentioned above, the water can be aerated and transferred to a settling pond for further treatment. Furthermore, if the DO concentration is more than 5 mg/L, the Fe^{3+} concentration is more than 25% of the total Fe and there is a high flow rate (greater than 200 mg/L), open limestone channels (OLC) may be used.

Most of the passive treatment systems mentioned above are followed by a settling pond to settle most of the suspended solids, and when the effluent meets the required water quality standards it can be discharged to the receiving environment. However, when the treated effluent does not meet the water quality standards, retreatment or chemical treatment through RAPS, wetlands, OLC, ALD, or other systems will be needed until the effluents meet the water quality standards. A periodic table for passive treatment, created by Gusek [59], has also been used in the selection of the type of passive treatment (Figure 2.4). From the passive treatment periodic table, it can be seen that high concentrations of Fe, Al, and As can be treated using anaerobic and oxidizing passive systems, whereas Mn can only be treated using oxidizing systems. SO_4^{2-} may also be potentially removed by means of anaerobic systems through microbial reactions. In South Africa, to date, the application of passive treatment for amelioration of contaminated mine water is mainly demonstrated at a pilot and laboratory scale. Therefore, the potential for demonstration of passive systems on a full scale for long-term treatment of AMD is substantial.

2.2.3 Active Treatment of AMD

Active treatment of mine water entails improving the water quality using techniques that requires continuous addition of artificial energy or (bio)chemical reagents, or both [14]. According to the Acid Rock Drainage Prediction Manual, Eger and Wagner, and Watzlaf *et al.* [15, 49, 53], treatment of AMD by conventional treatment technologies is expensive and a long-term commitment. Active treatment uses a range of chemicals such as limestone, soda ash, caustic soda, ammonia, hydrated lime, and pebble quicklime [14, 60]. The selection of the appropriate chemical and suitable active process is influenced by a range of factors (Figure 2.5) including the water chemistry (i.e., total dissolved solids (TDS), total

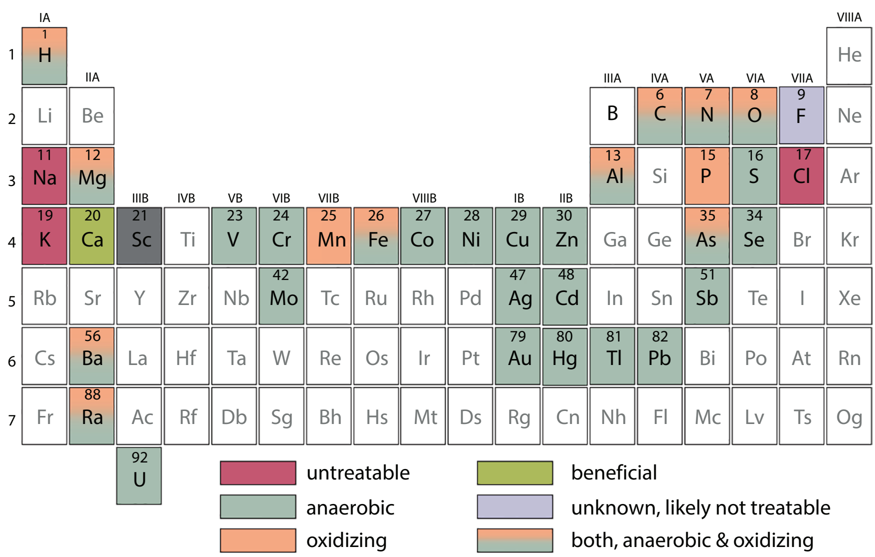

Figure 2.4 Periodic table for passive treatment (modified after Gusek [59]); image courtesy Christian Wolkersdorfer.

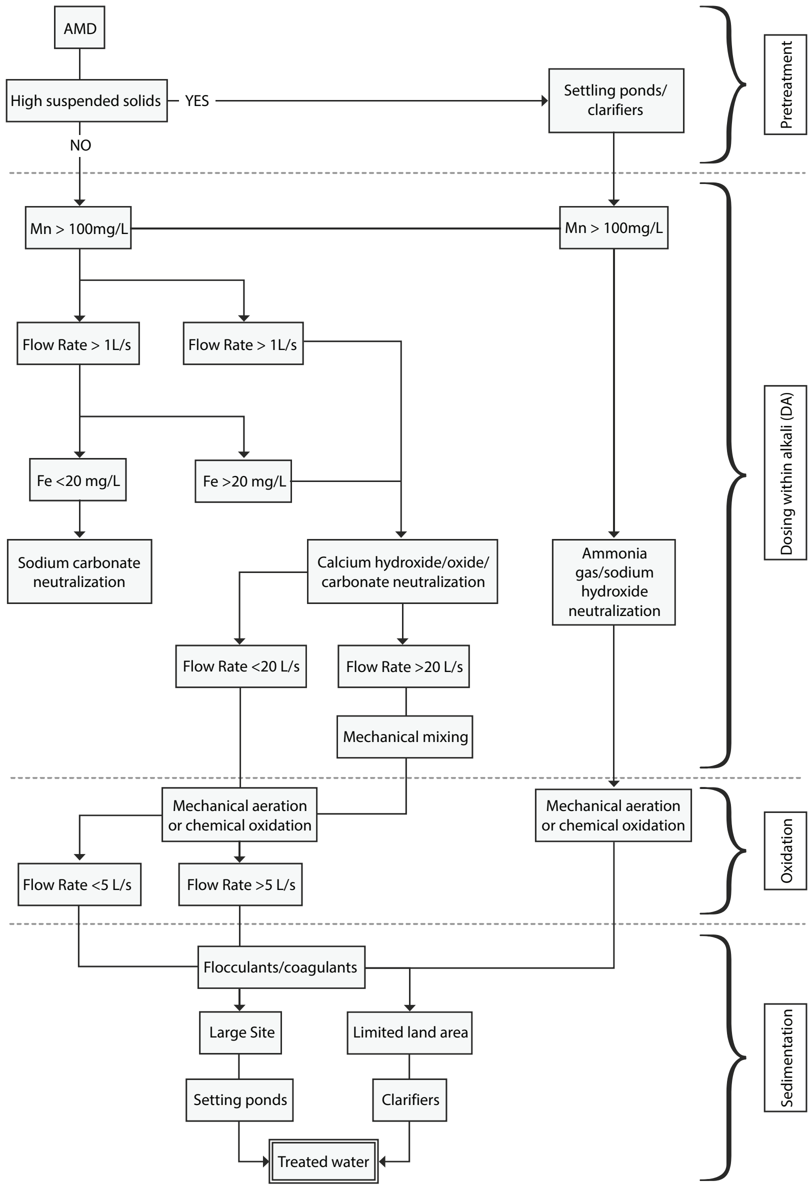

Figure 2.5 Flow chart for the selection of a site-specific active treatment system for AMD (modified after [47]).

suspended solids, and metal concentrations), quantity and flow rate, space, availability, and local climate [61–66]. Although active treatment can ameliorate AMD effectively, they are labor, energy, and maintenance-intensive and therefore not favored for abandoned mines.

There are different active treatment processes that are used for AMD remediation and some of those working at full scale are mentioned as:

a) Low density sludge (LDS): process plants that can accommodate AMD with any acidity loads. According to Taylor *et al.* [11], there are three main treatment stages involved. The first is the reagent mixing and dosing phase where a neutralizing reagent is mixed with AMD to produce a slurry. The second stage includes a reaction phase where mechanical stirrers are used to mix the slurry solution through one or more reactors. Mixing may also take aeration into account to oxidise any reduced metals. The third stage of treatment is the flocculation and clarification stage. This stage includes a thickener or clarifier tank where neutralized water from the second stage enters. For facilitation for sludge settling, a flocculant may be added. The disadvantages of LDS plants for AMD treatment include the large volumes of low-density sludge produced, storage needed for the sludge and the costs associated with sludge handling.
b) High density sludge (HDS): a treatment process that is similar to LDS and involves three stages of treatment, i.e., the reagent mixing stage, reaction stage, and the flocculation and clarification stage. This treatment process is better compared to LDS as the generated sludge contains enough alkalinity and is recirculated back into the treatment process along with the alkaline reagent. Therefore, the final sludge for disposal is concentrated and requires reduced storage space, also maximizing the sludge stability and density [11].
c) Pulsed carbonate reactors (PCRs): a treatment process centered around the principle of increasing the partial pressure of CO_2 in water intensely to improve the solubility of carbonate material such as limestone. Treatment includes CO_2 initially absorbed into AMD at atmospheric pressure and then palpitated over successive reactors and neutralized with calcium carbonate [11].
d) Electrochemical concentration technique: processes that use a combination of chemical, magnetic, electrical, and plasma techniques to recover metals from an AMD solution [11].
e) Biological mediation: a technique that takes AMD neutralization, sulfate reduction and redox control [67] into consideration. Micro bioreactor systems are used for chemical and biological processes [68].
f) Reverse Osmosis (RO): a treatment process that uses a semipermeable barrier (membrane) at a certain pressure to treat mine water. This semipermeable membrane, such as a cellophane-like semipermeable cellulose acetate membrane, impedes the flow of larger molecules (e.g., urea, glucose, and bacteria) and solutions (e.g., Na^+, Ca^{2+}, Cl^-) to pass through [69, 70]. The membrane only allows the passage of water. According to Feng *et al.* [71], membranes during RO processes have been shown to substantially reduce TDS, metals and metalloids, organic pollutants, viruses, bacteria, and other dissolved contaminants.
g) Ion exchange: a process where undesirable or potentially toxic ions in water are exchanged for desirable or less toxic ions [72]. Materials such as zeolites and resins are generally used for ion exchanges processes. According to Johnson and Hallberg [72], only ions with the same electric charge can be exchanged.

Currently, in South Africa, treatment of AMD on a bigger scale is being carried out in six active treatment plants of which three are situated in the East, West, and Central Rand Goldfields of Gauteng Province and three are situated in the coalfields in Mpumalanga Province. The HDS treatment plants in the East, Central, and West Rand Basin plants can treat 50,000 m^3/d, 82,000 m^3/d, and 110,000 m^3/d of mine water respectively, after which the treated water is released into adjacent rivers [73].

Two key-plan high-recovery precipitating reverse osmosis (HiPRO) treatment process plants exist in Mpumalanga Province: the eMalahleni Water Reclamation Plant (EWRP) and the Optimum Coal Water Reclamation Plant (OCWRP). In both cases, the treatment technology involves neutralization, reactors and clarifiers, multistage ultrafiltration, reverse osmosis, and sludge dewatering [74]. Implemented in the eMalahleni area in 2007, the EWRP treats AMD from several mines including Greenside Colliery, Kleinkopje Colliery, South Witbank Colliery, and Navigation Colliery and has been operating successfully since then [75, 76]. Its main aim is to treat AMD, produce high quality potable water for local municipality use and being safe for environmental release, with a current treatment capacity of 50,000 m^3/d [75]. On the other hand, the OCWRP was built in 2010 and has a capacity of 15,000 m^3/d presently. According to the Aveng Group [76], most of the reclaimed water is distributed to the local Hendrina municipality and the remaining is discharged into the Klein Olifants River. Because of the drinking water quality standard of the treated mine water discharge, the plant was bestowed with the prestigious Blue Drop Certification by the Department of Water Affairs (DWA) [77].

In 1997, the Brugspruit Water Pollution Control Works (BWPCW) plant eMalahleni, Mpumalanga Province was constructed by Department of Water Affairs and Forestry (DWAF) to protect Loskop Dam from negative effects of AMD [78]. This plant was treating AMD from the defunct and flooded underground coal mines towards the west and northwest of eMalahleni (Witbank), which started discharging in the mid-1990s [78, 79]. This AMD discharge was one of the contributors to the pollution of the water resources in the upper Olifants River catchment [78, 79]. Water was treated with sodium hydroxide to increase the pH and soda ash to increase the buffering capacity of the final effluent [19, 20]. Before unforeseen circumstances caused the treatment plant to fail, it could treat 10,000 m^3/d and is currently not operational [67].

2.2.4 Challenges With Current AMD Treatment

Passive treatment is capable of improving the water quality of polluted mine water. However, the long-term sustainability of these systems is a common problem and should be ensured by developing appropriate site-specific design criteria (Section 2.1). The depletion rate of the neutralizing agent and organic matter used in different systems is also a key problem [80]. Clogging, due to precipitate build-up and biofilms, is the leading drawback in these treatment techniques affecting the efficiency and longevity of such systems [11, 53]. Clogging results in the passivation of the alkaline substrate slowing down the dissolution rate. This challenge has been addressed by occasional maintenance where periodic flushing of the system is done. Another disadvantage associated with these treatment systems is minimal or no SO_4^{2-} and Mn^{2+} removal. The reasons for this limited or non-performance are lack of sulfate-reducing bacteria (SRB) for SO_4^{2-} reduction and the presence of Fe in the treatment system which competes for oxygen with Mn^{2+}, among others. Moreover, passive treatment systems can only accommodate low-flow volumes, with some exceptions, and cannot cope with high-flow volumes of mine water.

Challenges associated with the existing active treatment systems of AMD include the costs of operation and maintenance, especially in the case of those mines that reached end of life. The major challenge with the active treatment technologies is that they require constant addition of chemicals and artificial energy [81]. High-priced chemicals and operational resources are some of the factors that discourage the continuous active treatment of AMD. Furthermore, some of the neutralizing chemicals such as sodium hydroxide (NaOH) and anhydrous ammonia (NH_3) are hazardous. The extreme use of ammonia may result in challenges like denitrification and nitrification of receiving aquatic environments [82]. Storage and disposal of the slurry produced from the treatment plants are also considered a problem with the active treatment systems.

In the Witwatersrand basin, the mine water is currently being pumped and neutralized to keep the rising water levels under the environmental critical level (ECL). Neutralization is achieved with limestone or lime, or both, to reach a pH value that is suitable for discharge. This process adds alkalinity to the water, increases the pH and precipitates some of the metals as hydroxides. One of the challenges with the existing treatment plants in South Africa are the SO_4^{2-} concentrations in the treated water that are above the South African water quality standards acceptable for discharge [83]. The costs of implementation and operation of the treatment plants are also one of the predicaments of mine water treatment in the country. By the year 2020, R12.3 billion are anticipated to be spent on the implementation of treatment plants in the Eastern, Central, and Western Basins of the Witwatersrand [83, 84]. According to the studies, 67% of this amount will be or have been paid by the operating mining companies in these areas. The envisaged dilemma with these current plants is the continuation of receiving funding for maintenance and running the plants especially once the operating mines that are currently contributing, reach mine closure. Moreover, issues like vandalism are also a major challenge that may lead to failure of mine water treatment plants [67].

2.2.5 Value Recovery From AMD Treatment

Resource recovery and reuse is possible as a holistic sustainable approach in AMD treatment. Nonetheless, not many studies were carried out with regard to AMD-treated water reuse and resource recovery. In South Africa, many researchers have carried out studies on metal precipitation from AMD [3, 68, 86], but only a few have focussed on the recovery of valuable metals [87–89], sulfuric acid [90], and water for reuse [91, 92].

AMD is characterized by high concentrations of metals and metalloids and some of these constituents can be extracted through treatment for economic benefit and to achieve a circular economy. Several authors [65, 93] noted the possibility of recycling Fe-rich precipitates such as jarosite ($KFe_3(SO_4)_2(OH)_6$), schwertmannite ($Fe_{16}O_{16}(OH)_y(SO_4)_z.nH_2O$), goethite (FeOOH), and ferrihydrite ($Fe(OH)_3$) for products such as mineral pigments, depending on the variations in the major and trace metal chemistry. These Fe-hydroxides are acknowledged as sorbents of trace metals and consequently can control the kinetics of the trace metals (e.g., Zn, Co, and Ni) in the environment. Recovery of such trace metal species during remediation presents a case for offsetting treatment costs. Research around the recovery of rare earth elements (REEs) from AMD has also been done as a source for critical materials for batteries, magnets, and other electronic components. Recently, AMD and treated mine water via active and passive treatment were studied as likely economic sources of REE [65, 93–96]. Some of these REEs occur as sulfate species [65] and their recovery is a promising possibility that could potentially offset AMD treatment costs [97].

Partially treated mine water may be suitable for other applications such as in agriculture, sanitation and industries where high-quality water is not often required provided it is treated to acceptable concentrations for various pollutants [65, 73, 97–99]. The advantages of this approach include cost savings from a reduced treatment cost point of view as well as the availability of water as a resource [11, 68, 87].

2.3 Prediction of AMD

In mining environments where AMD may be generated, prediction plays an important role in mine planning, prior to the commencement of mining, environmental management during mining and closure planning during the late stages of mining. In addition, in mining legacy areas where no mine operator is present, predictive tools may be used to estimate the seriousness of current and future effects, as well as the duration of expected ongoing effects.

Three approaches for the prediction of AMD are commonly used:

a) Field measurements, including simple sampling and analysis, as well as controlled field experiments such as the construction and monitoring of lysimeters within the mining environment and field tests such as wall washing [100].
b) Numerical geochemical models, for example, PHREEQC [101], where known chemical parameters of specific minerals are used to predict the reactions between these minerals and solutions. Geochemical models may be coupled with flow models to predict the generation of AMD as well as its transport and fate in the environment.
c) Laboratory experiments, where samples of the material encountered in the mining project are exposed to laboratory-simulated environmental conditions, allowing researchers to monitor process and sample reaction products to develop predictive models of the likely behavior of the materials involved in the mining environment. Since the processes leading to the generation of AMD often operate over periods of decades and even centuries, these laboratory methods generally accelerate the reactions, allowing meaningful conclusions to be drawn in a manageable time-frame, typically days to weeks.

In practice, a meaningful AMD prediction exercise will combine all three of these approaches. Field observations and experiments may be used to develop a reliable conceptual model of the mining environment and to identify physical processes which are likely to influence, accelerate or retard the generation of AMD. A reliable conceptual model is essential in the design and parameterization of geochemical models if the results are to be at all relevant to the real-world situation. Likewise, laboratory tests need to be carefully selected to best represent the real-world conditions which will be experienced during the mining life cycle. A critical consideration for the prediction of mine water quality is that the results of the field investigations, laboratory tests, and numerical models should display sufficient consistency to represent the conditions on the mine and that they should be defined with reference to observed field conditions at all time.

These approaches have been well summarized in the Global Acid Rock Drainage (GARD) Guide [42], while detailed descriptions of laboratory methods have been provided as part of the Canadian Mine Environment Neutral Drainage (MEND) Programs [15]. The basic approach determines [27]:

a) Whether a given sample of material will generate acid drainage, or if it has sufficient neutralization potential to counteract the acidification by sulfide oxidation (e.g., acid-base accounting);
b) What the likely chemistry of the resulting reactions is (various leach tests); and
c) What the behavior of the material is likely to be over time (kinetic tests, including column tests, and humidity cell tests).

Additional laboratory tests such as the Mine Water Leaching Procedure [102] may be employed to determine the interactions between ore and mine residue leachates and other materials.

2.3.1 Limitations of Predictive Tools

The tools used to predict AMD have a number of limitations. In particular, they generally rely on simplified models of the orebody, the mine, and the environment where they exist. In the case of pre-mining predictive modeling, the modeling can also not accommodate changes in the mining programs when the mine operator has to adapt to new information gathered during mining, often rendering the pre-mining predictive models less relevant to the real-world conditions.

Orebodies and mines are complex environments, which are often difficult to reduce to manageable conceptual models. The resulting simplification often fails to provide an adequate prediction of the behavior of the source material, possible pollution dispersal pathways and discharge or fate in the environment. Particularly when these tools are applied in the early phases of a mining project, with the objective of developing mine closure plans and post-closure environmental management programs, the oversimplification may fail to adequately predict real outcomes. Changes in the initial mining program may exacerbate this problem.

While not an inherent quality of predictive modeling, a lack of interdisciplinarity in many environmental impact prediction exercises results in overly narrow predictions being made, with the prediction of water chemistry being done by geochemists and or chemists with insufficient involvement of hydrologists, hydrogeologists, and mining engineers. Constrained budgets in terms of both funding and available time will often exacerbate this problem. The prediction of AMD generation, transport and effect are then often treated as a problem defined by the chemistry of the ore and host rocks and their likely interactions with the environment.

Critical system components are often ignored or underemphasized. These include the topography of a mining area and its influence on the availability of water or oxygen in different parts of an underground or open-pit mine. For example, in the West Rand and Central Rand Goldfields of South Africa, extensive outcrop and near-surface underground operations were developed in the early stages of mining [103]. Within each of these goldfields, the underground workings of multiple mines are interconnected, resulting in water flow from mine to mine. Even if mines are allowed to flood and discharge to surface in the low-lying portions of these goldfields, as happened in the West Rand in 2002 [104], a substantial volume of the mine void will never flood, leading to the ongoing generation of juvenile acidity. It is therefore for the reasons above that people have started looking at alternative techniques to predict mine water quality for better decision-making.

2.4 Application of Artificial Intelligence for AMD Quality Prediction

2.4.1 Introduction

Artificial Intelligence (AI) is the study of making computers to perform functions or activities that are currently deemed "intelligent", such as learning, decision-making, solving problems, among others. The main aim of AI is to produce intelligent machines, computer programs, or embedded systems. Consequently, the field of AI is multidisciplinary in nature, combining various fields such as computer science, psychology, philosophy, and engineering.

The question of whether a machine is able to exhibit human-like intelligence has been a subject of debate for years. Many are against the idea of saying that some behaviors such as creativity, love, and moral values cannot be understood by machines. Others have accepted that machines can indeed exhibit aspects of human-like intelligence. This disagreement remains unresolved. In order to understand AI, it is important to define the concept of "intelligence". Intelligence may be defined in two ways [105]:

a) Intelligence is the ability to interpret and acquire knowledge and skills through a thought process, and
b) Intelligence is the ability to think and comprehend things using instincts.

The first definition does not include machines, whereas the second definition is more flexible to accommodate machines exhibiting intelligence. Thus, for a machine or someone to exhibit intelligence, the ability to think, learn, or understand is required. Thinking may be defined as "the activity of using the brain to consider a problem or to create an idea". Thus, intelligence may be defined as "the ability to think, learn and/or understand to solve problems and to make decisions" [105]. Humans, animals, and machines have this ability. Fundamentally, AI seeks to answer the question as to whether a machine is able to do things which at present are done by humans. The field of AI has been formulated in 1943 and since then has developed steadily until the present day. AI has many branches, all of which are connected and share commonalities and is widely used to build expert systems for natural language processing, robotics, speech, planning, and vision [106].

Uncertainty and subjectivity are inherent in all predictive modeling techniques as these assessments rely on expert opinions. These limitations have to be taken into consideration when formulating predictive intervening, especially if the results are intended to be used for critical applications such as decision-making. By quantifying and incorporating uncertainty and subjectivity, AI systems have been successfully used for prediction in fields such as robotics, science, and engineering [107].

The benefits of using AI for data processing and automation can potentially supplement human mind that has limited ability for processing data and susceptible to subjective bias, AI models can process huge amounts of data relatively faster with greater accuracy. Therefore, predictive models can help reduce computational cost while increasing computational speed, reliability, and consistency in addition to reducing any human-induced uncertainties [108, 109].

2.4.2 Different AI Techniques Used to Predict AMD Quality

The common AI tools used for predictive modeling of water quality can be classified into three board types, namely, the knowledge-driven, the data-driven, and the hybrid type.

According to Swain [110], knowledge-driven systems are computer programs that use knowledge (Expert) base with an inference engine meant to solve problems that typically entail substantial specialized human capability. The knowledge base comprehends an assembly of information while the inference engine infers interactions from the information instituted in the knowledge base. The knowledge-based systems moreover include an interface for users to be able to interrogate the system. Knowledge-driven AI techniques involve articulating computer-based systems that enable extracting and copying intellectual reasoning in making conclusions. Thus, the computer emulates human thought processes [110, 111]. The most common example of knowledge-driven techniques includes fuzzy inference systems, which are often used where the relationship between the input parameters and desired predicted variables is well understood.

Data-driven AI systems are computer programs that solve problems using information derived from data without explicit knowledge of the problem [112]. Modern-day data-driven AI approaches are mainly machine learning in nature. According to the literature, the widely used data-driven tools are regression analysis, artificial neural networks (ANNs), random forest (RF), decision trees, support vector machines (SVMs), radial base functions (RBFs), and genetic algorithms.

Maier and Dandy [112] used ANNs as a viable means of forecasting water quality parameters (salinity) in the Murray River at Murray Bridge (South Australia). The ANN results improved the 14 days forecasting better than the previously used real-time forecasting simulation. Bayatzadeh Fard [113] successfully used ANN and multi-output adaptive neural fuzzy inference systems (ANFISs) to estimate the distribution of (semi-)metals in groundwater of the Lakan lead-zinc mine with a high degree of accuracy.

SVM and back-propagation neural networks (BPNNs) were used to predict the concentration of Ni and Fe generated by the anthropogenic-activated pyrite oxidation in mining areas [114]. In this study, the SVM model provided a better and faster prediction of the Fe and Ni metals. Similar conclusions were also drawn by Tan *et al.* [115] regarding the superiority of the SVM over the ANN in water quality predictions. A hybrid method which is known as the real-value genetic algorithm support vector machine (RGA-SVM) was utilized to predict the quality of aquaculture water [116]. This proved to be an effective approach to predict aquaculture water quality when compared with the traditional SVM and back-propagation neural network models (BPNNs). A machine learning technique, in particular, regression tree induction, was applied to address the difficulty of inferring the chemical parameters from biological parameters of water quality [117]. This proved to be particularly important in enabling selective chemical monitoring of Slovenian River water quality.

Various AI algorithms such as knowledge-based systems, genetic algorithms, ANNs and fuzzy inference systems were used by Chau [118] to simulate and integrate flow and water quality measurements in coastal environments. The use of AI proved to be very useful in incorporating existing heuristic knowledge from various model developers and practitioners and furnished intelligent manipulation of the calibration parameters of numerical modeling systems.

Wavelet-neural network (WNN) and ANN techniques were used to predict water quality parameters (mineralization, temperature, and DO) in Hilo Bay, Pacific Ocean [119]. The outcome of the research shows that the WNN approach is superior to the ANN approach with over 0.98 correlation between model values and the actual values. The research also established that the approach managed to obtain good results even though some of the ocean data was missing due to a lack of regular acquisition or difficulty in data acquisition.

The application of AI for the prediction of mine drainage is not new. Several authors used machine learning techniques such as ANN [120], SVM [121], RBF [121], and K-mean [121] to model and forecast AMD quality using past physico-chemical parameters of a mining area. AI tools such as machine learning offer a rapid and cost-effective solution for mine water quality forecasting.

2.4.3 Limitations of AI Techniques in Prediction of AMD Quality

The AI techniques have their own limitations which include:

a) Time consuming processing and training of the model as optimization is heuristically and repeatedly performed until a good model or learning technique is obtained.
b) Most experts find it difficult to interpret and explain decisions made by AI models, suggesting its black box nature and limiting its successful application.

For any prediction, including mine drainage quality, a thorough investigation and understanding of the fundamental physical processes is compulsory. However, it is often challenging to involve domain expert knowledge directly into the data-driven approaches [122]. Hence, hybrid approaches are developed to mitigate this problem.

Prediction of mine drainage is very complex as the conditions which produce the drainage quality are normally nonlinear, dynamic, and change over time. In addition to this, acquiring good quality mine drainage data is difficult and often contains missing and erroneous values [122]. The approaches mentioned in the previous section often fail to learn the time-variant parameters leading to low accuracy and poor generalization, hence specially designed algorithms that can learn time series data are required. A recurrent neural network (RNN) is used for time series data learning but is mostly not successful when learning the long-term dependences [123], hence the long short-term memory (LSTM) is a specifically designed RNN to overcome this problem. Guazhou Water Source (China) project [124] tested the applicability of using LSTM to predict water quality of the Yangtze River in Yangzhou. The project results show that the trends in the water quality are in agreement with the actual measured values endorsing its potential for utilization as a powerful drinking water prediction tool.

Even with the availability of a well-trained and optimized model, the ability to interpret and analyze the results requires expert domain knowledge, and this can be only achieved by popularizing the predictive learning (PL) models among domain experts [122].

2.4.4 Case Study—Ermelo Coalfield, South Africa

The Ermelo Coalfield study investigates the application of a hybrid system, which combines LSTM and ANN to predict mine water quality with particular emphasis on sulfate concentration from an abandoned underground coal mine in Carolina Town, Mpumalanga Province of South Africa. The full details of this case study are presented in [125].

The methodology involves first the understanding of the likely factors contributing to mine water quality, approximated by the sulfate concentrations in the study environment [126]. According to [127], the most important external factors that contribute to AMD generation at an underground site are recharge (rainfall as a proxy), water table level fluctuations, soil temperature, and water pH. For the study area, the datasets were obtained from various governmental institutions, and hydrogeochemistry data was collected from the discharge test site between 1 November 2014 and 13 June 2018. The forecasting system can be divided into two sub-systems (Figure 2.6): LSTMs and ANN systems. The system architecture is designed to accept historical data (input parameters and output labels) for the training and optimization processes of the ANN system.

To improve the training and avoid under and overfitting, early stopping was used. Early stopping is whereby the training process is stopped when no further decrease in the training root mean square value is observed. LSTMs are used to predict the future values of each input variable (Figure 2.6). The blue dots represent the observation data, the black line is the LSTM fitting model for the observation data and the red line is the output prediction data for the four input parameters (Figure 2.6). Historic data spanning over 1,400 days was used for training and the next 350 days as testing.

The gradient descent optimizer algorithm with a batch size of 100 was used for training the ANN using the historic input parameters (pH, soil temperature, rainfall, and water table). During training, data is fed into the input layer which is connected to one or more "*hidden layers*" where the actual processing is performed by adjusting the weights "*connections*" using the back-propagation algorithm. In a sense, ANNs learn by example, in the same way, as a child learns to walk from observing adults walking. Thus, learning by neural networks may be viewed as a case whereby network weights are updated to produce the desired output, based on a set of

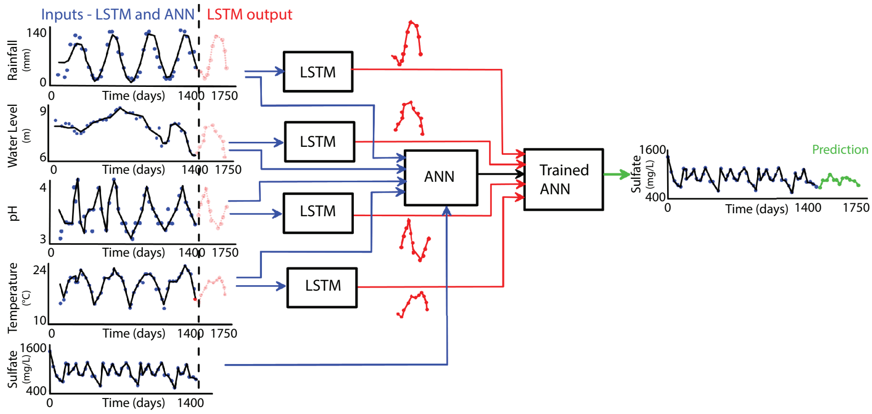

Figure 2.6 Mine water prediction system architecture showing the link between the input parameters, LSTM and ANN systems and the resultant predicted sulfate concentration for the Witkranz site (modified after [125]).

examples such as the beforementioned historical input parameters and the label output being the sulfate in this study. The output values generated by LSTM for each input are fed into the trained ANN model to forecast sulfate concentrations from June 2018 to May 2019 as depicted by the green line ("Prediction" in Figure 2.6). Future work includes testing and calibration of this preliminary AI model using more data collected at the discharge site.

2.5 Conclusions

Poor management of AMD poses a substantial environmental risk at both local and regional scales. Globally, this risk is currently being managed via a variety of interventions including a wide range of treatment technologies. These technologies are broadly categorized into active and passive systems. In the South African context, only active treatment systems are operating at a bigger scale to manage the environmental risk posed by AMD at the Witbank site and the Witwatersrand basins.

Prediction of mine water quality is critical for long-term mine planning and the application of AI techniques in this regard could play a pivotal role in achieving this objective, especially considering the successful application of these tools in other fields such as image processing and financial forecasting. However, in spite of frequently generating effective models, the use of AI for predicting AMD quality is strenuous considering the difficulty with integrating fundamental physical processes into the knowledge base model, the choice of suitable learning techniques and the assessment of the modeling results requires exceptional attention. Other limitations for delivering effective models include availability of limited and good quality data and reluctance to accept PL methods, among others [122].

Taking cognisance of the aforementioned positives and limitations, the case study presented in this chapter, investigated the application of a hybrid system, which combines LSTM and ANN to predict mine water quality with sulfate concentrations as a proxy from an abandoned underground coal mine in Mpumalanga province. A predictive preliminary AI prototype was developed that can be revised as and when new information is available. In conclusion, this chapter provides an overview of this field and, hopefully, will lead to more advances and intense research efforts on issues outlined above.

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