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Impact of design aspects on iron removal efficiencies from coal mine drainage in full-scale lagoons

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ABSTRACT

In response to the potential ecological problems caused by coal mine drainage, passive Mine Water Treatment Schemes (MWTS), consisting of settlement lagoons and aerobic wetlands, are developed to remove iron and other contaminants prior to discharge into the environment. Existing research has examined individual design aspects separately, addressing the effect of lagoons' design on treatment performance. However, long-term research lacks data on the design aspects of full-scale mine drainage lagoons, to ensure consistent iron removal and optimal treatment of the mine drainage. This study analysed and assessed the design aspects of five full-scale lagoons, alongside monthly iron concentrations spanning over a period of twelve years, aiming to evaluate lagoon treatment performance based on different design aspects. Correlation and regression analyses were conducted to offer a better understanding of the potential relationships between iron removal efficiencies and the various design aspects of lagoons.

Results indicated that the mean iron removal efficiencies of the lagoons studied, ranged from 25.12% to 92.85%, being impacted by the different design features. The correlation and multiple regression analysis results suggest that operational Water Levels, Surface Area, Aspect Ratio, layout and number of inlets and outlets, as well as shape of the lagoons affected iron removal (R^2 0.78, *p*-value <0.05). Lagoons with larger aspect ratio were observed to have performed better in removing iron. In addition, a reduction in operational water level was observed to lead to increased iron removal. Furthermore, the result of the regression analysis demonstrated that the age of the lagoon significantly affects its treatment performance. Overall, lagoons with mid-mid configuration, multiple inlets and outlets and aspect ratio of 4 are found to allow for better flow and contaminant spread within the system, ensuring better adsorption and optimal removal of iron, although subject to regular ochre removal. This study offers valuable insights to lagoons design engineers, research scientists, policy makers and MWTS operators to optimize treatment performance.

1. Introduction

As a key economic industry of a country, coal mining is associated with potential ecological problems, such as pollution of surface and ground water courses, river ecology growth limitation, and more (Gombert et al., 2019; Rinder et al., 2020; Setiawan et al., 2018). Coal mine wastewater discharge into waterways has been responsible for unnatural alterations to water quality, manifesting as elevated salinity levels, pH modification and higher amounts of heavy metals (Fleming et al., 2021). In addition, mine drainage contains elevated concentrations of a variety of contaminants such as Iron (Fe), Sulphates (SO_4^{2-}), dissolved Manganese (Mn) and Aluminium (Al) (Blanco et al., 2018; Jacob et al., 2022), as well as on occasions Arsenic, Cyanide, Nickel, Thallium, Zinc, and Uranium, which pose adverse environmental issues for receiving streams.

In response to the potential ecological issues brought about by coal mine drainage, passive Mine Water Treatment Schemes (MWTS) are developed to remove contaminants from coal mine-impacted waters prior to discharge into the environment. Passive MWTS, comprising settlement lagoons and aerobic wetlands are constructed with focus on

Acronyms: AR, Aspect Ratio; HRT, Hydraulic Residence Time; MWTS, Mine Water Treatment Schemes; PC, Principal Component; PCA, Principal Component Analysis; R.E, Removal Efficiency; RF, Random Forest; WL, Water Level.

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particularly iron removal, being the main contaminant in high concentrations. Iron, particularly in the form of pyrite, causes water discoloration and turbidity when present in high concentration, providing adsorption sites for other contaminants as well. Therefore, iron is the primary metal of concern in mine drainage and its removal is prioritized in the design of MWTS. Passive MWTS are designed with the objective to encourage ferrous iron (Fe^{2+}) oxidation to ferric iron (Fe^{3+}). Oxidations mostly occur in the lagoon converting Fe^{2+} to Fe^{3+}. Moreover, if a cascade is present in the MWTS, oxygenation will commence in the cascade initializing the conversion process of some of the Fe^{2+} present in the mine water to Fe^{3+} precipitates. This oxidation is followed by ferric iron hydrolysis to ferric oxyhydroxide (known as ochre). Ochre is a characteristic orange precipitate visible in water courses affected by iron contamination. Settlement lagoons are designed to facilitate the settling of ochre particles, allowing them to accumulate at the bottom of the lagoon (Banks et al., 2019; Khachatryan et al., 2021; Opitz et al., 2023).

The accomplishment of Fe^{2+} oxidation in lagoons is determined by two primary factors: the retention time of the mine water in the lagoon and the contaminant removal processes. The latter is influenced by manipulation of locally existing environmental conditions, as well as the design aspects of the lagoon. When these aspects are optimally combined, Fe^{2+} oxidation is encouraged, contaminant removal processes are improved, and the overall lagoon treatment performance is enhanced (Banks et al., 2019; Hedin et al., 2019). Given that passive MWTS require a substantial area of land for treatment to be considered effective, it is also important to select appropriate design aspects with high cost-effectiveness while ensuring optimal treatment performance (Guo et al., 2019; Opitz et al., 2021).

There have been few studies investigating the impact of individual design parameters - such as shape, aspect ratio (AR) [also referred to as length to width ratio], inlet and outlet configurations, design depth - and of the performance of lagoons (Ioannidou and Pearson, 2018; Li et al., 2018; Ma et al., 2020; Pat-Espadas et al., 2018; Skousen et al., 2017; Tran et al., 2022).

Previous research has shown that distinct mixed zones and dead zones are present in every treatment system, and their location and size varies as a function of its inlet-outlet configurations and system's shape, therefore, lagoon's shape can significantly affect the effective volume, dead zones occurrence and, the dispersion also the retention time (Nuel et al., 2017; Sabokrouhiyeh et al., 2017). Channel irregularities and irregularly shaped systems contribute to irregular flow fields, creating a preferential flow path due to sediments transport. This ultimately reduces the HRT of the lagoon, leading to decreased iron removal efficiency.

Water depth has been observed by previous researchers to directly or indirectly affect lagoon treatment performance. An important treatment process, i.e. sedimentation, is dependent on the water depth and water velocity, as well as the shape and size of particles within the lagoon (Sanchez-Ramos et al., 2017). Varying water depths induce different biochemical reactions, as a result of varying aerobic and anaerobic conditions. Therefore, water depth is indirectly affected by factors such as sediment redox potential which is impacted by changes in net oxygen supply rate, sediment oxygen demand, and water volume. An increase in water depth has been shown to increase the degree of short-circuiting, in addition large amounts of dead zones have been observed at deeper water depths compared to lower depths (Khatri et al., 2017; Le Bourre et al., 2020). A change in the water depth of a lagoon has also been observed to affect the HRT, water velocity, rate of sediment retention, and iron removal (Ma et al., 2020; Zhu et al., 2022).

Finally, surface area has been considered to affect lagoon's iron removal and overall treatment performance. Previous studies demonstrate that lagoons of larger surface areas, offer an increased possibility of contact between the wastewater particles and surfaces, such as organic matter and sediment particles which possess inherent electrostatic properties for adsorption, effectively binding ions present in the effluent, thereby reducing concentrations of iron and other contaminant on the wastewater (Feng et al., 2020; Li et al., 2019). Furthermore, in the lagoon, due to gravity, suspended solids and larger iron particles settle at the bottom forming a sludge layer. The larger the surface area, the longer the retention time and settling process, and reducing the possibility of resuspension of iron and other contaminants.

These previous studies examined individual design aspects separately, while comprehensive studies on interactions and impact of multiple design aspects on mine water treatment using regression analysis have not been widely investigated. Current research is also lacking an analysis of investigation of the best combination of design aspects of full-scale lagoons treating mine drainage to achieve consistent and optimum performance. Therefore, the aim of this study is to assess the influence of different design parameters on the iron removal of full-scale lagoons in passive MWTS over a 12-year period. Regression analysis conducted in this study aims to investigate iron removal from lagoons based on the design aspects combination and offers a guide for optimization of lagoon design, whilst reducing investments in time of field tests and land.

2. Material and methods

2.1. Schemes descriptions

The study was undertaken at five full-scale Passive Mine Water Treatment Schemes (MWTS) located within the north of England. Ten settlement lagoons in these full-scale schemes were assessed for their respective treatment performances. The investigated schemes vary in configuration, layout, and number of assets included. The overview of the schemes is presented as follows.

Site A consists of the cascade which flows into two parallel lagoons, as presented in Fig. 1a. This discharge is received by a cascade, flowing into a lagoon, subsequently feeding three wetlands connected in series, before the treated mine water is finally discharged (Fig. 1a).

Site B consists of a cascade, flowing into three parallel settlement lagoons, which individually flow into three separate wetlands (Fig. 1b). This is followed by another set of three wetlands, receiving flow from the previous wetlands. It is important to highlight that the purpose of the latter set of wetlands is for maintenance. The lagoons have one inlet and four outlets each, while the wetlands have four inlets and four uniformly distributed outlets.

Site C comprises of a cascade, two settlement lagoons connected in series and a wetland, as shown in Fig. 2a. This scheme has a sludge bed which receives flow from the second lagoon before flowing into the wetland, after which the treated flow is discharged.

Site D receives mine water directly into a lagoon after which the flow discharges in a long and narrow wetland (Fig. 2b) (no cascade is present). Finally, as presented in Fig. 2c, Site E consists of an aeration cascade, a settlement lagoon and three wetlands connected in series.

2.2. Data

This study employs data arising from the ten settlement lagoons presented in section 2.1. The data employed covers a period of twelve years, i.e. from January 2007 to September 2018. It should be noted however, that Site C includes data from January 2014 to September 2018. The dataset contains monthly records of ferric iron (Fe^{3+}). Design aspects of the MWTS were obtained from topographic maps, and included: shape, surface area, aspect ratio (AR), position of inlet and outlets (configuration), number of inlets and outlets. Iron removal is prioritized in the design of MWTS, hence the Fe^{3+} removal efficiency of the lagoons is calculated using eq. 1 (Li et al., 2020; Zhu et al., 2022).

$$Removal\ Efficiency\ (\%) = \frac{C_{in} - C_{out}}{C_{in}}\ x\ 100 \quad (1)$$

where C_{in} = influent concentration and C_{out} = effluent concentration.

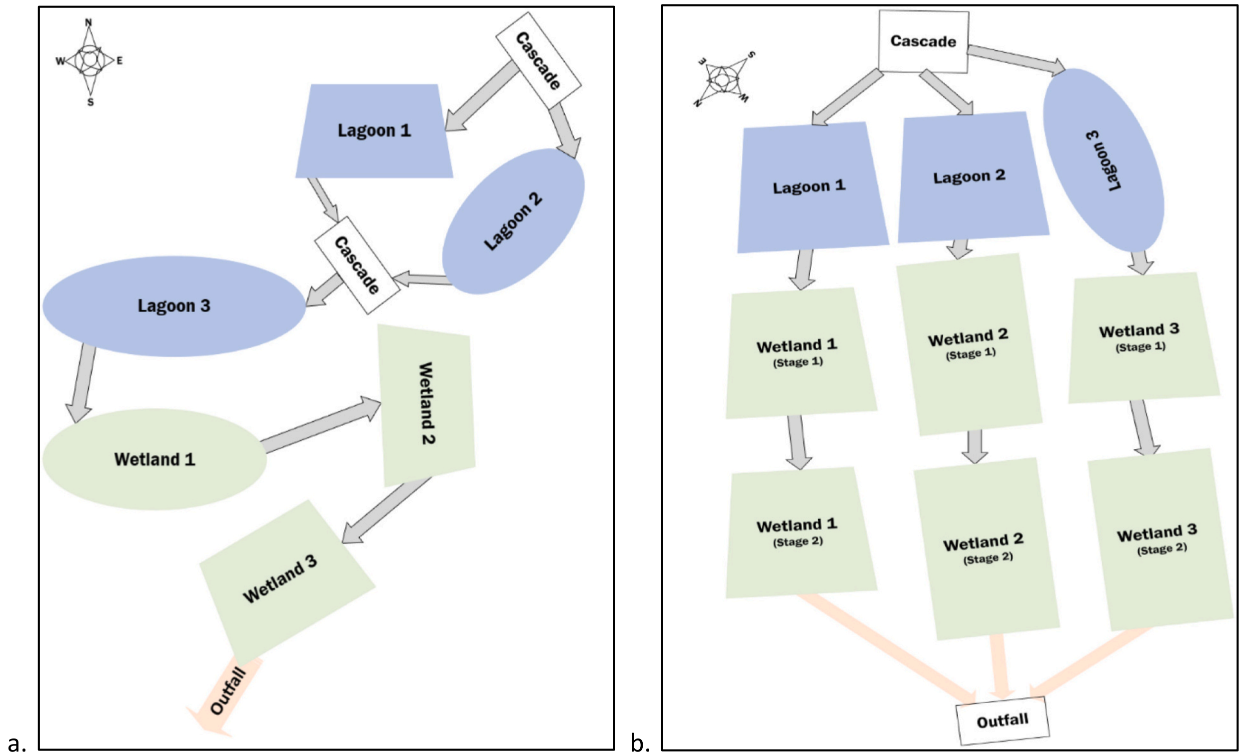

Fig. 1. Schematic Diagram of a) Site A MWTS and b) Site B MWTS (not drawn to scale).

In the UK, MWTS are strategically constructed adjacent to abandoned coal mines, known as collieries, which often contain significant amounts of iron sulphide minerals, such as Pyrite. Drainage from these areas contains high concentrations of unoxidized iron, which, if released directly into the environment, can contribute to acidity and ochre formation. Furthermore, regulatory bodies such as the Environment Agency in the UK enforce strict limits on iron concentration in treated mine water discharged into water bodies, as indicated in the Water Framework Directive (England & Wales) Regulations 2017, which is essential for preserving aquatic ecosystems, wildlife biodiversity and human health from the adverse effects of iron contamination. Moreover, iron potentially exists in association with other metals, providing adsorption sites for the metals. Therefore, effective iron removal from mine water also aids the removal of other metals and contaminants, contributing to an improved water quality.

2.3. Statistical methods

The influence that various design aspects of the ten lagoons (see section 2.1) might have on their treatment performance is explored by conducting statistical analyses (i.e. Principal Components Analysis and regression analyses). Univariate analysis was employed to calculate mean, minimum, maximum, standard deviation, standard error and range of the iron concentrations. Pearson correlation analysis was conducted among discharge concentrations and design aspects, so as to obtain the correlation coefficient and the degrees of significance between any pair of variables (design aspects and removal efficiencies). The level of significance was set to 0.05, which proves there is sufficient evidence to conclude that a significant linear relationship exists between the variables (Guo and Cui, 2022; Ilyas and van Hullebusch, 2020; Zolekar et al., 2021).

2.3.1. Data preprocessing

Prior to performing the Principal Components Analysis and regression analyses, the following data preprocessing steps were carried out.

a. <u>Categorical Variables transformation</u>: As regression models accept only numerical data, the categorical/non-numerical design aspects of this study (i.e. Shape and Configuration) were transformed into numerical values. Non-numerical variables can be transformed into numerical values via one-hot encoding and/or label encoding. Although one-hot encoding is a simple encoding method, (Cerda et al., 2018; Ul Haq et al., 2019), it also has some limitations, including potential risk of losing information due to resulting to a large number of categories, which invariably increases the dimensionality and complexity of the feature matrix.

Instead, label encoder assigns a unique integer between 0 and n-1 to each categorical variable of features and allows the variables to be handled as continuous data. Label encoder has been employed widely by researchers in transforming categorical variables (Lubis and Iqbal, 2022; Sakarkar et al., 2020; Sheikh et al., 2020). Unlike the one-hot encoding method, label encoding categorical data can be handled without losing any information, or increase in the number of categories, attributes that make label encoding less complex than one-hot encoding. Therefore, in this study, the categorical variables (i.e. Shape and Configuration) were transformed into numerical values using Python's scikit-learn LabelEncoder function (Lubis and Iqbal, 2022; Sakarkar et al., 2020; Weerasinghe et al., 2021).

b. <u>Data Standardization</u>: Standardization was performed to eliminate bias likely to arise from the various variables that were measured on significantly different units of measurements and might not equally contribute to model fitting. A standardized dataset with mean = 0, variance = 1 scale removes any biases present in the original variables. The dataset was standardized using Eq. 2 (Asadollah et al., 2021; Hai et al., 2020; Thippa et al., 2020).

$$z = \frac{x - \mu}{\sigma} \tag{2}$$

where x is the original value, z is the standardized value, σ is the standard deviation and μ is the mean.

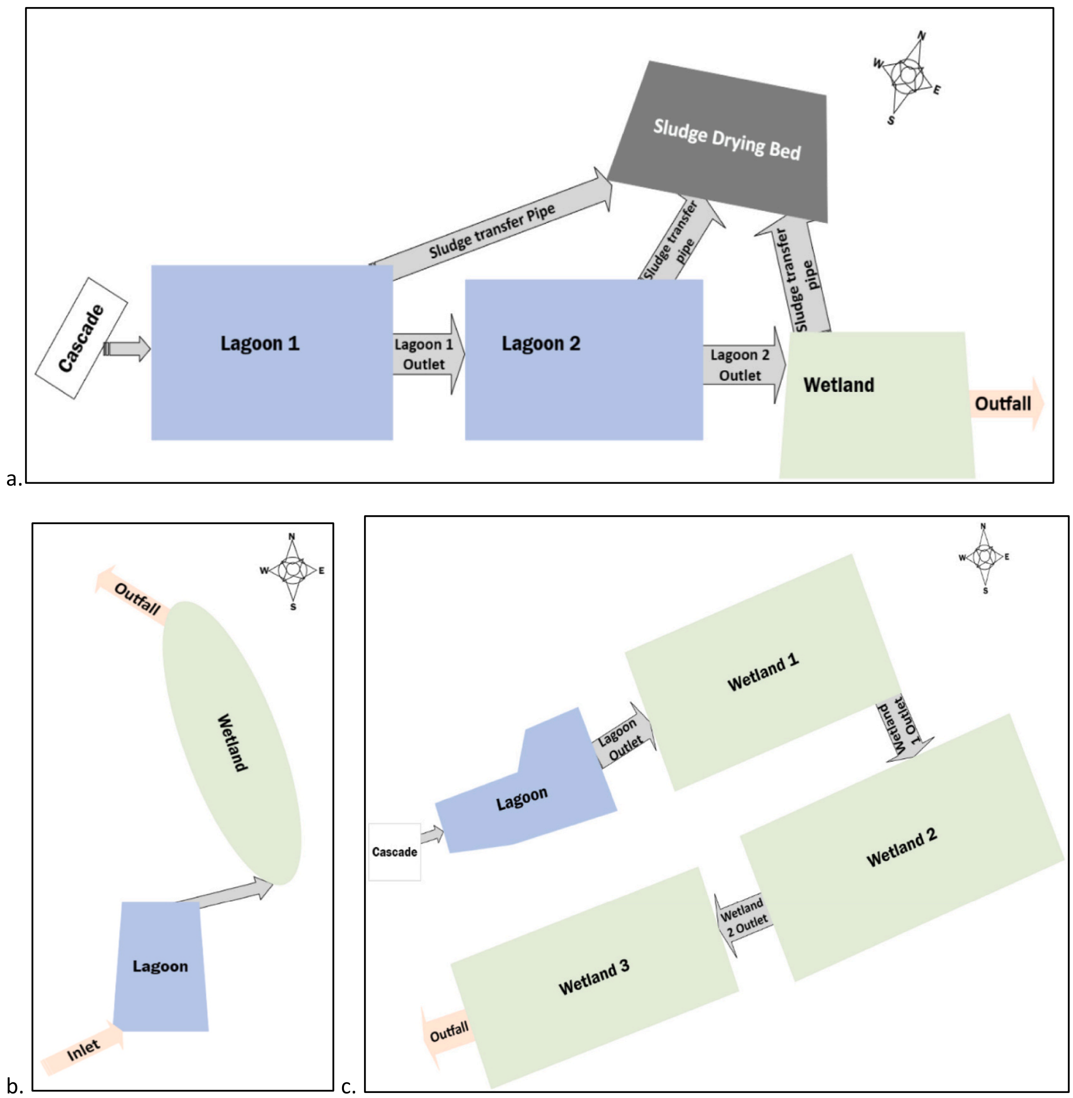

Fig. 2. Schematic Diagram of a) Site C MWTS b) Site D MWTS and c) Site E MWTS (not drawn to scale).

2.3.2. *Principal component analysis (PCA)*

PCA was conducted to help reveal the primary factors of influence controlling Fe removal from mine drainage. As a widely used dimensionality reduction method, PCA was performed to transform possibly correlated variables into a reduced set of uncorrelated variables, referred to as principal component (PC). Compared to the other available techniques for dimensionality reduction and feature selection, PCA captures the maximum amount of variance in the dataset, providing a comprehensive dataset summary while ensuring independence from model assumptions. In addition, PCA aids data visualization and simplifies interpretation of the dataset, thereby serving as a preprocessing step for subsequent machine learning algorithms, as the regression performed in this study. The PCs with variance summing up to approximately 80% of the dataset are selected and used to determine the factors strongly related to Fe^{3+} removal variation in the lagoons. Previous studies have shown that approximately 80% of the total variance is accurate enough and would capture important factors that significantly influence iron removal from the lagoons (Zhang et al., 2022; Zhu et al., 2022). The loadings of variables captured in each PC is then employed to observe and identify key patterns and relationships among the variables.

2.3.3. *Regression analysis*

In addition to the above-mentioned analyses, regression was performed to help achieve a better understanding on the relationships between iron removal efficiencies and design parameters of the lagoons. Seven design aspect features were used as independent variables in the PCA and regression analyses. These independent variables include: Water Level (WL), Configuration, Aspect Ratio (AR), Surface Area, Shape, Number of Inlets (Num_Inlets) and Number of Outlets (Num_Outlets). Month and year (of water sample collection) were also employed as independent variables.

Five regression models were implemented to examine the relationship among multiple design aspects and assess the significance of the design aspects to the lagoons' performance. The implemented models included: Random Forest (RF) regressor, Multiple Linear regression, XGBoost, Polynomial regression and Ridge regression. These five regression models have been selected since they have been utilised by other researchers to understand the roles of different physicochemical properties and design aspects in the removal processes of contaminants and have demonstrated satisfactory results. For instance, RF, Ridge regression and artificial neural network models recorded better performance with limited test data as indicated by higher R^2 in Guo and Cui (2022) study. These three models are also adept at preventing overfitting and exhibit robustness to data noise (Manasa et al., 2020; Sharafati et al., 2020). XGBoost is known to capture complex relationships that exist among dataset variables (Guo and Cui, 2022; Thippa et al., 2020).

Multiple Linear regression (MLR) was also selected in this study due to its relatively fast calculation and interpretation ability. Furthermore, from previous studies, Polynomial regression has been useful in capturing nonlinear relationship between variables, and lower order of variable is recommended to reduce the risk of overfitting (Ahmed et al., 2019), hence the use of order of two in this study. Therefore, the regression models employed in this research include RF Regression, MLR, XGBoost, Polynomial regression and Ridge regression.

The above-mentioned five regression models' efficiency was tested with four evaluation metrics which include: R-squared (R^2), mean squared error (MSE), root mean squared error (RMSE) and mean absolute error (MAE) to permit to select the best model (Asadollah et al., 2021; Breiman, 2001; Hai et al., 2020; Sharafati et al., 2020). The evaluation metrics are expressed in Eq. 3 to Eq. 6 (Asadollah et al., 2021; Islam Khan et al., 2021):

$$RMSE = \sqrt{\sum \left(y_{obs} - y_{pred}\right)^2 \Big/ n} \tag{3}$$

$$MSE = \sum \left(y_{obs} - y_{pred}\right)^2 \Big/ n \tag{4}$$

$$MAE = \sum \left(\left\|y_{obs} - y_{pred}\right\|\right) \Big/ n \tag{5}$$

$$R^2 = \left(\frac{\sum \left(y_{obs} - \overline{y_{obs}}\right)\left(y_{pred} - \overline{y_{pred}}\right)}{\sqrt{\sum \left(y_{obs} - \overline{y_{obs}}\right)^2 \sum \left(y_{pred} - \overline{y_{pred}}\right)^2}}\right)^2 \tag{6}$$

where y_{obs} = actual value, y_{pred} = predicted value, $\overline{y_{obs}}$ = average of the actual values, y_{pred} = average of the predicted values and n = total number of samples.

R^2, MAE, MSE and RMSE are important metrics for assessing the performance of regression models. While the proportion of variance explained by the model is measured by R^2, MAE, MSE and RMSE quantifies the models' prediction accuracy by calculating the average differences between actual and predicted values, as presented in eqs. 3–5. Higher R^2 values signifies a stronger fit while lower values of MSE, RMSE, and MAE indicate better performance (Asadollah et al., 2021; Islam Khan et al., 2021). In this study, the best model among the five tested models, was chosen based on its highest R^2 score and lowest MAE, MSE, and RMSE values for further analysis.

All statistical analyses were performed with Python 3.6.8 (Islam Khan et al., 2021; Sakala et al., 2019; Taoufik et al., 2022).

3. Results and discussion

This study aimed at observing the effect of lagoons' design aspects on iron removal and evaluating optimal design aspects combination for the future construction of full-scale mine drainage lagoons.

As discussed in Section 1, iron is the primary metal of concern in mine drainage in the UK, therefore, Fe^{3+} R.E was employed as a key performance indicator benchmark for MWTS (Banks, 2003; Johnston et al., 2007; Kusin et al., 2014; Opitz et al., 2020). Overall, Fe^{3+} R.E ranging between 50.97% and 98.98% was achieved by the studied schemes (lagoons and wetlands inclusive). Fig. 3 presents the overall performance of the schemes with respect to their iron removal, as well as their respective average influent and effluent iron concentrations.

The performance of the ten full-scale lagoons investigated in this study (see Fig. 3) were analysed using their respective Fe^{3+} removal efficiency. Column 3 of Table 1 presents the average removal efficiencies of the studied lagoons. The lagoons' names are listed in column 1, while the short form for each lagoon (which will be used for subsequent discussion) are presented in column 2. As observed in Table 1, the highest Fe^{3+} R.E was achieved by A-Lag3, B-Lag2 and C-Lag1 with 89.21%, 86.48% and 82.65% respectively. Fig. 4 presents the Fe^{3+} R.E of each of the lagoons, along with their average influent and effluent concentrations.

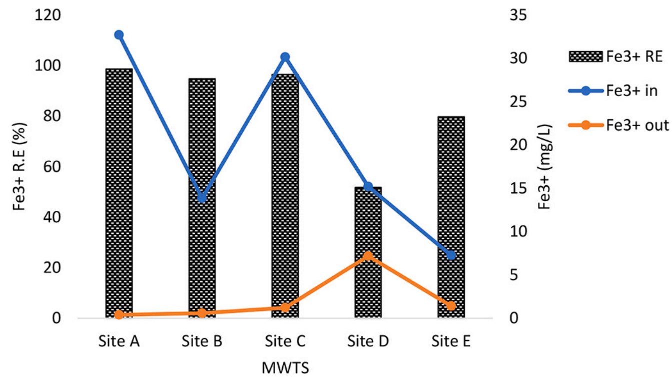

Fig. 3. Average Fe^{3+} removal efficiencies, influent Fe^{3+} and effluent Fe^{3+} concentrations from the schemes.

Table 1
Summary of Fe^{3+} R.E for the lagoons.

(1)	(2)	(3)
Asset	Short form	Fe^{3+} R.E (%)
SITE A-Lagoon 1	A-Lag1	54.94
SITE A-Lagoon2	A-Lag2	60.34
SITE A-Lagoon3	A-Lag3	89.21
SITE B-Lagoon1	B-Lag1	80.29
SITE B-Lagoon 2	B-Lag2	86.48
SITE B-Lagoon 3	B-Lag3	78.1
SITE C-Lagoon1	C-Lag1	82.65
SITE C-Lagoon2	C-Lag2	54.71
SITE D-Lagoon	D-Lag	13.72
SITE *E*-Lagoon	E-Lag	30.48

Site A MWTS has a cascade for oxygenation which initializes the conversion process of some of the Fe^{2+} present in the mine water to Fe^{3+} precipitates, before flowing into A-Lag1 and A-Lag2 which are connected in series (see Fig. 1a). The effluent from both lagoons then combines and flows into another cascade before emptying into A-Lag3, which achieved higher R.E of 89.21% compared to 54.94% (A-Lag1) and 60.34% (A-Lag2). Site B consists of 3 lagoons which are in parallel arrangement, and recorded R.E ranging between 78.1% and 86.48%.

Site C consists of 2 lagoons in serial connection, which despite having similar shape and inlet-outlet configuration, they achieved R.E of 82.65% (C-Lag1) and 54.71% (C-Lag2). The Num_Outlets in C-Lag1 and C-Lag2 were 4 and 2 respectively, and as discussed in section 3.3, the Num_Outlets play an important role in the lagoon's performance, thus contributing to the significant variation in R.E achieved.

Unlike the other schemes with multiple lagoons, Site D and Site E schemes consist of a single lagoon, achieving lower R.E, namely of 13.72% (D-Lag) and 30.48% (*E*-Lag) respectively. The D-Lag is of a smaller area than the other lagoons investigated in this study, which may potentially reduce the retention time of the mine water and iron removal (Dufresne et al., 2015; Shukla et al., 2021).

Overall, analysis of the design aspects presented in Section 3.1 provides an insight on how design aspects of the studied lagoons have affected their iron removal, and thus overall treatment performance, and how lagoon design could be improved to achieve higher iron removal.

3.1. Design aspects

The investigated lagoons were not only of varying influent iron composition, but also of varying geometry and configuration, as presented in Table 2. The lagoons short forms are listed in column 1 of Table 2, while the studied lagoons' shape, inlet-outlet configuration, number of inlets, number of outlets, AR, design depth, surface area and WL are presented respectively in columns 2 to 9 of Table 2.

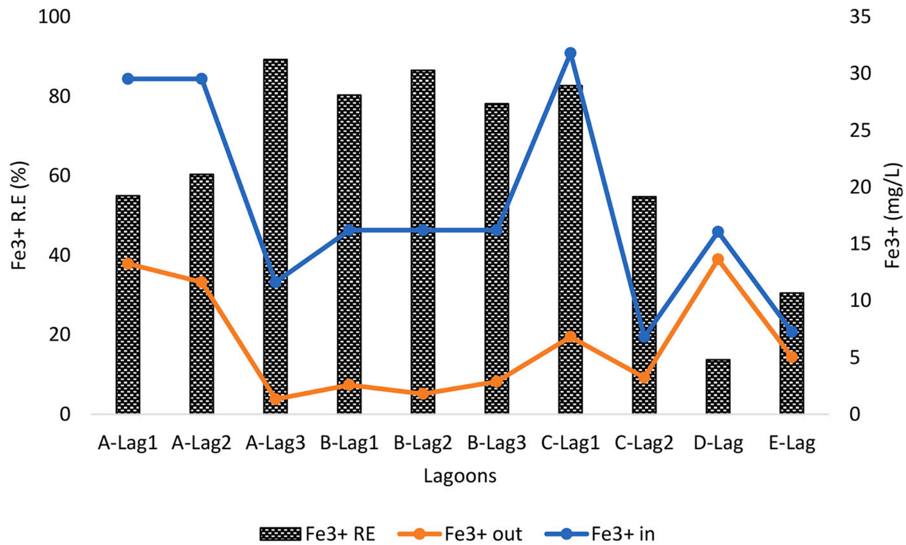

Fig. 4. Average Fe^{3+} removal efficiencies, influent Fe^{3+} and effluent Fe^{3+} concentrations from the Lagoons.

Table 2
Details of studied coal mine treatment lagoons.

1 Lagoons	2 Shape	3 Inlet-outlet configuration	4 No. of Inlets	5 No. of outlets	6 Aspect Ratio	7 Design Depth (m)	8 Surface Area (m^2)	9 Water Level (m)
A-Lag1	Trapezium	Mid-Corner	2	2	2	3.00	1314.60	2.00
A-Lag2	Oval	Corner -Corner	2	2	0.5	3.00	892.90	2.00
A-Lag3	Oval	Mid-Corner	1	2	4	3.00	1455.40	2.00
B-Lag1	Trapezium	Mid-Mid	1	4	2	3.00	2664.29	2.05
B-Lag2	Trapezium	Corner-Mid	1	4	2	3.00	3528.29	2.05
B-Lag3	Oval	Corner-Mid	1	4	3	3.00	2517.19	2.05
C-Lag1	Rectangle	Mid-Mid	1	4	3	3.00	1613.90	2.00
C-Lag2	Rectangle	Mid-Mid	2	2	3	3.00	1590.39	2.00
D-Lag	Trapezium	Corner-Mid	1	3	0.5	3.00	148.04	2.60
E-Lag	Trapezium	Mid-Mid	1	2	3	3.00	895.00	2.50

3.1.1. Surface area

Although C-Lag1 and E-Lag had similar AR, Configuration, Num_Outlets and design depth, they achieved notable variation in iron R.E, with C-Lag1 attaining a R.E of 82.65% and E-Lag 30.48% (see Table 1). The higher R.E of C-Lag1 could be due to its greater surface area (see Table 2). D-Lag recorded the lowest iron R.E of 13.72% but had the smallest surface area. Moreover, C-Lag1 with a larger surface area than C-Lag2, achieved higher R.E than C-Lag2, despite that both lagoons are of similar shape, WL and inlet-outlet configuration. It is therefore deduced that Fe^{3+} removal from the lagoons is dependent on the Surface Area, as also observed in Fig. 5a, and a larger surface area clearly results in a higher Fe^{3+} removal (see Fig. 5a). This relationship between surface area and Fe^{3+} removal is also supported by previous research which has demonstrated that a higher surface allows for better pollutants adsorption and is therefore expected to result to a higher Fe^{3+} removal rate (Li et al., 2018; Wan et al., 2015; Wolkersdorfer et al., 2016).

3.1.2. Water level

Iron removal from the lagoons appears to be also dependent on the WL, as illustrated in Fig. 5b. WL, denoted by dots in Fig. 5b, remained consistent when the R.E percentage, represented by bars, showed comparable values. However, a significant decrease in the R.E percentage was observed when the WL rose to 2.60 m for D-Lag. This relationship between WL and iron removal from the lagoon can be explained by the different biochemical reactions that occur under aerobic and anaerobic conditions (Chamberlain and Moorhouse, 2016; Guo et al., 2019; Liu et al., 2016). At lower WLs, a more oxygen-rich environment promotes aerobic processes that drive iron removal processes, while anaerobic conditions created by higher WLs could limit aerobic microorganisms' activities, resulting in reduced iron removal. Therefore, based on the findings of this study, it can be inferred that a higher WL results in a lower Fe^{3+} removal from the lagoons, confirming that WL variations play an important role in determining iron removal from lagoons.

For the design aspects, box plots were employed to observe the relationship between the design features and Fe^{3+} removal, as presented in Fig. 6. From the boxplots (see Fig. 6), a significant Fe^{3+} R.E difference is noted among the different aspects. Shape, AR, Num_Inlets and Num_Outlets are observed to have affected the Fe^{3+} concentration, as there was a significant difference among their respective categories.

3.1.3. Shape

A-Lag3 and B-Lag3 with oval lagoons were observed to have achieved higher Fe^{3+} R.E than rectangular lagoons. As presented in Figure 6Figure a, lagoons with oval shape overall attained a higher R.E range than rectangularly shaped lagoons. This can be explained by the fact that compared to trapezium and rectangular-shaped lagoons, an oval shape could improve the treatment performance by reducing potential formation of dead zones at the edges and corners (Nuel et al., 2017; Sabokrouhiyeh et al., 2017). In oval lagoons, dead zones, which would have been present along edges and corners of trapezium and rectangular-shaped lagoons, are replaced by regions of moving fluid, which promotes effective volume, and hence, higher iron removal.

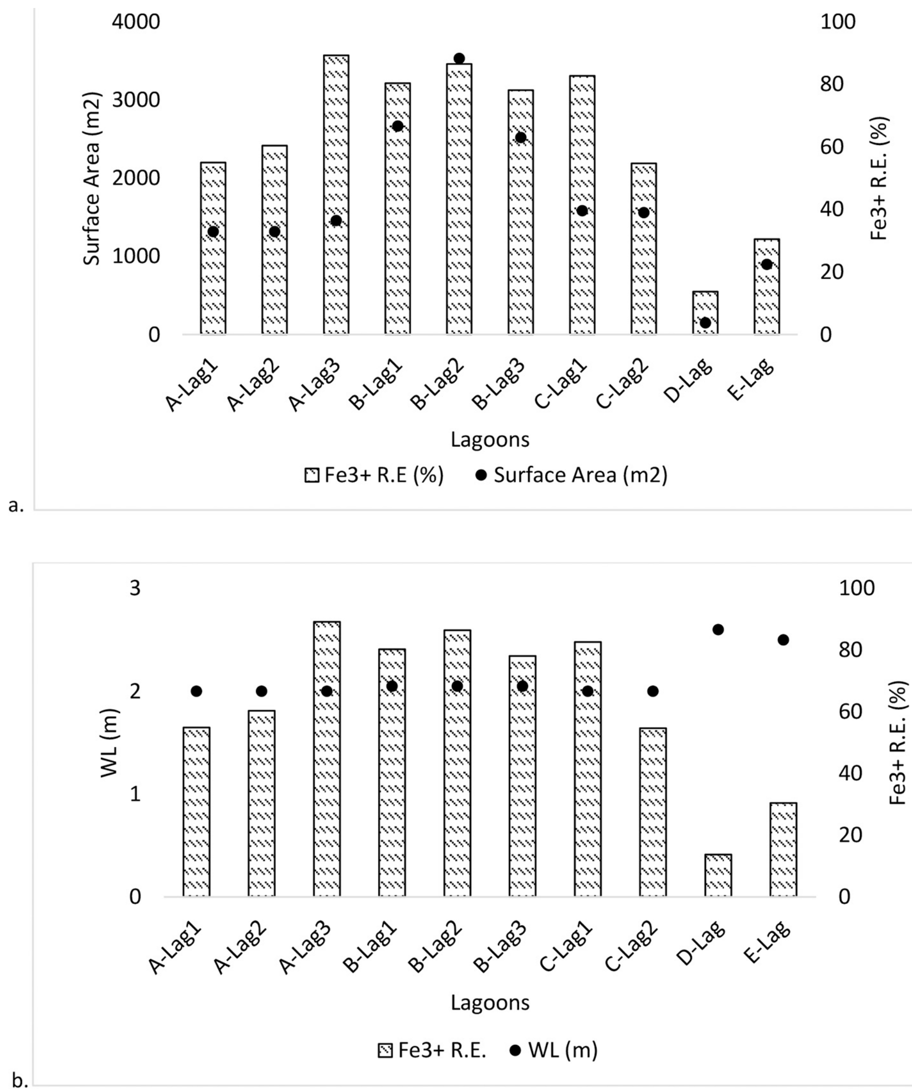

Fig. 5. Variation in Fe^{3+} removal efficiency in relation to a) Surface Area and b) WL for the lagoons.

3.1.4. *Aspect ratio (AR)*

The AR (which is the length-to-width ratio) of the lagoon is also observed to have an influence on iron removal. Although A-Lag2 was oval shaped, it however removed lesser iron compared to the other oval shaped lagoons (A-Lag3 and B-Lag3). This could be attributed to its lower AR of 0.5, against the AR = 4 of A-Lag3 and AR = 3 of B-Lag3. In addition, although B-Lag2 and D-Lag had similar shape and configuration, they achieved significantly different iron removal, i.e. 86.48% and 13.72% respectively. This significant difference in both lagoons could be attributed to D-Lag's smaller AR of 0.5 compared to B-Lag2 AR of 2. In Fig. 6b, lagoons with AR ≈ 4 were observed to have the highest average Fe^{3+} R.E, while AR of 0.5 recorded the least Fe^{3+} R.E.

Overall, lagoons with higher AR have performed better at removing Fe^{3+} (Fig. 6b), a finding that is in agreement with previous studies (Guo et al., 2019; Persson, 2000; Persson and Wittgren, 2003; Sabokrouhiyeh et al., 2017). According to Persson et al. (1999), to ensure optimal treatment in a system, the satisfactory design AR value should be approximately 4. However, recent studies have argued that the AR value of 4 will not promote good hydraulic efficiency (i.e. above 0.75) unless there is a uniform distribution of inflow achieved across the system's width, proving thereby the significance of inlet-outlet configuration (Liu et al., 2016; Ma et al., 2020; Persson et al., 1999), discussed in the next section.

3.1.5. *Inlet-outlet configuration*

Inlet-outlet configuration of the lagoons of the present study, does not appear to have a significant effect on Fe^{3+} removal, compared to the other design aspects presented in the previous sections. Fig. 6c presents the performance different inlet-outlet configuration alongside iron removal data. No significant relationship was observed between both variables, with mid-corner configuration resulting to the highest average Fe^{3+} R.E (Fig. 6c). This is contrary to existing studies which have demonstrated that mid-corner configuration excludes a larger region of the total volume from the flow circulation and treatment (Sabokrouhiyeh et al., 2017). Research has also suggested mid-mid configuration to be the best configuration, as it facilitates improved flow and spread of contaminant within the system, leading to enhanced adsorption and removal of contaminants (Ma et al., 2020; Okhravi et al., 2017). In addition, opposite corner-corner has been demonstrated to achieve better removal as it allows for larger effective volume to move from one corner to the other within the lagoon, thus reducing dead zones (Sabokrouhiyeh et al., 2017). In this study, lagoons with mid-mid configuration however had AR between 2 and 3 and the majority did not have multiple inlets.

3.1.6. *Number of Inlets*

The Num_Inlets in this study is observed to have had little effect on Fe^{3+} R.E, as presented in Fig. 6d. However, studies have revealed that

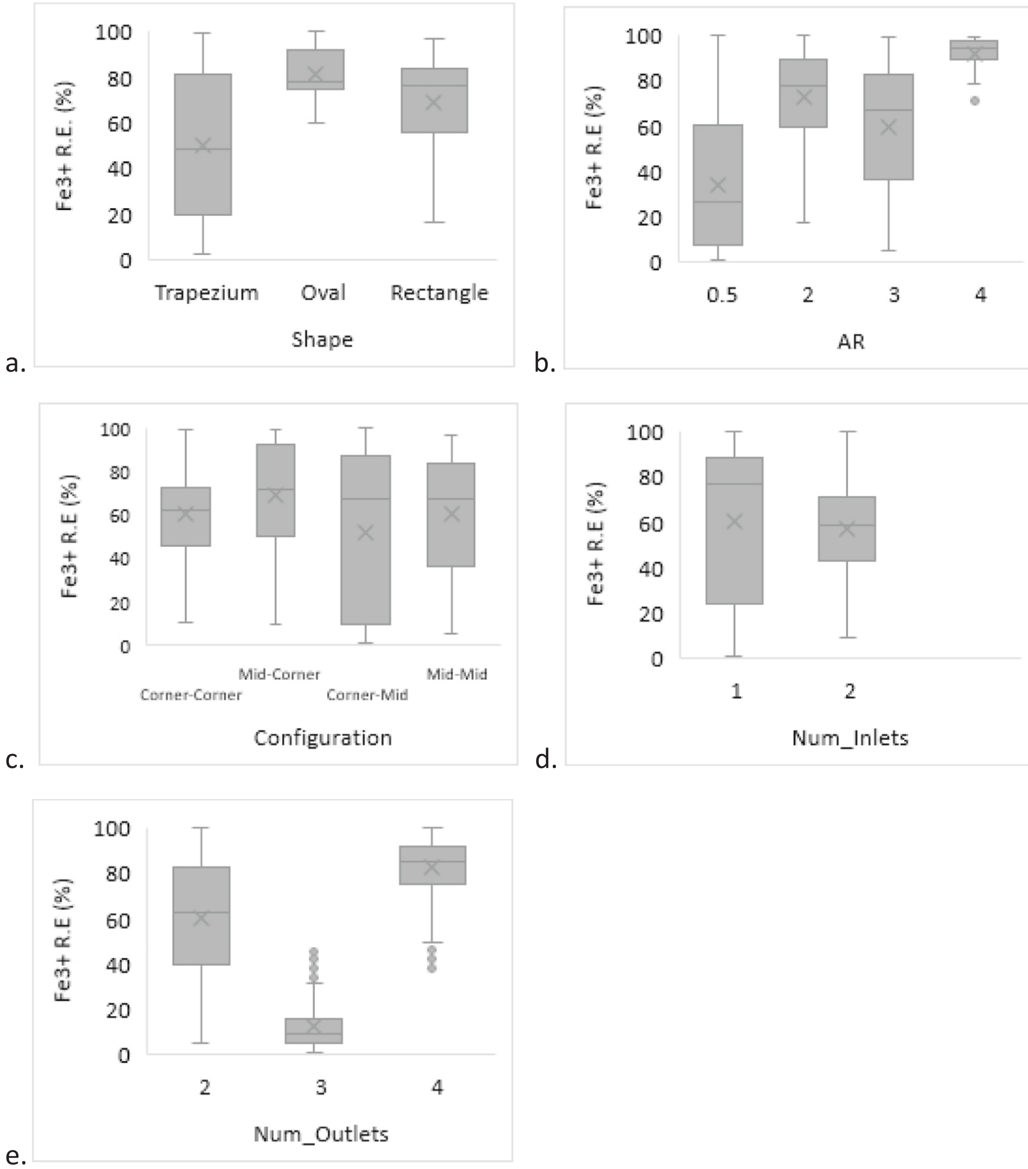

Fig. 6. Average Fe^{3+} removal efficiencies distribution in the Lagoons for different design parameters a) Shape and b) Aspect Ratio c) Inlet-outlet configuration d) Number of inlets and e) Number of outlets. For the box plots, vertical line within box = median, upper line = maximum, lower line = minimum and enclosed box = interquartile range, X = mean.

lagoons with single inlets are less effective at treating wastewater because they are less likely to experience short-circuiting, reduced removal efficiency and treatment performance (Okhravi et al., 2017; Sabokrouhiyeh et al., 2017). Lagoons with multiple inlets however encourage improved mixing conditions and flow distribution, utilizing the full lagoons' capacity in the treatment process (Ioannidou and Pearson, 2018; Ma et al., 2020; Okhravi et al., 2017).

3.1.7. *Number of outlets*

The Num_Outlets demonstrated a significantly greater effect on Fe^{3+} R.E from the studied lagoons (see Fig. 6e) compared to the Num_Inlets effect, suggesting significant variation between the respective categories investigated. Fig. 6e presents the performance of different Num_Outlets alongside iron removal; in particular, lagoons with 4 outlets can be observed to attain higher average Fe^{3+} R.E than lagoons with 2 outlets. D-Lag with 3 outlets however recorded the least Fe^{3+} R.E, which could be attributed to the lower surface area it occupies and higher AR compared to the other lagoons. Therefore, if D-Lag is regarded as an anomaly and excluded from the Num_Outlets analysis, it can be concluded that the higher the number of outlets, the better the iron removal from the lagoons.

Lagoons with single-point inlet and outlet configurations are less effective at removing iron, since they are likely to experience short-circuiting as water preferentially flows through the shortest path between the single inlet and outlet (Sabokrouhiyeh et al., 2017; Zhong et al., 2020). Studies have also revealed that systems with multiple inlets achieved increased dispersion, low dead volumes, utilizing the full system's capacity for the treatment process (Okhravi et al., 2017; Sabokrouhiyeh et al., 2017). Therefore, to reduce the occurrence of dead zones in a lagoon, and enhance iron removal, multiple inlets and outlets could be constructed, along with careful consideration of their respective positions which includes midpoint–midpoint, uniform–midpoint, corner–corner and corner-midpoint configurations. Strategic placement of inlets and outlets controls mine drainage flow, encouraging sedimentation of iron-rich particles. While some studies have observed midpoint-midpoint configuration to have a better performance due to reduced dead zones compared to the other types (Ma et al., 2020; Okhravi et al., 2017; Sabokrouhiyeh et al., 2017), others have indicated that lagoons with corner – corner configuration demonstrate improved treatment performance (Zhong et al., 2020).

In conclusion, considering all the findings discussed in the preceding sections (3.1.1 to 3.1.7), it can be inferred that designing lagoons with mid-mid or corner-corner configuration, multiple inlets and outlets, and AR $\approx$ 4, they would achieve higher iron removal from mine drainage flowing through them.

3.2. Principal components analysis (PCA)

PCA is employed to identify the primary factors influencing iron removal from mine drainage. The design features employed for the PCA analysis are: WL, AR, Number of Inlets, Number of Outlets, Shape, Configuration, Area. These features have been observed to have a significance of p-value <0.05 with Fe^{3+} R.E. The number of PCs was determined using the Kaiser criterion, which involves the selection of components with eigenvalues >1 (Cloutier et al., 2008; Zhang et al., 2022). Therefore, the first three principal components (PCs): PC1, PC2 and PC3 with eigenvalues of 2.188, 1.986 and 1.654 respectively were selected. These three PCs also captured 83.7% of the total variance in the dataset with PC1, PC2 and PC3 explaining 31.42%, 28.52% and 23.76% of the variance respectively. Thereby, the three PCs explained approximately 80% of the total variance, which is the recommended percentage accurate enough to determine the most influential factors (Zhang et al., 2022; Zhu et al., 2022). Fig. 7 shows the scree plot of the PCs, which indicates the variance contributed by each PC to the total variance of the original dataset.

The PCA loadings for the lagoons are presented in Fig. 8 in the form of a heatmap. The loading plot illustrates the level of influence each design aspect has on a PC. Loadings range from −1 to 1, and loadings closer to either −1 or 1, depicted in darker shades on the heatmap, indicate stronger influence of the design aspects with the PC, hence suggesting a pronounced relationship between those design aspects and iron removal from the lagoon.

It can be observed from Fig. 8 that Surface Area and AR exhibited high negative loadings on PC1, suggesting that they contribute to the primary source of variability in the lagoons' dataset. AR and Surface Area clustering together suggests that iron removal in some lagoons may be driven by the respective AR and Surface Area. In particular, although B-Lag2 and D-Lag are of similar shape, configuration, and single inlet-multiple outlets (see Table 2), they however achieved different iron removal, i.e. of 86.48% and 13.72% respectively. It is therefore suggested that D-Lag's smaller AR of 0.5 compared to B-Lag2 AR of 2, and a surface area of 148.04m^2 compared to B-Lag2's 3528.29 m^2, that D-Lag's lower AR and surface area led to a rather low Fe^{3+} R.E of 13.72% compared to B-Lag2's R.E of 86.48%.

WL and Shape indicated high negative loadings on PC2 while Num_Inlets suggest a high positive loading on PC2 (see Fig. 8). These three design aspects (WL, Shape, Num_Inlets) have been identified in section 3.1 to have varying effects on the amounts of iron removed from

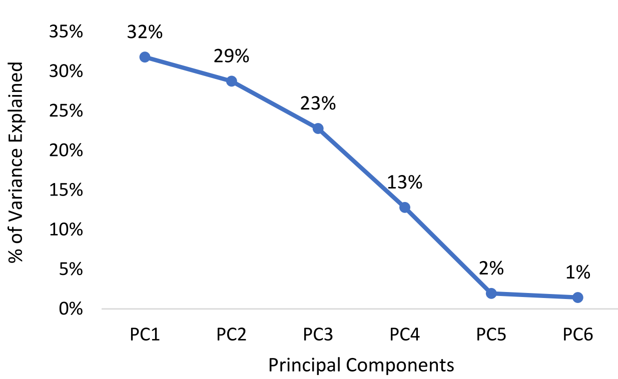

Fig. 7. Scree plot of the PCs.

the lagoon. This study has demonstrated that oval shaped lagoons perform better in removing iron than rectangular and trapezium shaped lagoons. In addition, higher WL has been observed to reduce Fe^{3+} removal as D-Lag and *E*-Lag with the highest WL recorded lower Fe^{3+} removal compared to the other lagoons. The Num_Inlets controls the WLs within the lagoon, while the shape affects the utilization of the effective volume and the retention time (Jenkins and Greenway, 2017; Wörman and Kronnäs, 2005).

In PC3, Configuration had high positive loading while Num_Outlets had a high negative loading (Fig. 8). This is supported by the clusters shown in Fig. 9, as some lagoons' performance may be distinguishable by their Configuration and Num_Outlets; for example, B-Lag1 and C-Lag1 both had mid-mid configuration and 4 outlets each and had similar Fe^{3+} R.E of 80.29% and 82.65% respectively.

The relationship among these variables and their contributions to PC1 and PC2 can also be visualized in a bi-plot to show the clusters that exist in the lagoon dataset (see Fig. 9). For instance, from the close proximity of AR and Surface Area in Fig. 9, it can be suggested that a significant relationship might be present between both variables, also supported by their relatively high loading values on the loadings plot (see Fig. 8). In addition, a relationship between Configuration and the Num_Outlets, and another relationship between shape and WL was observed, as these variables can be seen to cluster in Fig. 9.

3.3. Regression analysis

Regression analysis is performed to understand how each variable individually affects Fe^{3+} removal. Seven design aspects are used in the analysis: WL, Configuration, AR, Surface Area, Shape, Num_Inlets and Num_Outlets. Design depth was excluded from the regression as the depth for all studied lagoons is uniform (i.e. 3 m). Month (denoting seasonal variation) and year (of water sample collection) were also included in the regression analyses. Therefore, a total of 9 independent variables are used in the analysis, with Fe^{3+} R.E being the dependent variable.

Initially, five regression models are used to examine the relationship among these variables, and to assess the significance of the design aspects to the lagoons' performance (as presented in methods section). The five regression models were assessed for compliance to their respective assumptions. Furthermore, it was ensured that the assumption of no multicollinearity was met, which was examined using the variation inflation factor (VIF) and ensuring that the VIF for all variables were <10 (Artemiou et al., 2021; Rhoton, 2014; Thoe et al., 2014). Multicollinearity refers to occurrence of high correlations between one or two independent variables which could affect the reliability and accuracy of the regression results (Tabachnick and Fidell, 2001).

The best model is then selected using the evaluation metrics presented in Table 3. Overall, from Table 3, RF regression is observed to have achieved the highest R^2 and the lowest MAE, MSE and RMSE. Although other models also performed well, MLR and Ridge regression models proved to be less useful. Therefore, RF regression model was used for further analysis in this study.

The overall model fit of Random Forest is (R-squared value) is 0.7900, indicating that 79% of the variation in the dependent variable (Fe^{3+} R.E) can be explained by the independent variables. The RF regression coefficients, known as "importances" which signify both the strength and direction of the association between each independent variable and the dependent variable, were obtained and are presented in Table 4. For example, the coefficient for WL (0.5191) suggests that for 1 unit increase in WL, the dependent variable (Fe^{3+} R.E) is expected to increase by 0.5191 units, if all other variables remain unchanged; for every 1 unit increase in Num_Inlets, Fe^{3+} R.E increases by 0.1576 units; for every 1 unit increase in Surface area, Fe^{3+} R.E increases by 0.0156 units, all else being equal. Therefore, as in Table 4, WL is a more important factor affecting iron removal from lagoons compared to the number of inlets, whereas surface area is suggested to have a higher

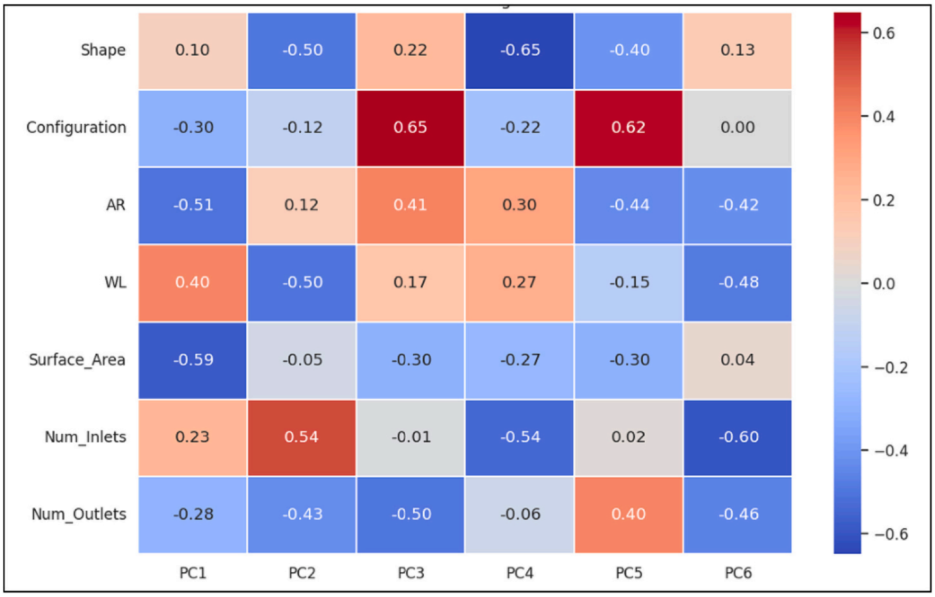

Fig. 8. PCA Loadings of the MWTS lagoons.

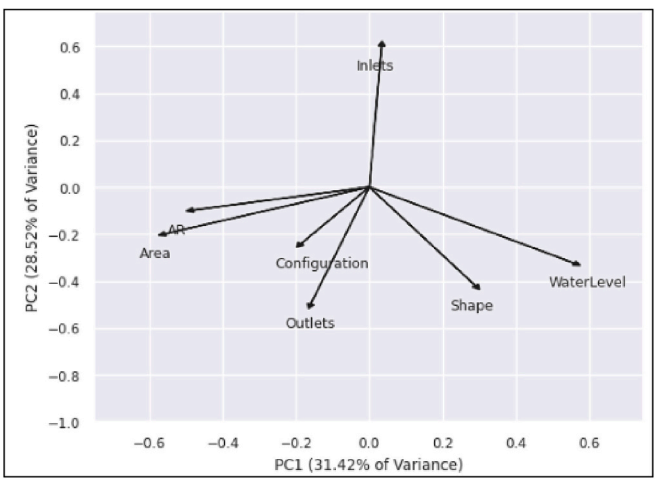

Fig. 9. PCA bi-plot for the MWTS Lagoons

Table 3
Different Regression models Evaluation Metrics (Lagoons).

Models	R^2	RMSE	MSE	MAE
Random Forest Regressor	0.7900	13.9919	195.7755	10.0783
Multiple Linear Regressor	0.7543	15.13479	229.0619	11.3611
XGBoost	0.7781	14.0208	196.5828	10.7704
Polynomial Regression (Degree = 2)	0.7623	14.8891	221.6861	11.1219
Ridge Regression	0.7542	15.13939	229.2012	11.3668

impact on iron removal than Configuration.

Num_Inlets was the next most important feature (after the WL), which significantly affects Fe^{3+} R.E compared to year and month (Table 4). The top 2 variables arising from the regression analyses, i.e. WL and Num_Inlets, were also grouped in the same PC (i.e. PC2) in the PCA loadings presented in Fig. 8.

Year is also an important feature to consider in the removal of Fe^{3+}. This suggests that as the older the lagoon, the more the deposition of ochre and sludge occur as time progresses, which impacts the lagoon's performance, particularly when the sludge is not regularly removed

Table 4
Regression coefficients of Random Forest (RF) Regression in Lagoons.

Variables	Importances
WL	0.5699
Num_Inlets	0.1576
Year	0.1147
Month	0.1059
Surface Area	0.0156
Shape	0.0106
AR	0.0101
Configuration	0.0086
Num_Outlets	0.0067

from the lagoon.

The best performing model (RF) is used with different number of variables in an order based on the regression coefficients values obtained on the initial run of the RF model (Table 4). The results, in terms of evaluation metrics, of using different number of features in the RF regression are presented in Fig. 10.

The regression best performance was obtained when all 5 dependent variables were included in the model. The R^2 of the RF regression model reduced slightly, when variables were removed one-by-one from the model, up till Model 5 (Fig. 10). Prior to the removal of Surface Area from the model, 79.18% of the variation in the dependent variable (Fe^{3+}) could be explained by WL, Num_Inlets, month, year and Surface Area. However, when Surface Area was removed, a sharp decrease in the R^2, and an increase in the other evaluation metrics can be observed (see Fig. 10a), compared to when other metrics like Year and Month were removed. A corresponding increase in MAE, MSE and RMSE values can also be noticed in Fig. 10 b-d. This indicates that Surface Area is an important design aspect to be considered when designing lagoons for Fe^{3+} removal from mine drainage.

On removal of Year from the model, R^2 increased to 0.7601, demonstrating that year/age of the lagoon has an impact on iron removal. The higher the year (of data collection), the older the lagoon. As the lagoon ages, the deposition of ochre and sludge increases with time, impacting the lagoon's performance, especially if the sludge is not removed from the lagoon on a regular basis (Kgari et al., 2016; Kusin, 2011; Tran et al., 2020; Wolkersdorfer et al., 2016). For example, without removal of sludge in 18 months of operation, the effective

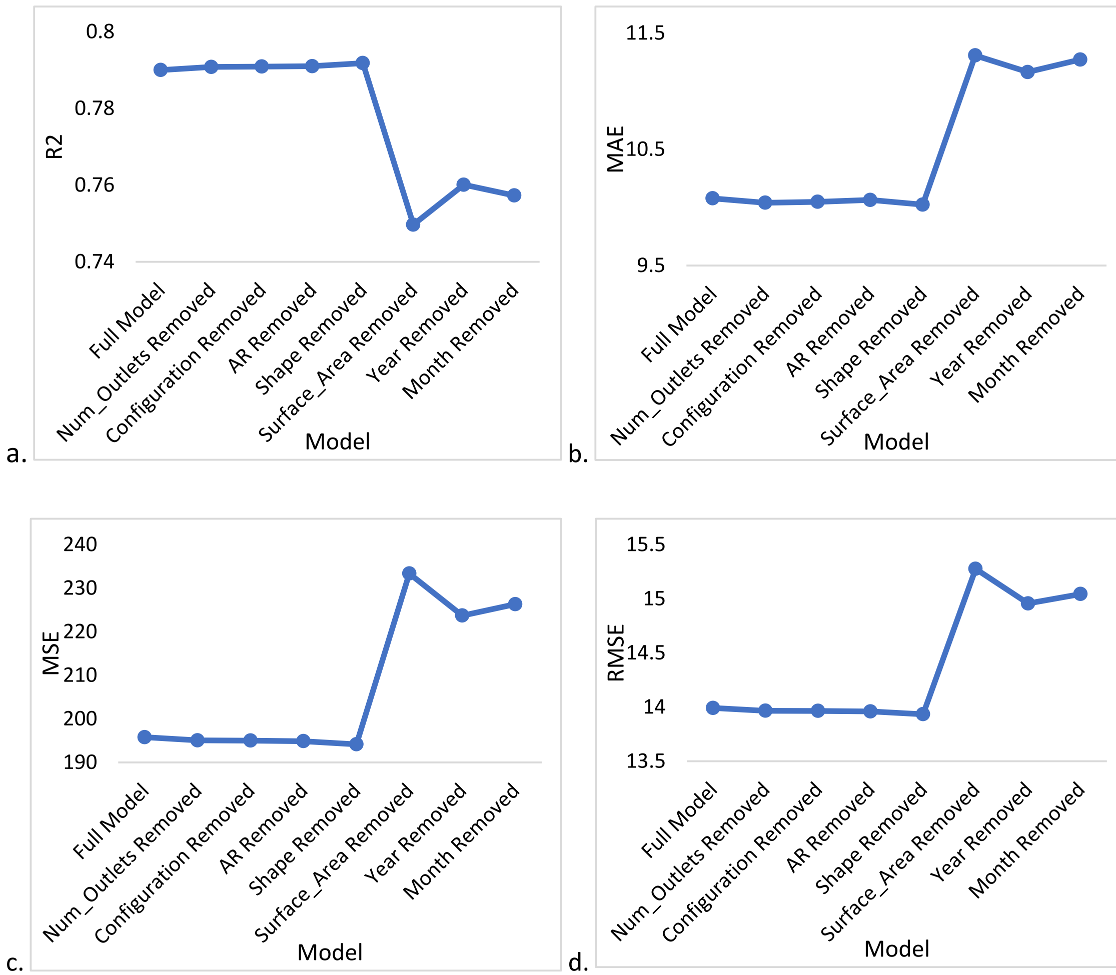

Fig. 10. Trends of evaluation metrics with variable removal from RF model a) R^2 b) MAE c) MSE and d) RMSE.

volume of a full-scale lagoon in a passive MWTS was found to have reduced by 39%, thus reducing at a rate of approximately 2.18% on a monthly basis (Kusin, 2011; Kusin et al., 2014).

Furthermore, although Num_Outlets demonstrated the least importance, the Num_Inlets should not be decided independent of the Num_Outlets. The Num_Outlets feature plays an important role in the lagoon's performance but depends on other design aspects, e.g. Configuration and AR, which were grouped together in PC3 due to their high loadings (Fig. 8). The use of single inlets and multiple outlets, or multiple inlets and single outlets has been observed to increase the creation of short-circuiting, reduce the effective volume, and reduce the treatment performance of the system (Okhravi et al., 2017; Su et al., 2009). However, in order to increase the performance of systems with single inlet or single outlet, the width of the inlet/outlet respectively should be increased, as previous studies have proved that widening an inlet or outlet improves the lagoon performance (Hendi et al., 2022).

Overall, the 5 variables included in the model prior to the removal of surface area were: WL, Num_Inlets, Month, Year, Surface Area. These variables are regarded to be influential variables to iron removal processes in lagoons. Among these, three variables represent key design aspects (namely WL, Num_Inlets, Surface Area), and should therefore be prioritized over other design aspects when combining aspects to optimize iron removal and treatment performance of full-scale lagoons treating mine drainage.

4. Conclusions

This study has investigated and assessed the influence of a variety of design aspects of 10 full-scale mine drainage lagoons on iron removal over a period of 12 years. Higher Aspect Ratios (AR) were observed to contribute to higher Fe^{3+} removal, with corner-corner configuration achieving minimum creation of dead zones, while multiple inlets formed a more uniform velocity field. In terms of the lagoon shape, oval shaped lagoons were found to perform better than rectangular and trapezium lagoons. A larger surface area resulted in a higher Fe^{3+} removal while a higher water level (WL) resulted in a lower Fe^{3+} removal from the lagoons.

From the principal component analysis three clusters emerged; one consisting of WL, shape and number of inlets; a second cluster comprising AR and surface area; and a third cluster consisting of configuration and the number of outlets. Design aspects within these three clusters shared common characteristics and collectively explained Fe^{3+} removal variation from the studied lagoons. Random Forest regression proved to be more effective in evaluating the relationship among the different design parameters, compared to Multiple Linear Regression and XGBoost Regression, Polynomial Regression and Ridge Regression. Results of the regression analyses demonstrated that WL, Num_Inlets and surface area were the most important features affecting Fe^{3+} removal from lagoons and should be given priority when addressing design aspects of lagoons. Other significant parameters, arising from the regression analyses, are age (year) due to increase of ochre and sludge with time; seasonal variation which influences microbial activity and other contaminant removal processes; and shape which determines potential formation of dead zones and effective volume utilised for treatment.

Finally, to attain improved lagoon treatment performance, multiple design aspects should be properly combined by positioning inlets and outlets in opposite corners, employing multiple inlets, and maintaining an AR ≈ 4.

Author contributions

All authors contributed to the study conception and design. Material preparation and data analysis were performed by Oluwanisola A. Okeleji and Vasiliki Ioannidou. All authors read and approved the final manuscript.

CRediT authorship contribution statement

Oluwanisola Ayodele Okeleji: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis. **Vasiliki G. Ioannidou:** Writing – review & editing, Supervision, Resources, Data curation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The authors do not have permission to share data.

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