## JOURNAL OF DEGRADED AND MINING LANDS MANAGEMENT

Volume 10, Number 1 (October 2022):3889-3904, doi:10.15243/jdmlm.2022.101.3889 ISSN: 2339-076X (p); 2502-2458 (e), www.jdmlm.ub.ac.id

### **Research Article**

## Declined peat heterotrophic respiration as consequences from zeolite amendment simulation: coupling descriptive and predictive modelling approaches

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Abstract

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#### Article history:

Received 11 June 2022 Accepted 4 August 2022 Published 1 October 2022

Keywords:

artificial intelligence CO<sub>2</sub> emission machine learning multivariate analysis pedotransfer modelling Nowadays, halting greenhouse gasses (GHG) emission is the world's major concern to mitigate global climate change. In oil palm cultivated tropical peatland, GHG emission is primarily constituted of CO<sub>2</sub> flux emitted from aerobic heterotrophic respiration (Rh), the natural degradation process of organic material in an oxidative environment. By coupling descriptive and predictive statistical approaches, this study attempted to gain an in-depth understanding of the effects of zeolite rates and incubation time on CO2 emission that came from aerobic R<sub>h</sub> in peat, as well as their decomposition process. This study found that zeolite amelioration up to 30% of the peat at field capacity and starting from the first month of observation (month-1) significantly restricted peat Rh, denoted by a reduced amount of observed CO2 flux (0.021 and 0.019-0.012 mg m<sup>-2</sup> sec<sup>-1</sup>, respectively). Both factors and several soil variables exhibited some non-linear relationships with Rh at different magnitudes and importance, showing the limitation of the traditional linear-based approach to interpreting their complex interrelationships, as well as predicting CO<sub>2</sub> flux. This study highlights the vital role of a polynomial (GAM) and artificial intelligence (Cubist and GBM) -based pedotransfer models in improving our understanding regarding the dynamic of the peat

**To cite this article:** Pulunggono, H.B., Hanifah, N., Nadalia, D., Zulfajrin, M., Nurazizah, L.L., Mubarok, H., Tambusai, N., Anwar, S. and Sabiham, S. 2022. Declined peat heterotrophic respiration as consequences from zeolite amendment simulation: coupling descriptive and predictive modelling approaches. Journal of Degraded and Mining Lands Management 10(1):3889-3904, doi:10.15243/jdmlm. 2022.101.3889.

decomposition process as affected by zeolite amendment.

### Introduction

Indonesian peatland contributes a considerable extent to the world's tropical peat and sequesters carbon at a huge volume (Kurnianto et al., 2014; Miettinen et al., 2017), as well as located closely to anthropogenic disturbance sources (Dohong et al., 2017; Page et al., 2022). Furthermore, greenhouse gas (GHG) emitted from Indonesian peatland is recently gained worldwide attention as a consequence of extensive landscape transformation from the natural peat-swamp forest into other land uses (Miettinen et al., 2017; Wijedasa et al.,

2017; Leifeld et al., 2019; Dadap et al., 2021). The changes in land use types, particularly for plantations, require drainage management to prevent prolonged waterlogging conditions, thereby resulting the deepening of groundwater levels (GWL). Oxic condition that occurs at the peat surface not only provides near-ideal conditions for growing oil palm seedlings or saplings but also generates a favorable environment for microorganism activity. This act, hence, will enhance the decomposition of peat material and increase GHG emissions (Cooper et al., 2019; Aditya Prananto et al., 2020; Xu et al., 2021). Consequently, mitigating peat decomposition in cultivated Indonesian peatland areas is urged to be done.

Managing aerobic heterotrophic respiration (R<sub>h</sub>) as low as possible is pivotal in oil palm cultivated peatland since GHG emission (in this case: total soil respiration/ $R_t$ ) is remarkably comprised of  $R_h$ , particularly at microsites that are far from the oil palm tree (Ishikura et al., 2018; Manning et al., 2019; Pulunggono et al., 2022a). Rh primarily consists of aerobic heterotrophic microorganism activity at the oxic zone above GWL, which requires oxygen to decompose organic materials and emits CO2 as their respiration result (Widiastuti et al., 2021). Peat material is commonly known as the primary source of decomposable organic matter; whereas lesser contributors of aerobic Rh also have been investigated, such as pruned fronds (Wakhid and Hirano, 2021), understory litters (Pulunggono et al., 2022a), or dead root fragments (Pulunggono et al., 2022b). Moreover, another R<sub>h</sub> fraction comes from an anoxic zone at a higher depth below GWL and unconnected pores, having a condition suitable for anaerobic decomposition, thus outgassing a negligible amount of CH<sub>4</sub> at a slower rate (Cooper et al., 2020). Furthermore, another GHG source is autotrophic respiration (R<sub>a</sub>) which originates from root-related respiration (Melling et al., 2013; Dariah et al., 2014; Sabiham et al., 2014). The contribution of R<sub>a</sub> might be low, offset by CO2 uptake during the oil palm photosynthesis process (Ishikura et al., 2018).

Previous reports quantifying declined R<sub>h</sub> as affected by peat surface waterlogging, either by a natural process (Desmukh et al., 2021) or artificially wetted (Ishikura et al., 2018; Manning et al., 2019). Other researchers suggested lowering soil temperature by increasing shading components through matured oil palm leaves (Jauhainen et al., 2014; Manning et a., 2019) and understory cover crops (Pulunggono et al., 2022a) and frond piles (Manning et al., 2019). Moreover, there is an indication that zeolite amelioration can also halt GHG emission and/or Rh of tropical peat materials, as reviewed by Santi et al. (2021). Zeolite possesses a high capacity to adsorb and hold a considerable amount of water and soil nutrients (Cataldo et al., 2021), store CO<sub>2</sub> and NH<sub>3</sub> (Megias-Sayago et al., 2019; Valencia et al., 2019), and reduce soil temperature oscillation (Badora, 2016). On the other hand, zeolite application in oil palm plantations was promising, owing to advanced zeolite synthesis from oil palm disposal (Khanday et al., 2016; Khanday et al., 2017; Kongnoo et al., 2017). Publications concerning zeolite amendment to improve soil health are abundant in mineral soil studies (Mondal et al., 2021; Szerement et al., 2021). Emerging studies regarding its application in tropical peat are also reported (Ahmed et al., 2015; Lim Kim Choo et al., 2020; Krishnan et al., 2021). Unfortunately, combating GHG emitted from  $R_h$  in oil palm cultivated tropical peat using zeolite are extremely scarce topic to be found.

There are large numbers of published reports on soil science domains, researching and reviewing the effect of zeolite amendment on soil health in particular, as well as on the environment and agriculture studies in general (Badora, 2016; Cataldo et al., 2021; Mondal et al., 2021; Morante-Carballo et al., 2021). As mentioned previously, its application in tropical peatland is considerably limited. Most of them are analyzed and interpreted with a traditional descriptive approach. Currently, there is developing interest emerging in agricultural and environmental studies regarding the usage of predictive modelling, especially artificial intelligence/AI (Liakos et al., 2018; Ye et al., 2020; Benos et al., 2021). Advanced predictive modelling based on AI is considered beneficial for interpreting soil data since they are not restricted by a particular set of rules and limitations. AI algorithm will automatically learn the pattern of the data, allowing the user to interpret the modelling results with an established theoretical framework or reveal new findings (Rossiter, 2018; Padarian et al., 2020). Compared to the linear-based model, the AIbased models can flexibly capture both linear and nonlinear relationships among the factors and soil variables with considerable accuracy, as shown in findings of the related fields (Bond-Llamberty, 2018; Holl et al., 2020; Adjuik and Davis, 2022; Pulunggono et al., 2022b).

Therefore, this study aimed to elucidate the effects of zeolite rates and incubation time on  $CO_2$  emission that came from peat  $R_h$ , as well as gain insight into concerning peat decomposition process by pairing descriptive and predictive statistical approaches.

Based on that, this study hypothesized that: (1) zeolite amendment in terms of its content and incubation time could restrict heterotrophic respiration ( $R_h$ ), as shown by decreasing trend of CO<sub>2</sub> emission, (2) the relationships between factors and soil variables used in this study with CO<sub>2</sub> emission are non-linear, and (3) AI-based pedotransfer models were beneficial to support common linear-based models and traditional descriptive approach, with respect to their accuracy and interpretability.

### **Materials and Methods**

#### Research site, peat sampling, and incubation

The peat material (0-20 cm) was collected compositely under oil palm cultivated peatland in Buatan Village, Koto Gasib, Siak Regency, Riau Province (0° 44' 44" N and 101° 46' 22' E), March 2021. The area undergoes 2,045 mm precipitation (May 2020 to April 2021) with an equatorial climate pattern and unclear precipitation difference between months (Pulunggono et al., 2022a). From a physiographic perspective, the study site is located on the back swamp of the Siak and Gasip rivers. The peatland surrounding the study site had a hemic-sapric maturity stage around five meters thick (Pulunggono et al., 2019). Their physical and chemical properties are summarized in Table 1.

Table 1. Peat properties used in this study.

| Type of analysis             | Value  | Status*     |
|------------------------------|--------|-------------|
| pH H <sub>2</sub> O -peat    | 3.21   | Very acidic |
| pH H <sub>2</sub> O -zeolite | 8.91   | -           |
| Organic C (%)                | 56.83  | Very high   |
| Peat water content (%)       | 432.65 | -           |
| Ash content (%)              | 2.30   | Low         |

Note: status referred to the technical guidelines of soil chemical analysis (Eviati and Sulaeman, 2009).

Immediately after being sampled, the peat material was packed and transported to the Soil Chemistry and Fertility Laboratory, Department of Soil Science and Land Resources, Faculty of Agriculture, IPB University. An approximately 2 kg of peat material was then incubated with zeolite inside a jar (d =15 cm; h = 18 cm) for three months. The zeolite rates varied from 0, 10, 20, 30, 40 to 50% with five replications, calculated based on peat weight at the field capacity, resulting in 30 experimental units in total.

### Laboratory analyses and CO<sub>2</sub> flux measurement

Laboratory analysis was conducted during the initial and every month of the incubation period. Actual peat acidity/APA was determined using pH H<sub>2</sub>O (1:1), peat water content/PWC was determined using gravimetric methods, and total peat acidity/TPA using BaCl<sub>2</sub>-TEA pH 8.2, and organic-C content was determined using lost on ignition/LOI method.

The CO<sub>2</sub> flux from each experimental unit was measured monthly using calibrated IRGA (Infrared Gas Analyzer) LI-830 with a closed-chamber method. A chamber (d =15 cm; h =18 cm) was installed to load gasses from the incubated peat inside the jar. The gas then flowed to the IRGA, which measured the gas every second for 2 minutes. The temperature in the chamber (T) was measured concurrently with the CO<sub>2</sub> measurement, followed by the measurement of the chamber height from the chamber lid to the surface of the peat material. The results were calculated using Madsen et al. (2009) equation:

$$fc = \frac{Ph}{RT} \frac{dC}{dt}$$

Fc represents the flux value (mg m<sup>-2</sup> sec<sup>-1</sup>), P is atmospheric pressure, h is the height from the chamber lid to the surface of the peat material, R is the gas constant (8.314 Pa m<sup>3</sup> °K<sup>-1</sup> mol<sup>-1</sup>), T is the temperature (°K), and  $\frac{dc}{dt}$  is the linear change in CO<sub>2</sub> concentration.

# Descriptive statistical analyses: LME-REML and PCA

Data collating, listing, and inspection were done using Microsoft Excel and Minitab 16. Prior to analysis, the data were inspected to omit missing values and outliers. A square root/sqrt transformation was applied to  $CO_2$  flux data to gain normalized distribution with respect to the Kolmogorov-Smirnov normality test.

To achieve reasonable perspective concerning the effects of zeolite rates and incubation time, as well as other related peat parameters to CO<sub>2</sub> flux, this study employed the linear mixed effect model/LME with restricted maximum likelihood/REML. At first, CO2 flux was plotted as a response and the entire parameters (zeolite rates, incubation time, T, PWC, APA, and TPA) were fed entirely into the general linear model (GLM type III) coupled with backward stepwise elimination/BSE (95% confidence interval) to obtain their effect to CO<sub>2</sub> flux variance. The elimination terms included the coefficient of determination (R<sup>2</sup>), Akaike information criterion/AIC, and Bayesian information criterion/BIC. The GLM-BSE analysis resulted from the consideration of zeolite rates and incubation time as fixed factors, whereas the others were seemingly favourable as random factors. Hence, LME-REML was performed to test the hypotheses, resulting in comparable R<sup>2</sup> and slightly higher performance of AIC and BIC terms than GLM-BSE model. Moreover, APA, PWC, and TPA were excluded from the model due to confounding/aliasing with the error terms. Lastly, Tukey's honestly significant difference/HSD test was chosen as post-hoc test to examine the grouping of the entire factors. All of the variance analyses were conducted using Minitab 16. In order to increase the clarity, the boxplot based on original metrics of CO<sub>2</sub> flux (mg m<sup>-2</sup> sec<sup>-1</sup>) was generated using tidyverse in the R environment (Wickham, 2022), equipped with a significant letter that was acquired from Tukey's HSD test.

This study also utilized principal component analysis/PCA as a multivariate analysis to complement LME-REML. A standard PCA was employed using factomineR (Husson et al., 2020) and factoExtra (Kassambara and Mundt, 2020) packages in the R environment to extract principal components/PCs, representing most of the variation of the entire data. This study considered PCA methods to reveal underlying relationships among CO<sub>2</sub> flux and the entire factors and parameters observed in this study since every PC contains certain parameters that contributed most to the dataset variances. Several groupings based on linear projection were also performed with respect to zeolite rate and incubation time.

# Predictive statistical analyses: pedotransfer models for CO<sub>2</sub> flux prediction

This study examined the performance of several pedotransfer models (summarized in Table 2) in predicting  $CO_2$  emission from peat materials incubated with zeolite. The entire pedotransfer models were developed under the R environment with the following general formula:

 $\label{eq:CO2} \begin{array}{l} CO_2 \mbox{ flux} \sim \mbox{ zeolite rate + incubation time + T + APA + PWC} \\ + \mbox{ TPA} \end{array}$ 

Unlike the sort-transformed form in LME-REML and PCA analyses, CO<sub>2</sub> flux was reversed back into its original value, allowing the model algorithm to learn the original relationships and pattern of the data. Meanwhile, organic C was discarded from the equation owing to higher missing data. The entire data was scaled and centred using min-max normalization to prevent the domination of variables that contain higher magnitudes and preserve their pattern. Moreover, the original datasets were randomized and then split into training (70%) and testing (30%) data. Both the training and testing data were separated into predictor matrices and response vectors for convenient use in training and validating the models. Most of the pedotransfer models were firstly trained and tuned using a common ML aggregator caret package (Kuhn et al., 2020), except for GAM and SVM-based models.

| Name                           | Abbreviation | Family     | Package         | Source                     |
|--------------------------------|--------------|------------|-----------------|----------------------------|
| Multiple linear regression     | MLR          | Linear     | stat            | R core team (2022)         |
| Logistic-linear model          | LogGLM       | Logistic   | stat, caret     | R core team, Kuhn et al.   |
|                                |              | binomial   |                 | (2020)                     |
| Multivariate adaptive          | MARS         | Polynomial | earth, caret    | Milborrow (2021), Kuhn     |
| regression spline              |              |            |                 | et al. (2020)              |
| Generalized additive model     | GAM          |            | mgcv, gam       | Wood (2021), Hastie        |
|                                |              |            |                 | (2022)                     |
| Cubist                         | Cubist       | Machine    | Cubist, caret   | Kuhn et al. (2022), Kuhn   |
|                                |              | Learning   |                 | et al. (2020)              |
| Tree regression                | TR           |            | rpart, caret    | Therneau et al. (2022),    |
|                                |              |            |                 | Kuhn et al. (2020)         |
| Random forest                  | RF           |            | Random          | Liaw and Wiener (2018),    |
|                                |              |            | Forest, ranger, | Wright et al. (2021), Kuhn |
|                                |              |            | caret           | et al. (2020)              |
| Gradient boosting machine      | GBM          |            | gbm, caret      | Greenwell et al. (2020),   |
|                                |              |            |                 | Kuhn et al. (2020)         |
| Support vector regression with | SVR1         |            | e1071           | Meyer et al. (2022)        |
| linear basis kernel            |              |            |                 |                            |
| Support vector regression with | SVRp         |            | e1071           | Meyer et al. (2022)        |
| polynomial basis kernel        |              |            |                 |                            |
| Support vector regression with | SVRr         |            | e1071           | Meyer et al. (2022)        |
| radial basis kernel            |              |            |                 |                            |
| Support vector regression with | SVRs         |            | e1071           | Meyer et al. (2022)        |
| sigmoid basis kernel           |              |            |                 |                            |

Table 2. Pedotransfer models used in this study.

The best performance model with particular hyperparameters setting that gained the lowest RMSE were selected using the combination of grid search and 5-fold cross validation (k-fold cross validation/KFCV) with ten replication to avoid model overfitting. The ensemble tree models (e.g., RF and GBM) were also trained separately using grid search and cross validation in ranger (Wright et al., 2021) and gbm (Greenwell et al., 2020) packages, respectively, exploiting their out-of-bag/OOB fraction. Similar to RF and GBM, grid search combined with 10-fold cross validation was also applied to separately train TR

model using rpart package (Therneau et al., 2022). To obtain the maximum model performance, the grid search-based tuning was repeated three to four times, each turn updated and narrowing the previous search ranges. The results of TR, RF, and GBM training using separated packages were then compared to caret's results thereby, the best model was selected by the lowest RMSE. GAM was left without much tuning since limited adjustment information in mgev package and a sufficient degree of freedom acquired at k = 4 for each predictor and REML as smoothing parameter estimation. The entire SVM-based model was tuned using grid search utilizing tune.svm function in e1071 package (Meyer et al., 2021).

Model evaluation was performed consisting of several performance metrics, i.e., root means square error/RMSE, mean absolute error/MAE, Bias, and coefficient of determination/R<sup>2</sup>. Model explainability or interpretability was approached divergently concerning their differences in complexity. To get uniform interpretability technique that works for all models, this study used several approaches, utilizing both local and global models agnostic methods that consisted of partial dependence/PD, individual conditional expectation/ICE, and permutation feature importance/PFI (iml package; Molnar and Schratz, 2022).

### Results

# The relationships between peat heterotrophic respiration with the entire factors and variables

According to LME-REML analysis in Figure 1.1, zeolite amendment, as determined by its rate, caused minimum and notably different  $CO_2$  flux emitted from maximum zeolite application (50% lower than control; 0.012 mg m<sup>-2</sup> sec<sup>-1</sup>). Amending zeolite up to 30 and 40% significantly decreased  $CO_2$  flux by 1.2 and 1.4 folds (0.021 and 0.014 mg m<sup>-2</sup> sec<sup>-1</sup>, respectively)

compared to control. Lower CO<sub>2</sub> flux was also emitted from peat amended by a lower zeolite percentage (10 to 20%; 0.025 and 0.023 mg m<sup>-2</sup> sec<sup>-1</sup>, respectively); however, their emissions did not statistically different from the control.

A significant effect of incubation time was also observed on  $CO_2$  emission, as shown in Figure 1.2. a significantly highest  $CO_2$  flux was emitted at the first observation (control; 0.037 mg m<sup>-2</sup> sec<sup>-1</sup>). The first and two months of incubation remarkably inclined  $CO_2$  flux by 1.4 and 1.5 folds (0.019 and 0.017 mg m<sup>-2</sup> sec<sup>-1</sup>, respectively) than control. A minimum  $CO_2$  flux (1.8 folds than control; 0.012 mg m<sup>-2</sup> sec<sup>-1</sup>) was pronouncedly emitted from the last month of incubation.

Generally, CO<sub>2</sub> fluxes had a negative correlation with T and APA (Figures 1.3 and 1.5). However, opposite relationships were recorded among CO<sub>2</sub> fluxes with PWC and TPA (Figures 1.4 and 1.6). A relatively flat trend was observed on CO<sub>2</sub> flux from 100 to 300% PWCs; furthermore, an inclined curve could be drawn from 300 to 500% PWCs. CO<sub>2</sub> emission seemingly had decreasing trend over the increase of both fixed factors, as shown in Figures 1.1 and 1.2. However, non-linear relationships were diversely observed from both fixed (Figures 1.1 and 1.2) and random factors (Figures 1.3, 1.4, 1.5, and 1.6).



Figure 1. The effect of the entire factors and peat properties on peat heterotrophic emission. The white asterisk and black horizontal line inside the boxplot indicate mean and median values, respectively; the black dashed line indicates means from the entire CO<sub>2</sub> flux data.

The zeolite treatment seems to have polynomial-based relationships with  $CO_2$  flux. Meanwhile, the relationships between  $CO_2$  flux and incubation time could be fitted with a Weibull-based curve. More complex relationships, as shown by more scattered points, emerged among  $CO_2$  flux with T, PWC, APA, and TPA, possibly could be determined by Poisson or quasiPoisson-based curve.

The effect of zeolite content and incubation time on T, PWC and APA were presented in Figure 2. The entire rate of zeolite application significantly increased PWC and APA compared to control; meanwhile similar effect on T was recorded on 20% of peat dry weight. PWC on 10% and 20% of zeolite applications were markedly different from control, whereas inconsiderably differences with both rates were observed at higher rates. Amending 10% of peat dry weight or higher chiefly affected APA, particularly at 30 and 50% zeolite application.

T, PWC, and APA were affected significantly by incubation time. Moreover, different effects were obtained, as shown by the up and down pattern for T and decreasing trends for PWC and APA. T was recorded inclined twice in the second and last months of observation. Both peaks exhibited insignificant differences from each other and notable differences with the first observation (month-0). PWC was remarkably different in every month of observation. APA' magnitudes remained less significant during the first three months of observation. Subsequently, a notable difference from the first observation was attributed to the last observation.



Figure 2. The effect of zeolite content and incubation time to T, PWC, and APA. The white asterisk and black horizontal line inside the boxplot indicate mean and median values, respectively; the black dotted line indicates means from T, PWC, and APA, respectively.

Descriptive multivariate analysis (in this study: PCA; Figure 3.1) showed five PCs that contributed to the variance of the entire dataset. The figure also depicted the first three PCs (PC1, PC2, and PC3) that mostly accounted for the dataset variance (46.7, 30.1, and 13.6%; respectively) with the eigenvalue more than 1, accumulating 90.5% of the total variance. PC1 was significantly loaded with the peat chemical properties, especially TPA and APA (Figure 3.2.1). Moreover, PWC and CO<sub>2</sub> flux remarkably correlated with PC2 (Figure 3.2.2). In Figure 3.2.3, PC3 only accounted T as its significant contributor.

After both significant first two PCs were plotted in the ordination diagram, gradual shifts were observed in the grouping of the observation points, either in zeolite content (Figure 2.3.1) or incubation time (Figure 2.3.2). These were the indication of both factors' significance in regulating the variances of the dataset, including  $CO_2$  emission variance. Several classes were significantly different, denoted by their less overlapped points (i.e., 0-all, 10-30 and 40, 30-50% zeolite content; 0-all, 1-3, and 2-3 months of observation; Figures 2.3.1 and 2.3.2). However, visual observation of both factors denoted overlapping observation points, indicating that some classes were not significantly different. In Figure 2.3.1, amending 20-30%, 30-40%, and 40-50% zeolites seemingly exhibited overlapping points. These results were partially different with grouping based on LME-REML analysis for  $CO_2$  flux (Figure 1.1), particularly for 30-40% zeolite application. Supporting the findings of LME-REML analysis, 1 and 2 months of observation were also visually overlapped (Figure 2.3.2).



Figure 3. Princical component analysis/PCA of peat heterotrophic emission with the entire factors and variables, exhibited the percentage of explained variances (2.1), variable contribution of the first three PCs (2.2.1, 2.2.2, and 2.2.3), and biplots of loading and observation plots, grouped by zeolite content (2.3.1) and incubation time (2.3.2). Note that the red dotted lines in Figures 2.2.1, 2.2.2, and 2.2.3 indicated the significant contribution of each variable loaded by their respective PC.

#### Pedotransfer modelling comparison of peat heterotrophic respiration as affected by zeolite amendment and incubation time

The entire pedotransfer models' performance was assessed using four evaluation metrics, shown in Figures 4 and 5. Generally, polynomial-based models (i.e., GAM and MARS) acquired the best performances in predicting  $CO_2$  flux, as indicated by their lowest RMSE (0.136 and 0.140, respectively) and MAE (0.101 and 0.111, respectively), as well as moderate Bias (0.34 and 0.35, respectively). ML-based models had also comparable RMSE and MAE, particularly for Cubist (0.140 and 0.111), GBM (0.141

and 0.111), and SVRr (0.144 and 0.106) models. Interestingly, several widely popular ML-based models gained the worst performances in this study, for instance, TR and RF, which possessed higher RMSE and MAE than simpler models (i.e., MLR and LogGLM).

According to Figure 4, the entire pedotransfer model showed positive values based on Bias. These indicated that they underestimated  $CO_2$  flux prediction compared to the actual  $CO_2$  flux. Interestingly, the high performer models (i.e., GAM, MARS, Cubist, GBM) based on both previous evaluation metrics failed to attain the lowest Bias. However, they reached a slightly lower value, about 60 to 20 percents from the

minimum Bias gained by LogGLM. Furthermore, based on  $R^2$  perspective in Figure 5, the entire pedotransfer models used in this study exhibited comparable results with strong confidence intervals, ranging from 0.55 to 0.69 (p<0.001). Both polynomial

(GAM) and ML (SVRr, Cubist, and GBM) -based models achieved best agreements ( $R^2 = 0.68$ -0.69). Except for TR, the entire polynomial and ML-based models attained higher  $R^2$  ( $R^2 \ge 0.64$ ) compared to MLR and LogGLM ( $R^2 = 0.62$ ).



Figure 4. RMSE, MAE, and Bias of several pedotransfer models used in this study.



Figure 5. Model agreement based on the coefficient of determination (R<sup>2</sup>) of several pedotransfer models used in this study. Note that the entire predicted and observed value of CO<sub>2</sub> fluxes were transformed to min-max normalization.

PDP and ICE methods employed in this study inferred both linear and non-linear relationships of each factor and soil variables' marginal effect on the predicted CO<sub>2</sub> flux (predicted.y in Figure 6) possessed by "the best performers" pedotransfer models compared to MLR. Predicted CO<sub>2</sub> flux had general decreasing trends over both factors (zeolite rate and incubation time). Soil temperature and peat water content had similar curve patterns to previous factors, except for GBM, which showed opposite slope directions. Other soil variables exhibited diverse and contrasting patterns over predicted CO<sub>2</sub> fluxes. The curve pattern of zeolite rate was similar all across the best performer pedotransfer models, except for GBM. GAM and GBM denoted a similar pattern, exhibiting a sharp dip of predicted CO2 fluxes during early observation, therefore, continued by decreasing trends with more moderated slopes at the middle and the end of observations. However, linear patterns that were relatively similar to MLR were shown by other ML-based pedotransfer models that also acquired higher R<sup>2</sup> and RMSE, for instance, Cubist and SVRr.

Interestingly, GAM as the best pedotransfer model in this study, shared closely a similar PDP pattern with MLR, particularly at zeolite content, soil temperature, and total peat acidity. Differently from the ordinary least square of MLR, restricted maximum likelihood/REML as smoothing parameter in polynomial-based algorithm of GAM successfully captured non-linear and opposite linear relationships of predicted  $CO_2$  fluxes to incubation time and actual peat acidity, respectively.



Figure 6. Partial dependence/PD (yellow lines) and individual conditional expectation/ICE (black lines) curves comparison of some of the best performer pedotransfer models used in this study compared to MLR model. Note that the data distribution is depicted by a rug in the x axis. T, PWC, APA, and TPA represent soil/peat

temperature, peat water content, actual peat acidity, and total peat acidity, respectively. All of the predictors and predicted values were min-max-transformed.

Feature importance based on MSE loss in Figure 7 exhibited that incubation time was the most important covariate for predicting  $CO_2$  flux, regardless of the model. Zeolite content and TPA were the second important covariates, respectively, accounting for nine and three of the entire pedotransfer models used in this

study. T was a moderately important covariate, owing to its middle position. Moreover, PWC and APA were the most unimportant covariates, as shown by their least position at utmost pedotransfer models in Figure 7.



Figure 7. Permutation feature importance/PFI plots based on MSE loss for the entire pedotransfer models used in this study.

### Discussion

This study demonstrated the importance of zeolite incorporation to halt heterotrophic respiration (R<sub>h</sub>) in tropical peat in the form of its rate and incubation time, supported by coupling descriptive statistical analyses (LME-REML and PCA; Figure 1) and advanced predictive-based pedotransfer modelling (Figure 7) approaches. By tailoring this combination approach, soil science and agricultural researchers are able to extract valuable information and gain understanding from various perspectives, as also pronounced by other researchers from diverse disciplines, such as material science (Bock et al., 2019), engineering (Patrick et al., 2019), as well as health and medical science (Basu et al., 2020; Ma, 2020). This study presents an initial stepping stone from the traditional approach into the multidimensional realm of analytics in soil science and agricultural studies.

Zeolite has a high water holding capacity/WHC, which can efficiently retain water (Nakhli et al., 2017; Mondal et al., 2021). In their intact natural environment, peat does not require zeolite application since they also have high WHC (Comeau et al., 2021) and are located in coastal or riverine back swamp areas that are periodically or permanently waterlogged (Sakabe et al., 2018). At the early stage of oil palm cultivation, the environmental impact associated with the high CO<sub>2</sub> flux could arise at the open peat surface due to the deepening GWL and rising of air and soil temperature, especially during the dry season (Ishikura et al., 2018). The combination of peat and zeolite as the high water-retaining agents holds much water could mitigate these issues by stabilizing R<sub>h</sub> (significantly lower at months-1 and 3; insignificant increment at month-2; Figure 1) and T under lower PWC as shown in Figure 2. With respect to T and PWC as affected by zeolite amendment, these findings corroborated with other research in mineral soil (e.g., Al-Busaidi et al., 2011; Baghbani-Arani et al., 2020; Karami et al., 2020; Baghbani-Arani et al., 2021).

The first observed T peak in Figure 2 is possibly attributed to the high amount of water initially contained by peat. Some researchers suggested that water exchange inside zeolite pores could generate the release of base cations into their surrounding environment (Mihok et al., 2020). This condition enhances the decomposition process of peat material adjacent to zeolite particles, thereby producing metabolic heat that appeared as a significant increase at months-1. Furthermore, the second T peak observed at the last observation seemingly occurred due to the water loss and continuing decomposition process throughout the remaining organic material. A half amount of water was lost during three months, generating a relatively ideal environment for R<sub>h</sub>. Nevertheless, the highest temperature observed in this study was 30% lower than the maximum temperature reported by the zeolite experiment using different organic materials (i.e., Venglovsky et al., 2005; Ramos et al., 2018), indicating peat and zeolite combination successfully suppress excessive Rh in peat, especially while a particular amount of nutrients were added into a drier peat environment.

The prominent characteristic possessed by zeolite in order to restrict GHG emission is high available pores. These properties promote high air and water-filled pore space, whereas the latter had previously discussed. The abundance of air-filled pore spaces combined with a particular mechanism provides zeolite crystal and ample storage to trap CO<sub>2</sub> under certain conditions (De Baerdemaeker and De Vos, 2013; Kumar et al., 2020). However, the CO<sub>2</sub> uptake capacity of zeolite is markedly reduced under high humidity or water content (Kolle et al., 2021), which significantly constrains its functionality when applied in a peat environment during the rainy season. This also partially explains the reason for higher  $CO_2$ emissions, with the highest PWC that is observed in the first month of observation. Based on these facts, an improved zeolite performance concerning CO<sub>2</sub> entrapment is considered to occur under a prolonged dry season.

Based on the result of this study, long-term zeolite application is important in oil palm cultivated tropical peatland. Three months of incubation could significantly restrict peat R<sub>h</sub>, shown by the flattening trend over the first and second months in Figure 1b. In the field, the zeolite amendment combined with appropriate management of drainage and agronomic practice could minimize the microbial activity in decomposing peat materials. Moreover, good drainage management results stabilized GWL, hence, preserving PWC at its moist condition at long period. Thus, matured oil palm trees, understory covers, and pruned fronds piles provide thick shading and coverage at each microsite, preventing direct atmospheric exposure to the peat material at the surface. Both practices maintain air and soil temperature stabilization, hence, minimizing R<sub>h</sub> and CO<sub>2</sub> flux (Jauhainen et al., 2014; Manning et al., 2019; Pulunggono et al., 2022a).

By combining all evaluation metrics, this study found that polynomial and ML-based pedotransfer models were considered promising to predict CO<sub>2</sub> flux emitted from tropical peat materials as affected by zeolite amelioration rather than using widespread MLR technique (e.g., Nurzakiah et al., 2021; Pulunggono et al., 2022a; Figures 4 and 5). These findings were caused by their flexibility in capturing non-linear relationships among Rh with its predictors, which in this study were markedly related to zeolite amendment. The CO<sub>2</sub> flux emitted from incubated peat material was the result of biological processes that originated from microbial R<sub>h</sub>. Some published reports revealed the importance of factors and variables used in this study in controlling microbial respiration, therefore suggesting their non-linear relationships with CO<sub>2</sub> emissions. Previous reports indicated that zeolite addition could boost CO2 emission from composted sludge (Awasthi et al., 2016) and duck manure (Wang et al., 2014), contrastingly with inhibitory effects found in this study (Figures 1 and 6), as well as other composting experiment using swine (Bautista et al., 2011), cattle mixtures (Lim et al., 2017), and chicken manures (Peng et al., 2019). Kučić et al. (2013) found that CO<sub>2</sub> gas emitted from grape and tobacco wastes mixture incubated with zeolite was strongly affected by incubation time with non-linear decreasing trend over time, similarly to other reports conducted using various types of organic manures or sludge (e.g., Wang et al., 2014; Awasthi et al., 2016; Wang et al., 2020). Hirano et al. (2009) and Jauhainen et al. (2014) reported a close relationship between soil temperature with R<sub>h</sub> in tropical peatland, similar to this study (Figure 7). However, their relation seemingly appeared as non-linear, concerning the lower R<sup>2</sup> and correlation found by Marwanto et al. (2014) and Batubara et al. (2019).

This study also provides examples and comparisons of pedotransfer models trained with different techniques. Single splitting and single splitting with grid search were performed on GAM and SVR, respectively. Meanwhile, other pedotransfer models (i.e., MLR, LogLM, MARS, Cubist, TR, RF, and GBM) were trained and tuned with repeated kfolds cross-validation/KFCV methods using training data (70% of the entire data). KFCV performed in this study provides 50 randomized models, trained and tuned separately using 80% of the training data and internally tested using the remainder 20% data. Furthermore, the tuning process of some tree-based ensemble ML models used in this study (i.e., RF and GBM) was more complex. They perform a stochastic approach, employing a random subspace method which requires random resampling on the training data, subsequently averaging the entire constructed sub-trees (Ho, 1998; Breiman, 2001) or additively validated each sub-trees using out-of-bag data and gradient descent (Friedman, 2001). Both first models acquired the lowest RMSE and MAE (Figure 4), as well as the highest  $R^2$  (Figure 5), whereas common best-performers (e.g., RF and GBM) followed behind them. More simplified and explainable models (i.e., MLR, LogLM, and TR) were at the least. These agreement metrics obtained by GAM and SVR were possibly biased since they only computed on a single instance. These results were supported by other polynomial-based pedotransfer models, i.e., MARS, which trained using KFCV method, obtaining agreement metrics similar to ML-based models. The biased model that relied on the single instance was vulnerable to overfitting, could not compensate for outliers, and may fail to generalize on real-field deployment. Some research also noted that KFCV approach was weak in mitigating overfitting, particularly when applied to evaluate models with limited samples size. Nested KFCV sufficiently provides the best-unbiased estimates and reliable model compared to all approaches used in this study, as well as more robust to outliers according to previous findings and reviews (Tabe-Bordbar et al., 2018; Vabalas et al., 2019; Maleki et al., 2020; An et al., 2021). Unfortunately, nested-based techniques cannot be explored in this study due to the limitation of observation data. Based on the above explanation, this study considered Cubist and GBM as the most reliable AI-based pedotransfer model, regarding their predictive performance and relatively unbiased design for model development.

Contrasting with this study, Nurzakiah et al. (2021) reported considerably higher  $R^2$  (0.91) of CO<sub>2</sub> flux than predicted from MLR-based pedotransfer model. A similar method with lower  $R^2$  (0.14-0.49) was also reported by Pulunggono et al. (2022a), who utilized different variables to predict CO<sub>2</sub> flux. Molnar (2022) stated that evaluating models with training data is somewhat problematic since they utilized the same dataset that was used for training the model, which is considered prone to over-optimistic estimation. This is because the models are forced to predict from and compare their prediction with the data they previously learned, not from the new unseen data.

### Conclusion

Utilization of tropical peatland potentially generated considerable R<sub>h</sub>, thereby enhancing organic material degradation and boosting GHG emissions into the atmosphere. Through this simulation study, zeolite could be used as a potential amendment to restrict R<sub>h</sub> from tropical peat material, as shown by decreasing trend of CO2 flux affected by zeolite content and incubation time. Both factors significantly controlled CO<sub>2</sub> flux with linear and non-linear patterns, based on the evidence of descriptive (LME-REML and PCA) and predictive pedotransfer-based modelling (GAM, Cubist, and GBM) statistical approaches. Zeolite amelioration at 30 to 50% of peat field capacity and the entire months of observation (except for month-0) significantly reduced CO2 fluxes (0.021-0.012 and 0.019-0.012 mg m<sup>-2</sup> sec<sup>-1</sup>, respectively). Besides the factors, T and TPA were the soil variables that nonlinearly govern  $CO_2$  flux, whereas other variables were less important. This study provides the initial attempt to disclose the importance of pairing descriptive and predictive modelling analyses, particularly while factors and variables had complex and non-linear relationships.

### Acknowledgements

The authors thanked the Indonesian Oil Palm Plantation Fund Management for this research funding. The authors also acknowledged the support and assistance of management and field staff of Astra Agro Lestari Tbk. during the fieldwork.

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