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Research Paper

Multi-objective machine learning for compost maturity and ammonia-risk trade-offs with external CO2 emissions modeling

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ABSTRACT: *Composting can recycle biodegradable organic residues into agronomically useful amendments, but operational decisions must balance product stabilization against nitrogen loss and atmospheric emissions. Most machine-learning studies of composting have modeled maturity or emissions separately, limiting their usefulness for process-level decision support. This study developed a reproducible Python workflow for multi-objective compost assessment using open data. A primary matched compost dataset was used to model maturity score and ammonia-related risk, while a second external Dryad dataset of compost-amended field plots was used to test whether the same modeling workflow could be extended to CO2 flux prediction in a related environmental context. Target-specific feature sets were used to reduce information leakage, and models were evaluated using held-out test data and cross-validation. The maturity model achieved excellent predictive performance (test R2=0.992; cross-validated R2=0.990±0.003). The ammonia-risk model also performed strongly (test R2=0.780; cross-validated R2=0.829±0.059). External CO2 prediction was moderately successful (test R2=0.606; cross-validated R2=0.736±0.065), reflecting the greater heterogeneity of field emissions data. Pareto screening of the matched maturity and ammonia outcomes identified non-dominated candidate profiles that jointly support high compost maturity and lower ammonia-related risk. The results show that leakage-aware, multi-objective machine learning can translate compost monitoring data into practical trade-off information, while external CO2 modeling can provide complementary environmental context when interpreted separately from active compost-process optimization.*

KEYWORDS: *compost maturity, ammonia risk, CO2 flux, machine learning, Pareto optimization, environmental monitoring*

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I. INTRODUCTION

Food waste and other biodegradable residues remain major management challenges for municipalities, agriculture, and the food industry. Composting is a practical treatment option because it converts unstable organic matter into a more stable soil amendment while diverting organic waste from landfill disposal. However, composting performance is not defined by decomposition alone. Operators must balance several objectives, including rapid stabilization, product maturity, nitrogen retention, odor control, and greenhouse-gas mitigation.

These objectives can conflict. Operating conditions that accelerate organic-matter degradation and improve maturity can also increase ammonia volatilization, reducing the fertilizer value of the final product and contributing to air-quality concerns [1], [2]. Broader environmental performance is also influenced by carbon-related emissions and greenhouse-gas dynamics from composting and compost-amended systems [3]. A maturity-only optimization strategy may therefore overlook important environmental costs. A more useful decision-support question is: which operating conditions can maintain high maturity while reducing ammonia-related risk?

Machine learning has become increasingly common in composting research, including maturity prediction, sensor-based process monitoring, and gaseous-emission forecasting [4], [5], [6]. Nevertheless, much of the literature remains organized around single targets. Some studies focus on maturity indicators such as germination index or C/N ratio, whereas others focus on emissions or downstream environmental effects. Fewer studies explicitly frame compost management as a multi-objective trade-off problem. This gap limits the direct operational value of predictive models.

The present study addresses that gap by developing a reproducible Python workflow centered on the following research question: which available operating and quality profiles are predicted to produce mature compost while minimizing ammonia-related risk, and how far can this workflow be extended to external CO2 prediction? The workflow was designed for transparent implementation in common Python environments and for use with open datasets.

Two datasets were used for complementary purposes. The first dataset contained compost-process and quality variables, including maturity score and ammonia-related measurements, which allowed direct matched modeling of maturity and ammonia risk [5]. This dataset formed the core multi-objective analysis. The second dataset contained greenhouse-gas fluxes from compost-amended field plots and was used only as an external environmental module for CO2 modeling [7]. Because the two datasets were collected in different experimental contexts, they were not merged.

The contribution of this work is twofold. First, it demonstrates leakage-aware multi-objective modeling of compost maturity and ammonia-related risk using matched outcomes. Second, it evaluates the feasibility of adding external CO2 prediction as a complementary environmental layer. The study therefore aims to provide a realistic decision-support workflow rather than to claim universal optimization across all composting and field-emissions outcomes.

II. MATERIALS AND METHODS

2.1 Study design

The study used a two-dataset design with clearly separated objectives. Dataset A supported the primary matched analysis of compost maturity and NH3 risk. Dataset B supported an external analysis of CO2 flux in compost-amended field plots. This design avoided an artificial merge between datasets collected at different scales and under different environmental conditions.

2.2 Datasets

Primary matched compost dataset

Dataset A was the open Compost-Dataset associated with sensor-based compost maturity and gas-emission monitoring. It contained 452 observations and variables describing process conditions and compost quality, including day, temperature, moisture content, pH, C/N ratio, ammonia, nitrate, total nitrogen, total organic carbon, electrical conductivity, organic matter, T value, germination index, and maturity score [5]. After preprocessing, two primary targets were retained:

1. **Maturity score**, defined directly from the provided score variable.
2. **NH3 risk, defined from the ammonia measurement and predicted using feature sets that excluded the ammonia variable itself.**

External CO2 dataset

Dataset B was a Dryad dataset containing greenhouse-gas flux measurements from field plots receiving compost amendments [7]. The dataset included CO2 flux, treatment identifiers, year, plot, block, and related contextual variables. This dataset was not treated as an active composting-process control dataset; instead, it was used to evaluate whether the modeling workflow could be extended to a related environmental outcome.

2.3 Preprocessing and leakage control

Preprocessing was carried out in Python using pandas, NumPy, scikit-learn, and XGBoost. Numeric conversion, feature cleaning, and missing-value handling were performed separately for each dataset. Categorical fields in the external dataset were encoded before model fitting. Each target was modeled with a target-specific predictor set to reduce information leakage.

For Dataset A, the maturity model excluded the maturity score from the predictors. The NH3-risk model excluded the ammonia measurement and any variables that directly reconstructed the NH3 target. This was essential because exploratory analyses showed that proxy-like target definitions can inflate performance when target-defining variables remain in the input matrix. For Dataset B, the CO2 flux variable was excluded from the predictors, while treatment, time, plot, block, and other contextual variables were retained when available.

2.4 Model development

Separate models were trained for each outcome. Candidate learners included random forest and XGBoost regressors, which were selected because they can capture nonlinear effects and interactions without requiring strong parametric assumptions. Hyperparameters were tuned conservatively to limit unnecessary complexity. The general prediction task was expressed as

$$\hat{y} = f(x_1, x_2, \ldots, x_p),$$

where $\hat{y}$ is the predicted target, $x_1, \ldots, x_p$ are input features, and $f(\cdot)$ is the fitted machine-learning model.

Three final targets were retained:

1. maturity score, the primary compost-quality outcome;
2. NH3 risk, the primary ammonia-related environmental-risk outcome; and
3. CO2 flux, the secondary external environmental outcome.

2.5 Model evaluation

Performance was evaluated using a held-out test split and k-fold cross-validation. The main metrics were coefficient of determination (R^2), mean absolute error (MAE), and root mean squared error (RMSE):

$$R^2 = 1 - \frac{\sum_{i=1}^{n} \quad (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} \quad (y_i - y^{-})^2},$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n} \quad |y_i - \hat{y}_i|,$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} \quad (y_i - \hat{y}_i)^2}.$$

Here, y_i is the observed value, $\hat{y}_i$ is the predicted value, and y^{-} is the mean observed value. Cross-validation stability was assessed using the mean and standard deviation of fold-level R^2. Residual patterns and actual-versus-predicted plots were inspected to identify systematic model failure.

2.6 Feature interpretation

For the tree-based models, feature importance values were extracted and ranked. These rankings were used descriptively to identify which compost attributes and contextual variables contributed most strongly to maturity, NH3 risk, and CO2 prediction. Feature importance was interpreted as an explanatory aid rather than as proof of causality.

2.7 Multi-objective screening

Pareto-based screening was applied only to the matched primary outcomes. The objectives were to maximize predicted maturity score and minimize predicted NH3 risk:

$$max\ maturity\_score, \qquad min\ nh3\_risk.$$

Candidate profile A was considered to dominate candidate profile B if

$$Maturity_A \geq Maturity_B, \qquad NH_{3,A} \leq NH_{3,B},$$

with at least one strict inequality. Non-dominated profiles formed the practical recommendation set.

III. RESULTS AND DISCUSSION

3.1 Primary matched outcomes: maturity and NH3 risk

The strongest evidence came from the matched-outcome analysis using Dataset A. The maturity model achieved a test R2 of 0.992 and a cross-validated R2 of 0.990 ± 0.003. The NH3-risk model achieved a test R2 of 0.780 and a cross-validated R2 of 0.990 ± 0.003. These values indicate that the leakage-aware workflow captured stable relationships between the available compost variables and the two primary management-relevant outcomes.

Table 1: Headline predictive performance of the final reported models.

Outcome	Best model	Test R^2	Test MAE	Test RMSE
Maturity score	XGBoost	0.992	1.068	1.451
NH3 risk	Random forest	0.780	485.998	739.863
CO2 flux	Random forest	0.606	1.581	2.216

Figure 1 summarizes test-set R2, and Figure 2 shows observed-versus-predicted values for the two primary outcomes. Maturity predictions clustered closely around the one-to-one line, whereas NH3 risk showed greater scatter. The larger NH error is expected because ammonia-related processes are sensitive to pH, temperature, moisture, nitrogen transformations, and unmeasured operational conditions. Even so, the model retained enough predictive structure to support screening and trade-off analysis.

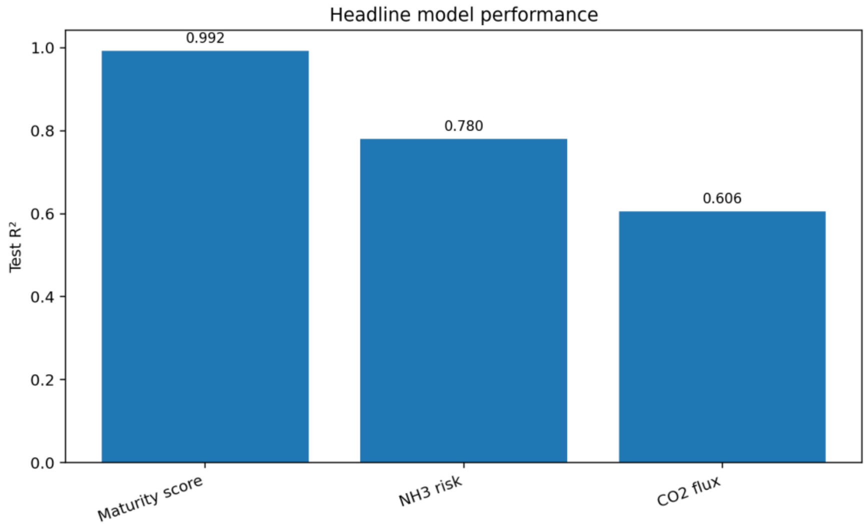


Figure 1: Headline test-set values for the final reported outcomes.

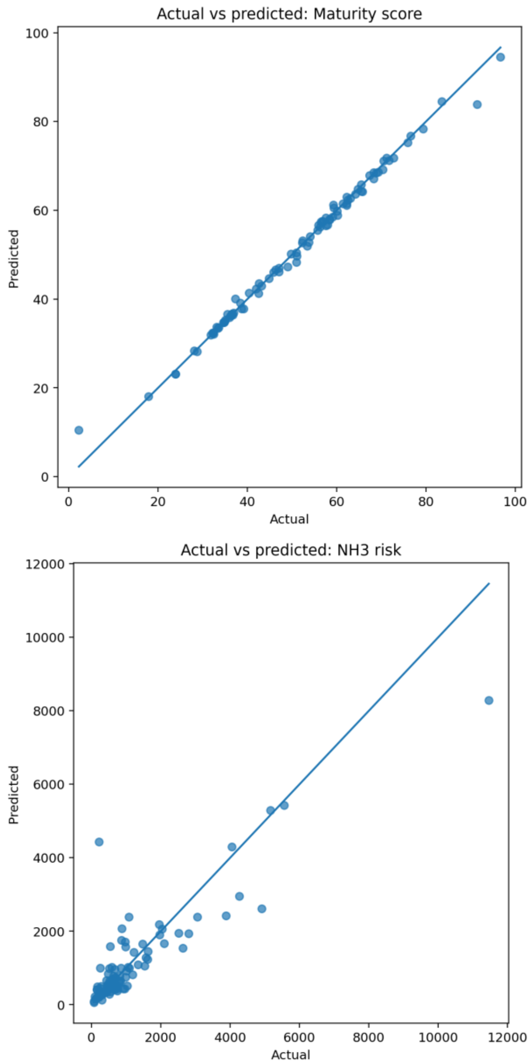


Figure 2: Actual-versus-predicted plots for the primary matched outcomes: (left) maturity score and (right) NH3 risk.

A key methodological improvement was the use of target-specific predictor sets. This avoided direct inclusion of target-defining variables and made the reported performance more defensible than exploratory models that might contain leakage. For applied environmental machine learning, this distinction is critical because high apparent accuracy can otherwise result from duplicated measurements rather than from generalizable process relationships.

3.2 Cross-validation stability

Cross-validation supported the robustness of the primary results. The maturity model showed minimal fold-to-fold variation, indicating that the relationship between maturity score and the available process-quality variables was highly stable. The NH3 model showed more variability but remained within a useful predictive range. The external CO2 model also showed acceptable cross-validated stability despite being trained on a more heterogeneous field dataset.

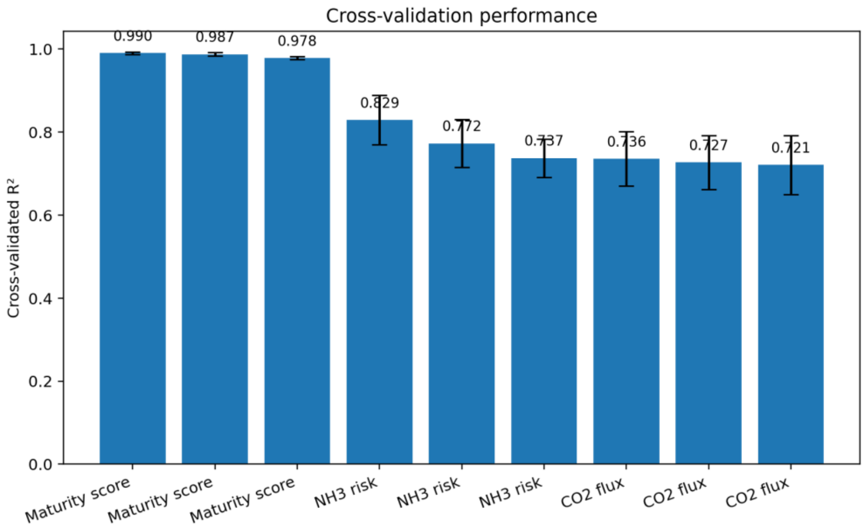


Figure 3: Cross-validated values (mean standard deviation) for the final reported models.

These patterns support a tiered interpretation: maturity prediction was the strongest and most reproducible result; NH3 risk prediction was the main secondary matched result; and CO2 prediction served as a supporting external extension rather than as part of the same matched optimization problem.

3.3 Feature importance and environmental interpretation

Feature-importance rankings indicated that maturity prediction was driven by established compost-quality indicators, especially germination index and T value, followed by pH, nitrate, and related chemical properties. This is consistent with the role of phytotoxicity reduction, nitrogen transformation, and organic-matter stabilization in maturity assessment [4], [8]. For NH3 risk, important predictors included pH, C/N ratio, nitrate-related information, moisture, and temperature-related variables. These drivers are environmentally plausible because ammonia volatilization and nitrogen transformation are strongly influenced by substrate chemistry and process conditions [1], [2].

These results suggest that the models were not merely statistical black boxes. The most informative variables aligned with known composting mechanisms. However, feature importance is not causal identification; rather, it indicates which measured variables were most useful for prediction within the available datasets.

3.4 Pareto-based decision support

The multi-objective component focused on the matched primary outcomes. Figure 4 shows the Pareto-recommended candidate profiles in terms of predicted maturity score and predicted NH3 risk. Because these profiles were non-dominated, no other candidate in the screened set simultaneously achieved higher predicted maturity and lower predicted NH3 risk.

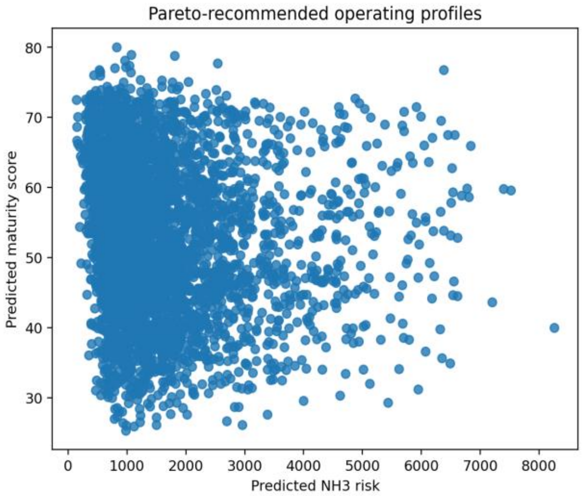
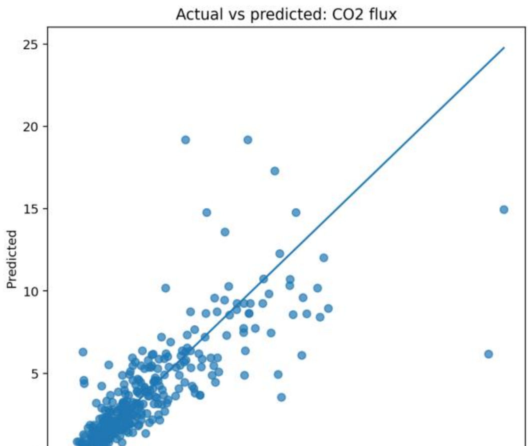


Figure 4: Pareto-recommended operating profiles for the matched primary objectives: maximizing maturity score and minimizing NH3 risk.

This step converts model outputs into decision-support information. Instead of presenting a single optimum that may depend on arbitrary weighting, Pareto screening provides a shortlist of defensible trade-off profiles. Operators or researchers can then select among these profiles according to site-specific priorities, such as maturity thresholds, nitrogen-retention goals, odor constraints, or regulatory requirements.

3.5 External CO2 module

The external CO2 model achieved a test R2 of 0.606 and a cross-validated R2 of , indicating moderate predictive success. Figure 5 presents the actual-versus-predicted relationship and treatment-level CO2 comparison.



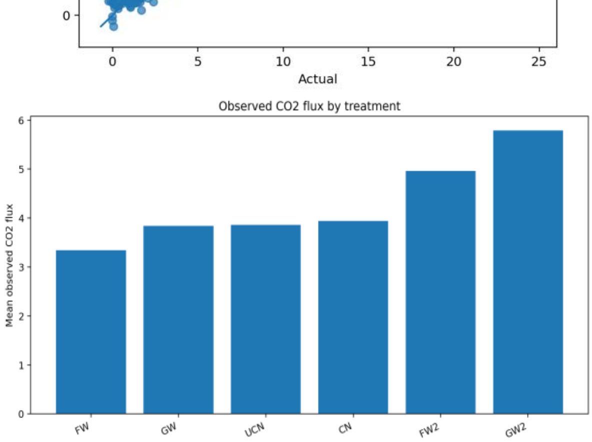


Figure 5: External CO2 results: (left) actual-versus-predicted CO2 flux and (right) observed mean CO2 flux by treatment in the Dryad field dataset.

The CO2 result should be interpreted as an external environmental module, not as a fully matched extension of the maturity–NH3 optimization. The Dryad data describe field-plot greenhouse-gas fluxes after compost amendment, whereas Dataset A describes active compost-process and quality variables. The CO2 analysis therefore demonstrates portability of the modeling workflow to a related target, but it does not support a claim of unified optimization across maturity, ammonia, and CO2 in one experimental system.

3.6 Comparison with previous studies

The findings are consistent with the growing use of machine learning in composting research. Wan et al. [4] showed that machine-learning models can predict maturity-related indicators such as germination index and C/N ratio with high accuracy. Khandakar and colleagues developed a sensor-based and interpretable machine-learning approach for compost maturity prediction and gas-emission monitoring [5]. Rosik et al. [6] further demonstrated that machine-learning models can predict gaseous emissions during early-stage composting with biochar addition.

The present study extends this literature by making the trade-off structure explicit. Its novelty is not a new algorithm, but a decision-oriented workflow combining matched outcome modeling, leakage control, interpretable feature ranking, and Pareto screening. This combination is relevant for environmental monitoring because it links predictive performance to management choices rather than reporting isolated model scores.

3.7 Limitations

Several limitations should be acknowledged. First, the study relied on two open datasets from different contexts, which prevented full integration of maturity, NH3, and CO2 into one matched experimental framework. Second, some operational variables of practical interest, such as aeration rate, turning frequency, bulking-agent characteristics, and energy use, were not jointly available with all target outcomes. Third, the external CO2 dataset reflected field-plot conditions after compost amendment rather than active compost-process control. Finally, the Pareto front should be interpreted as a screening result within the available candidate profiles, not as a universal optimization landscape.

Despite these limitations, the workflow is useful because many composting applications first need to determine whether compost has reached an acceptable maturity level and whether ammonia-related losses can be reduced. A model that jointly screens maturity and ammonia-related risk can support process planning, monitoring, and experimental design, while the external CO2 module broadens the environmental perspective without overstating the available evidence.

IV. CONCLUSIONS

This study developed a reproducible Python workflow for multi-objective compost-process modeling using open data. The strongest result was the matched prediction of compost maturity and NH3 risk. With target-specific feature sets, the maturity model achieved excellent performance and the NH3 model achieved strong predictive performance, supporting the use of machine learning as a decision-support tool for balancing compost quality and ammonia-related environmental risk.

The external CO2 analysis provided a secondary extension. It showed that carbon-related emissions can be modeled with moderate success in a related compost-amended field dataset, but it should not be interpreted as part of the same matched compost-process optimization problem. Future work should prioritize larger open datasets that jointly measure maturity, ammonia indicators, CO, operating conditions, feedstock properties, and management actions within the same composting systems.

Overall, leakage-aware multi-objective modeling can help convert compost monitoring data into practical trade-off guidance. By identifying non-dominated profiles, the proposed workflow provides a transparent way to balance product maturity with ammonia-risk reduction and to incorporate additional environmental modules as suitable matched data become available.

V. STATEMENTS AND DECLARATIONS

Competing interests The authors declare no competing interests.

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Author contributions Conceptualization: [BL]; methodology: [BL]; software: [BL]; formal analysis: [BL]; writing—original draft: [BL]; writing—review and editing: [BL]. All authors reviewed and approved the final manuscript.

Data availability The data analyzed in this study are available from the public Compost-Dataset repository and from the Dryad dataset with DOI https://doi.org/10.5061/dryad.hhmgqnkr0.

Code availability Code used for preprocessing, modeling, evaluation, and visualization is available from the corresponding author upon reasonable request.

Ethics approval Not applicable.

Consent to participate Not applicable.

Consent for publication Not applicable.

Use of AI tools Large language model assistance was used for language refinement and grammatical editing. All scientific content, analysis, and conclusions were developed by the author.

Ethical responsibilities statement All authors have read, understood, and complied as applicable with the statement on Ethical Responsibilities of Authors in the journal instructions.

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