https://doi.org/10.30970/apmicro.2026.63

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MACHINE LEARNING-ASSISTED PREDICTION OF BACTERIAL INACTIVATION BY COBALT FERRITE-ACTIVATED HYDROGEN PEROXIDE

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Abstract. Hydrogen peroxide activated on cobalt ferrite is a promising non-chlorine option for continuous-flow water disinfection, but bacterial survival depends nonlinearly on oxidant dose, initial load, and contact time. This study compared Weibull and Gompertz equations with ten supervised machine-learning algorithms using 208 individual *Escherichia coli* observations collected at 3, 6, and 10 mM H_2O_2. Gradient boosting and random forest performed best; their averaged model reached a group-based R^2 of 0.963. Independent experiments at 4 mM H_2O_2 confirmed good interpolation, supporting dose-contact-time selection within the tested range.
Keywords: *Escherichia coli*; hydrogen peroxide; cobalt ferrite; continuous-flow disinfection; machine learning.

Reliable control of flow-through water disinfection requires a model that links the initial microbial load, oxidant dose, and residence time to the number of viable cells remaining after treatment. Cobalt ferrite is attractive as a heterogeneous Fenton-like catalyst because it activates H_2O_2 and can be used as a stable fixed bed in continuous flow (Danyliuk et al., 2025; Tatarchuk et al., 2024). Recent studies also demonstrate the broader potential of ferrite-assisted peroxide treatment and machine-learning approaches for predicting disinfection performance (Huang et al., 2025; Tran et al., 2024). The aim of this study was to determine whether conventional kinetic equations or data-driven models can more reliably predict *E. coli* inactivation across a variable operating window.

Granulated $CoFe_2O_4$ (0.8–1.0 mm) was placed in a 100 cm × 12 mm stainless-steel packed-bed reactor. *E. coli* ATCC 35218 suspensions were treated with 3, 6, or 10 mM H_2O_2 at initial bacterial loads of $1.0 \cdot 10^3$–$5.0 \cdot 10^4$ CFU/L and six nominal contact times from 0.46 to 27.64 min. Viable bacteria were enumerated on Endo agar after 24 h at 37 °C. Replicates were retained as individual observations, giving 208 data points. Weibull and Gompertz models and ten supervised machine-learning algorithms were evaluated. Random forest (RF) and gradient boosting (GB) were selected for detailed analysis, including group-based five-fold cross-validation in which each of 28 complete kinetic curves was kept within a single fold. An averaged RF + GB model was then tested against an independent 4 mM H_2O_2 dataset that had not been used for training.

The classical models captured only parts of the inactivation trajectory. The Weibull model described the initial decline most closely at 3 mM H_2O_2, but its error increased with peroxide concentration and contact time. The fitted Weibull exponent n = 0.42 indicated substantial heterogeneity in bacterial resistance and the presence of a more resistant

subpopulation. The Gompertz model also performed satisfactorily at 3 mM in the early stage but systematically overestimated survival at 6–10 mM, with mid-phase relative errors exceeding 400 % under the strongest oxidative conditions. Its accuracy improved at the longest exposure time (27.6 min).

The ensemble algorithms were substantially more robust. In group-based validation, R^2 values were 0.915 for RF, 0.961 for GB, and 0.963 for the averaged RF + GB model; the corresponding MAE values were 3214, 2229, and 2018 CFU/L, while RMSE decreased from 4635 for RF to 3055 CFU/L for the combined model. RF tended to overestimate and GB to underestimate residual bacterial numbers at longer contact times, so averaging their predictions reduced directional bias. At 3 and 6 mM H_2O_2, errors of the combined model were mostly within ±10% during the first 10 min. Even at 10 mM, late-stage errors remained within ±18 %, lower than those of the individual models. Independent validation at 4 mM confirmed good interpolation: at an initial load of $1.62 \cdot 10^4$ CFU/L, errors were ≤ +10 % at 0.46–1.7 min and reached about −15 % at longer contact times. Larger percentage errors at the lower starting load occurred mainly when residual bacterial counts were very low, so small absolute deviations produced large relative errors.

Thus, cobalt ferrite-activated H_2O_2 produces distinctly nonlinear bacterial inactivation kinetics that are not adequately represented by a single classical equation over the full operating range. GB showed stronger generalization, while the RF + GB average provided the most balanced prediction. Within the tested domain, the ensemble approach offers a practical basis for estimating the H_2O_2 dose and contact time required to reach a target residual bacterial count. Further validation is needed before extrapolating the model to other reactor geometries, water matrices, catalyst batches, or peroxide ranges.

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