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Biochar Stability Revealed by Infrared Spectroscopy and Machine Learning

MONICA A. MCCALL[1,2], JONATHON S. WATSON[1], JONATHAN S.W. TAN[1,3] AND MARK A. SEPHTON[1]

[1]Imperial College London
[2]Grantham Research Institute on Climate Change and the Environment
[3]Viridien Satellite Mapping

Biochar is a carbon-rich, environmentally recalcitrant material with significant potential for climate change mitigation. Its carbon sequestration efficacy is primarily determined by stability, the resistance to degradation in soil, which is commonly assessed through H:C and O:C molar ratios. However, these measurements are expensive, resource-intensive, and destructive, creating a need for rapid and accessible stability estimation methods. This research combines Fourier-transform infrared spectroscopy (FTIR) with predictive modeling to estimate H:C and O:C molar ratios. Multiple lignocellulosic feedstocks were pyrolyzed at highest treatment temperatures (HTT) ranging from 200-700°C (5°C/min heating rate), followed by FTIR and elemental composition analysis of the resulting biochars. Several machine learning models, including Partial-Least-Squares, Elastic Net, Random Forest, and Support Vector Machines, were developed and trained on the FTIR spectra. Models underwent hyperparameter optimization and various data preprocessing evaluations. When applied to unseen test data from new feedstock and temperature treatments, several models achieved high predictive accuracy (R^2 values) and low root-mean-square-error (RMSE) for both molar ratio predictions. Feature importance analysis identified the most influential spectral ranges and associated chemical signals for predictions. The results of this study demonstrate that FTIR data can serve as a rapid and accurate proxy for biochar stability assessment, particularly valuable when pyrolysis conditions or feedstocks are unknown. These advancements support data-driven biochar deployment for optimized carbon sequestration and climate mitigation strategies.

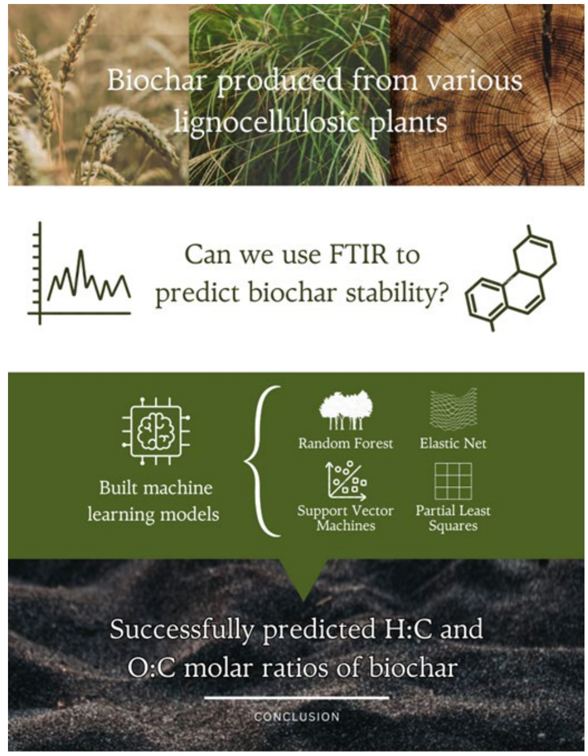

Figure 1: Graphical Abstract