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Exploratory Data Analysis of Biochar Composites Production Parameters for Supercapacitor Applications

Fernanda M.L. Toledo (PG),^{1,2} Amauri J. De Paula (PQ),³ Odair Pastor Ferreira (PQ),² Luiz Henrique Dall 'Antônia (PQ).^{1*}

fernandatoledo@uel.br; luizh@uel.br

¹Laboratory of Eletrochemistry and Materials (LEMA), Chemistry Department, UEL; ²Laboratório de Materiais Funcionais Avançados (LaMFA), Chemistry Department, UEL; ³Solid-Biological Interface Group, Chemistry Department, ITA.

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Highlights

Exploratory analysis is a rational approach for materials design. Data mining of scientific abstracts identifies trends in biochar synthesis and processing. Agricultural waste is the most common biomass.

Abstract

Until now, materials chemistry has been guided mainly by exploratory strategies for materials development. Scientists have focused on trial-and-error methods, which often result in low efficiency and lead to greater expenditure of time and experiments. However, recent advances in data science and machine learning (ML) provide the possibility to adopt rational design approaches. Therefore, this work proposes to extract and analyse data from scientific abstracts to identify trends and correlations that could guide the production of biochars modified with nanoparticles for supercapacitor applications.

For this purpose, a database was created with 544 scientific abstracts collected from *Web of Science using the keywords 'biochar' and 'supcapacitor'*. A Python script was performed with Regular expressions (Regex) to extract the process parameters and results from abstracts, such as the presence of post-treatments, the type of biomass, year of publication, specific capacitance, energy density, power density, and surface area values. The collected data were used to generate density plots, bar charts, and pie charts to identify the trends.

The preliminary results show that publications on this topic started in 2013 and have been increasing since. Most studies used agricultural waste as biomass. It was also observed that 43,2% of the abstracts reported some type of post-treatment. The density plots showed that most specific capacitance values were between 0 and 500 F g⁻¹, while the energy and power density distributions were concentrated in the ranges of 0 - 50 Wh kg⁻¹ and 0 - 500 W kg⁻¹, respectively. Surface area data were widely distributed, reaching values below 3500 m² g⁻¹.

These preliminary findings highlight key trends in the synthesis and characterization of biochars for supercapacitor applications. The analysis demonstrates the potential of literature data treatment to reveal patterns that can guide more rational strategies for the design and optimization of biochar materials.

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