

Adsorptive Removal of Pharmaceutical Contaminants from Wastewater using Magnetic Biochar Composites: A Sustainable Water Restoration

Abstract

The increasing presence of pharmaceutical contaminants in aquatic environments has become a major environmental concern due to their persistence, potential ecotoxicity, and incomplete removal during conventional wastewater treatment. This thesis focuses on the development of sustainable biochar-based adsorbents derived from waste biomass for the efficient removal of pharmaceutical pollutants from water, coupled with adsorption modelling, machine-learning prediction, fixed-bed column evaluation, and life cycle assessment (LCA). Accordingly, a novel magnetic biochar (GC-MBC) was synthesised from waste green coconut shells through a one-step FeCl_3 -assisted pyrolysis process. The adsorbent exhibited a high surface area ($680 \text{ m}^2/\text{g}$), well-developed porosity, abundant surface functional groups, and favourable magnetic properties, enabling efficient adsorption and easy recovery. Batch adsorption experiments demonstrated excellent paracetamol removal performance, with a maximum adsorption capacity of 217 mg/g . Adsorption followed the Freundlich isotherm and the pseudo-second-order kinetics and involved mechanisms such as pore filling, hydrogen bonding, π - π interactions, and n - π interactions. Life cycle assessment further confirmed the environmental sustainability of the process. Additionally, magnetic biochar derived from waste sawdust was subsequently developed for cephalexin removal. The synthesised adsorbent had a surface area of $611.9 \text{ m}^2/\text{g}$ and efficiently adsorbed cephalexin, achieving a maximum capacity of 143.9 mg/g . Adsorption equilibrium and kinetic data were well represented by the Langmuir isotherm and pseudo-second-order model, respectively. Statistical physics modelling provided molecular-level insights into the adsorption mechanism. Moreover, the environmental impact assessment revealed that natural gas-based electricity substantially reduced the environmental burden associated with adsorbent production compared to coal and diesel-based alternatives. Moreover, the simultaneous removal of paracetamol and cephalexin from binary solutions was investigated using FeCl_3 -activated magnetic biochar derived from green coconut shell. Adsorption capacities decreased in the binary system because of competitive adsorption between the pharmaceuticals. Statistical physics models successfully described the adsorption behaviour and revealed that the process was predominantly governed by physisorption mechanisms, including hydrogen bonding, electrostatic attraction, π - π interactions, and van der Waals forces. To predict adsorption efficiency, machine learning approaches such as random forest (RF), gradient boosting (GB), support vector machine (SVM), and artificial neural network (ANN) were employed. Among these models, ANN demonstrated the highest predictive accuracy, with R^2 values exceeding 0.99 for both pharmaceuticals. Furthermore, Fe-Mg layered double oxide magnetic biochar (LDO@MBC) was synthesised and applied for the removal of ofloxacin. The adsorbent exhibited a high surface area of $908.4 \text{ m}^2/\text{g}$ along with excellent magnetic properties. Statistical physics modelling indicated a double-layer adsorption mechanism involving multiple molecules per active site, while thermodynamic analysis confirmed that the adsorption process was spontaneous, entropy-driven, and primarily controlled by physical interactions. Environmental impact assessment of both adsorbent synthesis and wastewater treatment demonstrated low overall environmental burdens, particularly when adsorbent reuse was considered.

In addition, the practical applicability of biochar-based adsorbents was further evaluated by developing sodium alginate-based LDO-biochar composite beads (B-LDO@BC) for paracetamol removal under both batch and continuous-flow conditions. Adsorption kinetics followed the pseudo-second-order model, whereas equilibrium data were best described by the Langmuir isotherm, with a maximum adsorption capacity of 36.45 mg/g . Packed-bed column

studies revealed the significant influence of bed depth and influent flow rate on breakthrough behaviour and removal efficiency. The Thomas and Yoon–Nelson models successfully predicted column performance, demonstrating the potential of the developed adsorbent for continuous wastewater treatment applications.

Keywords: *Wastewater treatment, Pharmaceutical wastewater, Magnetic biochar, Paracetamol removal, Cephalexin adsorption, Ofloxacin removal, Machine learning, Life cycle assessment, Sustainability*