

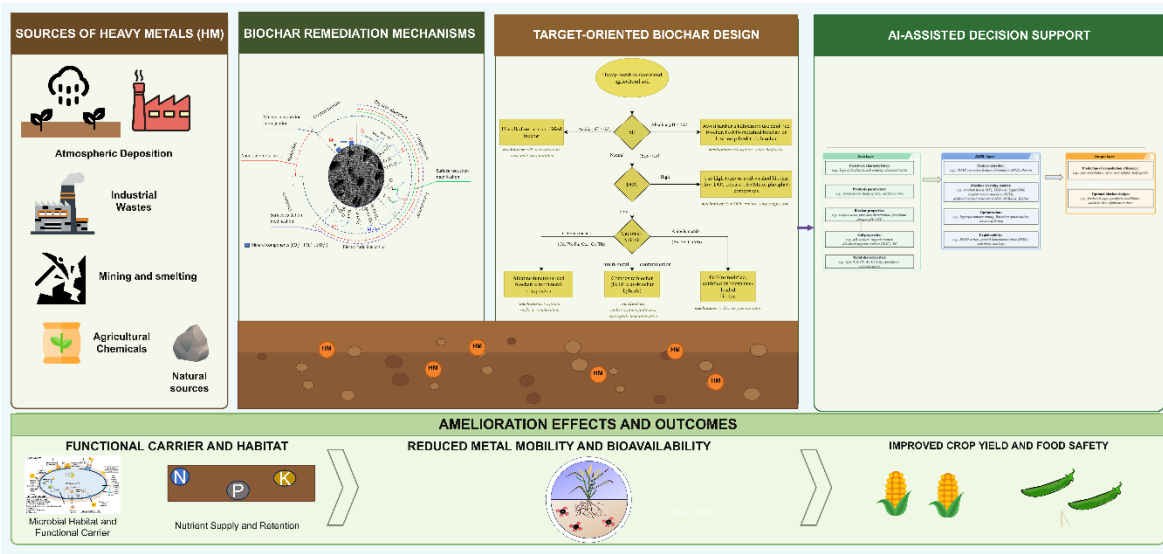
Biochar-Based Approaches for Heavy Metal Remediation in Agricultural Soils: Mechanisms, Optimization, and Emerging AI Applications

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GRAPHICAL ABSTRACT



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Heavy metal contamination in agricultural soils poses persistent risks to crop safety and food-chain exposure. Although biochar is widely proposed—and increasingly applied—as a remediation amendment, field performance remains highly variable across soil constraints, metal speciation, and biochar designs. This review addresses this uncertainty by translating immobilization pathways (sorption/ complexation, precipitation, and redox-mediated stabilization) into a decision-oriented “mechanism–lever–endpoint” framework, thus linking mechanistic hypotheses to controllable engineering strategies such as feedstock selection, pyrolysis windows, and mineral/composite design. Beyond established plant–microbe interactions, there is a critical assessment of under-synthesized biochar–soil fauna pathways, with a focus on earthworms, and a reconciliation of conflicting evidence by highlighting boundary conditions that shift biological responses. Agronomic trade-offs and environmental risks are considered, associated with biochar production and application, emphasizing failure modes relevant to long-term soil health and remediation reliability. To support decision-grade deployment under heterogeneous evidence, a bias-aware AI-assisted workflow is outlined, which stresses standardized reporting, interpretability, and leakage-safe validation. Overall, the review integrates engineering options with biological synergies into a practical roadmap for more predictable and site-specific remediation in agricultural soils.

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Keywords: Biochar; Agricultural soils; Heavy-metal immobilization; Modification strategies; Machine learning (ML)

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INTRODUCTION

Heavy-metal contamination in agricultural soils remains a persistent food-safety challenge because risk is governed not only by total metal concentration, but more directly by metal bioavailability at the soil–plant interface and subsequent transfer along the food chain (Lawal *et al.* 2021). Unlike natural geochemical backgrounds, modern soil pollution is increasingly dominated by heterogeneous anthropogenic inputs—including mining, smelting, wastewater irrigation, and agrochemical use—thereby creating contamination

profiles that rarely respond to uniform remediation strategies (Fei *et al.* 2022; Qin *et al.* 2021). Consequently, controlling bioavailability has become as important as reducing total metal concentrations. Remediation strategies that specifically minimize bioavailability and maintain long-term stability under variable soil conditions are especially needed.

Conventional organic amendments such as compost and manure are widely used in agricultural soils, but their remediation performance may be limited by rapid decomposition, variable composition, and, in some cases, dissolved organic carbon (DOC)-mediated metal mobilization (D. Chen *et al.* 2022; Xu *et al.* 2025). In this context, biochar has progressed from a general soil amendment to an increasingly engineerable material platform for farmland remediation (Aziz and Kareem 2023). Unlike more labile amendments, biochar is a thermochemically transformed carbonaceous material whose pore architecture, surface chemistry, alkalinity, and mineral associations can be more deliberately tuned through feedstock selection, pyrolysis conditions, and post-modification. Its remediation efficacy arises from coupled interactions—including surface complexation, precipitation, and, in some cases, redox-mediated stabilization—making it particularly relevant for heavy-metal immobilization under diverse soil constraints (Ji *et al.* 2022; Gusiatin and Rouhani, 2023). A central research gap persists. There needs to be a transition from trial-and-error experimentation to rational, context-specific biochar design. Despite a rapidly expanding literature, biochar engineering is still frequently pursued through ad hoc testing, and many existing reviews emphasize either synthesis routes or broad application benefits without clearly identifying which engineering lever is most appropriate under specific soil–metal scenarios (Venkatachalam *et al.* 2023). Much less attention has been paid to a practical decision framework that explicitly links mechanistic soil cues to controllable engineering levers. Without such a framework, the field risks remain reliant on fragmented case-by-case evidence with limited predictive power.

Artificial intelligence (AI) is increasingly being explored as a decision-support layer for decoding high-dimensional interactions among pyrolysis parameters, soil properties, and immobilization outcomes (Nguyen *et al.* 2024). However, the reliability of AI in this domain remains constrained by fragmented reporting, data bias, weak validation practices, and the inclusion of descriptors that are not always directly aligned with remediation goals. Accordingly, this review advances a mechanism-centered and decision-oriented perspective on biochar-based heavy-metal remediation. Specifically, the authors (1) develop a decision-oriented framework linking immobilization mechanisms to controllable engineering levers across soil and metal contexts; (2) evaluate integrated biochar–plant–microbe strategies by identifying synergy pathways and boundary conditions; (3) critically assess the role of AI in biochar design and remediation prediction, with emphasis on remediation-relevant variables and validation challenges; and (4) highlight risk-aware deployment, arguing that success should be judged not only by short-term immobilization, but also by long-term stability and ecological safety. This review is therefore structured from mechanistic soil controls to biochar design and optimization, and finally to AI-assisted decision support for more predictable remediation outcomes.

SOURCES, PATHWAYS, AND BIOAVAILABILITY OF HEAVY METALS IN AGRICULTURAL SOILS

Understanding the sources, transformation pathways, and bioavailability of heavy metals is essential for rational biochar-based remediation. This is because these controls determine which immobilization mechanisms and material properties are most appropriate under specific soil conditions. Heavy metals contamination in farmlands seldom stems from a single origin (Fig 1). Most sites exhibit mixed-source legacies in which geogenic backgrounds intersect with anthropogenic inputs (Table S1). In practice, contamination is assessed against local geochemical backgrounds or regulatory thresholds, not a universal rule (Rothwell and Cooke 2015). Attention typically centers on topsoil, which exchanges rapidly with air and water and directly interfaces with crop roots (O'Connor *et al.* 2018). This context makes it necessary to understand metal provenance, transport, and bioavailability before selecting biochar-based remediation strategies intended to deliver predictable field performance.

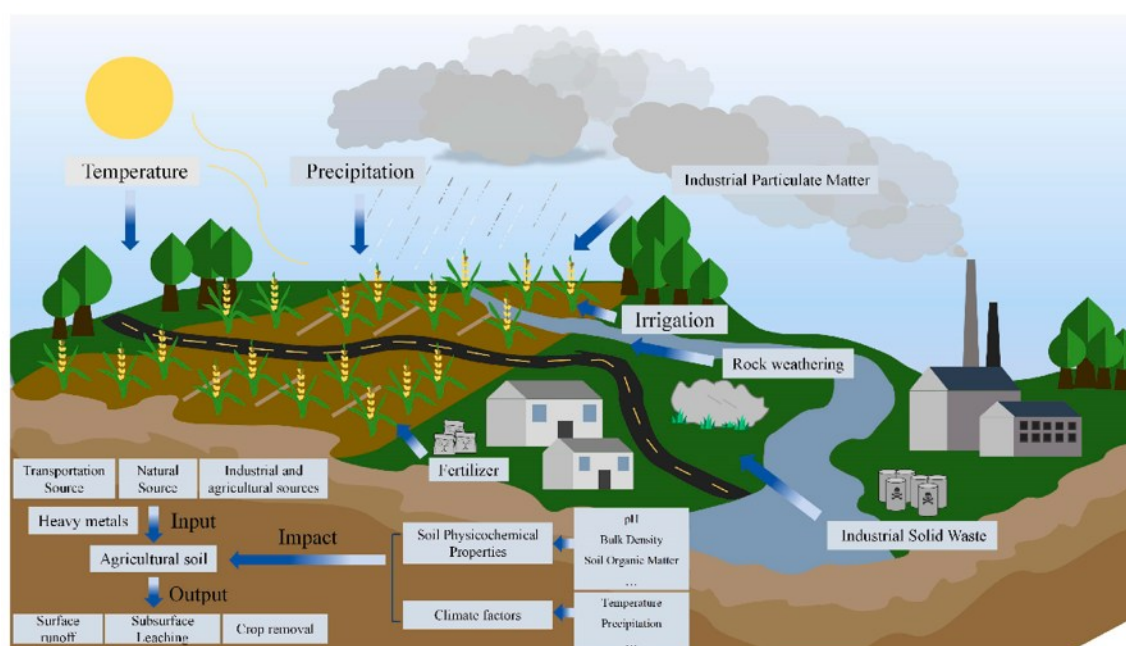


Fig. 1. Major sources and pathways of heavy metals into agricultural soils (Zhao *et al.* 2025, under CC BY 4.0 license)

Sources and Entry Routes

Natural inputs arise from weathering of parent materials, volcanic and aeolian deposition, and lithological anomalies (Zhang and Wang 2020). While natural processes establish background levels and can locally contribute substantially, anthropogenic sources generally dominate contemporary enrichment patterns. Major human-derived inputs include mining and smelting, wastewater irrigation, agrochemical applications (fertilizers, pesticides, fungicides with trace-metal impurities), organic amendments such as manure and sewage sludge, industrial emissions, traffic, and mismanaged solid wastes (Joshi and Gururani 2023). Once released, metals are transferred to agricultural soils through multiple pathways, atmospheric deposition (Qiao *et al.* 2023), irrigation with contaminated water (Joshi and Gururani 2023), runoff and leaching from tailings or waste sites, and direct

inputs through fertilizers and amendments (Zhang and Wang 2020). The relative contribution of these pathways varies across regions and land-use histories, yet their convergence commonly results in cumulative and persistent enrichment in farmland soils. This source heterogeneity partly explains why uniform amendment strategies often perform inconsistently across sites and why remediation design must remain context-specific.

Transformations and Controlling Factors in Soils

After entering soils, metals repartition among soil solution, exchange sites, and more specific associations such as surface complexation on Fe/Al/Mn (hydr)oxides and co-precipitation with carbonates or phosphates (Dhiman *et al.* 2023). In agricultural systems, a biologically mediated fraction may also be transferred into plant tissues, from which metals can later re-enter the soil through residue return and decomposition (Tan *et al.* 2023). The pH remains the primary regulator of cationic metal mobility (Zhang *et al.* 2022), while redox potential (Eh) dictates speciation and the stability of Fe/Mn phases; under flooded or reducing conditions Fe/Mn oxide dissolution can release previously sorbed ions and convert As(V) to the more mobile As(III) (Yu *et al.* 2024). In addition to these inorganic controls, dissolved organic carbon (DOC) often complexes Cu and other trace metals, sometimes enhancing mobility. Over time, aging and occlusion processes progressively reduce lability as ions diffuse into micro-/mesopores or become encapsulated within recrystallizing minerals (Li and Gong 2021). Ultimately, total metal concentrations are often poor predictors of environmental risk; instead, risk depends more directly on the fraction that remains chemically labile and biologically accessible. These physicochemical controls also define the design requirements for remediation, including whether performance is more likely to depend on alkalinity, mineral-assisted sorption, redox buffering, or suppression of DOC-mediated mobilization.

Bioavailability: Concept and Measurement

Bioavailability denotes the fraction of a metal that is accessible for biological uptake over relevant timescales (Xu *et al.* 2022); it is method- and organism-dependent. Operational proxies interrogate different processes. Researchers can choose between simple extractions (*e.g.*, CaCl₂, NH₄NO₃, DTPA/EDTA), sequential extraction schemes that partition operational pools, diffusive gradients in thin films (DGT) for labile supply, and direct porewater or isotopic-exchange approaches (O'Connor *et al.* 2018; Zhu *et al.* 2023). Method choice should be decision-oriented and locally calibrated to soils and crops; for example, organic amendments such as compost can lower plant burdens mainly by shrinking the labile pool, not by changing totals (D. Chen *et al.* 2022). Linking measurement to management is therefore essential, because remediation should target the chemical pool that actually drives ecological exposure and food-chain risk. For biochar-based remediation in particular, success should be judged mainly by reductions in labile and biologically relevant pools rather than by changes in total concentrations alone.

Implications for Risk and Management

Elevated labile fractions of heavy metals can impair seed germination, plant growth, photosynthesis, and cellular homeostasis in crops and pose human-health risks through food-chain transfer (Angon *et al.* 2024; Rai *et al.* 2023). Source control remains the primary mitigation strategy wherever feasible. However, when *in-situ* remediation is required, effective intervention depends on aligning material choice with the soil's governing chemical constraints rather than relying on trial-and-error amendment application. In practical terms, the mobility-limiting factors of different contaminants dictate the required remediation functions: acidic soils contaminated with cationic metals generally require stronger pH buffering and precipitation-promoting capacity, redox-dynamic environments require greater stabilization against speciation shifts, and DOC-rich systems demand materials capable of limiting ligand-assisted remobilization. These site-specific cues provide the conceptual basis for the mechanism–lever–endpoint framework developed in the next section. By linking the soil constraints summarized here to the engineered biochar properties and immobilization pathways discussed later, remediation strategies can be designed in a more predictable and field-relevant manner.

ENGINEERING BIOCHAR FOR HEAVY-METAL REMEDIATION: PROPERTIES, MODIFICATION LEVERS, AND PROCESS DESIGN

Biochar performance in agricultural soils is governed by engineerable physicochemical attributes—pore architecture, surface functional chemistry, and alkalinity/surface charge—that map onto the dominant immobilization pathways in soils (sorption, surface complexation/co-precipitation, and redox interactions) (Ibrahim *et al.* 2022). Feedstock and thermochemical history set the baseline, whereas post-synthesis modification extends the design space for site-specific remediation. A process view is therefore essential: from soil cues, to property targets, modification choices, and field-ready materials and metrics.

Pore Architecture and Accessible Surface

Physical sorption contributes meaningfully when the pore network provides both capacity (internal surface) and accessibility (mass-transfer pathways) (Hou *et al.* 2024; Xing *et al.* 2023). The IUPAC classification—micropores (< 2 nm), mesopores (2 to 50 nm), and macropores (> 50 nm)—is useful operationally: micropores often supply the majority of internal surface (capacity), mesopores facilitate diffusion toward microporous domains, and macropores support transport and biotic colonization (Leng *et al.* 2021). Critically, overly deep “dead-end” pores may trap pollutants without proportionate risk reduction, whereas connected mesopores improve utilization of internal sites (Krebsbach *et al.* 2023). Brunauer–Emmett–Teller (BET) surface-area values are often misleading; Sinha *et al.* (2019) reported that BET surface area, together with pore-size distribution, is necessary to interpret performance beyond a single ‘surface area’ value. According to comprehensive reviews on biochar porosity engineering (Li *et al.* 2016), and consistent with the empirical patterns summarized in Table S2, BET surface area generally increases with pyrolysis temperature, although substantial variability remains due to feedstock characteristics and processing conditions. Reported values can range from less than 10 m²/g in some low-temperature chars (below 350 °C) to more than 400 m²/g in high-temperature or physically activated biochars.

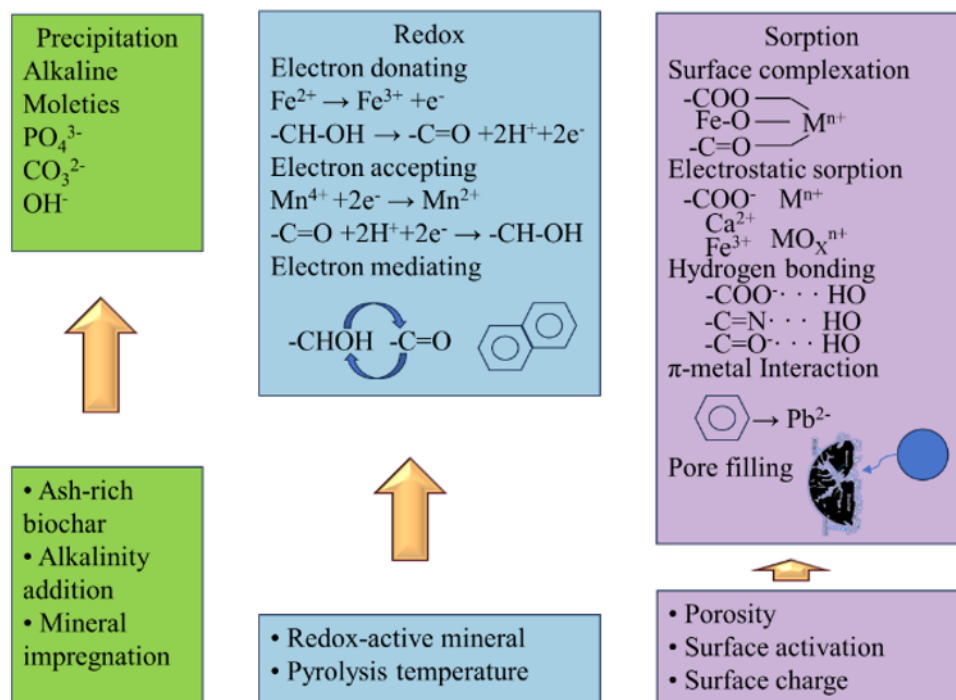
Pyrolysis window and feedstock co-determine these traits, and studies consistently show that increasing microporosity and accessible surface area enhances immobilization of target metals in soils (Souza *et al.* 2023; Yakout *et al.* 2015). However, gains in microporosity may trade off with accessibility, especially in dense carbons with tortuous structures.

Design implications: prioritize (i) micropore development to maximize capacity, (ii) mesoporous pathways to facilitate diffusion, and (iii) avoidance of excessive tortuosity that limits accessibility. Importantly, BET surface area and pore-size distribution (PSD) data should always be interpreted in the context of soil conditions, since factors such as moisture, DOC, and texture constrain the effective utilization of internal sites in the field.

Surface Functional Groups and Chemical Interactions

Functional groups (O-, N-, P-, S-, and Si-containing moieties) mediate chemisorption *via* surface complexation, hydrogen bonding, and coordination, thereby shrinking the labile pool that drives exposure (Flórez *et al.* 2024). Oxygenated groups, such as -COOH, phenolic -OH, and carbonyls, dominate cation binding (J. Chen *et al.* 2024); N-bearing motifs and other heteroatom sites modulate affinity and electron density. Although typically less abundant, P, S, and Si functionalities also contribute *via* complexation or by nucleating co-precipitates (D. Luo *et al.* 2023; M. Luo *et al.* 2023). Group abundance originates from feedstock biochemistry and systematically declines with increasing pyrolysis temperature—a trade-off between reactive surface chemistry and carbon stability, as illustrated in Fig. 2 (He *et al.* 2022). Thus, aligning functional-group composition with soil chemistry and target metal speciation is a key design principle.

(a)



(b)

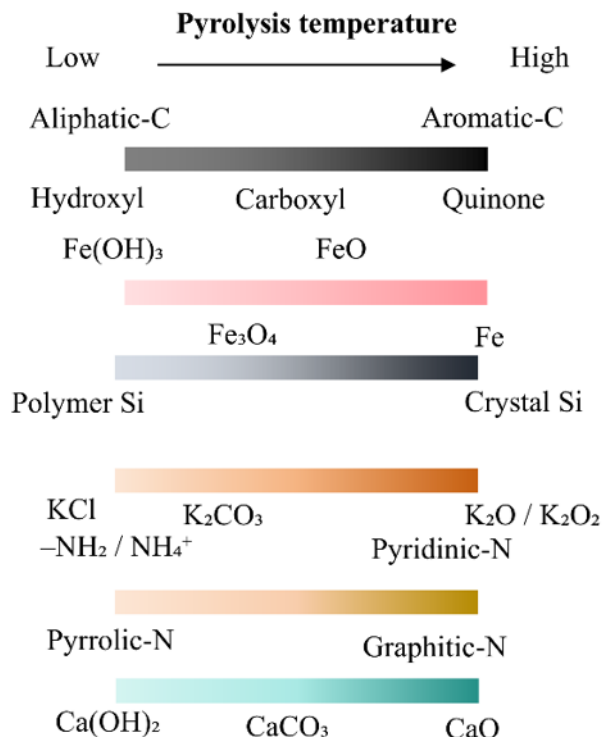


Fig. 2. Temperature-driven biochar reactive sites and heavy-metal immobilization mechanisms. (Barszcz *et al.* 2024; Nguyen *et al.* 2024). (a) Major immobilization pathways of heavy metals by biochar, including precipitation, redox-mediated transformation, surface complexation, electrostatic sorption, hydrogen bonding, π -metal interactions, and pore filling. These pathways are regulated by engineering levers such as alkalinity adjustment, mineral impregnation, redox-active minerals, porosity, surface activation, and surface charge. (b) Pyrolysis temperature drives the evolution of biochar reactive moieties, including the transition from aliphatic to aromatic carbon structures, the transformation of oxygen-containing functional groups, nitrogen species, silicon forms, and mineral phases. Matching these temperature-dependent functional-group and mineral “palettes” to metal speciation and soil chemistry is central to effective biochar design, rather than relying only on bulk O content or BET-derived surface metrics.

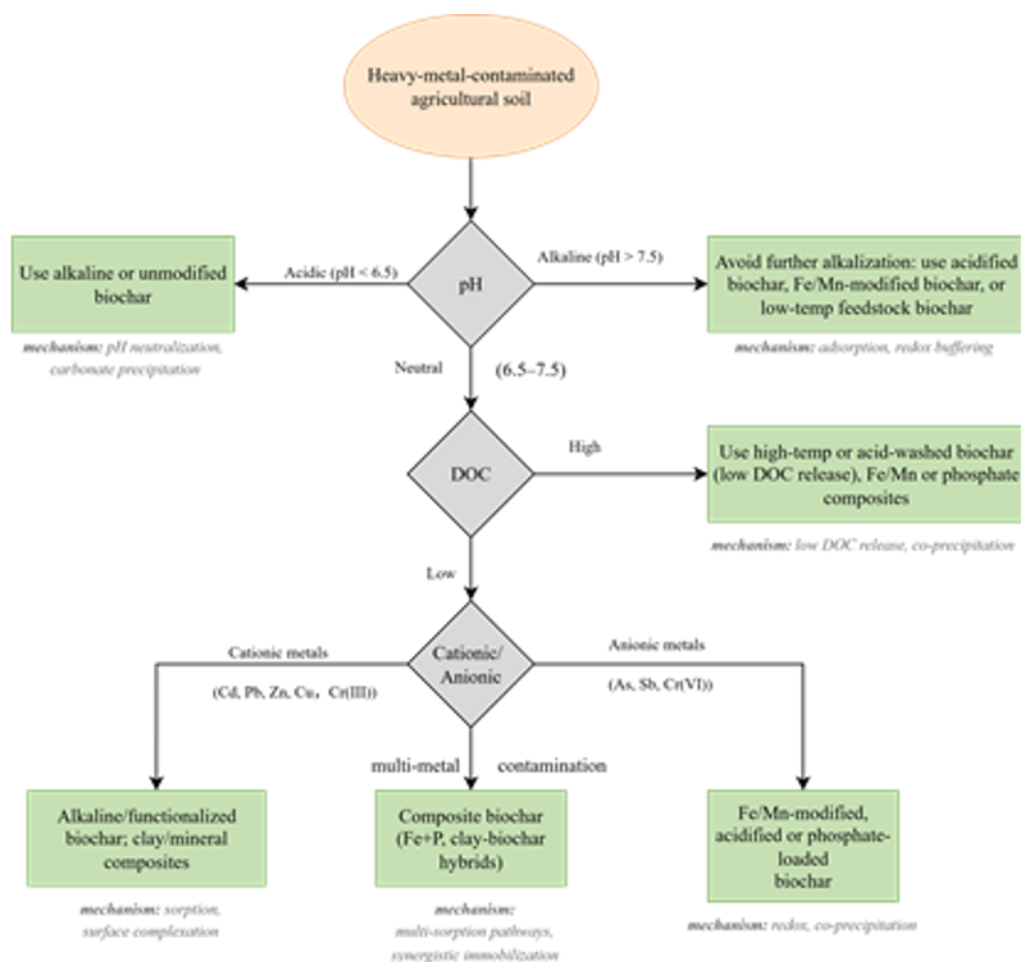


Fig. 3. Decision framework linking soil conditions and contamination types to biochar modification strategies

Alkalinity, pH, and Surface Charge (pH_{pzc})

Soil and biochar pH jointly control metal speciation and sorption thermodynamics. Increasing pH generally lowers the solubility of many cationic metals and promotes hydroxide formation and carbonate-related precipitation, whereas acidification can remobilize carbonate- or hydroxide-associated metals (Kicińska *et al.* 2022; Z. L. Li *et al.* 2022). The point of zero charge (pH_{pzc}) frames electrostatics: at $\text{pH} > \text{pH}_{\text{pzc}}$ surfaces are negatively charged and promote uptake of metal cations; at $\text{pH} < \text{pH}_{\text{pzc}}$ positively charged surfaces can retain oxyanions (e.g., HAsO_4^{2-} , HCrO_4^-) (El-Wakil *et al.* 2022). Representative values in Table S2 show that biochar pH can vary widely, ranging from about 5.26 to 13.15 depending on feedstock and pyrolysis conditions. In general, pH tends to increase with pyrolysis temperature, although substantial variability remains due to feedstock composition and ash content. With increasing pyrolysis temperature, biochar alkalinity tends to rise and pH_{pzc} can shift upward, while cation-exchange capacity often declines due to loss of acidic groups—an important trade-off to report and leverage (Joshi *et al.* 2023).

Design implications

For acidic soils with cationic metals, alkaline/ash-rich chars raise pH and provide basic exchange sites; for oxyanion risks (*e.g.*, As, Cr(VI)), pH control around pH_{pzc} and provision of specific inner-sphere sites are more decisive than bulk alkalinity alone. Practitioners should balance the benefits of alkalinity against potential losses in cation exchange capacity (CEC) and functionality toward anions.

Engineering Biochar via Physical/chemical Modification: Toolbox, Mechanisms, and Trade-offs

Post-synthesis modification expands the design space of biochar by enabling selective tuning of surface chemistry, porosity, and charge properties beyond what feedstock and pyrolysis alone can achieve (Ravindiran *et al.* 2024). Strategies include physical and chemical activation, mineral loading, heteroatom enrichment, and biological functionalization. Each method offers distinct advantages but also introduces trade-offs that may constrain field applicability (Wen *et al.* 2023). A critical evaluation of these approaches is essential to translate laboratory improvements into reliable remediation strategies.

Physical activation (steam/ CO_2)

Physical activation enhances surface area and pore volume through controlled gas–solid reactions, typically using steam or CO_2 . Steam activation tends to produce higher microporosity, while CO_2 yields a more balanced micro–mesopore network that facilitates diffusion. Reported increases in BET surface area often correlate with improved sorption in batch experiments (Zhang *et al.* 2021). Under optimized physical activation conditions, BET surface area can exceed $400 \text{ m}^2/\text{g}$; for example, almond shell biochar reached $436 \text{ m}^2/\text{g}$ (Fan *et al.* 2022; Table S2).

However, reliance on BET alone can be misleading: larger surface areas do not necessarily translate to improved immobilization in soils, because DOC, colloids, and soil texture can constrain site accessibility (He *et al.* 2024). Over-activation may collapse micropores and strip oxygen functionalities, weakening chemisorption (Han *et al.* 2020; Manning *et al.* 2023). Physical activation is best viewed as a capacity-enhancing baseline that is particularly effective in neutral to slightly alkaline soils with cationic metals. In DOC-rich soils, pore blocking reduces efficacy unless combined with mineral phases to outcompete DOC binding.

Chemical activation (acid/base routes)

Chemical activation modifies the carbon matrix and surface chemistry *via* acid or alkali treatments. Acid activation (*e.g.*, H_3PO_4 , H_2SO_4 , HNO_3) removes ash, introduces oxygenated groups, and lowers pH_{pzc} , thereby enhancing inner-sphere complexation with Cd^{2+} and Pb^{2+} (Murtaza *et al.* 2022). Base activation (*e.g.*, KOH, NaOH) etches microporosity and increases surface area, sometimes boosting sorption capacities by an order of magnitude (Chen *et al.* 2021).

Nonetheless, acid activation may lead to leaching of phosphate or sulfate, contributing to eutrophication (Cui *et al.* 2022), while base activation can strip oxygen functionalities and leave residual ions (K^+ , Na^+) that elevate soil salinity. Many studies emphasize surface area increases without evaluating soil-relevant endpoints (Vijay *et al.* 2021). Acid routes are better suited for neutral–alkaline soils with cationic metals, whereas base routes are effective in acidic soils but limited against oxyanions. For complex or DOC-rich systems,

chemical activation alone is insufficient and should be combined with mineral or heteroatom modification.

Mineral loading and composite formation (Fe/Al/Mn oxides, phosphates, clays)

Incorporating mineral phases introduces high-affinity sorption sites *via* complexation, ligand exchange, and co-precipitation. Fe/Al oxides enhance retention of oxyanions (As, Cr), while phosphate-rich additives promote cation precipitation (Alam *et al.* 2020; Zheng *et al.* 2020). Mn-oxide and MgO composites offer rapid Pb removal with high capacities (Ling *et al.* 2017), and magnetic composites facilitate recovery and reuse (Song *et al.* 2021).

Despite their promise, mechanistic attribution is often oversimplified. Reported improvements may reflect unwashed residues rather than true sorption (Liu *et al.* 2022). Stability is a concern: Fe/Al phases may dissolve under anoxic conditions, and phosphate composites can leach nutrients. Excessive loading may block pores and reduce accessibility. These risks highlight the need for systematic reporting of mineral phase identity, crystallinity, and leaching behavior—data that remain scarce in current literature. Taken together, mineral loading and composite formation can substantially expand the functional range of biochar for target-specific remediation, particularly in systems requiring oxyanion retention or mineral-assisted precipitation. However, their practical value depends on careful control of loading intensity, phase stability, and leaching risk under soil-relevant conditions.

Heteroatom enrichment (n, s, p motifs)

Doping with nitrogen, sulfur, or phosphorus alters electron density and surface charge, introducing donor sites that enhance metal affinity. N-doping (pyridinic, graphitic N) improves binding with transition metals (Kasera *et al.* 2022), while sulfur motifs form strong complexes with Pb²⁺ and Hg²⁺ (Yin *et al.* 2022). P-enrichment promotes precipitation with Cd²⁺ and Zn²⁺ (Peiris *et al.* 2023).

However, attribution to heteroatoms is often speculative. Many studies fail to distinguish true heteroatom–metal coordination from indirect effects such as pore restructuring or mineral residues (Y. Sun *et al.* 2024). S- and P-enriched chars may suffer from functional group instability during aging, while N-enrichment may increase NO₃[−] release. Rigorous mechanistic confirmation using advanced spectroscopy and aging trials is therefore still needed.

Biological modification strategies

Microbial residues and live consortia introduce sorption-active moieties and create micro-environments that complement carbon–mineral scaffolds. Phosphate-solubilizing bacteria (PSB) coupled with biochar enhance Pb immobilization *via* local phosphate release (H. Chen *et al.* 2019), while biologically treated residues improve Cd binding efficiency (Tao *et al.* 2021).

Yet, translation from solution systems to soils remains uncertain. DOC, competing ions, and redox dynamics constrain microbial survival and functionality. Exogenous inocula may disrupt native communities, and extreme pH/salinity limits persistence. Biological modification is best suited for moderate contamination where immobilization and soil–biota recovery are joint goals, but robust field evidence is still limited.

Modification decision map

Figure 3 illustrates a decision framework linking soil–metal scenarios to suitable biochar modifications. The first determinant is soil pH. In acidic soils (pH < 6.5), alkaline or unmodified biochars are effective through pH neutralization and carbonate precipitation (S. Liu *et al.* 2025). Physical or chemical activation (*e.g.*, steam, alkali) can further increase sorption capacity, but those processes may erode functional groups and generate persistent free radicals (PFRs) or reactive oxygen species (ROS), raising ecological concerns (Z. Zhao *et al.* 2025). In alkaline soils (pH > 7.5), acidified or Fe/Mn-modified biochars, or low-temperature feedstocks are preferred to avoid further alkalization, though excessive mineral loading may destabilize under reducing conditions or increase nutrient leaching (Lin *et al.* 2025; L. Liu *et al.* 2023).

The second decision point is DOC. In high-DOC soils, high-temperature or acid-washed biochar, combined with Fe/Mn or phosphate composites work together to minimize DOC release and enhance co-precipitation (Ahmed and Aidi 2025; T. Sun *et al.* 2024). Heteroatom doping (N, P, S, Si) improves selectivity but raises questions regarding long-term stability and dopant fate (J. Zhao *et al.* 2025; Yang *et al.* 2025). When DOC is low, metal speciation becomes decisive. For cationic metals (Cd, Pb, Zn, Cu, Cr(III)), functionalized biochar or clay/mineral composites enhance immobilization, while anionic metals (As, Sb, Cr(VI)) require Fe/Mn-modified, acidified, or phosphate-loaded biochar (Ahmed and Aidi 2025). Multi-metal contamination favors composite hybrids (Fe–P, clay–biochar) to exploit multiple immobilization pathways (Wang *et al.* 2025).

Biological modifications provide eco-friendly synergies with microbes or enzymes, but results remain inconsistent in field soils due to competition and abiotic variability (Fakhar *et al.* 2025).

Despite these advances, key gaps remain. Cross-comparison under standardized matrices and long-term validation are scarce; climate and soil aging can reverse remediation benefits (Dimitriadou *et al.* 2025). Standardized reporting of pore architecture and functional groups would enable reliable meta-analyses (Schmidt *et al.* 2021). Integration with AI offers opportunities to optimize multi-parameter designs across soils, feedstocks, and metals, though robustness depends on training data quality (Ge *et al.* 2025). Overall, Fig. 3 and Supplementary Table S2 provide a foundation for aligning soil–metal conditions with targeted engineering routes. However, the limitation of single-route optimization becomes especially evident in multi-metal systems. In a Cu-, Zn-, As-, Cd-, and Pb-contaminated soil, nZVI@BC was shown to simultaneously engage multiple mechanisms, including surface adsorption, electrostatic attraction, ion exchange, co-precipitation, oxidation-reduction, and complexation, with competitive and synergistic interactions observed among metals (Song *et al.* 2022). Likewise, in Cd-, Cr-, and Pb-contaminated soil, a biochar- and bentonite-supported nZVI composite promoted the co-existence of adsorption, reduction, co-precipitation, and complexation during simultaneous immobilization (Jin *et al.*, 2023). These studies support a key inference: under mixed-contaminant conditions, multifunctionality is often observed as an emergent property of composite or modified materials rather than as a fully controlled active-site design. This pattern suggests that, rather than assuming that a single engineered active site can be reliably matched to heterogeneous field conditions, a more practical route may be to combine complementary functionalities—either within one multifunctional biochar or across blended biochar systems—to broaden coverage across cationic and oxyanionic metals.

In practice, such an approach could involve either multifunctional biochars carrying multiple reactive moieties within the same material, or blended amendment systems composed of contrasting biochars or biochar-based composites with different dominant functions, so that more than one immobilization pathway can be deliberately engaged. Function-specific modification illustrates the same principle at a narrower scale. For instance, phosphorus-loaded biochar-assisted phytoremediation was reported to enhance metal immobilization in Cd-, Cr-, and Pb-contaminated soils, mainly through precipitation- and complexation-related processes, while also improving selected soil physicochemical properties (Serrano *et al.*, 2024). Although multifunctional and composite biochars are already well represented in the literature, explicit blended-biochar strategies remain comparatively underexplored. Integrating multiple functionalities within a single biochar may also increase preparation complexity and cost, which may limit routine use but still make such materials attractive for targeted remediation scenarios where broader functional coverage justifies the added engineering burden. A portfolio-style approach may therefore provide a pragmatic route for multi-metal remediation by broadening functional coverage rather than maximizing a single mechanism.

ADDITIONAL ADVANTAGES OF USING BIOCHAR FOR REMEDIATING HEAVY METALS IN SOIL

Crop toxicity due to heavy metals primarily results in reduced yields and the excessive accumulation of these metals. Crops that are subjected to heavy metal contamination may have reduced enzyme activity, deterioration of chlorophyll pigments, and impaired nutrient uptake, among other physiological effects (Hafeez *et al.* 2023). On the other hand, heavy metal accumulation in crops can transfer through the food chain to affect human health (Mwelwa *et al.* 2023). This section reviews studies focused on increasing crop yields and reducing the accumulation of heavy metals.

Increasing Crop Yields

Biochar may support crop productivity in heavy-metal-contaminated soils by improving soil physical and chemical conditions and thereby alleviating stress at the root–soil interface. However, these benefits are not uniform and should not be generalized across all biochars. A more meaningful interpretation requires comparison across feedstock type, application rate, and thermochemical history, because these factors often influence whether biochar improves or constrains soil functioning.

A first distinction concerns feedstock type. In many cases, lignocellulosic biochars, such as those derived from crop residues, are associated with improvements in pore architecture, aggregate stability, and water retention, which may indirectly support crop growth. For example, rice-straw biochar was reported to improve bulk density, porosity, aggregate stability, and soil hydraulic pathways, thereby contributing to a more favorable air–water balance in soil (Wu *et al.* 2023; Ramezanzadeh *et al.* 2023). By contrast, waste-derived biochars, such as sludge biochar, may also improve physical properties, but their effects often appear to be more strongly influenced by ash content, mineral composition, and greater feedstock heterogeneity. Xin *et al.* (2023) found that sludge biochar altered particle-size distribution, decreased bulk density, and increased total porosity by 1.2 to 11.5%. In addition, waste-derived biochars often contain higher initial nutrient and ash contents, and ion-exchange processes during metal sorption may release certain nutrient

ions into the soil solution. Under some conditions, this mechanism may contribute to improved nutrient availability and crop performance, although the magnitude of this effect remains strongly context-dependent. Taken together, the available evidence suggests that lignocellulosic biochars are often linked to structural and hydraulic improvements, whereas waste-derived biochars may exert stronger mineral-related or liming effects, albeit with greater variability across feedstocks.

A second determinant is application level. At low-to-moderate levels, biochar often improves plant-available water, porosity, and root-zone conditions, which may contribute to better crop performance. For instance, all treatments considered by Šurda *et al.* (2024) significantly increased plant-accessible water content and porosity in sandy soil, while X. Chen *et al.* (2023) showed that a 2% application rate exerted a more pronounced positive effect on water retention in medium-grained soils than in coarse-grained soils. However, higher application levels do not necessarily yield proportionally greater benefits. Z. Chen *et al.* (2024) observed that when biochar application exceeded 4%, saturated permeability declined by approximately one order of magnitude. The effect was attributed to pore filling within clay intra-aggregate spaces during repeated freeze–thaw cycles. These findings suggest that dosage may act as a threshold-dependent factor: moderate rates are often beneficial, whereas excessive rates may impair permeability or aeration under certain soil conditions.

A third consideration is thermochemical history, especially pyrolysis temperature, although the evidence in this subsection is less systematically reported than feedstock and dosage effects. In general, pyrolysis temperature influences the balance between short-term reactivity and longer-term persistence, and may therefore affect nutrient dynamics, water relations, and the durability of agronomic benefits (He *et al.* 2022; Joshi *et al.* 2023). However, the available literature does not support a universal ranking of low- versus high-temperature biochars for crop-yield improvement, because temperature effects are typically mediated by feedstock type, particle size, soil texture, and application rate. Pyrolysis temperature should therefore be interpreted as a modifying factor rather than as an independent predictor of agronomic performance.

Beyond these broad comparisons, the evidence on soil hydraulic responses remains mixed. Biochar may enhance water retention and hydraulic conductivity by increasing mesoporosity and improving pore connectivity, but under other conditions it may reduce permeability by clogging fine pores or altering the packing arrangement between soil particles and biochar particles. Faloye *et al.* (2024), for example, reported significant improvements in saturated hydraulic conductivity in biochar-amended soils, attributing this to increased mesopore development. In contrast, Z. Chen *et al.* (2024) found decreased permeability under specific high-rate application and freeze–thaw conditions. Similar variability has been reported for shrinkage, cracking, and air permeability, all of which appear to depend on the interaction between soil texture, biochar particle size, pore structure, and amendment rate.

Overall, the yield-related benefits of biochar are best understood as context-dependent co-benefits rather than universal outcomes. Lignocellulosic biochars are often associated with physical improvement and water regulation; waste-derived biochars may provide stronger chemical or liming effects but with greater variability; moderate dosages are generally more reliable than excessive applications; and pyrolysis temperature appears to influence the balance between reactivity and persistence. Accordingly, improvements in crop yield should be interpreted through a comparative framework that considers feedstock

origin, dose, thermochemical history, and soil constraints together, rather than through isolated case studies.

Based on such findings, the main advantages of biochar in this context include improved soil physical functioning, enhanced water regulation, and potential support for crop performance, whereas the main limitations include variability across feedstocks, threshold-dependent dosage effects, and inconsistent hydraulic responses under different soil conditions.

Reducing the Accumulation of Heavy Metals

Some studies attribute the reduction in heavy metal accumulation in crops following biochar application to its ability to decrease the bioavailability of heavy metals in soil (Fig. 4).

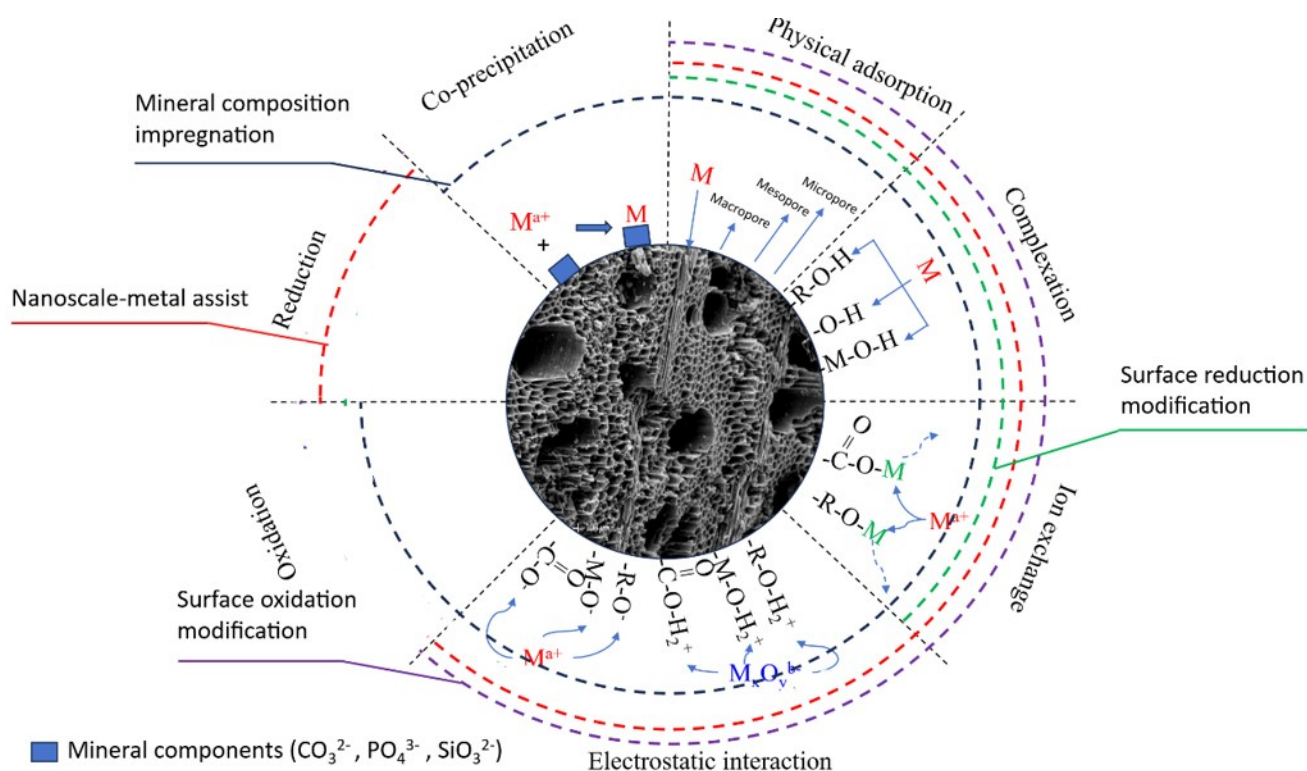


Fig. 4. Proposed mechanisms for heavy-metal adsorption and immobilization by biochar modified from (W.-H. Chen *et al.* (2022) and Wang *et al.* (2019) ions between pyrolysis temperature, elemental composition, and resulting reactive moieties of biochar; implications for pollutant removal mechanisms. (Adapted based on the scientific framework reported by He *et al.* 2022).

Notably, plant uptake does not always scale linearly with bulk-soil bioavailability indices, because rhizosphere processes and physiological barriers can dominate under certain conditions. In this context, the impact of biochar on crop metal accumulation should be understood as a coupled soil-rhizosphere-plant process rather than as a simple consequence of reduced extractable metal pools alone. Other studies further suggest that biochar may influence plant physiological and biochemical responses under metal stress, thereby contributing to lower uptake and accumulation. Haider *et al.* (2022) summarize that biochar application can regulate stress-induced antioxidant responses in plants. Biochar application may also affect membrane-associated transport and cell permeability.

Biochar also enhances ATPase activity, which is linked to the synthesis of soluble proteins and nucleic acids, which can aid in metal contamination control. Additionally, biochar reduces ROS formation under metal stress, thereby alleviating oxidative damage in polluted soils. Through these combined effects, biochar may support metabolic and enzymatic activity and reduce contaminant transfer into plant tissues. Overall, many studies report simultaneous yield benefits and reduced metal accumulation following biochar amendment; however, the magnitude and consistency of these responses vary with soil constraints, metal chemistry, biochar properties, and management context (Haider *et al.* 2022; Y. H. Liu *et al.* 2023).

While these agronomic co-benefits motivate interest in biochar as a multifunctional amendment, farm-scale remediation decisions are typically made in the context of alternative organic inputs and practical trade-offs.

A complementary perspective is to contrast engineered biochar with more labile organic amendments commonly used in farming systems (*e.g.*, compost or manure). Biochar, as a thermochemically transformed and increasingly “engineerable” carbon material, can be tailored toward sorption, complexation, and precipitation functions through feedstock choice, pyrolysis conditions, and post-modification. A practical advantage of this functional tunability is that targeted functions can be deliberately strengthened to improve reproducibility, whereas organic amendments often exhibit greater variability in composition and reactivity across feedstocks and composting maturity. At the same time, engineered biochar should not be treated as synonymous with activated carbon, although partial overlap can occur. Biochar remains defined by the thermochemical conversion of biomass and its broader agronomic or environmental functional context, whereas activated carbon is more commonly regarded as a more intensively processed sorbent optimized primarily for high surface area and adsorption performance (Subramanian *et al.* 2025). Some strongly activated or post-modified biochars may enter an overlapping functional space, but many engineered biochars retain design goals extending beyond sorption alone. While biochar may provide ancillary agronomic co-benefits (*e.g.*, liming), its key engineering distinction lies in its relative persistence, which supports longer-lived immobilization when governing mechanisms remain stable. In contrast, conventional organic amendments contribute more directly to nutrient supply and stimulation of biological activity, but their impacts on metal immobilization are often more dynamic; increases in dissolved organic carbon (DOC) and competing ligands may either attenuate or enhance metal mobility depending on soil redox–pH trajectories (Xu *et al.* 2025). Nevertheless, organic amendments can serve as practical, low-intensity options for mildly contaminated soils; for example, compost has been reported to reduce Cd phytotoxicity while improving wheat growth in specific case studies (Ahmad *et al.* 2025). Taken together, these contrasts underscore that remediation in agricultural soils is inherently multi-objective, requiring a balance between food-safety risk reduction and fertility management. Outcomes are strongly contingent on baseline soil constraints, contamination severity, and management context. Accordingly, strategy selection benefits from calibration to local conditions and may include integrated approaches that combine sorption-oriented biochars with nutrient-oriented organic inputs where appropriate. In this context, the main advantages of biochar are its relative persistence, engineerability, and potential to simultaneously reduce crop metal uptake and support agronomic performance, whereas its main limitations lie in context-dependent effectiveness, variability across feedstocks and soils, and the possibility of unintended trade-offs under field conditions. However, regardless of the pathway chosen, introducing amendments—especially

engineered materials—into soil can generate environmental trade-offs and unintended consequences, which are critically evaluated in the following section.

ENVIRONMENTAL AND OPERATIONAL RISKS OF BIOCHAR APPLICATION

Biochar is widely promoted as a cost-effective and multifunctional amendment for agricultural soils. However, its production and application are not without environmental and operational risks (Long *et al.* 2024; Yao *et al.* 2024). A critical assessment of these risks—ranging from pollutant formation during pyrolysis to unintended ecological perturbations in field soils—is essential for translating laboratory promise into safe and scalable remediation practices.

Risks during Biochar Preparation

Thermochemical conversion of biomass can generate polycyclic aromatic hydrocarbons (PAHs) and dioxins, both of which pose environmental and health concerns (Hale *et al.* 2012). PAHs are formed during pyrolysis and related thermochemical processes, with concentrations strongly influenced by feedstock type, production method, residence time, and temperature. Reported total PAH concentrations in biochars vary widely; for example, Hale *et al.* (2012) reported values of 0.07 to 3.27 $\mu\text{g g}^{-1}$ for slow-pyrolysis biochars, compared with 0.3 $\mu\text{g g}^{-1}$ for a fast-pyrolysis biochar and 45 $\mu\text{g g}^{-1}$ for a gasification biochar. In that study, the highest PAH concentrations in slow-pyrolysis materials were generally observed in biochars produced in the 350 to 550 °C range, while higher pyrolysis temperatures often resulted in lower total PAH concentrations. Excessive activation or poorly controlled processing can also favor PAH accumulation (Weidemann *et al.* 2018).

Dioxin formation is mainly associated with feedstocks rich in chlorine and with low-temperature processes such as hydrothermal carbonization. Studies indicate that chars produced at 200 to 300 °C pose the highest risk of generating chlorinated congeners with elevated toxicity (Sobol *et al.* 2023). Regulatory frameworks such as the European Biochar Certificate (EBC) set a limit for PCDD/F (dioxins and furans) at 20 ng/kg dry matter (I-TEQ, EBC guidelines) (Grafmüller *et al.* 2024). However, compliance with this threshold and transparent reporting of dioxin/furan levels in biochar products is still uneven across studies.

Overall, feedstock choice, pre-treatment, and pyrolysis control are decisive for minimizing contaminant formation, yet these aspects are insufficiently standardized across studies.

Risks during Biochar Application

Although biochar is widely promoted for heavy-metal immobilization and soil remediation, its application stage poses several risks that depend heavily on soil chemistry, biochar feedstock and production conditions, and field management practices. Key risks include:

Secondary release of heavy metals

Biochar can act as a transient sink rather than a permanent fix: under acidic pH or fluctuating redox conditions, adsorbed metals (*e.g.*, Cd, Pb, Zn) may re-mobilize. At the same time, such re-mobilization does not necessarily imply irreversible loss of retention,

as released metal ions may be re-adsorbed by biochar or associated mineral phases as the system continues to equilibrate, provided that sufficient sorption capacity remains and local chemical conditions remain favorable. A column experiment using maize straw-derived biochar pyrolyzed at 600 °C showed increased mobility of Cu, Pb, Zn, and Cd in a highly acidic soil (pH ~4 to 5) when large biochar doses were applied, while soils with moderate to high pH showed much reduced remobilization (Jia *et al.* 2021). Additionally, a 3-year field experiment in paddy soil revealed that biochar amendment significantly decreased exchangeable Cd fractions, but the study also suggested that biochar aging and soil buffering capacity are crucial for ensuring long-term immobilization (Sun *et al.* 2023).

A management lesson provided by the forementioned studies is to select feedstocks with low inherent heavy-metal content; combine biochar with stabilizing mineral phases (*e.g.*, iron or manganese oxides), especially in acid or redox-variant soils; and implement leaching tests under site-relevant conditions and monitor over multiple seasons.

PFRs and redox toxicity

Biochar, especially from certain biomass sources and pyrolysis conditions, frequently contains environmentally persistent free radicals. These radicals can catalyze ROS formation, with potential to damage microbial cells or soil fauna. Alfei and Pandoli (2024) reported that biochars commonly contain abundant carbon- and oxygen-centered radicals, whose relative abundance varies with feedstock type and pyrolysis temperature. However, field data quantifying ecological impacts of PFRs (*e.g.*, on microbial oxidative stress, plant health) remain sparse and inconsistent.

The management lesson in this case is to employ harmonized protocols for quantifying PFR concentration; avoid pyrolysis conditions that maximize radical formation without controlling quenching; investigate aging or post-treatment (*e.g.*, natural oxidation, steam, or light exposure) to reduce reactive radical concentrations before widespread field application.

Soil microbiome perturbations

Biochar modifies soil microhabitats through changes in pH, adsorption of inhibitory molecules, or altering moisture and substrate availability. While many lab-scale, short-term studies report increased microbial biomass or enzyme activities, longer-term or field scale work reveals shifts in community composition and function that may be detrimental (*e.g.*, nitrification/denitrification reductions). Bolan *et al.* (2024) reported positive or negative effects, depending on biochar rate, feedstock, and soil type.

The management lesson here is to use moderate biochar amendment amounts; co-apply buffering amendments (organic matter, compost) to offset potential adverse pH or substrate effects; and include multi-season microbial community and functional enzyme monitoring in field trials to detect delayed or cumulative effects.

Agrochemical interactions (pesticide/herbicide interception)

Biochar's sorptive properties can reduce off-site losses of agrochemicals, but they may also decrease pesticide bioavailability and thereby compromise pesticide efficacy under field conditions. A global meta-analysis (J. Wang *et al.* 2024) covering 58 studies (386 observations) found that high-adsorption biochars generally reduced pesticide residues in organisms (plants, earthworms) by 66%, but they had no consistent effect on soil pesticide concentrations. Effects depended strongly on soil properties (*e.g.*, organic matter, texture) and biochar characteristics. Another study with rice straw biochar showed

that atrazine, simazine, and prometryn had decreased half-lives in biochar-amended soils, but adsorption also competes with microbial degradation, meaning that timing and dose remain important (Singh *et al.* 2024).

Taken together, these findings indicate that agrochemical interactions should be considered as a practical management risk of biochar application, particularly where reduced pesticide efficacy may offset other agronomic benefits. Accordingly, biochar-pesticide compatibility should be tested under field conditions, with attention to application timing, dose, environmental fate, and crop protection outcomes.

Intrinsic contaminants in certain biochars

Biochars derived from manures or wastes often have higher ash content and background heavy-metal burdens. For example, in the three-year field trial in paddy soil, biochar application reduced Cd in rice organ uptake, but the study also showed that some Cd remained in more mobile soil fractions, and immobilization efficiency declined over time with aging and under lower biochar dosages (Sun *et al.* 2023)

The management lesson to be shared from the reported work is to require feedstock screening for metal content, ash composition; to certify batches; to use higher pyrolysis temperature or modifications (washing, mineral amendment) to immobilize resident contaminants; and to track mobile and bioavailable metal fractions, not only total metal content.

Summary

Collectively, these findings underscore that the efficacy of biochar depends not just on immediate sorption or immobilization but on long-term stability, soil buffering, and management under realistic field conditions. Risks may be magnified in acidic, redox-variable, high-DOC, or low-buffer soils. Regulatory or certification frameworks (*e.g.*, European Biochar Certificate) should increasingly require performance-based monitoring (leachability, PFR reactivity, pesticide interception effects, microbial function over time) rather than just compositional limits.

These limitations highlight the importance of moving beyond biochar as a stand-alone amendment and exploring integrated strategies with biological and agronomic partners, which are discussed in the next section.

EMERGING APPLICATIONS: INTEGRATING BIOCHAR WITH BIOLOGICAL AND AGRONOMIC APPROACHES

Biochar is widely applied as a low-cost and environmentally friendly amendment for pollutant removal and soil remediation (Gong *et al.* 2022). As has been detailed, its primary function in contaminated soils is stabilization rather than degradation—shrinking labile metal pools *via* sorption, surface/co-precipitation, and pH/charge effects (Mukherjee *et al.* 2022). Building on these mechanisms, integrating biochar with microorganisms, plants, or soil fauna can enhance remediation efficiency through synergistic pathways (Xiang *et al.* 2022). An at-a-glance summary of representative pairings, mechanisms, and suitable soil–metal contexts is provided in Table S3.

Biochar Alone for Heavy Metal Immobilization

Biochar used as a stand-alone amendment has been widely investigated for heavy-metal immobilization, but its efficacy remains highly soil-specific (Guo *et al.* 2020). As discussed earlier, the main mechanisms include sorption, surface or co-precipitation, and pH buffering, although their relative importance varies with metal speciation, soil chemistry, and biochar properties. Case studies nonetheless confirm that stand-alone biochar can be effective under suitable conditions. For example, Li *et al.* (2018) reported nearly 98% removal of Cr(VI) using H₃PO₄-activated corncob biochar. In such applications, performance is shaped largely by the interaction between biochar's thermochemical history (*e.g.*, pyrolysis temperature) and feedstock origin, with higher-temperature chars often showing greater capacity for redox-mediated Cr(VI) transformation.

This redox dimension is particularly relevant for chromium, because biochar has been reported to participate in the transformation of highly toxic Cr(VI) to the less toxic and more readily immobilized Cr(III). Such participation may occur through electron-shuttling roles in microbially mediated systems, as well as through electron-donating or electron-mediating functions under abiotic conditions (Ren *et al.* 2023; Xu *et al.* 2021). In biochar-based composites, this transformation may be further enhanced, with biochar functioning mainly as an electron mediator while redox-active Fe species serve as the principal electron donors (Dai *et al.* 2025). Even so, converging evidence indicates that mineral-modified or composite biochar generally outperforms stand-alone materials in both capacity and stability (L. Sun *et al.* 2022; Tan *et al.* 2023).

The practical value of stand-alone biochar lies in its relative simplicity, lower modification burden, and ability to provide baseline immobilization under favorable soil conditions. However, its main constraint is the limited reliability of performance under multi-metal contamination, redox-variable environments, or otherwise heterogeneous field conditions. These limitations motivate the exploration of integrated strategies (see Table S3), which are discussed in the following subsections. Accordingly, long-term field validation remains necessary to determine when stand-alone biochar is sufficient and when more engineered or integrated systems are required.

Biochar and Microorganisms Synergistic Remediation

Compared with direct microbial loading discussed in the section on biological modification strategies, where biochar is pre-loaded or surface-modified with biomass, synergistic remediation systems emphasize the *in-situ* co-functioning of biochar and soil microbiota. Here, biochar acts less as a passive carrier and more as a catalyst for functional hotspots in which physicochemical stabilization and biological transformation converge. Within biochar pores and on its surfaces, microorganisms accelerate biomineralization (*via* localized carbonate/phosphate release), drive redox conversions (*e.g.*, Cr(VI) → Cr(III)), and secrete extracellular polymeric substances (EPS) that complex metals into less labile forms; co-localization further creates co-sorption hotspots and shifts community composition toward metal-tolerant guilds (Garg *et al.* 2025; Manikandan *et al.* 2023; Shan *et al.* 2021) (Fig. 5).

Different biochar–microbe interaction modes can be compared in terms of their dominant remediation functions and practical limitations. In the simplest systems, co-application with beneficial microbial inoculants, such as phosphate-solubilizing bacteria (PSB), may enhance immobilization beyond either component used alone. For example, PSB co-applied with biochar improved Pb and Cd immobilization more effectively than

single-component treatments (Lai *et al.* 2022). A second category involves functionally modified biochars that appear to favor beneficial microbial guilds or sustain microbial activity under stress conditions. Phosphorus-modified biochar, for instance, was reported to promote beneficial microbial communities and maintain remediation performance under contamination stress (Y. C. Wang *et al.* 2024). A third category includes redox-active or composite systems, in which biochar and microorganisms may jointly facilitate detoxification through coupled electron-transfer processes and redox transformation pathways (Manikandan *et al.* 2023). Taken together, these studies suggest that biochar–microbe systems may be most effective when they combine physicochemical immobilization with biologically mediated transformation, rather than relying on either pathway alone.

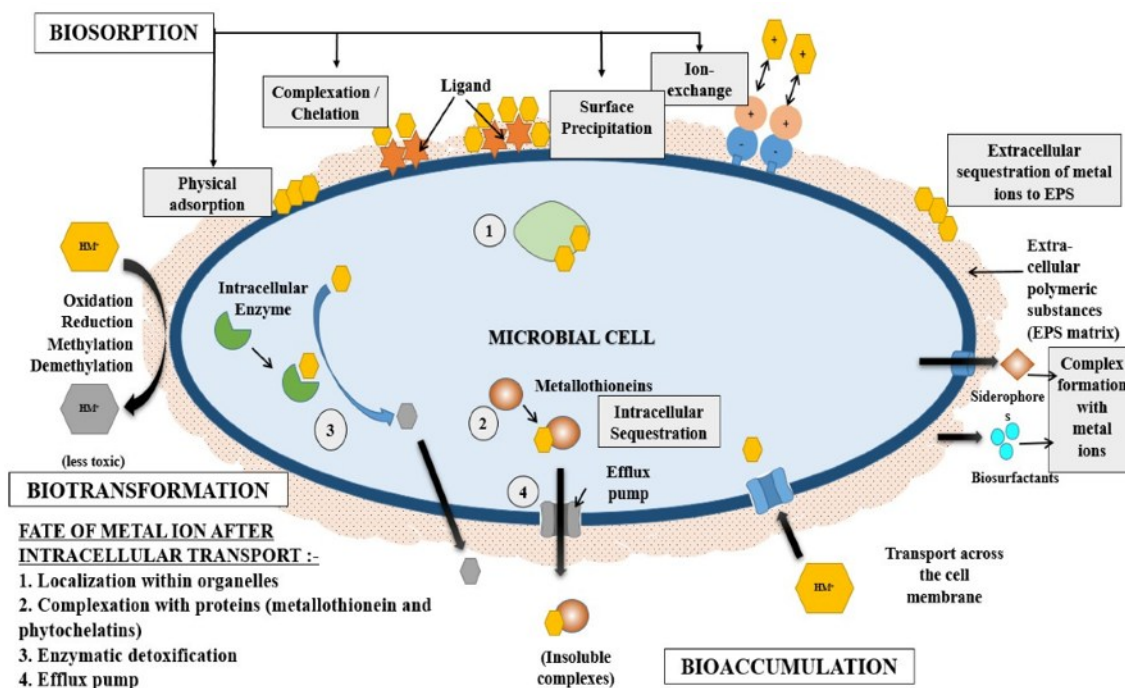


Fig. 5. Mechanisms of heavy-metal bioremediation by *Bacillus* species immobilized on biochar (Manikandan *et al.* 2023, under CC BY 4.0 license)

At the same time, these advantages should not be overgeneralized. The persistence of exogenous inocula under fluctuating pH, moisture, and redox conditions remains uncertain, and competition with native microbial communities may offset intended benefits. In addition, positive responses observed in controlled systems do not always translate directly to heterogeneous field soils, where contamination history, soil texture, and DOC dynamics may simultaneously affect microbial establishment and metal mobility. In particular, DOC may play a dual role by supporting microbial activity as a carbon source while also enhancing metal mobility through complexation under some conditions. Thus, the apparent success of biochar–microbe consortia often depends not only on amendment design, but also on ecological compatibility and environmental stability. Co-application systems mainly strengthen immobilization efficiency. Functionally modified biochars mainly support microbial persistence under stress, whereas redox-active composites are more relevant where detoxification through electron-transfer pathways is required.

Overall, biochar–microorganism synergistic remediation is promising because it may couple immobilization, transformation, and ecological recovery within the same system. However, the current evidence remains stronger for proof-of-concept performance than for field reliability. Future studies should therefore prioritize multi-season validation, direct comparison with non-biological amendment systems, and joint monitoring of microbial community dynamics and labile metal pools. Such work will be essential to determine when microbial synergy provides a robust remediation gain and when it remains conditional on site-specific constraints.

Biochar and Phytoremediation Integrated Techniques

Beyond the general agronomic benefits of biochar summarized earlier, its integration into phytoremediation systems specifically enhances remediation efficiency by modifying the rhizosphere environment—reducing the labile fraction of metals, stimulating root-associated enzymes, and supporting plant stress tolerance. For example, P. Sun *et al.* (2022) observed that combined biochar–plant treatments increased Pb immobilization by 12 to 18% compared with either treatment alone. Similarly, ferrate-modified biochar improved ryegrass tolerance in petroleum–zinc co-contaminated soils, enhancing hydrocarbon degradation while limiting Zn accumulation (M. R. Zhang *et al.* 2024). Mushroom-derived biochar co-applied with *Medicago sativa* also reduced bioavailable Cd by 44% in multi-metal soils while sustaining plant establishment (A. D. Wang *et al.* 2023).

Overall, biochar–plant combinations exhibit strong synergistic effects, enhancing both contaminant immobilization and plant productivity. However, most evidence stems from short-term pot experiments, and the efficiency of these systems under field-scale, multi-season conditions remains underexplored. Future work should clarify crop-specific responses, long-term ecological trade-offs, and the economic feasibility of large-scale deployment.

Biochar–soil Fauna synergistic Remediation

Soil fauna, particularly earthworms, can facilitate heavy metal remediation through bioaccumulation, biotransformation, stimulation of microbial activity, and enzyme release (C. Zhang *et al.* 2024). When combined with biochar, these processes can be synergistic. Biochar additions have been reported to elevate earthworm metallothionein levels, enhancing Cd tolerance (Luo *et al.* 2024), while vermicomposting systems integrating biochar produce “vermibiochar,” which is enriched with enzymes and organic ligands that further stabilize metals (Rehman *et al.* 2023). Such combinations can substantially reduce the bioavailability of toxic metals. For instance, Alsamhary (2023) documented a 60% reduction in Cd bioavailability when biochar was co-applied with *Eisenia fetida*. Nevertheless, findings remain inconsistent. Certain studies suggest that some earthworm species may actually increase heavy metal mobility by stimulating nitrification and lowering soil pH, thereby undermining biochar’s immobilization capacity (J. Wang *et al.* 2023). These contrasting outcomes indicate that biochar–earthworm systems are context-dependent, influenced by factors such as soil chemistry, biochar type, and species-specific earthworm behavior.

In summary, biochar–animal synergistic approaches represent an innovative frontier in remediation research, offering potential co-benefits for soil fertility and structure. However, their mechanisms remain poorly understood, and evidence from long-

term field trials is scarce. Future studies should prioritize mechanistic elucidation, species selection, and ecological risk assessments before recommending widespread adoption.

ARTIFICIAL INTELLIGENCE FOR BIOCHAR-BASED HEAVY-METAL REMEDIATION IN SOILS: FROM MATERIAL DESIGN TO DECISION SUPPORT

Artificial intelligence (AI) is increasingly being explored as a decision-support tool for addressing the complexity of soil-biochar-metal interactions in agricultural remediation systems (Balakumar *et al.* 2025). In contrast to conventional empirical or regression-based approaches, AI enables the integration of heterogeneous datasets, supports efficient parameter optimization, and delivers robust predictive capabilities for highly nonlinear systems (Ahmed and Aidi 2025). Within the domain of biochar-based soil remediation, AI applications are converging along two principal axes: (i) the rational design and process optimization of biochar materials (Zhou *et al.* 2024), and (ii) the prediction, monitoring, and adaptive control of remediation performance (Li *et al.* 2024). This integration is conceptually illustrated in Fig. 6, while representative AI/machine learning (ML) implementations in biochar research are summarized in Table S4. Importantly, although AI offers data-driven accuracy and risk minimization, its practical deployment in biochar remediation remains at an early stage, highlighting the need for systematic frameworks and field-level validation (Guo *et al.* 2025).

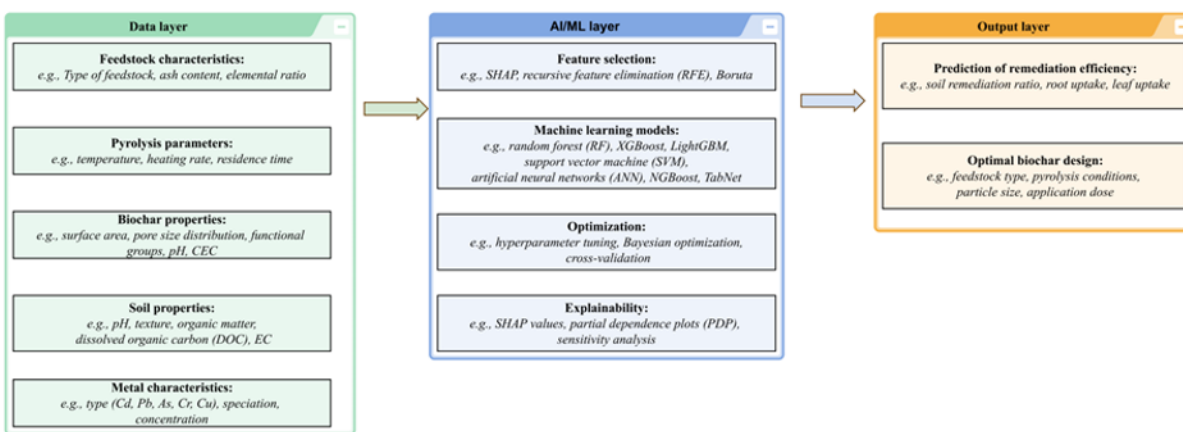


Fig. 6. Workflow of AI-assisted modeling for biochar-based heavy-metal remediation in soil

AI-driven Biochar Design and Process Parameter Optimization

Optimizing pyrolysis conditions to produce biochar with tailored physicochemical properties—such as yield, specific surface area (SSA), carbon content, and pore architecture—remains a critical challenge owing to the complex, nonlinear interplay between feedstock composition and pyrolysis parameters (*e.g.*, temperature, residence time, heating rate) (M. Liu *et al.* 2025). Traditional trial-and-error approaches are not only labor-intensive and costly but also prone to local optima, which can limit generalizability and scalability (M.-W. Chen *et al.* 2023). This bottleneck has constrained the wider deployment of biochar in environmental and agricultural applications. In response, AI-driven methodologies are reshaping this paradigm by systematically exploring high-dimensional design spaces, uncovering hidden interactions, and enabling rapid *in silico*

screening (Jiang *et al.* 2025). These advances can accelerate discovery, reduce experimental overhead, and lay the foundation for predictive, knowledge-guided biochar engineering.

Across recent studies, tree-based ensembles such as Random Forest (RF), Extreme Gradient Boosting (XGBoost), and Gradient Boosting Decision Trees (GBDT), as well as neural networks (NNs), generally outperform linear baselines for predicting yield, SSA, and composition from proximate/ultimate analyses, lignocellulosic features, and reactor parameters. For instance, Uppalapati *et al.* (2025) found that XGBoost attained a test R^2 close to 0.89, which was markedly higher than the 0.44 obtained by the linear model Lasso Regression. Beyond point prediction, model interpretability has increasingly become standard practice because it enables the identification of key variables, supports more efficient optimization of biochar design and application strategies, and helps align data-driven findings with plausible physicochemical explanations rather than leaving models as opaque black boxes (Freiesleben *et al.* 2024; Murdoch *et al.* 2019). Among various approaches, SHapley Additive exPlanations (SHAP) is widely used, as it not only ranks features by importance but also characterizes how changes in feature values shift model outputs, thereby revealing structured patterns in the available data (Lundberg and Lee 2017). In practice, SHAP values, partial-dependence profiles, and permutation importance frequently highlight pyrolysis temperature, ash content, elemental composition, and residence time as influential drivers of predicted yield (Uppalapati *et al.* 2025), SSA, and functional-group-related indicators—patterns that are broadly consistent with established pyrolysis chemistry.

Multi-objective optimization is increasingly used to navigate trade-offs among yield, SSA, energy input, and environmental performance. For instance, yield-and-SSA joint modeling with ensembles (Hai *et al.* 2023) and SSA–Total Pore Volume (TPV) modeling with gradient boosting (Li *et al.* 2023) exemplifies data-driven design approaches for pore-structure engineering. Collectively, the studies summarized in Table S4 suggest several recurring contributions of AI/ML to biochar research. Across diverse datasets, nonlinear models such as Random Forest, XGBoost, and neural networks often outperform linear baselines in predicting biochar yield, SSA, and composition, indicating an improved ability to capture complex interactions among feedstock composition, pyrolysis conditions, and (where included) soil-context variables. Despite heterogeneity in experimental sources, these works converge on a broadly similar set of predictive inputs—proximate and ultimate composition, lignocellulosic fractions, and reactor parameters—suggesting the emergence of a core variable framework for biochar modeling. Furthermore, many studies emphasize not only predictive accuracy but also interpretability, increasingly adopting SHAP and related techniques to identify dominant predictors and to contextualize model behavior in ways that are consistent with known pyrolysis mechanisms. Taken together, these contributions position AI/ML as a promising and knowledge-oriented toolset for guiding biochar design and informing soil remediation strategies.

AI-assisted Prediction and Control of Heavy-Metal Immobilization

The efficiency of biochar-mediated immobilization is difficult to predict because of nonlinear interactions among biochar properties, soil chemistry, metal speciation, and application strategies (Zand and Abyaneh 2020). Such complexity introduces uncertainty that may cause environmental risks, for example, ineffective immobilization or unintended remobilization (Dong *et al.* 2025). To address these challenges, AI models—including RF, GBDT, Support Vector Regression (SVR), ANN, and emerging deep or hybrid

architectures—are increasingly employed to integrate diverse covariates and provide data-driven forecasts of immobilization outcomes across metals and soil contexts.

Studies summarized in Table S4 suggest that models emphasizing controllable variables (biochar traits and application conditions) typically explain more variance than those centered primarily on intrinsic metal properties. Random-forest frameworks trained on consolidated soil datasets (Guo *et al.* 2023; Palansooriya *et al.* 2022) report strong cross-validated performance and commonly use SHAP and Partial Dependence Plots (PDP) to identify leverage points for design-for-remediation. Extensions to soil–plant systems (Li *et al.* 2024) further indicate promise for predicting crop uptake and bioaccumulation (BAF), although available training data remain dominated by pot experiments and short-term studies. Table S4 provides representative sample sizes, performance metrics, and validation strategies across these implementations.

Importantly, moving from prediction toward practical monitoring and control will require models that remain reliable under field heterogeneity and changing conditions and that can support operational decisions (*e.g.*, amendment selection and dosing) with transparent uncertainty. AI has also been explored for predicting broader soil-process responses to biochar amendment, including greenhouse-gas emissions such as N₂O, showing that its utility may extend beyond remediation efficiency alone (Wang *et al.* 2024). Although such applications fall outside the core focus of heavy-metal immobilization, they help situate AI-assisted remediation within the wider context of biochar-soil interactions. These considerations motivate the critical challenges discussed next, including data bias, leakage-safe validation, and lab-to-field transferability.

Critical Challenges: Data Bias, Model Reliability, and Validation Gaps

While AI offers substantial potential for biochar remediation research, translation from modeling to agronomic decision support remains constrained by three recurring bottlenecks.

Data limitations constitute a structural constraint on AI credibility in biochar-based remediation. Recent methodological analyses have highlighted that reported accuracy can be systematically inflated in small-*n* settings, consistent with the higher susceptibility of small datasets—typical of current biochar research—to overfitting and optimistic performance estimates (Vabalas *et al.* 2019). Literature-derived datasets are also likely enriched for “successful” outcomes, whereas null or unfavorable results are less frequently reported (publication bias), which may lead training data to over-represent best-performing scenarios and under-sample boundary conditions and failure modes critical for risk-aware deployment (Saidi *et al.* 2025). Robustness is further weakened by heterogeneity and incompleteness: key descriptors (*e.g.*, pore-volume distributions, mineral phases, surface functional group metrics) are often missing or measured inconsistently across studies, introducing measurement bias and forcing imputation or feature exclusion. Finally, dataset imbalance (over-representation of particular feedstocks or soil types) and inconsistent outcome definitions (different extraction protocols) create domain-shift and label-inconsistency risks when models are applied beyond their training distribution (Miftahushudur *et al.* 2025). Together, these data constraints place a practical ceiling on model reliability and motivate the need for stringent validation and uncertainty-aware reporting.

Beyond data quality, methodological pitfalls in model development pose major risks to generalizability. A pervasive issue is study-structure leakage, where random splits place samples derived from the same study or experimental series (sharing feedstock, soils,

treatment settings, and measurement protocols) into both training and test sets (M.-W. Chen *et al.* 2023). This can inflate apparent performance by evaluating interpolation within familiar experimental regimes rather than true transferability. The problem may be compounded by adaptive data analysis, in which a fixed test set is repeatedly leveraged—explicitly or implicitly—during model selection and hyperparameter tuning, yielding overly optimistic estimates and overfitting to dataset-specific idiosyncrasies (Saidi *et al.* 2025). Accordingly, leakage-safe evaluation (*e.g.*, grouped/blocked cross-validation such as leave-one-study/site/feedstock-out, and external tests where available) is essential for credible claims of generalization. Moreover, interpretability tools such as SHAP require cautious application. Attributions are model- and feature-set-dependent: different choices of input representation (*e.g.*, inclusion/exclusion of correlated covariates, feature engineering, encoding, and preprocessing) can lead to substantially divergent importance rankings even on the same underlying dataset. Therefore, SHAP results should be interpreted primarily within the context of a specific modeling pipeline rather than as universally comparable “mechanistic truth,” and cross-model comparisons should be grounded in harmonized feature sets and leakage-safe validation designs (Freiesleben *et al.* 2024; Murdoch *et al.* 2019).

Finally, a critical lab-to-field generalization gap persists. Much of the available training evidence is derived from short-term, laboratory-scale incubation studies, often using homogenized and/or spiked soils (Vijay *et al.* 2021). Such datasets do not fully capture field heterogeneity and, crucially, long-term biochar aging processes (*e.g.*, surface oxidation, mineral deposition, and pore clogging). Consequently, AI models trained predominantly on short-term “fresh-biochar” conditions may overestimate remediation performance when transferred to aged biochars or long-contaminated field soils (Cui *et al.* 2024). This gap highlights that data representativeness can be as important as algorithmic sophistication; future research should prioritize integrating field-scale and long-term datasets, and where appropriate, adopt transfer learning or domain-adaptation strategies to calibrate lab-trained models to field realities. In parallel, decision-grade deployment requires uncertainty-aware outputs and explicit statements of domain applicability when extrapolating across soils, climates, and aging states.

Collectively, these bottlenecks imply that AI in biochar remediation is currently best positioned as bias-aware, uncertainty-calibrated decision support—rather than a universal predictor—until leakage-safe validation and field-scale evidence have become more mature.

CONCLUSION AND OUTLOOK

Conclusions

Biochar has evolved from a simple soil amendment to an increasingly engineerable material platform for environmental remediation. This review has systematically evaluated the state of the art in biochar engineering, highlighting that heavy-metal immobilization is often shaped by a coupled interplay among pore architecture, surface functional groups, and redox-active components. In this review these pathways have been consolidated into a “mechanism–lever–endpoint” logic (Fig. 3), bridging mechanistic hypotheses with practical design and synthesis choices under soil–metal constraints.

However, the inherent complexity of soil–biochar–metal interactions increasingly limits trial-and-error optimization and encourages “black-box” deployment—both in material selection (*e.g.*, overlooking long-term risks such as remobilization) and in model development (*e.g.*, overconfident performance claims under leakage-prone validation). In this context, AI can be a powerful decision-support layer for navigating high-dimensional design spaces and for prioritizing candidate strategies that merit field testing. Yet, it is important to emphasize that neither high sorption capacity nor high predictive accuracy is sufficient for decision-grade use. Risk-aware deployment therefore benefits from a dual-validation mindset: validating materials for durability and ecological safety over time, and validating models for leakage-safe transferability with uncertainty-aware reporting.

Outlook

To transform biochar-based remediation from an empirical practice to a precision science, future research must address critical gaps through a coordinated paradigm shift. Future research should prioritize the following areas:

Standardization for data-driven discovery

The current fragmentation of data hinders the application of advanced analytics. Establishing universal reporting standards for pyrolysis conditions, feedstock properties, and functional parameters is a prerequisite. High-quality, standardized datasets are essential to unlock the full potential of Machine Learning (ML) meta-analyses, ensuring that predictive models are robust and transferable across different soil types.

From soil immobilization to food safety prediction

Current research predominantly focuses on reducing the extractable fraction of metals in soil (*e.g.*, TCLP/DTPA methods). However, reduced bioavailability in soil does not always linearly correlate with reduced accumulation in crop tissues due to the complexity of the soil-root-shoot barrier. A critical future direction is to shift the prediction target from “soil availability” to “edible tissue accumulation.” Integrating AI models with plant physiology data will make it possible to predict heavy metal concentrations in grains or fruits directly. This shift is essential for bridging the gap between geochemical remediation and actual human health risk assessment.

Embedding computational toxicology for “safe-by-design” composites

While modifying biochar with nanomaterials or metal oxides enhances efficiency, it may inadvertently increase cytotoxicity or ecological risks. Future computational frameworks must integrate computational toxicology. By incorporating molecular descriptors of loaded materials into predictive ML models, researchers can achieve multi-

objective optimization. This may involve simultaneously maximizing heavy metal immobilization while minimizing the intrinsic toxicity of the engineered biochar. Such a “Safe-by-Design” approach prevents the “regrettable substitution” scenario where a remediation material becomes a new pollutant.

From single-route optimization to AI-guided multifunctional design

A further priority is to move beyond single-route optimization toward AI-guided design of multifunctional or complementary-function biochars for mixed-contaminant systems. Rather than seeking a single optimal active site for a given field condition, future models should aim to identify combinations of reactive moieties, mineral phases, or blended amendment strategies that broaden functional coverage across cationic and oxyanionic metals. Progress in this direction will depend on standardized descriptors of surface chemistry, pore architecture, and mineral loading, as well as mechanistically informed training data and long-term validation under heterogeneous field conditions. Such frameworks could ultimately support multi-objective optimization of remediation efficiency, stability, cost, and environmental safety.

Long-term field validation and aging mechanisms

Most current knowledge is derived from short-term incubation studies. There is an urgent need for multi-season field trials to decipher the aging mechanisms of engineered biochars. Understanding how surface oxidation, pore clogging, and interactions with soil organic matter affect the long-term stability of immobilized metals is crucial for regulatory approval and commercialization.

Take-home Message

The traditional trial-and-error paradigm in biochar remediation is increasingly insufficient for addressing field-scale complexity. The next frontier involves a paradigm shift toward intelligent precision. Future research should harness AI not only to optimize immobilization efficiency but also to predict crop safety and screen for ecological toxicity *via* computational toxicology. By integrating the “soil-plant-human” continuum into data-driven frameworks, it may be possible to engineer biochars that are not only effective in theory but also safe, predictable, and compliant in reality.

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SUPPLEMENTARY INFORMATION

Table S1. Origins of Heavy Metals in Agricultural Soil

Location	Contamination	Method	Sources and contribution level	Reference
Northeast Yunnan province, China	As, Zn, Pb, Ni, Cd, Cu, and Cr	Positive matrix factorization (PMF)	Smelting activities 37.11%, fertilizer and industrial sewage application 23.69%, agrochemical utilization 19.69%, and atmospheric deposition 19.51%	Guanghui Guo <i>et al.</i> 2023
Northwestern Guizhou province, southwest China	Cr, Cu, Ni, Pb, Cd, Zn, Hg, and As	PMF	Natural sources accounted for 27%, smelting activities 14.5%, agricultural activities 20.9%, mixed sources of traffic emissions and smelting-related activities 19.8%, and atmospheric deposition 17.8%.	Li <i>et al.</i> 2022
Northern Guangdong province, China	As, Hg, Cd, Cr, Pb, Zn, Cu, and Ni	PMF	Atmospheric deposition 19.3%, anthropogenic and geogenic sources 65.5%, and soil parent materials 15.2%.	Shi <i>et al.</i> 2022
Kaifeng, China.	Pb, Zn, and Cu	UNMIX	Industrial and agricultural activities 61.74%, sewage irrigation and atmosphere deposition 28.14%.	Chen <i>et al.</i> 2022
Southeast Spain	Cr, Cu, Fe, Mn, Ni, Pb, Zn, and Cd	PCA	parent rock 56%, anthropogenic component 14%, fertilizers 12%.	Micó <i>et al.</i> 2006
Lake Chilwa catchment in Malawi, southern Africa.	Zn, Pb, Ni, Cr, Cu, and Cd	PCA	Agrochemicals (manure, inorganic fertilizers, and pesticides) account for 49%, whereas weathering and leaching of the parent rock material account for 35%.	Mussa <i>et al.</i> 2020
Kwara state, Nigeria.	Pb and As	PCA	Anthropogenic 68%, geologic sources 23%.	Elemile <i>et al.</i> 2023
Lintong district of Shaanxi province, China	Cr, Mn, Co, Ni, Cu, Zn, As, and Pb	Spatial distribution - principal component analysis (SD-PCA)	Agriculture sources 65.5%, traffic sources 17.9 %, natural pollution sources 11.1%.	Liu <i>et al.</i> 2023
Western part of Yangzhou city, Jiangsu province, China	Ni, Zn, Cu, Pb, Cr, As, and Cd	PMF	Anthropogenic activities: 34%; parent material weathering: 65%;	Qi <i>et al.</i> 2024
Southwest of Nanyang city, Henan province, China	As, Cr, Mn, Ni, Zn, Pb, Hg, Cd, and cobalt	PCA	Natural sources 41%, agricultural sources 16%, Industrial emissions and transportation sources 13%.	(Dong <i>et al.</i> 2023
Qingcheng district, Guangdong province, China	Sn, Zn, P, As, and Cd.	PCA	Anthropogenic activities 28.9%, medium acidic granites 28.6%, geological origin 15.9%, and calcium-alkaline materials 11.17%.	Luo <i>et al.</i> 2023

Table S2. Physicochemical Properties of Biochar Prepared from Different Feedstocks Under Various Pyrolysis Conditions

Feedstock	Pyrolysis Temp. (°C)	Pyrolysis time	pH	C (%)	O (%)	H (%)	N (%)	O/C (molar ratio)	H/C (molar ratio)	BET surface area (m ² /g)	Total pore volume (cm ³ /g)	Average pore size (nm)	Reference
Wheat straw	450°C	2h	9.81±0.12	62.3	14.6	2.99	1.43	52.7		2.38	40.4	0.009	Lian <i>et al.</i> 2023
Rice husk	450°C	2h	9.62±0.23	52.7	10.7	2.68	0.85			3.19		0.015	
Pig manure	450°C	2h	8.34±0.14	40.4	14.2	3.11	2.06			3.83		0.029	
Oyster shells	450°C	2h	10.63±0.22	13.6	30.3	0.22	0.30			6.03		0.018	
Phyto-remediation residue	750°C	0.5h	13.15	27.56		0.92	1.20					0.0624	Z. Li <i>et al.</i> 2024
<i>Gigantochloa levis</i>	300°C	2h	5.89±0.018	55.73		3.6	3.00		0.065	0	0	0	Abdul Halim <i>et al.</i> 2024
	450°C	2h	6.38±0.027	70.91		2.57	3.1		0.036	10	0.005	1.79	
	600°C	2h	7.97±0.059	79.9		1.84	2.97		0.023	147	0.079	2.14	
<i>Melaleuca cajuputi</i> trees	300°C	2h	5.26±0.089	65.84		4.39	2.68		0.067	1	0.079	1.06	
	450°C	2h	6.04±0.046	74.97		3.2	2.43		0.043	25	0.01	1.66	
	600°C	2h	9.05±0.035	85.09		1.78	2.40		0.021	358	0.155	1.73	
Rubber powders and <i>Ginkgo biloba</i> leaves 5 : 2	700°C	2h		71.84	2.49	0.29	0.43	0.026	0.048			16.49	Zhang <i>et al.</i> 2023
	800°C	2h		61.31	1.87	0.16	0.33	0.20	0.030			13.90	
	900°C	2h		67.47	1.52	0.26	0.20	0.017	0.046			6.076	
Apricot shells	300°C	3h		65.14	28.21	5.24	0.19	0.44		3.19	0.0243		Fan <i>et al.</i> 2022
	400°C	3h		67.27	28.02	2.99	0.12	0.42		160.40	0.0771		
	500°C	3h		84.52	10.15	3.38	0.13	0.12		110.44	0.0725		
	600°C	3h		83.53	11.48	2.46	0.13	0.14		370.34	0.1009		
	700°C	3h		88.57	6.40	2.03	0.17	0.07		326.01	0.1045		
	800°C	3h		89.64	4.71	1.2	0.08	0.05		435.98	0.1207		
Coconut shell	300°C	3h		65.51	28.80	4.74	0.16	0.44		4.03	0.0288		
	400°C	3h		77.31	17.39	4.04	0.07	0.23		7.86	0.0579		
	500°C	3h		84.82	10.39	3.24	0.16	0.12		24.83	0.0701		
	600°C	3h		89.51	6.18	2.42	0.12	0.07		320.42	0.0943		
	700°C	3h		89.15	6.95	1.75	0.17	0.08		198.92	0.0996		
	800°C	3h		91.30	4.80	1.25	0.06	0.05		415.13	0.1269		
Peanut shells	300°C	3h		60.16	26.58	5.08	2.10	0.44		4.06	0.0244		
	400°C	3h		66.48	19.62	3.58	1.62	0.30		66.86	0.0593		
	500°C	3h		76.84	9.59	1.93	1.08	0.13		22.43	0.0560		

Walnut shells	600°C	3h	77.72	7.80	2.36	1.38	0.10	71.47	0.0804
	700°C	3h	75.33	7.79	1.81	1.14	0.10	184.17	0.0773
	800°C	3h	76.54	5.29	1.31	0.56	0.07	439.82	0.1109
	300°C	3h	61.53	31.13	5.26	0.26	0.51	5.09	0.0261
	400°C	3h	65.77	29.01	3.04	0.23	0.44	95.44	0.0700
	500°C	3h	83.10	11.30	3.39	0.17	0.14	112.71	0.0720
	600°C	3h	87.73	7.18	2.37	0.14	0.08	329.30	0.0966
	700°C	3h	86.83	7.41	1.80	0.10	0.08	249.93	0.0894
	800°C	3h	89.33	4.69	1.33	0.10	0.05	454.17	0.1114

Table S3. Recent Studies on Agricultural Soil Remediation by Biochar

Heavy metals	Type of Biochar	Integrated Methods	Results	References
Cd	Sulfur(S)-Chicken manure biochar(CMB)(SCMB), hydroxyapatite - CMB(HCMB) and MnFe ₂ O ₄ -CMB(MCMB)		DTPA-extractable Cd (mg·kg ⁻¹) of CK, CMB5%, SCMB5%, HCMB5%, CMB5% are 0.82,0.72,0.55,0.63,0.72, respectively. Similarly, Cd in shoot of brassica chinensis are 0.67,0.66,0.53,1.17,0.54, respectively.	L. Sun <i>et al.</i> 2022
Cd	Chitosan-Modified Biochar(β-CD/C-BC)		Conversion of HMs in soil into a residual state (from32 % to 82 %)	Lin <i>et al.</i> 2024
Cd	Fe-Mn oxide-modified biochar		When compared to soil that has simply been treated with biochar (BC), Fe and Mn loaded on BC-FM enhanced the removal efficiency of CaCl ₂ extractable Cd in soil and Cd in pore water, with maximum removal rates at 67.9% and 77.8%, respectively.	Tan <i>et al.</i> 2023
Cd	Ca-modified biochar (CBC)	low-Cd cultivars of Liyu16 and Sanbei218	Following the addition of CBC, the Cd level in the grains of the low-Cd cultivars of Liyu16 and Sanbei218 was dramatically reduced by 37.55–50.80% and 23.60–51.20%, respectively.	Sun <i>et al.</i> 2023
Cr, As, Cd, and Pb	Biochar	<i>A. ferrooxidans</i>	The average decrease of heavy metals in soil was as follows: combined treatment (28.42%) > biochar (22.35%) > <i>A. ferrooxidans</i> (18.94%). All three treatments reduced the content of heavy metals in lettuce (26.19–84.42%),	Yang <i>et al.</i> 2023
Pb and Cd	Rice husk biochar	phosphorus-solubilizing bacteria (PSB)	Combined remediation significantly increased the acid-soluble and non-bioavailable fraction of Pb/Cd by 5/15 times and 14/5.8 times in contaminated soil.	Lai <i>et al.</i> 2022
Pb	<i>Enteromorpha prolifera</i> biochar at 400 °C and 600 °C BC and BC6)	<i>Brassica juncea</i> (BJ)	Pb immobilization rates of biochar-plant treatments (BJBC4 and BJBC6) were 12.47% and 11.38% higher than biochar treatment (BC4, BC6), and 17.66% and 16.28% plant treatment (BJ).	P. Sun <i>et al.</i> 2022
Cd, Pb, and Zn	Rice straw biochar		The Cd, Pb, and Zn bioavailability assessed by DTPA decreased 32%	de Lima Veloso <i>et al.</i> 2022)
Cd,Cr,Pb	(i) activated coffee husk biochar (BAC), (ii) nonactivated biochar coffee husk (BSAC), (iii) activated sugar cane leaf biochar (BAA), and (iv) nonactivated biochar sugar cane leaf (BSAA). Biochar, loaded with phosphorus (P),	<i>Lolium perenne</i>	The utilization of biochar contributes to an 11.6% enhancement in the retention of HM in plant organs.	Serrano <i>et al.</i> 2024
Cd	Rice husk biochar	Vermi-cyanobacterial	Quantity of Cd (60.3%) was removed.	Alsamhary 2023

Table S4. Summary of AI/ML Applications in Biochar Research

Application Domain	Models Evaluated	Best Model	Dataset Size (n)	Input Variables	Predicted Out-puts	Performance Metrics (R^2 , RMSE, etc.)	Validation Method	Limitations / Remarks	Reference
Biochar yield and carbon content	Random Forest (RF), multiple linear regression, decision tree.	Random Forest (RF)	245 datasets for biochar yield, 128 datasets for C-char	12 variables grouped into: (i) structural components (lignin, cellulose, hemicellulose, ash), (ii) elemental composition (C, H, O, N), (iii) particle size, (iv) pyrolysis conditions (heating rate, highest treatment temperature, residence time)	Biochar yield, carbon content in biochar	Yield : $R^2=0.85$, RMSE=3.40	80:20 training-test data split, 5-fold cross-validation	Dataset compiled from literature (heterogeneous experiments, data digitized); potential bias due to inconsistent feedstock/pyrolyzer conditions; no external validation beyond 80:20 split	Zhu <i>et al.</i> 2019
Biochar yield & Composition	Multi-Layer Perceptron Neural Network (MLP-NN); Adaptive Neuro-Fuzzy Inference System (ANFIS)	MLP-NN (ReLU, 14 neurons, 1 hidden layer)	226 datasets	Feedstock proximate (FC, VM, ash), ultimate (C, H, O, N), pyrolysis conditions (PT, HR, RT); sulfur & lignocellulosic data excluded due to missingness	Biochar yield (%), proximate composition (FC, VM, ash), ultimate composition (C, H, O, N)	Yield: $R^2 = 0.964$, RMSE = 3.4; Proximate avg: $R^2 = 0.914$, RMSE = 4.4; Ultimate avg: $R^2 = 0.887$, RMSE = 1.8	Train/test splits (80/20, 70/30, 60/40); cross-comparison with literature	Dataset compiled from heterogeneous literature → variable quality and missing data; mean imputation applied; no external validation beyond random splits; scope limited to feedstocks with ash $\leq 15\%$	Li <i>et al.</i> 2022

Biochar design & Process optimization	Multiple Linear Regression (MLR), Decision Tree (DT), Random Forest (RF), Support Vector Machine (SVM), K-Nearest Neighbor (KNN)	Random Forest (RF)	292 data points	proximate analysis (MC, VM, AC, FC), ultimate analysis (C, H, N, S, O), lignocellulosic fractions (Cellulose, Hemicellulose, Lignin), pyrolysis parameters (Temperature, Residence time, Heating rate, Particle size)	Biochar total yield (%), specific surface area (SSA, m ² /g)	Yield (RF, test): R ² = 0.855, RMSE = 3.119; SSA (RF, test): R ² = 0.804, RMSE = 4.322	Train/test split 80:20; feature selection by PCC + feature importance ranking	Data compiled from heterogeneous literature; possible bias due to variability of experimental setups; only agricultural biomass in N ₂ atmosphere; no validation under other inert gases or with activating agents	Hai <i>et al.</i> 2023
Biochar design & Pore structure engineering	Random Forest (RF), Gradient Boosting Regression (GBR)	GBR (single- & multi-target)	169 data-sets (39 bio-mass feedstocks, from 30 published papers); for yield-only models, n=152 (due to missing data)	Biomass proximate (VM, Ash, FC), elemental (C, H, N, S, O), pyrolysis parameters (T, RT, HR)	Yield (%), Specific surface area (SSA, m ² /g), Total pore volume (TPV, cm ³ /g)	GBR (test): Yield R ² =0.94, RMSE=4.25; SSA R ² =0.92, RMSE=46.53; TPV R ² =0.91, RMSE=0.06. Multi-target GBR average test R ² =0.90	80/20 train–test split; hyperparameter tuning with 5-fold cross-validation	Dataset relatively small; compiled from heterogeneous literature → possible bias; only three pyrolysis variables considered (T, RT, HR); external validation absent; TPV–SSA relationship weak/inconsistent	Li <i>et al.</i> 2023
Biochar design & Property prediction	Random Forest (RF), Gradient Boosting Decision Tree (GBDT), LightGBM, AdaBoost, XGBoost	XGBoost	622 datasets	Proximate composition (VM, Ash, FC), elemental composition (C, H, N, O), pyrolysis parameters (Temperature, Retention Time, Heating Rate), biomass type	Biochar yield (%), Specific surface area (SSA, m ² /g)	Yield (test): R ² =0.79, RMSE=8.41; SSA (test): R ² =0.92, RMSE=45.21 (Table 2 & 3)	Train/test split 70:30; hyperparameter tuning via grid search; 5-fold cross-validation	Dataset compiled from heterogeneous literature; missing data filled (linear interpolation); limited to reported features (S excluded); no external/independent validation; performance on yield lower (R ² =0.79) than SSA (R ² =0.92)	Zhou <i>et al.</i> 2024
Biochar design & Process optimization	Random Forest (RF), XGBoost	XGBoost	355 datasets	Biomass elemental composition (C, H, O, N, S, FC, VM, Ash); lignocellulosic (cellulose, hemicellulose, lignin); HHV; pyrolysis temperature	Biochar yield (%), Carbon content (wt%)	XGBoost: Train R ² = 0.98, Test R ² = 0.91; RMSE = 1.06–4.79 (yield, C content)	80/20 train–test split; 5-fold CV; hyperparameter tuning (grid search)	Data compiled from heterogeneous studies; missing values mean-imputed; unstable variables (sample mass, heating rate, residence time)	Xu & Du 2024

								removed; no external validation	
Biochar production from aquatic biomass (hydro-thermal carbonization HTC & pyrolysis carbonization PLC)	Random Forest Regression, Extreme Gradient Boosting (XGB), AdaBoost, Gradient Boosting Regression (GBR), Extra Trees Regression (ETR)	RFR (hydro-char yield, N recovery, energy recovery, residual S) XGB (energy density, pyrochar yield, N recovery pyrochar)	586 data points total (425 HTC; 161 PLC)	Feedstock elemental composition (C, H, N, O, S); proximate analysis (volatile matter, moisture, ash, fixed C); process conditions (temperature, time, biomass concentration)	Hydrochar yield; Pyrochar yield; N recovery; Energy density; Energy recovery Residual S	$R^2 = 0.89\text{--}0.98$ (RFR, hydrochar properties); $R^2 = 0.84\text{--}0.94$ (XGB, pyrochar properties & energy density); RMSE = 2.81–7.75 depending on target	Train–test split (80/20); 5-fold CV; Hyperparameter tuning	Outputs limited (did not include SSA, pH due to lack of AB data); <8% missing values imputed; potential variability from different experimental methods; external validation limited	Yuan <i>et al.</i> 2024
Soil heavy-metal immobilization by biochar	SVR, Neural Network (NN), Random Forest (RF); plus updated RF after feature selection	RF (updated RF best on test set)	152 data points for immobilization model (after imputing missing SA); total collected = 162; separate SA sub-model built	20 inputs grouped as: pyrolysis T; biochar properties (pH, SA); composition (C, H, N, O, ash); atomic ratios (H/C, O/C, [O+N]/C); operational (biochar rate, time, available HM); soil (pH, EC); HM property (electronegativity).	HM immobilization efficiency (%) in soils (Cu, Zn, Pb, Cd, Fe, Ni, Mn).	Preliminary RF: train $R^2 = 0.95$, test $R^2 = 0.91$; RMSE(train) = 7.35, RMSE(test) = 10.54. Updated RF (with 14 features): train $R^2 = 0.95$, test $R^2 = 0.92$; RMSE(train) = 7.54, RMSE(test) = 9.92..	Standardization; 85% train / 15% test split; 5-fold CV for hyperparameter tuning.	Literature-compiled and heterogeneous; SA imputed (see SA sub-model); soil EC records with missing data excluded; only limited external check via a GUI with 8 new points (most errors <30%), no true field-scale validation.	Palansooriya <i>et al.</i> 2022

Soil remediation & heavy-metal immobilization	Linear Regression (LR), Support Vector Regression (SVR), Gradient Boosting Decision Trees (GBDT), Random Forest (RF)	RF	844 data points	20 inputs: Biochar properties — Temperature (T), pH_BC, EC_BC, SSA, CEC_BC, Ash, C, N, O, H; Soil — pH_soil, EC_soil, CEC_soil, clay, silt, sand, OC; Experiment — Rate_BC, Time, HM_soil. Feature selection retained 9 key inputs (C, N, O, pH_BC; pH_soil, OC, CEC_soil; HM_soil, Rate_BC).	HM immobilization ratio (%) in bio-char-amended soil (Cd, Cu, Pb, Zn)	Combined model (RF): Train R^2 = 0.90; Test R^2 = 0.87; RMSE = 4.4; MAE = 2.18 (Table 3). Per-metal RF (Table 4) test R^2 : Cd 0.81; Cu 0.84; Pb 0.82; Zn 0.81.	Random 80/20 train–test split; 5-fold CV; grid search for hyperparameters. External check with 10 literature data points, prediction error < 20%.	Literature-compiled, heterogeneous sources; variables standardized; SHAP/PDP used for interpretation; no true field-scale validation; external check limited to 10 points.	Guo <i>et al.</i> 2023
Soil remediation & heavy-metal immobilization (soil–plant environment)	Linear Regression (LR), Partial Least Squares (PLS), Support Vector Regression (SVR), Random Forest (RF)	RF	211 data-sets (94% pot, 6% field experiments)	14 variables: experiment scale, crop type, application rate, feedstock, pyrolysis T, clay, silt, sand, soil pH, soil OC, crop duration, total HM in soil, available HM in soil, HM species	Immobilization efficiency (%); CCU (change in crop uptake); BAF (bioaccumulation factor)	Immobilization (RF): R^2 = 0.5924, MAE = 0.1556, MSE = 0.0596, RMSE = 0.2441; CCU (RF): R^2 = 0.7338; BAF (RF): R^2 = 0.6997	5-fold cross-validation only (no independent train/test split)	Literature-compiled; dataset dominated by pot studies (94%); missing agronomic/biochar factors; relatively low R^2 under CV indicates weak generalizability and possible overfitting; no external validation	X. Li <i>et al.</i> 2024