JOURNAL OF THE ROYAL LAUREATES ACADEMY

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ADSORPTION MECHANISMS AND PERFORMANCE EVALUATION OF HYBRID MATERIALS: ISOTHERM MODELLING, KINETIC ANALYSIS, AND ENVIRONMENTAL APPLICATIONS

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ABSTRACT

Hybrid adsorbents are increasingly investigated for water purification because their combined chemical and structural properties can support the removal of diverse pollutants. Nevertheless, evaluating these materials requires more than measuring the percentage of contaminant removed. Adsorption mechanisms, equilibrium relationships, mass-transfer rates, and the effects of operating conditions must be examined to establish reliable performance. This paper reviews the mechanisms involved in pollutant adsorption by hybrid materials and evaluates the role of equilibrium isotherms and kinetic models in interpreting experimental data. Langmuir, Freundlich, Temkin, and other isotherm models are discussed alongside pseudo-first-order, pseudo-second-order, intraparticle-diffusion, and related kinetic approaches. The importance of nonlinear regression, model validation, and consistency between experimental observations and theoretical assumptions is emphasized. Environmental applications involving toxic metals, dyes, pharmaceutical residues, and other water pollutants are considered. The paper also identifies challenges associated with competing contaminants, regeneration, real-water performance, and translation from laboratory experiments to continuous treatment systems.

Keywords: Hybrid materials, adsorption mechanisms, adsorption isotherms, kinetic modelling, mass transfer, pollutant removal, water purification.

I. INTRODUCTION

The release of toxic pollutants into water environments creates persistent risks for aquatic ecosystems and human populations. Industrial effluents, mining operations, agricultural runoff, household wastewater, and pharmaceutical discharges may contain heavy metals, synthetic dyes, pesticides, organic micropollutants, and inorganic ions. Because these substances differ in their molecular structures, charge, solubility, and chemical reactivity, no single treatment process performs equally well under all conditions. Adsorption has consequently attracted substantial attention as a flexible separation method that can be adapted to different pollutant classes. Its performance, however, depends on the interaction between the contaminant, the adsorbent surface, and the surrounding solution.

Hybrid materials combine two or more components to provide complementary adsorption properties. These may include porous carbon, mineral supports, metal oxides, polymers, silica, and other functional materials. Their pollutant-removal behaviour may involve electrostatic attraction, ion exchange, surface complexation, hydrogen bonding, hydrophobic interactions, pore filling, and, in some cases, precipitation or redox processes. The relative importance of these mechanisms depends on the material composition, solution pH, pollutant speciation, and operating conditions. Therefore, a high removal percentage does not, by itself, reveal how a hybrid material captures a pollutant or whether the observed removal can be attributed exclusively to adsorption.

Equilibrium and kinetic models provide complementary approaches for interpreting adsorption experiments. Isotherm models describe the relationship between the amount of pollutant adsorbed and its equilibrium concentration under specified conditions. They can help estimate adsorption capacity and characterize the shape of the equilibrium relationship. Kinetic models describe changes in pollutant uptake over time and are used to investigate the rate of adsorption and possible mass-transfer limitations. However, model equations are mathematical representations rather than direct observations of molecular mechanisms. A good statistical fit does not automatically establish that the physical assumptions of a model are correct. Critical reviews of adsorption modelling have highlighted the importance of

understanding model assumptions, validation procedures, and the limitations of common fitting practices (Wang & Guo, 2020; Tran et al., 2017).

A comprehensive performance evaluation should therefore combine material characterization, controlled adsorption experiments, equilibrium and kinetic modelling, and assessment under realistic water-treatment conditions. It should also consider regeneration, material stability, competitive adsorption, and the possibility of secondary pollution. This paper examines the mechanisms and modelling approaches used to evaluate hybrid adsorbents, explains how isotherm and kinetic results should be interpreted, and discusses their relevance to environmental applications. The central argument is that reliable assessment requires consistency between experimental design, model assumptions, statistical validation, and the practical requirements of water treatment.

II. ADSORPTION MECHANISMS AND EQUILIBRIUM ISOTHERM MODELLING

The adsorption of pollutants by hybrid materials can involve several mechanisms operating simultaneously. Electrostatic attraction occurs when surface charges and pollutant charges favour association, while electrostatic repulsion may reduce uptake under other conditions. The charge of a hybrid surface depends on its chemical composition and solution pH, whereas the charge and speciation of the pollutant may also change with pH. Ion exchange occurs when contaminant ions replace ions associated with the adsorbent, while surface complexation involves interactions between pollutant species and functional groups or reactive sites. These mechanisms are particularly relevant to the interpretation of inorganic pollutant removal, although their relative contributions must be established using appropriate experimental evidence.

Organic pollutants may interact with hybrid surfaces through hydrogen bonding, hydrophobic interactions, aromatic interactions, and pore filling. Carbon-rich materials can provide porous structures and aromatic surfaces, while polymeric or mineral components may introduce additional functional groups. The molecular size of the pollutant relative to the pore structure can influence whether internal adsorption sites are accessible. Surface functionalization can increase affinity for particular contaminants, but excessive modification may obstruct pores or reduce the accessibility of existing sites. A material's adsorption mechanism should

therefore be interpreted in relation to its chemical composition, pore structure, and the properties of the target compound rather than inferred from a single characterization result.

Adsorption equilibrium is commonly described using isotherm models, which relate the equilibrium concentration of a pollutant in solution to the amount retained by the adsorbent at a specified temperature. The Langmuir model is frequently used to represent adsorption on a surface with a finite number of equivalent sites and an assumed monolayer capacity. Its usefulness lies in providing an estimate of maximum adsorption capacity under the assumptions of the model. However, many hybrid surfaces are chemically and structurally heterogeneous, and adsorption may involve multiple types of sites. Consequently, a Langmuir fit should not be taken as conclusive proof that adsorption occurs exclusively as a uniform monolayer.

The Freundlich model is an empirical relationship often used to represent adsorption on heterogeneous surfaces. It allows adsorption intensity to vary across the concentration range, making it useful for describing systems that do not conform closely to the Langmuir assumptions. Nevertheless, the Freundlich model does not provide a finite saturation capacity in its conventional form and may be unsuitable for extrapolation beyond the measured concentration range. Other models, including Temkin, Sips, Redlich–Peterson, and Dubinin–Radushkevich, may provide alternative descriptions of equilibrium behaviour. Their usefulness depends on the characteristics of the dataset and whether the added parameters improve meaningful interpretation rather than simply producing a better numerical fit.

Model selection should involve more than comparing correlation coefficients. Researchers should examine residual patterns, parameter uncertainty, the plausibility of estimated values, and the agreement between predicted and observed adsorption capacities. Nonlinear regression is often preferable to linearized transformations because transforming equations can alter the error structure and disproportionately weight certain parts of the dataset. The equilibrium experiments should span a sufficiently broad concentration range and use replicated measurements where feasible. Temperature, pH, adsorbent dosage, ionic strength, and equilibrium criteria should be reported clearly because isotherm parameters are conditional on the experimental system rather than universal constants for a material.

Equilibrium modelling becomes especially challenging when the adsorbent encounters mixtures of pollutants. Competing ions or organic compounds may occupy the same sites,

modify surface chemistry, or influence the activity of the target contaminant. An isotherm derived from a single-solute solution may therefore overestimate the performance achievable in a complex effluent. Competitive adsorption studies and tests using actual water samples are important for determining whether the observed equilibrium relationship remains useful outside controlled laboratory conditions. Isotherm models are most valuable when treated as tools for organizing experimental evidence, comparing materials under consistent conditions, and informing process design—not as substitutes for mechanistic proof or real-water validation.

III. KINETIC ANALYSIS, MASS TRANSFER, AND MODEL VALIDATION

Adsorption kinetics describe the rate at which pollutants move from the liquid phase to the adsorbent and become retained. In a typical experiment, rapid initial uptake may occur when many adsorption sites are available and the concentration gradient between the solution and surface is high. The rate may subsequently decrease as sites become occupied, the concentration gradient diminishes, or transport into internal pores becomes increasingly important. This pattern is common but not universal; the shape of the uptake curve depends on the adsorbent structure, pollutant properties, mixing conditions, and experimental design. Kinetic measurements are essential for estimating contact time and assessing whether a material could be practical in a treatment process.

The pseudo-first-order model and pseudo-second-order model are widely applied to adsorption datasets. These models relate uptake over time to the difference between the adsorption capacity at equilibrium and the capacity at a given time. The pseudo-first-order equation is often useful for describing systems in which the rate follows a first-order relationship with the remaining uptake capacity. The pseudo-second-order model has been widely used across many adsorption studies, but its frequent use does not establish that it is universally superior or that chemisorption is necessarily the controlling mechanism. Critical analyses have identified potential biases associated with model fitting and validation practices, emphasizing the need to evaluate competing models rather than selecting a model solely because it is commonly reported (Wang & Guo, 2020).

Diffusion-based models provide additional insight into transport limitations. The intraparticle-diffusion model examines whether uptake follows a relationship with the square root of time, which may indicate the influence of transport within pores. A linear segment in

an intraparticle-diffusion plot does not necessarily mean that intraparticle diffusion is the only rate-controlling step. If the fitted line does not pass through the origin, additional processes may be involved. External film diffusion, pore diffusion, surface interactions, and changes in concentration gradients can operate sequentially or simultaneously. Accordingly, kinetic interpretation should consider the full uptake curve, experimental mixing conditions, particle dimensions, and the suitability of the assumed transport model.

Model fitting procedures can strongly affect the conclusions drawn from kinetic data. Linearization changes the statistical structure of the observations and may lead to different parameter estimates from those obtained by fitting the original nonlinear equation. Researchers should therefore consider nonlinear regression, examine residuals, and report uncertainty in fitted parameters. A high coefficient of determination is not sufficient evidence that a model is physically appropriate. It is also important to distinguish equilibrium capacity measured experimentally from capacity estimated by the fitted model. Inconsistent equilibrium definitions, insufficient sampling during the rapid initial stage, and a limited number of time points can weaken model reliability.

Experimental conditions must be designed to reveal the adsorption rate rather than confound it with unrelated processes. Mixing intensity can influence external mass transfer, while particle size can affect diffusion distances. Adsorbent dosage and initial concentration influence the number of available sites relative to the quantity of pollutant. Temperature and solution composition may change both diffusion and equilibrium behaviour. Measurements should cover the initial uptake period and extend sufficiently close to equilibrium to establish the final capacity. Replicate experiments, appropriate blanks, and consistent sampling procedures improve the reliability of the resulting kinetic dataset.

A robust kinetic evaluation compares alternative models and considers whether their assumptions are compatible with the material and experimental system. Kinetic constants should not be compared uncritically across studies conducted at different temperatures, pH values, concentrations, or adsorbent dosages. Where possible, batch kinetic analysis should be supplemented with continuous-flow column experiments. Column studies provide information about breakthrough, dynamic capacity, and the effects of residence time and flow rate. Such measurements are especially important because a material with rapid uptake in a well-mixed laboratory vessel may still experience practical limitations when incorporated into a packed bed or filtration unit.

IV. ENVIRONMENTAL APPLICATIONS AND INTEGRATED PERFORMANCE EVALUATION

Hybrid adsorbents have potential applications in treating water contaminated by toxic metals, dyes, pharmaceutical compounds, pesticides, and selected inorganic pollutants. The most suitable hybrid depends on the target contaminant and the chemistry of the water. Metal-containing or mineral-based surfaces may offer binding sites for particular inorganic species, while carbon-rich structures may be useful for some organic compounds. Polymer-supported adsorbents can facilitate recovery and handling, and selected magnetic hybrids may enable separation through magnetic collection. Nevertheless, the success of each approach must be established for the relevant contaminant and operating conditions. Reviews of adsorption applications emphasize the diversity of available materials and the need to relate adsorbent characteristics to the pollutant being treated (Somashekara et al., 2023).

The evaluation of toxic-metal removal requires particular care because dissolved metal concentrations can decrease through precipitation, complexation, or other processes in addition to adsorption. Experimental controls should establish whether the observed removal is attributable to the adsorbent. Changes in pH may affect both the surface chemistry and the chemical form of the metal. For dyes and pharmaceutical residues, solution absorbance or other analytical signals may be affected by pH, degradation, or matrix interference. Reliable studies should therefore use suitable analytical methods, calibration procedures, and controls to distinguish actual contaminant removal from measurement artefacts or non-adsorptive processes.

Performance metrics should include adsorption capacity, removal efficiency, equilibrium time, material recovery, and stability over repeated cycles. Removal efficiency describes the proportion of pollutant removed from solution, whereas adsorption capacity expresses the amount retained per unit mass of adsorbent. These measures answer different questions and should not be used interchangeably. A high percentage removal can result from using a large adsorbent dosage even when the mass-specific capacity is modest. Conversely, a material with a high estimated capacity may not achieve the required residual concentration under the conditions of a practical treatment system. Both metrics should be reported alongside initial concentration, final concentration, solution volume, adsorbent mass, and experimental uncertainty.

Regeneration and reuse influence the overall environmental and economic performance of a hybrid adsorbent. Desorption procedures may restore binding sites, but they can also alter surface chemistry, damage the support, or cause the loss of active components. A meaningful reuse assessment should include several adsorption–desorption cycles, changes in capacity, material mass loss, and the quality of the regenerated adsorbent. The concentrated desorption solution must also be managed safely. Where pollutants are recoverable, regeneration may create an opportunity for resource recovery; where they are hazardous or difficult to recover, controlled treatment or disposal may be necessary. Initial adsorption capacity alone is therefore an incomplete measure of material sustainability.

Real-water testing is essential because natural and industrial waters contain competing ions, dissolved organic matter, suspended solids, and variable pH. These components may occupy adsorption sites, block pores, or alter surface interactions. The results of single-solute laboratory tests should be treated as an initial screening stage rather than definitive evidence of field performance. Subsequent evaluation should use multicomponent solutions and representative water samples, followed by continuous-flow experiments where appropriate. For treatment-system design, the influence of flow rate, bed depth, residence time, and breakthrough behaviour must be understood in addition to equilibrium capacity.

Future performance evaluation should integrate material characterization, isotherm analysis, kinetic modelling, toxicity assessment, regeneration studies, and economic considerations. Researchers should report experimental procedures and modelling choices transparently, including nonlinear fitting methods, uncertainty, and the criteria used to select the best model. Standardized reporting would make it easier to compare materials and identify which differences arise from material properties rather than experimental conditions. Life-cycle and techno-economic assessments can further establish whether the benefits of a hybrid material justify its production and operating requirements. The strongest candidates will be those that demonstrate consistent contaminant removal, manageable regeneration, minimal secondary pollution, and practical performance in realistic treatment systems.

V. CONCLUSION

The evaluation of hybrid adsorbents requires an integrated understanding of adsorption mechanisms, equilibrium relationships, kinetic behaviour, and practical operating conditions. Hybrid materials may combine complementary surface groups, porous structures, and

reactive components, enabling their application to a range of water pollutants. However, their performance cannot be understood solely through removal percentages or a single characterization technique. Electrostatic interactions, ion exchange, surface complexation, hydrogen bonding, hydrophobic interactions, and pore filling may contribute differently depending on the adsorbent and pollutant. Mechanistic conclusions should therefore be supported by multiple forms of experimental evidence and appropriate controls.

Isotherm models provide a useful means of describing equilibrium adsorption and estimating material performance within a measured concentration range. Langmuir, Freundlich, Temkin, and more flexible models each have assumptions and limitations. Similarly, pseudo-first-order, pseudo-second-order, and diffusion-based kinetic models help describe uptake over time but do not independently prove the underlying molecular mechanism. Reliable model selection requires examination of residuals, parameter uncertainty, experimental coverage, and consistency between model assumptions and observed behaviour. A statistically acceptable fit should not be confused with direct mechanistic evidence.

Environmental applications introduce additional complexity because real water contains competing substances and may vary in pH, ionic strength, and contaminant composition. A material that performs well in a single-solute batch experiment may exhibit lower capacity or different kinetics under practical conditions. Performance evaluation should therefore progress through controlled experiments, multicomponent testing, real-water assessment, and continuous-flow studies. Regeneration, stability, leaching, recovery of spent adsorbents, and secondary-waste management should be considered alongside adsorption capacity and contact time.

Further research should emphasize reproducible experiments, transparent model validation, realistic operating conditions, and integrated assessments of safety and cost. Combining equilibrium and kinetic modelling with material characterization and process-scale testing can improve the reliability of adsorbent selection and treatment design. Hybrid materials are promising candidates for environmental remediation, but their practical value depends on demonstrating durable performance, safe operation, and economic feasibility. A rigorous evaluation framework is therefore essential for translating laboratory adsorption results into effective and sustainable water-treatment technologies.

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