



SCHOLARLY PUBLICATIONS

School of Chemical Engineering

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Journal Name: Coordination Chemistry Reviews

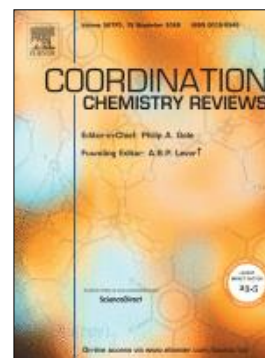
IF: 25.6

Title: Function-oriented engineering of framework materials for advanced sonocatalytic energy and environmental applications

Author: Kumar R.; Choi K.-W.; Abdullah; Biswas G.; Sathish S.; Acharyya S.S.; Chakraborty S.; Tripathy S.K.; Prabhu S.M.; Jeon B.-H.

Details: Volume-567, November 2026

Abstract: Sonocatalysis is a rapidly emerging advanced method that uses acoustic cavitation to produce localized extreme conditions and reactive radical species that accelerate chemical reactions. Sonocatalysis offers numerous benefits over conventional catalysis and advanced oxidation processes, which include enhanced mass transfer, flexible reactor design, and operation in dark or murky environments. This review delineates a systematic framework correlating to cavitation mechanisms, charge transfer pathways, ultrasonic operational parameters, and structure–property relationships in catalysts. The sonocatalysts are classified as carbon-derived supports, graphitic carbon nitride, biomaterials, and carbon-free materials, including semiconductor-based materials, metal and metal-oxide systems, and heterostructured multifunctional composites. A comparative analysis highlights the distinct contributions of each category to radical generation, defect modulation, energy harvesting, recyclability, and scalability. Recent advances in piezoelectric polarization, plasmon-coupled activation, heterojunction engineering, and sonophotocatalytic hybrid architectures substantially expanded sonocatalysis toward pollutant degradation, H₂ production, CO₂ conversion, biomass valorization, disinfection, and biomedical applications. However, significant scientific challenges remain in the sonocatalysis system, related to the mechanistic understanding, energy efficiency, catalyst durability, reactor scalability, and industrial applicability. Operando spectroscopy, computational modeling (including density functional theory and machine learning-based approaches), microfluidic sonoreactor engineering, and techno-economic assessment are essential for advancing sonocatalysis from laboratory-scale studies to practical implementations. This review provides a comprehensive overview of the rapidly evolving materials, mechanistic pathways, applications, and scale-up challenges of sonocatalysis.



URL: <https://www.sciencedirect.com/science/article/abs/pii/S0010854526007721?via%3Dihub>





SCHOLARLY PUBLICATIONS

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Journal Name: Journal of Colloid and Interface Science

IF: 9.6

Title: Field-induced tubular assembly of ionic microgels: Evidence for shape anisotropy from small-angle neutron scattering studies

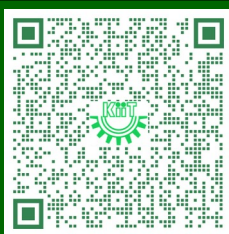
Author: Brijitta J.; Radulescu A.; Pal A.; Gulotta A.; Mohanty P.S.; Schurtenberger P.

Details: Volume-724, 15th December, 2026

Abstract: We report the AC electric field-induced directed assembly of 10 mol% crosslinked ionic microgels at various effective volume fractions, investigated using confocal microscopy and small-angle neutron scattering. At low effective volume fractions, in an electric field, the microgels form strings, tubes, and islands of body-centered-tetragonal structures. While tubular structures have previously been reported for intrinsically anisotropic particles such as ellipsoids or bowl-shaped colloids, analogous assemblies have not been observed for initially isotropic hard or soft particles. Small-angle neutron scattering experiments under the so-called zero-average contrast conditions were carried out to obtain the single-particle size and structure as the microgels align along the direction of the field. The $P(r)$ analysis of the small-angle neutron scattering data reveals a clear signature of elongated ellipsoidal particles. A fuzzy-ellipsoid model was thus employed to fit the data, yielding aspect ratios ranging from 1.93 to 2.46 depending on the field strength and effective volume fraction. We therefore propose that the tubular assemblies observed at low effective volume fractions arise from field-induced shape anisotropy of the microgels. Our results demonstrate how external electric fields can dynamically induce particle anisotropy in initially spherical soft colloids, thereby enabling the formation of new self-assembled structures that are typically associated with anisotropic building blocks. We discuss the experimental phase diagram and compare our observations to the theoretical phase diagram for soft dipolar spheres.



URL: <https://www.sciencedirect.com/science/article/pii/S0021979726012877>





SCHOLARLY PUBLICATIONS

School of Chemical Engineering

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Journal Name: Journal of Environmental Chemical Engineering

IF: 7.5

Title: Can reactor design-hydrodynamics interplay intensify the photocatalytic bacterial inactivation? A CFD study

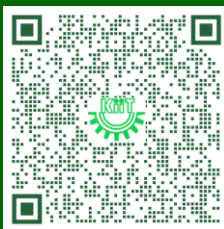
Author: Mahapatra G.C.; Mishra P.; Chakraborty S.; Banerjee S.; Mishra A.; Chowdhury S.; Kumar R.; Jeon B.-H.; Lundborg C.S.; Tripathy S.K.

Details: Volume-14, Issue-5, October 2026

Abstract: Implementation of scalable photocatalytic inactivation systems still remain limited due to the absence of information regarding the impact of reactor design on bacterial inactivation. To elucidate the fundamental understanding of hydrodynamics, photocatalyst dispersion, and efficiency in batch and continuous flow reactors, this work combines computational fluid dynamics (CFD) and photocatalytic inactivation of *Escherichia coli* (*E. coli*), using Fe-doped ZnO nanoparticles (Fe/ZnO NPs) as visible-light-responsive photocatalysts in batch stirred tank reactor (BSTR) and continuous flow helical tube reactor (CFHTR). The key variables that influenced the process efficiency were identified by systematically running the reactions with varying catalyst and bacterial loading, flow rate, and pH. Total inactivation of *E. coli* was achieved within 60 min at a low catalyst loading (25 mg/L) in CFHTR, while the BSTR required 210 min at higher catalyst loading (1000 mg/L). The role of reactive oxygen species (ROS) in inactivation which induces membrane disruption was investigated by metabolic activity analysis and electron microscopy. To relate photocatalytic stress with the regulation of resistance genes in both of the reactor modes, parallel genomic profiling of *E. coli* genes was conducted. The CFD analysis suggested that the synergistic impact of velocity, turbulence kinetic energy and its gradient along with eddy viscosity varies with the change in the reactor design and hence, intensify the inactivation efficiency. Furthermore, a user-friendly, menu-driven simulation tool is developed to facilitate efficient optimization and performance evaluation of the proposed system. Findings of this study may help to design and upscale photocatalytic inactivation systems for water treatment.



URL: <https://www.sciencedirect.com/science/article/abs/pii/S2213343726030484?via%3Dihub>





SCHOLARLY PUBLICATIONS

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Journal Name: Hydrometallurgy

IF: 6.3

Title: Extraction and recovery of V (V) from citrate leachate of spent catalyst containing impurities (Mg and Fe) using tricapryl methyl ammonium chloride

Author: Mohapatra A.S.; Mohanty C.K.; Sanjay K.; Parhi P.K.

Details: Volume-244, October 2026

Abstract: A systematic investigation was carried out for the selective extraction and recovery of vanadium from a citric acid-mediated leach liquor of spent catalyst using a mixture of Aliquat 336 and 2-Octanol. Prior to extraction, iron was efficiently removed at pH_e 4.0 via slaked lime precipitation. Extraction equilibrium studies indicated that vanadium was predominantly extracted as the $[\text{VO}(\text{C}_6\text{H}_5\text{O}_7)]^{2-}$ anionic complex by Tricapryl methyl Ammonium Chloride (Aliquat 336). The association of 2 mol of aliquat 336 was confirmed from the slope analysis method with extraction of vanadium from citrate media as $\text{CH}_3\text{R}_3\text{N}_2\text{VOC}_6\text{H}_5\text{O}_7\text{]org}$. Vanadium extraction was quantitative under conditions of pH 6.0 ensuring no co-extraction of magnesium. Extraction isotherm examined using 0.6 M Aliquat 336 + 10% (v/v) 2-octanol at A: O = 8:1 in two stages leading to attaining 5 folds enrichment of vanadium during extraction. FTIR analysis confirmed the successful coordination of vanadium in the organic phase. Stripping of vanadium using NaOH at an aqueous-to-organic (A:O) ratio of 1:5 yielded a concentrated strip solution containing 47.2 g/L vanadium, representing almost eightfold enrichment compared to the initial leachate. Final precipitation and calcination of the strip solution produced high-purity V_2O_5 , confirmed by XRD analysis. This study demonstrates a clean, efficient, and environmentally benign method for the selective recovery of vanadium from spent catalyst leachates using ionic liquid-based solvent extraction.



URL: <https://www.sciencedirect.com/science/article/abs/pii/S0304386X26001702?via%3Dihub>





SCHOLARLY PUBLICATIONS

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Journal Name: Frontiers in Chemical Engineering

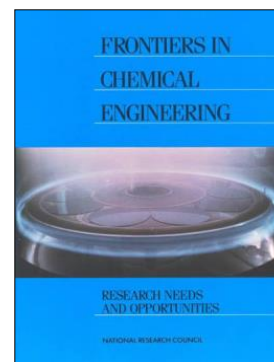
IF: 4.0

Title: Biofunctional hydrogel adsorbents for sustainable downstream dye purification and circular wastewater management

Author: Patra S.; Panda A.; Chakraborty P.; Basu A.; Sengupta A.; Khan G.A.; Nayak J.; Chakraborty S.; Banerjee S.; Tripathy S.K.

Details: Volume-8, July 2026

Abstract: Introduction – Although the use of clay–alginate composites and activated clays as adsorbents has been thoroughly examined for the removal of dyes, very few studies have addressed the effect of reactor hydrodynamics on the efficiency of the process. In this research, efforts were made to fill the knowledge gaps by adopting an approach combining batch adsorption tests, fixed-bed column studies, breakthrough modeling, and computational fluid dynamics (CFD) simulation in order to create connections between flow characteristics and mass transfer and adsorption kinetics involved in the removal of malachite green (MG) dye using mesoporous AC@SA hydrogel beads. Methods – Mesoporous hydrogel beads possessed pore sizes in the range of 3–10 nm and exhibited a negative zeta potential of –8 mV (mean). Batch adsorption tests, fixedbed column studies, breakthrough modeling, and CFD simulations were conducted to evaluate adsorption performance and investigate the influence of reactor hydrodynamics on the adsorption process. Results – Maximum MG dye removal efficiency was observed to be around 90% in batch adsorption tests at 50 g L⁻¹ adsorbent dose, pH 7, and 150 rpm after about 120–150 min contact time. Column experiments showed an increase in bed height from 6 to 14 cm increased the breakthrough time from about 18 to 32 min, while increasing the influent dye concentration and flow rate reduced breakthrough times. The Thomas model showed excellent agreement with experimental data ($R^2 \approx 0.99$), with adsorption capacities reaching 21.28 mg g⁻¹ and rate constants ranging from 0.22 to 0.33 ml mg⁻¹ min⁻¹. Further simulations by CFD revealed that a flow rate of 10 ml min⁻¹ would ensure uniformity of velocity, lower turbulence, controlled eddy viscosity, and stable hydrodynamic conditions, hence maximized adsorption.



URL: <https://www.frontiersin.org/journals/chemical-engineering/articles/10.3389/fceng.2026.1895352/full>





SCHOLARLY PUBLICATIONS

School of Chemical Engineering

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Journal Name: Environmental Engineering Research

IF: 3.6

Title: Coupling adsorption (batch plus column) experiments, CFD modeling, and molecular docking for efficient dye remediation using Zinc-activated Phosphogypsum beads

Author: Panda, A; Mishra, S; Jena, S; Patel, JK; Banerjee, S; Borah, D; Kumar, R; Khan, MA; Jeon, BH; Chakraborty, S; Tripathy, SK

Details: Volume-31, Issue-4, August 2026

Abstract: This study proposes a sustainable method for malachite green (MG) removal using zinc-treated phosphogypsum (PG) beads. Phosphogypsum, a phosphate-fertilizer by-product, was activated with ZnCl_2 and thermally treated to enhance porosity, surface acidity, and available binding sites. Characterization through XRD, FTIR, BET, and zeta potential confirmed the structural and surface modifications enabling superior adsorption performance. Batch and column studies revealed that pH, adsorbent dosage, flow rate, and bed height strongly influenced MG removal, achieving over 90% efficiency at 7 cm bed height and 10 mL/min flow rate. Kinetics followed a pseudo-second-order model, with the Temkin isotherm indicating chemisorption. Thomas and Yoon–Nelson models fit well ($R^2 = 0.98$), while Clark showed the best breakthrough prediction ($R^2=0.99$). Adams–Bohart provided only moderate agreement. CFD simulations confirmed that the 7 cm bed height generated the most uniform flow, longest residence time, and minimal channeling, enabling efficient MG transport to active sites. Stable turbulence and porosity profiles enhanced external mass transfer, supporting the high experimental removal efficiency (>90%). Molecular docking showed strong electrostatic attraction between MG cations and negatively charged Si-O^- , Al-O^- , and S-O^- groups on ZnCl_2 -treated PG beads.



URL: <https://www.eeer.org/journal/view.php?doi=10.4491/eeer.2025.722>

