



Reticular framework architectures for coagulation-flocculation and colloidal separation: Mechanistic insights, structure-performance correlation, and AI-guided discovery

Asma Sohail^a, Badrul Mohamed Jan^{a,b,**}, Nazeri Abdul Rahman^c, Mahar Diana Hamid^a, Rabia Ikram^{d,e,*}

^a Department of Chemical Engineering, Faculty of Engineering, Universiti Malaya, 50603 Kuala Lumpur, Malaysia

^b Center for Energy Sciences (CES), Faculty of Engineering, Universiti Malaya, Malaysia

^c Department of Chemical Engineering, Faculty of Engineering, Universiti Malaysia Sarawak, Malaysia

^d Department of Mechanical Engineering, Faculty of Engineering, Universiti Malaya, 50603 Kuala Lumpur, Malaysia

^e Department of Chemistry, Faculty of Science, Universiti Putra Malaysia (UPM), Serdang 43400, Selangor, Malaysia

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ABSTRACT

The controlled destabilization of colloidal systems remains a central challenge in water purification and related separation processes. Although reticular framework architectures (RFAs), including covalent organic frameworks (COFs) and metal-organic frameworks (MOFs), have been extensively explored for adsorption-driven separations, their role in active coagulation-flocculation remains comparatively underdeveloped. This review critically evaluates RFAs as emerging coordination-based coagulants and flocculants, emphasizing their limited but rapidly growing application space and identifying key mechanistic and design constraints. A unified mechanistic framework is developed by integrating colloidal science with RFAs chemistry, describing pollutant removal through charge regulation, adsorption bridging, and pore-mediated aggregation within the Derjaguin-Landau-Verwey-Overbeek (DLVO) theoretical framework. Unlike conventional coagulants, which primarily rely on nonspecific charge neutralization, RFAs enable structurally programmable and coordination-driven interactions that enhance selective aggregation and floc formation. The structure-performance relationships governing coagulation performance are critically analyzed with respect to framework topology, surface chemistry, porosity, and interfacial electrostatics. In addition, emerging data-driven approaches, including artificial intelligence (AI), are highlighted as powerful tools for accelerating the design and optimization of next-generation reticular coagulants across large chemical spaces. Overall, this review establishes a mechanistic and design-oriented foundation for RFAs in coagulation-flocculation systems and identifies key challenges related to stability, mechanistic ambiguity, and scalability that must be addressed for practical deployment in advanced separation technologies.

1. Introduction

Managing colloidal stability is fundamental to three closely linked areas of research: the treatment of aquatic environments, the control of colloidal aggregation processes in biological systems (as a mechanistic

analogy), and the engineering of advanced separation materials [1]. In all these systems, the central objective is the controlled and rapid transition of dispersed matter into stable, retrievable aggregates. To address the growing complexity of these aggregation systems, nanostructured materials have emerged as attractive candidates because

Abbreviations: MOFs, Metal-organic frameworks; COFs, Covalent organic frameworks; POPs, Porous organic polymers; AI, Artificial intelligence; MIL, Materials of Institute of Lavoisier; UiO-66, Universitetet i Oslo-66; DLVO, Derjaguin-Landau-Verwey-Overbeek; D_f, Fractal dimensions; ZIFs, Zeolitic imidazolate framework; ZIF-8, Zeolitic Imidazolate Framework-8; GO, Graphene oxide; θ, Surface coverage; PBO, *p*-phenylene benzobisoxazole; PVA, Polyvinyl alcohol; PIC, Polyferric iron-based coagulants; RFAs, Reticular framework architectures; QDs, Quantum dots; EDL, Electrical double layer; SEM, Scanning electron microscopy; TEM, Transmission electron microscopy; CuTCPP, Cu(II)tetrakis(4-carboxyphenyl)porphyrin; GPP, Gelatin methacrylate/poly(ethylene glycol) diacrylate/polyacrylamide.

* Corresponding author at: Department of Mechanical Engineering, Faculty of Engineering, Universiti Malaya, 50603 Kuala Lumpur, Malaysia.

** Corresponding author at: Department of Chemical Engineering, Faculty of Engineering, Universiti Malaya, 50603 Kuala Lumpur, Malaysia.

E-mail addresses: badrules@um.edu.my (B.M. Jan), raab@um.edu.my (R. Ikram).

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