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Molecular Dynamics Simulation Studies for Fouling of polyvinylidine (PVDF) Membrane

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Membrane fouling is an undesirable formation of deposits on membrane surfaces and it is considered a major problem in most brackish, seawater, and waste water reclamation applications. In order to understand membrane-fouling phenomenon, molecular dynamics simulation was carried out. We carried out adsorption of bovine serum albumin (BSA) on poly(vinylidene fluoride) (PVDF) surfaces in an aqueous environment. MD simulation was carried out in the presence and absence of excess ions in order to understand effect of ions on adsorption process. The adsorption process involved diffusion of protein to the surface and dehydration of surface–protein interactions, followed by adsorption and denaturation. Although adsorption of BSA on PVDF surface was observed in the absence of excess ions, denaturation of BSA was not observed during the simulation (1 μs). Basic and acidic amino acids of BSA were found to be directly interacting with PVDF surface. Simulation in a 0.1 M NaCl solution showed delayed adsorption of BSA on PVDF surfaces in the presence of excess ions, with BSA not observed in close proximity to PVDF surface within 700 ns. Adsorption of Cl^- on PVDF surface increased its negative charge, which repelled negatively charged BSA, thereby delaying the adsorption process. Results are consistent with experimental finding that states that fouling was reduced in presence of ions. These results will be helpful for understanding membrane fouling phenomena in polymeric membranes and fundamental advancements in these areas will lead to a new generation of membrane materials with improved antifouling properties and reduced energy demands.

Biography:

Abdul Rajjak received his PhD from Tohoku University Japan. After PhD, he joined Kyoto University, Japan and National University of Singapore as a postdoctoral fellow. At King Abdullah University of Science and Technology, he did his research on enzyme-catalyzed reactions using computational chemistry. Later in 2013, Abdul Rajjak joined Kobe University Japan as a Research Assistant Professor. He worked there on computational studies on polymeric membrane for water treatment. Since September 2017, he is working with King Fahad University of Petroleum and Minerals as a Assistant professor. His area of research interest is computational studies, polymeric membranes, catalysis, drug designing.