Implementation of a multilayer statistical physics model to interpret the adsorption of food dyes on a chitosan film

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Abstract

This paper reports the application of an advanced multilayer model to study the adsorption of food dyes FD&C blue No. 2, acid red 18, FD&C red No. 2, and FD&C yellow 5 from aqueous solutions with a chitosan film. These dyes' adsorption mechanisms were discussed and analyzed at 298–328 K and pH 4–7 via statistical physics calculations. Physicochemical parameters were utilized to explain the dye adsorption at the molecular scale. Modeling results showed dye aggregation phenomena where each functional group of chitosan film adsorbed several dye molecules simultaneously at different tested temperatures. Aqueous solution temperature reduced the dye adsorption capacities, attributed to the exothermic nature of dye removal. The chitosan film was more effective for the adsorption of dye FD&C yellow 5. The estimated adsorption energies for dye-chitosan film and dye-dye interactions confirmed an exothermic physisorption associated with van der Waals forces and hydrogen bonding. This study's results contributed to expanding the knowledge on the adsorption mechanisms of dye molecules using biopolymers like chitosan.

Keywords

Adsorption, Food dyes, Chitosan film, Multilayer model

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