

Investigating the effect of constant heat flux on the adsorption of doxorubicin by bio-MOF-11 biocarrier using molecular dynamics simulation

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Abstract

This study aimed to investigate the effect of constant heat flux on the adsorption of doxorubicin by bio-MOF-11 biocarrier using molecular dynamics simulation. The research explores the behavior of drug molecule and carrier under different thermal conditions to understand the underlying mechanisms of adsorption. The modeled samples were made of bio-MOF-11 structure, trisodium phosphate buffer (as a drug), and aqueous environment in the presence of NaCl. Technically, the atomic interaction among various atoms inside a computational box was described using a Universal Force Field. The findings of this study could contribute to the development of more effective drug delivery systems and advance the understanding of the adsorption process in carriers. The present outputs predicted the external heat flux was an important parameter in the atomic evolution of the drug-MOF system. The 0.3 W/m^2 value of heat flux was optimum for drug diffusion into the MOF sample. Numerically, the number of diffused drug particles and diffusion coefficient converged to 335 and $73.19 \text{ nm}^2/\text{ns}$ (respectively) in the optimum value of heat flux. So, it was concluded that heat flux implementation to the drug-MOF system and changing this external parameter manipulated the drug adsorption (drug delivery) procedure in the designed system for various clinical applications.