عنوان مقاله:

Co-Solvent Effects on Self-Diffusion Coefficient of Drugs in Supercritical Carbon Dioxide: a Molecular Dynamics Viewpoint

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خلاصه مقاله:

The diffusion coefficient of the propranolol, phenazopyridine and methimazol in triplesystems including drugs, carbon dioxide and co-solvent was calculated by moleculardynamics simulation. Methanol, Ethanol and Propanol were used as co-solvents.Density of designed systems was calculated at 65 ° C and pressures 122, 152, 182,213, and 243 bar. There is a good agreement between the calculated density valuesand the experimental values of density. The results show that with increasing pressure,the error in the density values is reduced. Thus, the molecular dynamics simulationwas carried out under supercritical (65 ° C, 243 bar) and subcritical (25 ° C, 1 bar)conditions. Calculating the diffusion coefficients of various system componentsindicates that the supercritical carbon dioxide diffusion coefficient is larger than thediffusion coefficient under subcritical conditions. The results also show that propanolhas a greater effect on the diffusion coefficient of drugs, especially phenazopyridine.The diffusion coefficient of alcohols in the supercritical conditions is greater than theirdiffusion coefficient in subcritical conditions.

کلمات کلیدی:
Alcohol; Transport Phenomena; Diffusion Coefficient

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