World Academy of Science, Engineering and Technology
International Journal of Mechanical and Industrial Engineering
Vol:11, No:07, 2017

Heat Capacity of a Soluble in Water Protein: Equilibrium Molecular Dynamics Simulation

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Abstract : Heat transfer is of great importance to biological systems in order to function properly. In the present study, specific heat capacity as one of the most important heat transfer properties is calculated for a soluble in water Lysozyme protein. Using equilibrium molecular dynamics (MD) simulation, specific heat capacities of pure water, dry lysozyme, and lysozyme-water solution are calculated at 300K for different weight fractions. It is found that MD results are in good agreement with ideal binary mixing rule at small weight fractions. Results of all simulations have been validated with experimental data.

Keywords : specific heat capacity, molecular dynamics simulation, lysozyme protein, equilibrium
Conference Title : ICHTA 2017 : International Conference on Heat Transfer and Applications
Conference Location : Amsterdam, Netherlands
Conference Dates : July 10-11, 2017