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A GREEN STRATEGY TOWARDS THE MISCIBILITY STUDIES OF STYROFOAM IN ORGANIC AND INORGANIC SOLVENTS BY USING MATERIALS MODELLING AND SIMULATION METHOD

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ABSTRACT

For chemical industries environmental consideration is an issue. It is required to control the operational inputs to reduce and minimize emissions including air pollutant and global warming gasses such as CO2 and Per-fluorinated chemicals/gasses (PFC's). Therefore we need to look for the solutions that aid to limit the waste (solid and liquid chemicals), and to reduce them by recycling methods. This paper focuses on the topic that introduces the miscibility studies of Styrofoam cup (polystyrene foam) in water (inorganic solvent) and in acetone (organic solvent) by using Materials Studio Software. The structures of Styrofoam cup, water and acetone were constructed prior to the calculation of miscibility. Optimization was carried out on the models and the energy of the built structures was reduced to the minimum levels in which the most stable state of the materials was achieved. Two miscibility tests, blending energy and mixing energy, were done on the optimized structures. In blending test, acetone was proven as a better solvent to dissolve the Styrofoam cup as compared to water. The temperature range of 0–56^{o} C was used in the mixing energy analysis. Results showed that the miscibility of the Styrofoam cup-acetone system was higher than the Styrofoam-water system at all temperatures. Besides, both systems also showed improvement of miscibility at elevated temperature.

KEYWORDS: Miscibility Studies, Environmental Impact Sustainability, Materials Studio, Styrofoam Decomposition Method, Binding Energy, Mixing Energy