Understanding the third phase formation using molecular dynamics simulations

Since *n*-dodecane is employed as a diluent and tetraoctyldiglycolamide (TODGA) is proposed as a ligand for the solvent extraction of trivalent actinides, it is quite likely that the solvent phase (TODGA/*n*-DD) undergoes a number of changes in the structure of TODGA and *n*-dodecane upon radiolytic degradation. Therefore, it is necessary to understand the aggregation behaviour of different diglycolamides in various diluents. For this purpose, the diglycolamides ranging from tetrahexyldiglycolamide to tetradodecyldiglycolamide have been prepared and diluted in different *n*-paraffins such as *n*-octane to *n*-tetradecane and studied for the extraction of nitric acid in 0.2 M tetraalkyldiglycolamide in *n*-paraffin. The aggregation results obtained from DLS experiments were validated by molecular dynamics simulation studies. It was observed that the size of the clusters obtained from MD simulations was in good agreement with the experimental results. (Collaboration: Fuel Chemistry Division, IGCAR)

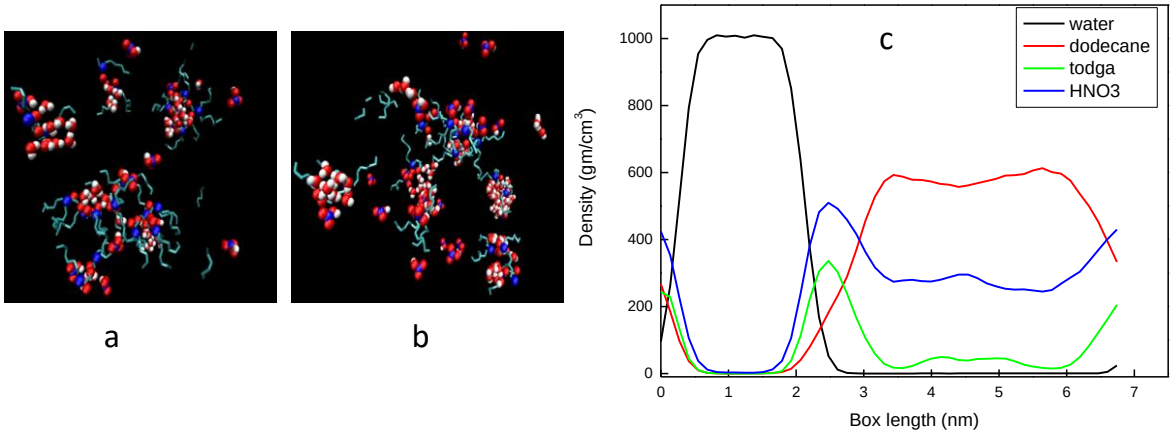

Figure: The snapshots of MD simulation of aggregates formed after equilibration with nitric acid (Aqueous phase: 3.5 M HNO_3). Organic phase: (a) 0.2 M TODGA/*n*-octane (b) 0.2 M TODGA/*n*-tetradecane. (c) Accumulation of TODGA and HNO_3 at the inter-phase leading to third phase formation.