

Thermal Energy Storage Based on Molten Salts Containing Nano-Particles: Dispersion Stability and Thermal Conductivity Using Multi-Scale Computational Modelling

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Abstract : New methods have recently been introduced to improve the thermal property values of molten nitrate salts (a binary mixture of NaNO₃:KNO₃ in 60:40 wt. %), by doping them with minute concentration of nanoparticles in the range of 0.5 to 1.5 wt. % to form the so-called: Nano-heat-transfer-fluid, apt for thermal energy transfer and storage applications. The present study aims to assess the stability of these nanofluids using the advanced computational modelling technique, Lagrangian particle tracking. A multi-phase solid-liquid model is used, where the motion of embedded nanoparticles in the suspended fluid is treated by an Euler-Lagrange hybrid scheme with fixed time stepping. This technique enables measurements of various multi-scale forces whose characteristic (length and timescales) are quite different. Two systems are considered, both consisting of 50 nm Al₂O₃ ceramic nanoparticles suspended in fluids of different density ratios. This includes both water (5 to 95 °C) and molten nitrate salt (220 to 500 °C) at various volume fractions ranging between 1% to 5%. Dynamic properties of both phases are coupled to the ambient temperature of the fluid suspension. The three-dimensional computational region consists of a 1µm cube and particles are homogeneously distributed across the domain. Periodic boundary conditions are enforced. The particle equations of motion are integrated using the fourth order Runge-Kutta algorithm with a very small time-step, Δt, set at 10⁻¹¹ s. The implemented technique demonstrates the key dynamics of aggregated nanoparticles and this involves: Brownian motion, soft-sphere particle-particle collisions, and Derjaguin, Landau, Verwey, and Overbeek (DLVO) forces. These mechanisms are responsible for the predictive model of aggregation of nano-suspensions. An energy transport-based method of predicting the thermal conductivity of the nanofluids is also used to determine thermal properties of the suspension. The simulation results confirm the effectiveness of the technique. The values are in excellent agreement with the theoretical and experimental data obtained from similar studies. The predictions indicate the role of Brownian motion and DLVO force (represented by both the repulsive electric double layer and an attractive Van der Waals) and its influence in the level of nanoparticles agglomeration. As to the nano-aggregates formed that was found to play a key role in governing the thermal behavior of nanofluids at various particle concentration. The presentation will include a quantitative assessment of these forces and mechanisms, which would lead to conclusions about nanofluids, heat transfer performance and thermal characteristics and its potential application in solar thermal energy plants.

Keywords : thermal energy storage, molten salt, nano-fluids, multi-scale computational modelling

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