Simulation Study of the thermal physical properties of Molten Salt based Nanofluids

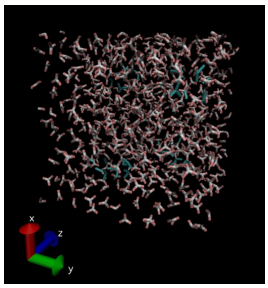

Figure: Simulation Screenshot

Challenges

To study the thermal physical properties of molten salt based nanofluids using molecular dynamics (MD) simulation.

Background

Molten salts are often used in solar energy storage and other applications and they are playing an increasingly more important role. For a heat storage material, the specific heat capacity is the most important property; it determines how much heat can be stored in a certain amount of substance. By doping a eutectic of salts with nanoparticles at less than 1% weight concentration, specific heat capacity enhancements of up to 57% have been reported. Some suggested that the interaction between nanoparticle and salt atoms at particle surface caused the enhancement and the larger surface-to-volume ratio and greater solid/liquid interface that nanoparticles provided strengthened the interaction. Others proposed a nanolayer theory in which they claimed that the formation of a special nanolayer in the adjacent liquid region around the nanoparticles had thermal properties different from either liquid or solid salt. MD simulation uses numerical methods to examine the dynamics of atomic-level phenomena that cannot be observed directly, which makes it a suitable tool to study the physical properties of nanofluids.

Results

In our simulations, with the introduction of nanoparticles, the specific heat capacity of molten salt based nanofluids was enhanced and the enhancement was concentration dependent which was in good agreement with experiments. The assumption of specific heat capacity based on equilibrium model of mixtures cannot explain this anomalous enhancement. Along with the nanostructures we observed using scanning electron microscope, a better understanding of the mechanism of the enhancement was gained. Other than by experiments, the thermal physical properties were studied from atomic-level. This will provide a new way of studying molten salt based nanofluids.

Molecular systems consist of a vast number of particles, which makes it very resource and time consuming. With the help of BEAR system, it's very fast for me to finish my simulations. The parallel computing capability makes it even more efficient. The best thing is that you are remotely doing your computations. As a result, after submitting your job on BEAR you can do whatever you are supposed to do on your own computer without being worried that anything you are doing is possible to interrupt the simulation.

Case study

Client Profile

Geng Qiao
Birmingham Centre for Energy Storage
School of Chemical Engineering_University of Birmingham
B15 2TT

Contact Details

Email : GXQ471@bham.ac.uk

Product Used

LAMMPS

Contributors

Professor Yulong Ding
Dr Alessio Alexiadis