

## Molecular Dynamics Studies of Homogeneous Condensation and Thermophysical Properties of HFC-1336mzz(Z)

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**Abstract :** The Organic Rankine Cycle (ORC) plays an important role in converting low-temperature heat sources into electrical power by using refrigerants as working fluids. The thermophysical properties of working fluids are essential for designing ORC. HFO-1336mzz(Z) (cis-1,1,1,4,4,4-hexafluoro-2-butene) considered as working fluid and have almost 99% low GWP and relatively same thermophysical properties used as a replacement of HFC-245fa (1,1,1,3,3-pentafluoro-propane). The environmental, safety, healthy and thermophysical properties of HFO-1336mzz(Z) are needed to use it in a practical system. In this paper, Molecular dynamics simulations were used to investigate the Homogeneous condensation, thermophysical and structural properties of HFO-1336mzz(Z) and HFC-245fa. The effect of various temperatures and pressures on thermophysical properties and condensation was extensively investigated. The liquid densities and isobaric heat capacities of this refrigerant was simulated at 273.15K to 353.15K temperatures and pressure 0.5-4.0MPa. The simulation outcomes were compared with experimental data to validate our simulation method. The mean square displacement for different temperatures was investigated for dynamical analysis. The variations in potential energies and condensation rate were simulated to get insight into the condensation process. The radial distribution function was simulated at the micro level for structural analysis and revealed that the phase transition of HFO-1336mzz(Z) did not affect the intramolecular structure.

**Keywords :** homogenous condensation, refrigerants, molecular dynamics simulations, organic rankine cycle

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