Journal of Molecular Liquids
Volume 373, 1 March 2023, 121232

The combustion process of methyl ester-biodiesel in the presence of different nanoparticles: A molecular dynamics approach

Ying Chen [a], As'ad Alizadeh [b], Azher M. Abed [c], Navid Nasajpour-Esfahani [d], Ghassan Fadhil Smaisim [e f], Salema K. Hadrawi [g h], Hussein Zekri [i j], Roozbeh Sabetvand [k], Davood Toghraie [l]

Show more

https://doi.org/10.1016/j.molliq.2023.121232

Abstract

Today, the problems, such as the environmental pollution caused by the consumption of fossil fuels, which have disrupted the ecological conditions and created environmental risks, as well as the limited reserves of fossil fuels, have caused countries worldwide to pay more attention to this type of energy. Biofuels are a type of fuel obtained from biomass sources. Biodiesel is one of the fuels produced from natural and renewable sources, which does not harm the environment. On the other hand, the presence of nanoparticles in alternative fuels is particularly important because adding nanoparticles reduces the ignition delay. This study investigated the effect of different nanoparticles, such as copper oxide (CuO) and aluminium oxide (Al_2O_3), on methyl ester-biodiesel (as base fluid) fuel's combustion performance. The following investigated the effects of different volume fractions of CuO nanoparticles. This research used the molecular dynamics (MD) simulation, and the LAMMPS software package. The results show that CuO nanoparticles had better thermal performance than Al_2O_3 nanoparticles. By adding Al_2O_3 and CuO nanoparticles to the base fluid, the heat flux of the simulated nanofluid converged to a numerical value of 2410.31 W/m^2 and 2410.31 W/m^2, respectively. Because CuO nanoparticles show better thermal performance than Al_2O_3 nanoparticles, the effect of the volume fractions of CuO nanoparticles on the thermal performance of the studied nanofluid was investigated. For this purpose, CuO nanoparticles with atomic ratios of 1%, 2%, 3%, 5% and 10% were added to the base fluid. The results reveal that the heat flux in atomic samples reached 4448.89 W/m^2 in the presence of 10% CuO nanoparticles. It is expected that by optimizing this process, the combustion performance of fuels will be improved, fuel consumption will be optimized, and the emission of pollutants will be reduced.