Journal of Molecular Liquids
Volume 391, Part A, 1 December 2023, 123265

Computational study of palladium percentage and oxygen ratio effects on air-methane catalytic combustion in a helical microchannel: A molecular dynamics approach

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https://doi.org/10.1016/j.molliq.2023.123265

Abstract

Combustion is an exothermic chemical process between an explosive substance and an oxidizing agent that is accompanied by heat generation and chemical change of raw materials. Catalysts are used in a combustion process for various reasons, including the speed at which the material reaches equilibrium. Catalysts are chemicals that increase the rate of reaction in chemical processes. The present research investigates the influence of palladium percentage and oxygen ratio on air-methane catalytic combustion in a helical microchannel. For this purpose, the atomic behavior and combustion performance of the simulated sample in the presence of excess oxygen and oxygen deficiency is reported by the molecular dynamics (MD) method. The potential functions used in this paper were Lennard-Jones, the embedded atom model (EAM), and Coulomb. It is concluded that increasing palladium percentage in limited ratios improves the atomic and combustion performance of the simulated structure, and this enhancement is greater in the presence of excess oxygen. In the presence of excess oxygen, the numerical value of maximum density, velocity and temperature converged from 0.138 atom/Å^3, 0.33Å/ps and 523K to 0.144 atom/Å^3, 0.36Å/ps and 539K, respectively with increasing palladium percentage from 1% to 4%. And by increasing the palladium ratio to 10%, these numerical values decrease to 0.137 atom/Å^3, 0.31Å/ps and 530K. Moreover, in the presence of oxygen deficiency, heat flux, thermal conductivity, and combustion efficiency of atomic samples reached 2049W/m^2, 1.23W/m.K and 90% after rising palladium to 4%, and it decreased to 2035W/m^2, 1.19W/m.K and 86% by adding 10% palladium. Therefore, the results indicate that the oxygen and the catalyst (palladium) ratios can benefit the combustion process. These results can optimize the atomic performance and combustion performance of structures essential for use in various industries.