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Molecular dynamics simulation of gasification technology to produce hydrogen from biomass at different initial pressures in the presence of platinum catalyst

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Abstract

Biomass is a renewable source of energy obtained from biological materials. Gasification technology is commonly used to produce hydrogen (H_2) from biomass. This method is based on the partial oxidation of the input materials and their conversion into synthetic gas. After gasification, the biomass is converted into a gas consisting of H_2, carbon monoxide (CO), carbon dioxide (CO_2), and other compounds. This research investigates the number of H_2 molecules ($n(H_2)$) and CO molecules (n(CO)) in the basic structure at a temperature and pressure of 1 bar and 1800 K. Additionally, the effect of initial pressure (IP) changes on the $n(H_2)$ and n(CO) produced with a 10% volume fraction of platinum (Pt) catalyst was evaluated using molecular dynamics (MD) simulation. The results demonstrate that the produced $n(H_2)$ and n(CO) increase from 559 to 146 to 586 and 165, increasing the Pt nanocatalyst ratio from 1% to 10%. Furthermore, the $n(H_2)$ and n(CO) increase from 586 to 165 to 598 and 175, respectively, by increasing the IP from 1 to 5 bar. Also, the results reveal that the combustion efficiency (CE) increases from 62% to 66% with increasing IP from 1 to 5 bar. The application of this research is to study the production of hydrogen and carbon monoxide from biomass using gasification technology. This information can be useful for improving the efficiency of biomass gasification for hydrogen production.