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Performance and emissions characteristics of an intensified membrane reactor for steam methane reforming and H₂ separation/in-situ-combustion for power generation

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ABSTRACT

This study numerically examines the characteristics of hydrogen separation and in-situ hydrogen-air combustion in a palladiumbased membrane reactor for combined steam methane reforming (SMR), hydrogen separation, and power generation. The combustion and emissions (mainly NO_x) characteristics of the generated H_2 -air suspended flames associated with this promising intensified process are well investigated. A monolith structure membrane reactor was considered, where hydrogen is extracted from methanereformed exhaust flow in the feed sides and combusted on the permeate sides of the reactor, aided by water vapor obtained from the heat recovery process. A three-dimensional (3D) computational fluid dynamics (CFD) model is employed in the numerical simulation, considering a reduced mechanism for H₂-air combustion in the permeate sides of the membrane reactor. The study explores the effects of design and operational parameters on membrane reactor performance and emissions characteristics, including gas reactor temperature, feed gas concentrations, operating pressure, feed gas flow rates, and flow configuration (co-current vs counter-current), to determine the optimal conditions for maximizing hydrogen yield. Additionally, the formation of NO_x due to the high temperatures generated during the hydrogen combustion is assessed to evaluate the environmental impact of this highly-intensified reactor of multiple processes, which integrates hydrogen separation and in-situ hydrogen combustion for power generation. Increased feed pressure and hydrogen concentration on the feed side led to a higher hydrogen permeation flux on the permeate side, with the permeated hydrogen being concentrated near the membrane. Additionally, the in-situ combustion of hydrogen on the permeate side results in the formation of thermal NO_x due to the elevated temperatures of the combusted gases. This proposed configuration introduces a novel approach in the field of process intensification, with the potential for scale-up to the industrial scale.