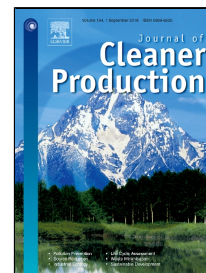


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# On the effects of fuel type, fuel mixing and Sulphur content on the performance of a high-temperature membrane reactor adapting liquid fuel: A numerical study

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## Abstract

The study investigates numerically oxygen permeation and combustion and emission characteristics of a button-cell high-temperature membrane reactor (HTMR) handling different grades of liquid fuels including methanol ( $\text{CH}_3\text{OH}$ ), ethanol ( $\text{C}_2\text{H}_5\text{OH}$ ), benzene ( $\text{C}_6\text{H}_6$ ), n-octane ( $\text{C}_8\text{H}_{18}$ ) and gas oil ( $\text{C}_{16}\text{H}_{29}$ ). Effects of mixing different grades of fuels on the HTMR performance are also investigated. A disc-shaped  $\text{La}_2\text{NiO}_4$  (LNO) ceramic membrane is used. A plain orifice atomization model is used for numerical calculations of liquid fuel atomization. Fuel is introduced along with  $\text{CO}_2$  at sweep inlet and air is introduced at fed inlet of the membrane reactor. 2-D axisymmetric mesh was constructed, and simulations were performed using Ansys-Fluent Workbench 15.0. All calculations were performed at fixed inlet gas temperature of 1173 K, fixed inlet fuel temperature of 300 K and fixed molar fuel concentration of 5% in the vapor phase. For single fuel operation, the highly reactive light oxygenated alcohol fuels resulted in stoichiometric combustion with better oxygen flux compared to rich combustion and low oxygen flux for heavier fuels. Gas oil fuel showed poor fuel evaporation, poor mixing with the sweeping gas, and low reaction rate. Trying to improve the performance of the HTMR while burning heavy fuels, three mixtures of three fuels containing gas oil fuel were tested. The compositions of the mixtures 1, 2 and 3 are 2% $\text{C}_6\text{H}_6$ /2% $\text{C}_8\text{H}_{18}$ /1%  $\text{C}_{16}\text{H}_{29}$ , 2% $\text{CH}_3\text{OH}$ /2% $\text{C}_8\text{H}_{18}$ /1% $\text{C}_{16}\text{H}_{29}$  and 2% $\text{CH}_3\text{OH}$ /2% $\text{C}_6\text{H}_6$ /1% $\text{C}_{16}\text{H}_{29}$ . The results showed better performance of the HTMR when burning gas oil fuel in a mixture than burning it purely. Mixtures 1 and 2 resulted in about three times and mixture 3 resulted in about six times the oxygen flux value when using pure gas oil fuel. The maximum temperature with the reactor has been improved from 1208 K for gas oil fuel to 1383 K, 1372 K and 1557 K for mixtures 1, 2 and 3. Using methanol as fuel additive significantly improve the performance of the HTMR, even better than burning it alone, and enables the use of heavier fuels in HTMR applications. Based on that, the performance of the HTMR was evaluated while burning mixtures of two fuels, one of them is methanol. Three mixtures were considered (mixtures 4, 5 and 6) with the compositions of 4% $\text{CH}_3\text{OH}$ /1% $\text{C}_6\text{H}_6$ , 4% $\text{CH}_3\text{OH}$ / 1% $\text{C}_8\text{H}_{18}$  and 4% $\text{CH}_3\text{OH}$ /1% $\text{C}_{16}\text{H}_{29}$ . Mixing methanol with benzene (mixture 4) resulted in the highest obtained oxygen permeation flux among the tested ranges of pure and mixed fuels. Locations where sulfates compounds are created within the HTMR with respect to the membrane are calculated for proper control of membrane operation while utilizing heavy gas oil fuel with Sulphur content.

**Keywords:** High-temperature membrane reactor (HTMR); oxygen separation membranes; oxy-fuel combustion; liquid fuel; carbon capture.

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