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Thermodynamic and Kinetics Modeling of H_2 Production by Dry Reforming of Ethanol with $CaCO_3$ as CO_2 Source

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ABSTRACT

A viable alternative to fossil fuels is to make use of H_2 from renewable sources as an energy carrier or as a clean fuel. Steam reforming of hydrocarbons is the conventional process to produce H_2, with the drawbacks that presents low efficiency combined with high operational costs and CO_2 being emitted into the atmosphere. An alternative to this process is the dry reforming of hydrocarbons, which employs CO_2 to produce hydrogen-syngas and the use of ethanol as a renewable feedstock which would prevent CO_2 emission into the atmosphere. One innovative approach is the use of a solid carbonate to serve as a source of CO_2 for this process. Thus, exposing the solid carbonate to high temperatures (reaction temperature), this decomposes emitting CO_2, which is used as raw material along with ethanol (ETOH) to produce hydrogen-synthesis gas. The present work aims to perform a thermodynamic and kinetic simulation study to explore reaction conditions close to equilibrium for a high syngas-H_2 production, under the dry reforming of ETOH. $CaCO_3$ was used as source of CO_2 for the reaction system. The thermodynamic study was performed using the HSC software and the studied conditions were: T = 300-1000 °C, $CaCO_3$/ETOH molar ratio = 1-5. Results showed that at T ≥ 755 °C and $CaCO_3$/ETOH ≥ 3, a free carbon formation syngas is produced. Maximum H_2 production was obtained at 855 °C and $CaCO_3$/ETOH ≥ 3, while the highest concentration of H_2 was produced at 755 °C. Furthermore, a process and kinetics simulations were performed through ASPEN-Plus and CKS, respectively and based on experimental data taken from the literature for the dry reforming of ETOH. Results indicate that at 900 ºC and $CaCO_3$/ETOH = 0.9 ratio, the estimated value of H_2 purity was very similar to that obtained by the thermodynamic equilibrium analysis.

Keywords: CO_2 dry reforming; thermodynamic analysis; kinetics modelling.