

## BIOMASS-DERIVED COMPOUNDS AS RAW MATERIALS FOR HYDROGEN PRODUCTION UNDER SUPERCRITICAL CONDITIONS

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Hydrogen has become an attractive alternative energy source; depending on the raw material used for its production, hydrogen can be considered renewable, promoting the hydrogen economy. In that sense, the use of biomass-derived compounds as substrate for hydrogen production, via reforming with water under supercritical conditions, offers numerous advantages over the traditional steam reforming of fossil fuels, with higher production rates and without catalyst poisoning. This work considers hydrogen-rich gas production via supercritical water reforming (SCWR) using different materials (glucose, glycerol, bio-oil) as feedstock.

The phase behavior of the compounds involved in this chemical transformation (glycerol, glucose, H<sub>2</sub>O, H<sub>2</sub>, CH<sub>4</sub>, CO, CO<sub>2</sub>) is studied to define the supercritical region to carry out the process. The Group Contribution with Association Equation of State (GCA-EoS) thermodynamic model was chosen to investigate the phase behavior of the reactive system and the produced gases. The GCA-EoS model, takes into account molecular self and cross-association effects, and shows accurate results in predicting phase behavior of asymmetric and polar systems at high pressures and temperatures, required for the SCWR process. With the aim of examine the optimal conditions for maximizing hydrogen production in each case, equilibrium calculations were also performed, using the Gibbs free energy minimization method; the operating parameters investigated were the reactor feed (water to glycerol mole ratio), temperature and pressure (near or supercritical conditions). In general terms, hydrogen conversion close to theoretical values is achieved feeding dilute solutions, at temperatures > 900 K, and pressure has a little effect on gas yields.

**Keywords:** supercritical water, phase behavior, glycerol, hydrogen, conversion.

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