Process Modelling, Thermodynamic Analysis and Optimization of Dry Reforming, Partial Oxidation and Auto-Thermal Methane Reforming for Hydrogen and Syngas Production

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ABSTRACT
In this work, process modelling, thermodynamic analysis and optimization of stand-alone dry and partial oxidation reforming of methane as well as, the auto-thermal reforming processes were investigated. Firstly, flowsheet models were developed for both the stand-alone systems and auto-thermal reforming process using ASPEN HYSYS®. Furthermore, thermodynamic studies were conducted for the stand-alone and auto-thermal reforming processes for temperatures range of 200–1000°C and pressure range of 1–3 bar using Gibbs free energy minimization methods which was also performed using ASPEN HYSYS®. The simulation of the auto-thermal reforming process was also performed at 20 bar to mimic industrial process. Process parameters were optimized in the combined reforming process for hydrogen production using desirability function. The simulation results show that 84.60 kg/h, 62.08 kg/h and 154.7 kg/h of syngas were produced from 144 kg/h, 113 kg/h and 211 kg/h of the gas fed into the Gibbs reactor at $CH_4/CO_2/O_2$ ratio 1:1:1 for the stand-alone dry reforming, partial oxidation reforming and auto-thermal processes respectively. Equilibrium conversion of CH_4, CO_2, O_2 were thermodynamically favoured between 400 and 800°C with highest conversions of 100%, 95.9% and 86.7% for O_2, CO_2 and CH_4 respectively. Highest yield of 99% for H_2 and 40% for CO at 800°C was obtained. The optimum conditions for hydrogen production were obtained at CH_4/CO_2, CH_4/O_2 ratios of 0.634, 0.454 and temperature of 800°C respectively. The results obtained in this study corroborate experimental studies conducted on auto-thermal reforming of methane for hydrogen and syngas production.

KEYWORDS: process modelling; thermodynamics; reforming; equilibrium conversion; Gibbs free energy minimization

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