

## Thermodynamic analysis of carbon dioxide reforming of methane in view of solid carbon formation

### Abstract:

A thermodynamic equilibrium analysis on the multi-reaction system for carbon dioxide reforming of methane in view of carbon formation was performed with Aspen plus based on direct minimization of Gibbs free energy method. The effects of CO<sub>2</sub>/CH<sub>4</sub> ratio (0.5-3), reaction temperature (573-1473 K) and pressure (1-25 atm) on equilibrium conversions, product compositions and solid carbon were studied. Numerical analysis revealed that the optimal working conditions for syngas production in Fischer-Tropsch synthesis were at temperatures higher than 1173 K for CO<sub>2</sub>/CH<sub>4</sub> ratio being 1 at which about 4 mol of syngas (H<sub>2</sub>/CO = 1) could be produced from 2 mol of reactants with negligible amount of carbon formation. Although temperatures above 973 K had suppressed the carbon formation, the moles of water formed increased especially at higher CO<sub>2</sub>/CH<sub>4</sub> ratios (being 2 and 3). The increment could be attributed to RWGS reaction attested by the enhanced number of CO moles, declined H<sub>2</sub> moles and gradual increment of CO<sub>2</sub> conversion. The simulated reactant conversions and product distribution were compared with experimental results in the literatures to study the differences between the real behavior and thermodynamic equilibrium profile of CO<sub>2</sub> reforming of methane. The potential of producing decent yields of ethylene, ethane, methanol and dimethyl ether seemed to depend on active and selective catalysts. Higher pressures suppressed the effect of temperature on reactant conversion, augmented carbon deposition and decreased CO and H<sub>2</sub> production due to methane decomposition and CO disproportionation reactions. Analysis of oxidative CO<sub>2</sub> reforming of methane with equal amount of CH<sub>4</sub> and CO<sub>2</sub> revealed reactant conversions and syngas yields above 90% corresponded to the optimal operating temperature and feed ratio of 1073 K and CO<sub>2</sub>:CH<sub>4</sub>:O<sub>2</sub> = 1:1:0.1, respectively. The H<sub>2</sub>/CO ratio was maintained at unity while water formation was minimized and solid carbon eliminated.