

Abstract

Process synthesis deals with the development of synthesis tools to help improve process efficiencies, energy efficiency, capital and operating expenses for the process industries. In recent years, researchers have focused on process synthesis tools such as the ‘Attainable Regions’ technique, and many other complex mathematical formulations have been developed for different applications. All these tools assist the design engineer to identify all possible outputs, by considering only the given feed specifications and permitted fundamental processes.

This work contributes to the development of a process synthesis tool in the form of systematic graphical techniques that look at the processes of coal gasification and coal-methane co-gasification. This tool is also used to look for opportunities to improve efficiencies of these processes and to reduce carbon dioxide emissions.

By making a few reasonable assumptions; the mass balances, the energy balance and reaction equilibria around a gasifier can be set up. This thesis deals with how these balances are set up; also looks at what effect the feed composition and choice of reactor conditions (temperature and pressure) may have on the possible gasifier product.

This tool is used to analyse; the partial pressures of components through the gasifier, reaction equilibria, reaction paths and syngas composition ($\text{CO}:\text{H}_2$ and $\text{CO}_2:\text{H}_2$ ratios) given certain operating conditions and the results were found to be consistent with literature.

The traditional requirement of a $\text{CO}:\text{H}_2$ ratio of 2 for Fischer Tropsch (FT) synthesis is explored. Of biggest interest is a proposed new FT chemistry as proposed by Patel et al. This chemistry

proposes setting a $\text{CO}_2\text{:H}_2$ ratio of 3 as the target for FT synthesis. Some optimisation work is also done on the possible syngas composition for both the traditional and proposed chemistry routes.

Coal and methane co-gasification is also explored using this tool and the results are shown to be consistent with literature.

The result of this approach shows that we can work in a stoichiometric subspace defined by the energy and mass balance. Furthermore we can show that gasification is energy and not work limited which has implications for the design and operation of these units.