Synopsis

Economies have become increasingly reliant on the use of fossil fuels as the primary energy source in order to meet energy demands of a growing population. The combustion of fossil fuels results in greenhouse gas (GHG) emissions, particularly carbon dioxide (CO_2). This has resulted in CO_2 emissions increasing at a rate that is detrimental to climate. To curb the detrimental effects of these emissions, whilst providing for the energy requirements of the population, a carbon negative energy source should ideally be introduced into the energy mix.

In this dissertation, a P-Graph superstructure approach is utilized to encompass a wide array of CO_2 reaction pathways that produce methanol (MeOH) and dimethyl ether (DME), both of which have proven to be prominent in the energy industry. A total of 85 reaction pathways were simulated using Aspen Plus ® software. These case studies were then analyzed from an environmental and economical perspective, in order to determine the most viable pathways to produce the aforementioned products. The framework developed was able to systematically reduce the search space from 85 possible scenarios, to 6 viable case studies, which is a 93% reduction in the original search space. The use of a $CuO/ZnO/Al_2O_3$ catalyst at 240^oC and 80 bar pressure, was found to be the most viable option to produce MeOH. The most viable scenario for the production of DME, on the other hand, is to produce MeOH over the aforementioned catalyst, and then further dehydrate the MeOH over an Al/Si catalyst at 400^oC and 25 bar pressure. The production of MeOH is deemed to be more feasible than the production of DME.

With the most viable reaction pathway being known as the production of MeOH via a $CuO/ZnO/Al_2O_3$ catalyst, the focus is shifted outside of the framework, to the optimization of this reaction pathway. Post-optimization, it is found that the use of a $CuO/ZnO/Al_2O_3$ (TMC-3/1 industrial ZA Tarnow) catalyst at 201^oC and 29 bar pressure, is the most viable reaction conditions involved in the direct hydrogenation of CO_2 to MeOH. This pathway is able to yield a 97.69% conversion of CO_2, thereby exhibiting the highest environmental and economic benefits after optimization.

This dissertation details the systematic framework used in the synthesis and analysis of the P-Graph when arriving at the reduced search space, as well as the optimization procedure that is followed for the most viable reaction pathway.