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Modelling water removal from Fischer-Tropsch products using glycerol.

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ABSTRACT

The focal point of this dissertation was to study the removal of water from a Fischer-Tropsch (FT) product stream using glycerol. The Fischer-Tropsch reaction forms water as one of the products, and the concentration of water keeps on increasing with increasing conversion. Therefore there is a need to remove water from the FT product stream in order to prevent a decline in catalyst activity and to keep the concentration of water within acceptable limits. Glycerol was found to be suitable for the removal of water from an FT product stream because of its property to attract moisture and to hold it.

The process to remove water from an FT product stream using glycerol was synthesized and simulated on Aspen Plus under typical operating conditions of a commercial Fischer-Tropsch process. The simulation was conducted by contacting a typical reactor product stream with liquid glycerol. Three thermodynamic property models were used for the process simulation on Aspen Plus, namely the NTRL model (Non Random two Liquid), UNIQUAC model (Universal QuAsi Chemical), and UNIFAC model (Universal Functional Activity Coefficient).These models were chosen based on their ability to predict thermodynamic data when non is available and their suitability to simulate the system under investigation.

The simulation results from Aspen Plus showed that the removal of water from the FT product stream using glycerol was a possibility; all the thermodynamic property models predicted the same outcome. The general outcome of the simulation process was that the ability of glycerol to remove water from a Fischer-Tropsch product stream increased with pressure at a constant temperature and the amount of water it removed decreased with temperature at constant pressure.

The Aspen simulation results suggest that 91.3% of the water was removed by the glycerol at a pressure of 50 bar and a temperature of 180˚C, and 5% of the water can be removed by glycerol at 10 bar and 300˚C. The recovery of hydrocarbons by glycerol was found to be insignificant for hydrocarbons with a low carbon number (C_1–C_4). However, it was found about 40% of hydrocarbons with carbon numbers C_{10}–C_{15} were recovered into the liquid stream with glycerol because at these conditions the heavy hydrocarbons exist as a liquid rather than as a vapour phase. The process simulation also predicted that about 99% of water can be removed when the flow rate of glycerol is increased to twice the molar flow rate of water. The NTRL model was found to best fit literature data and also predicted simulation results better than the other two models.

When the simulation of the process was performed without the recycle stream of glycerol, the temperature of glycerol fed into the process had an effect on the exit temperature of the tail gas stream. When the glycerol feed temperature was low, the exit temperature of the tail gas stream was found to be lower than the FT operating temperature. However, when the process was simulated with a recycle stream of glycerol, the tail gas was found to be at a temperature that did not require the stream to be heated if it were to be recycled to the FT reactor for further reactions to take place in order to increase conversion. Furthermore recycling glycerol did not have a significant influence in improving water recovery.