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Interaction between reaction and phase equilibria in the Fischer-Tropsch reaction.

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ABSTRACT

The aim of the thesis is to describe the behaviour and performance of the Fischer–Tropsch (FT) reactor by considering the dynamic interaction between reaction equilibrium and vapour–liquid equilibrium (VLE) inside the reactor. There may be an equilibrium set up between species of either an olefin precursor or the olefins themselves which leads to the Flory-type distribution found in the FT reaction. Experimental results obtained show that VLE is attained inside an FT reactor. The measured vapour and liquid compositions (K-values) can be sufficiently described by Raoult's law. Hydrocarbons with carbon number greater than 18 deviates from Raoult's law. The deviations from Raoult's law are due to diffusion limitations. Elaborate thermodynamic models could be used given the pure component parameters with relevant mixing rules for a higher degree of accuracy.

VLE can explain the observed two-alpha product distribution in FT reactors. This further predicts a relationship between the two values of alpha that is consistent with the measured experimental results. Experimental results show that the average residence time increase with carbon number and the higher carbon number products have a longer residence time in the reactor. Products with a chain length of 22 and higher have the same residence time as the liquid. This suggests that VLE is the predominant cause for chain length dependencies of secondary olefin reactions in FT synthesis and diffusion limited removal of products is only significant for products with carbon number greater than 17.

A mathematical model to describe the behaviour and performance of an FT reactor by considering the dynamic interaction between reaction and VLE was developed. The model results show that the rate of formation of component hydrocarbons is dependent on either the reaction rate or stripping rate, depending on which one is rate-limiting. Furthermore, that at steady state, the rate of formation of hydrocarbons is given by the stripping rate. Modelling an

FT reactor as a reactive distillation column can explain a rate increment when the reactor is switched from Batch to CSTR mode and is also consistent with the observed two-alpha positive deviation product distribution observed experimentally and industrially.