CHAPTER VI

CONCLUSION

The incorporation of ethylene in the conventional Fischer-Tropsch synthesis in the past had only been utilized for the purpose of studying the reaction mechanism. Studies with the objective to develop reliable rate equations for the modified Fischer-Tropsch reaction based on kinetic considerations have not been reported. Thus, the primary goal of this study was to fill this void by developing suitable rate equations that could be utilized for reactor modeling and optimization studies on a real biomass indirect liquefaction conversion system.

Complicated theoretical models including a large number of nonlinear parameters usually will result in an excellent fit to experimental data, but it can also easily lose theoretical justification, i.e., physical meaning. The ultimate test will be that if the model will successfully extrapolate and interpolate beyond or within the range of the data of which it was obtained. Thus, the simplest theoretical model that makes sense from the mechanistic point of view is generally adequate and more desirable.

A rather simple theoretical kinetic model of the Eley-Rideal type based on the rate-determining step being the reaction between ethylene molecule and adsorbed hydrogen atom, not only fits the data of justified kinetic experiments very well, but also describes the nature of the reaction fairly adequately. The model also takes into account the effect of the inherent mass diffusion effect on the ethylene molecules. The mechanism was proposed based on various evidence of recent research in surface science. However, this model certainly is not the only one and proof for or against it may only come from other fields of science such as surface chemistry, surface physics and energetic spectroscopy as well as the extrapolation capability. In any case, this rate equation should provide a useful basis for future studies of reactor modeling and optimization experiments.

Since a broad spectrum of hydrocarbon products are produced by the synthesis reactions, some of them may not easily be identified. Thus a kinetic study based on individual chemical species is formidable. Therefore, almost all the kinetic studies of the Fischer-Tropsch and related syntheses were done based on net forward reaction, namely correlating the reaction rate with only reactant species. The kinetic model obtained from this study, although it takes into account the stepwise addition of methylene intermediate to the growth of the chain, bears the same drawback of being unable to predict the selectivity of the reaction. This can be remedied by either developing a separate product distribution model for experimentation, or employing those commercial gradientless reactors to run experiments under more realistic conditions.

There is also room for the refinement of this model. For example, use high purity component gases, improved operating controls for temperature, pressure and mass flows, and accurate on-line GC/MS analysis. Reports from current research of heterogeneous catalysis have shown that there may be a strong interaction between the cobalt metal and alumina support. Therefore, catalyst characterization must be emphasized.

For most precise kinetic studies, the rate of reaction should be expressed in terms of the turnover number. Unfortunately, the nature of active sites of almost all the reactions is still a mystery, not to mention how to count the active sites. Nevertheless, available techniques such as selective chemisorption and temperature programmed desorption and reaction enable one to count the number of metal atoms exposed to the reactant molecules, and to study the kinetics of some of the very elementary reactions in detail.