SUMMARY

In this report, the published and the unpublished non-proprietary data and calculations available on various scale units were used to carry out a review of several aspects of reaction kinetics and reactor performance. The material was divided into the following categories:

- Hydrodynamic, mixing and mass transfer behavior of various size reactors.
- Lumped kinetic models based on distillation or extraction fractions.
- Hydrogen consumption kinetics and its dependence on reactor temperature, pressure and catalyst concentration.
- Thermal behavior of adiabatic reactors.

The performance of a coal liquefaction reactor depends not only on the intrinsic kinetics but also on prevailing hydrodynamic, mixing and mass transfer characteristics. The scale-up of the reactor also depends on how faithfully one can predict or reproduce its characteristics in larger sized reactors. Many "non-adjustable" parameters including gas and slurry holdup, axial and radial mixing, gas-liquid mass transfer coefficients, radial and axial distribution of the catalyst, and the intraparticle diffusion inside the catalyst particles, affect the performance of coal liquefaction reactors. For a proper design, these "non-adjustable" parameters, should be expressed as a function of "adjustable" parameters including superficial gas and slurry velocities, reactor diameter and length, and the physical properties of fluids and solids. The first section analyzes the vast literature for simple air-water, two and three-phase bubble column reactors, and discusses the suitability of existing correlations for coal liquefaction reactors. The

design parameters discussed are; flow regimes, bubble dynamics, phase holdups, gas-liquid mass transfer coefficients, and backmixing in gas, liquid, and solid phases. Based on the available literature, suitable correlations are recommended for the evaluation of non-adjustable parameters along with their limitations. Some of the hydrodynamic models frequently used for bubble column reactors are discussed with their application to coal liquefaction reactors.

In the next section, kinetic models for coal liquefaction are evaluated. Numerous efforts have been made in the literature to evaluate and model the kinetics of coal liquefaction. Since there are many chemical species present during liquefaction, kinetic modeling involving individual chemical species is impossible. Generally, in indirect coal liquefaction, lumped fractions have been defined either on an extraction basis or on a boiling point (distillation fraction) basis. A number of kinetic models based on lumped parameter fraction have been proposed. In the first part of this section, product characterization of coal liquefaction reactors is described. The two types of characterization techniques; one based on the solubilities in different solvents, and the other based on the boiling points of fractions, are explained highlighting their relative advantages and limitations. The mechanism of coal liquefaction is briefly outlined followed by a detailed analysis of kinetic models for donor solvent coal liquefaction. The models are divided into three categories: rate models, lumped models, and correlation models, the most popular being the lumped kinetic model. Many investigators have proposed different reaction pathways. These pathways are tabulated along with the type of coal and solvent, pressure and temperature, and the type of catalyst. All these models however, have a basic drawback, that the applicability of these models is

restricted to the experimental data on which the model is based. Some of the models based on relatively large data bases are critically evaluated along with their limitations. Finally, the application of correlation models is discussed pointing out their relevance in identifying the major process variables.

The last section is divided into two subsections, namely, hydrogen consumption kinetics and the thermal behavior of coal liquefaction reactors, although it should be noted that they are interrelated. Hydrogen consumption is one of the major operating costs in direct coal liquefaction. Hydrogen consumption depends on reaction temperature, hydrogen partial pressure, nature and concentration of catalyst (recycle ash content in the case of the SRC-II process) and slurry residence time. Few experimental and theoretical studies have been carried out studying the effect of these "adjustable" parameters on the hydrogen consumption. All these studies are critically analyzed highlighting their relevance in application to the thermal behavior of the reactors. Large scale reactors have a smaller surface to volume ratio and they will be operated under non-isothermal and probably close to adiabatic conditions. The prediction of temperature distribution in large scale reactors is important for two reasons: (1) a wide temperature distribution will affect the performance in the reactor; and (2) a highly backmixed adiabatic slurry reactor may lead to multiple steady states and problems with reactor start up and control. It is important to know the thermal behavior of a large scale reactor as a function of reaction operating conditons including reactor inlet temperature, pressure, slurry residence time, nature of coal, solvent, and concentration of coal and catalyst in the slurry phase. In the first part, the background literature on multiple steady states is surveyed. Different thermal models relevant to coal liquefaction reactors are outlined

highlighting the relative advantages and limitations. The thermal behavior of the SRC-II reactor is discussed with the possibility of existence of multiple steady states, and the ways to control them. In the final part, the thermal inertia of high pressure reactors is briefly outlined, along with the caution to be exercised in carrying out these experiments in small scale units.