1. INTRODUCTION AND MOTIVATION

Synthesis gas (mixture of carbon monoxide and hydrogen) from coal is one of the most abundant and reliable sources of energy and chemicals. Fischer-Tropsch (FT) Chemistry is an acknowledged route for clean utilization of coal-derived synthesis gas in production of fuels and chemicals. Based on reaction engineering considerations and economics (i.e., from the heat transfer and high volumetric productivity viewpoints), slurry bubble column reactors (SBCR) operated at high gas velocities in churn turbulent flow regime are the preferred reactors for commercialization of FT synthesis.

Reliable data and tested models or theory for design and scale-up of SBCR for FT synthesis are currently not available. In response to this need, the Department of Energy (DOE) initiated the Hydrodynamics Initiative which focuses on advancing the state of the art in understanding the fluid dynamics of slurry bubble columns and replacing empirical design methods with a more rational approach.

As a part of this initiative DOE has awarded the DE-FG-26-99FT40594 grant for a collaborative effort between Washington University (WU), Ohio State University (OSU) and Air Products and Chemicals, Inc. (APCI) to advance the knowledge and understanding of the hydrodynamics of FT SBCR. The overall goals of this grant are: to search and select a system that simulate the microstructure of FT waxes and mimic their hydrodynamics at low temperature and pressure up to 10 atm, to study the microstructure of the gas-liquid-solid mixtures in a comparable fluid to FT waxes in 2 inch diameter column and develop a fundamental understanding as to how important the physical and fluid dynamic properties can be "finger-printed" via various diagnostic techniques (such as particle image velocimetry, PIV) or laser doppler anemometry (LDA), optical probe, dynamic gas disengagement (DGD) and differential pressure fluctuation technique) and to measure large scale hydrodynamic parameters at high pressure and high gas velocity in a 6 inch diameter slurry bubble column using computed tomography (CT) and computer automated radioactive particle tracking (CARPT) . CARPT and CT are the only non-invasive techniques that can provide information on slurry velocity and density profiles in the whole column. Such data provides a firm scientific and engineering basis for scale-up and design of FT SBCR. The resulting findings can be utilized as a benchmark to validate the computational fluid dynamic codes.

This grant enables a unique integration of the expertise of the two universities (WU and OSU) and industry (APCI) towards achieving the goals set as a part of the DOE Hydrodynamics Initiative. This study complements well the work in progress at CREL-WU, OSU, Iowa State University (ISU) and Sandia National Laboratory, Contract No. DE-FC-22-95PC95051, related to the LaPorte Advanced Fuels Demonstration Unit (AFDU) operated by Air Products with the Department of Energy funding.

1.1 Slurry Bubble Column Reactors (SBCR)

A slurry bubble column reactor (SBCR) is a cylindrical vessel in which gas is sparged through a batch slurry (liquid and small particles) or a flowing slurry (Figure 1.1). The gas superficial velocities are order of magnitude larger than those of the liquid so that it is the gas that governs the fluid dynamics of the system. Small slurry particles follow the liquid phase in SBCR. It is well known that fluid dynamics (phase velocities and holdup distribution) affect the phase mixing and transport (gas-liquid interfacial area, transport coefficients) between the phases, and hence, to a large extent affect the conversion and selectivity as shown in Figure 1.1. If the reaction involves phase volume changes (e.g. gas is either consumed or produced), the phase mixing, and transport parameters are affected along the column. Thus quantitative knowledge of fluid dynamics is essential for rational and predictive reactor design and scale-up.

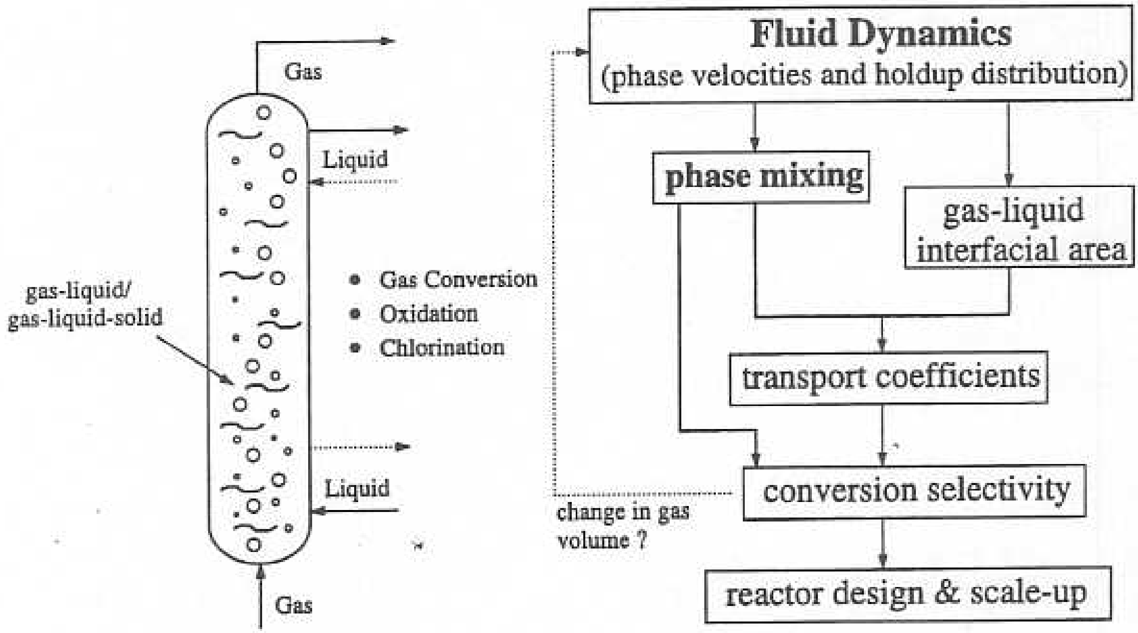

Figure 1.1. Slurry bubble column and the integrated effects of the phase mixing and transport on the reactor design and scale-up.

1.2 Overall Objectives

The overall objectives of this cooperative university (WU and OSU)-industry (APCI) research is to advance the understanding of the hydrodynamics of FT SBCR via advanced diagnostics techniques. The goals set for these projects are as follows:

TASK 1: Literature Review

- Physicochemical properties and their effect on the hydrodynamics of bubble columns.
- Models used to predict FT reactor performance.

TASK 2: Based on Task 1, identify the range of intrinsic properties (density, viscosity and surface tension) of the fluids used for the FT synthesis.

- Identify a solvent that, at room temperature and pressure up to 200 psig, will mimic the hydrodynamics of FT wax (at FT reaction conditions).
- Measure the intrinsic properties (density, surface tension, viscosity) of the identified solvent at room temperature and pressure up to 200 psig in a 2" diameter column.
- Identify the particle type and size to be used.

TASK 3: Using the identified system (solvent-particle-air), perform the following investigation on the hydrodynamics in a 2" diameter column:

- Using Laser Doppler Anemometer (LDA) or Particle Image Velocimetry (PIV) investigate the effect of reactor pressure on the flow field and turbulent parameters.
- Using Δp fluctuation measurements to identify the flow regime transition and investigate the effect of reactor pressure on the flow regime transition.
- Overall gas holdup.
- Bubble size and bubble rise velocity using optical probe.

TASK 4: Using the identified system in Task 2, investigate the hydrodynamics in a 6" diameter column via CT and CARPT techniques. The following will be measured:

- Phase distribution profiles using CT/CARPT/ Δp
- Flow field and turbulent parameters using CARPT
- Overall gas holdup

TASK 5: Evaluate scale-up procedure for slurry bubble column. Develop additional correlations, if needed.

TASK 6: As a case study, examine the available CFD and mechanistic models against the newly obtained data.

TASK 7: Final report.

1.3 Accomplishments During the First Year

The first year was dedicated to the technical review preparation of the experimental facilities and the advanced measurement techniques. A new correlation was developed to predict the liquid-solid mass transfer coefficient in high pressure bubble column based on the atmospheric pressure data. The accomplishments were as follows:

1. Technical review of the variable affecting SBCR performance, some aspects of bubble dynamics and hydrodynamic properties and the physical properties of FT waxes and catalyst have been performed.
2. Preparation of the experimental facilities and the advanced measurement techniques. The preparation includes the following units:
   - High pressure (up to 3000 psi) and high temperature (up to 250°C) 2-inch diameter slurry bubble column set-up.
   - High pressure (up to 200 psi) 6-inch diameter slurry bubble column set-up. Two facilities will be used; one for computer automated radioactive particle tracking (CARPT) and computed tomography (CT) techniques and another one for pressure drop measurements. The later facility consists of a 6-inch diameter column equipped with 6- windows and 15 ports along the column.
   - Particle Image Velocimetry (PIV) and Laser Doppler Anemometry (LDA) for 2" slurry bubble column facility.
   - CARPT and CT for 6-inch slurry bubble column facility.
   - Techniques to measure in situ the intrinsic density, viscosity and surface tension of the liquid phase that will be used for hydrodynamics investigation which mimic the hydrodynamics of FT waxes.
3. Identify the solvent that mimic FT waxes at FT operating conditions and the gas and solid phases to be used in the hydrodynamics investigation.
4. Development of a new procedure to estimate the mass transfer coefficient at high pressure based on atmospheric pressure data.

1.4 Plan for the Next Year

The following represents an outline of the tentative plan set for the next year (July 1, 2000 to June 30, 2001).

- Measure in situ the intrinsic properties (density, viscosity, surface tension) of the identified solvent that has properties within the range of FT waxes properties.
- Initiate the experimental investigations of the hydrodynamics using the identified system in 2-inch diameter column via LDA or PIV, optical probe and dynamic pressure drop measurements.
- Initiate the experimental investigation of the hydrodynamics using the identified system in 6"-inch diameter column via CARPT, CT and dynamic pressure drop measurements.
- Continue the hydrodynamic parameters modeling and initiate the computational fluid dynamic (CFD) work using the available codes (e.g. CFDLIB, Fluent).