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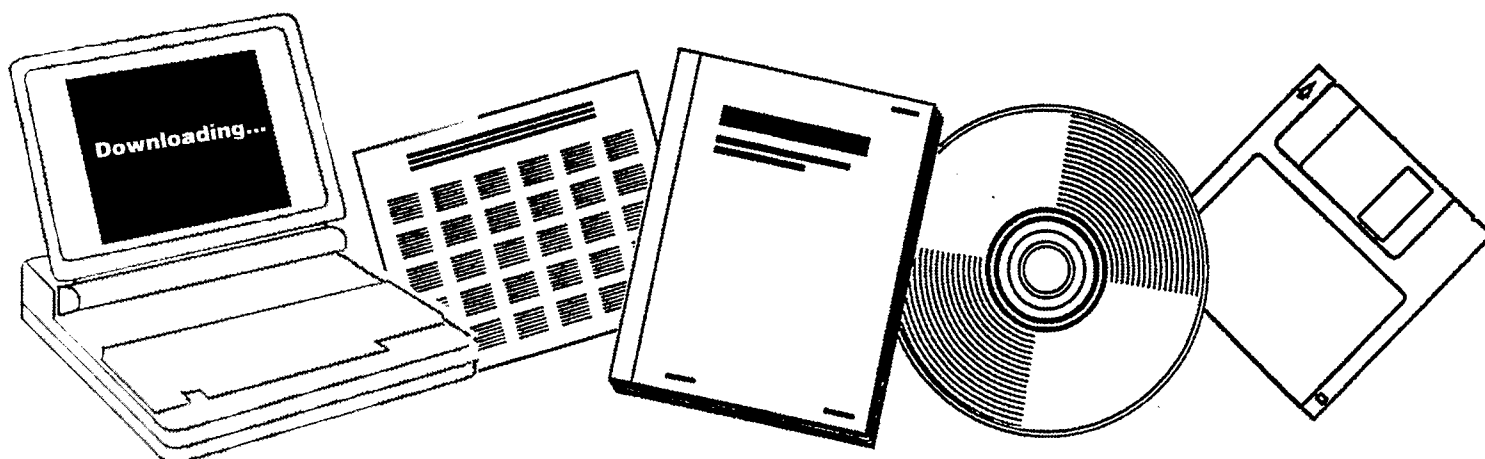
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**NOVEL EXPERIMENTAL STUDIES FOR COAL
LIQUEFACTION. QUARTERLY PROGRESS REPORT,
APRIL 1, 1985-JUNE 30, 1985**

PITTSBURGH UNIV., PA

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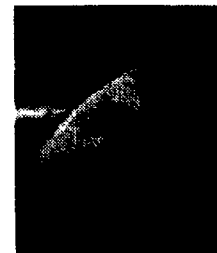
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Quarterly Progress Report

Novel Experimental Studies
for Coal Liquefaction

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Task 1: Thermal Behavior of Slurry Reactors Used for Indirect Coal Liquefaction

The conversion of synthesis gas to liquid products is usually carried out with the reactants in the gas phase and a solid catalyst. Because of relatively poor heat transfer from the gas to the solid, the reaction sites may overheat with loss of selectivity and activity. Slurry reactors in which the catalyst is suspended in a liquid medium, and the gases are bubbled through the slurry, have intrinsically better heat transfer characteristics and appear promising for indirect liquefaction.

In Task 1 the thermal behavior of slurry reactors is being studied. Of particular interest is the determination of multiple steady states if they exist. Previous work with a ruthenium catalyst has shown that two distinct steady states can be found for identical operating conditions. Other catalysts and operating conditions are being studied.

The slurry reactor has been modified to permit better control and measurement of the amount of liquid in the reactor, to simplify piping, and to improve instrumentation.

During the last quarter, some related runs were made using the slurry reactor and a Cu-ZnO catalyst (United H-18C). Runs were made at pressures of 250, 500, 750 and 1000 psi; temperatures of 220 C, 240 C, 260 C, two compositions; and three flow rates. Not all combinations were tested. Results are now being analyzed.

During the next quarter, the reactor will be run to determine thermal requirements with a different Fischer-Tropsch type catalyst.

Task 2: Coal Liquefaction under Supercritical Conditions

Supercritical fluid extraction is an attractive process primarily because the density and solvent power of a fluid changes dramatically with pressure at near critical conditions, and during the extraction of coal, the density of a supercritical fluid should also change the extractability of the coal. During the first part of this project a non-reacting supercritical fluid, toluene, was studied to determine the effect of density on the coal extraction/reaction process. Extractions were carried out for 2 to 60 minutes at reduced densities between 0.5 and 2.0 and at temperatures between 647 and 698 K. The data obtained can be explained by the hypothesis that coal dissolution precedes liquefaction reactions and that the degree of dissolution depends upon solvent density and temperature. A kinetic model shows that higher solvent densities result in faster conversion rates and in higher total conversions. Figure 1 shows how the model fits the experimental data. A complete copy of the submitted paper was included in the last quarterly report.

A second factor that makes supercritical extraction attractive is high mass transfer rates. At high pressures, mass transfer rates in a supercritical fluid are much higher than in a liquid, despite the fact that the supercritical fluid has liquid-like solvent powers. In this quarter we have been building an apparatus to measure mass transfer rates for naphthalene extraction by carbon dioxide. It has been constructed and pressure tested (Figure 2) and experiments will begin in late July or August. We are interested in determining how mass transfer coefficients vary with solvent density since these parameters will influence the design of extraction or reaction processes which utilize supercritical fluids. The kinetic model which was developed in the first quarter is based upon the assumption that

mass transfer resistances are negligible at the supercritical conditions employed. However, measured diffusion coefficients have shown a dramatic decrease as solvent pressure is increased and a similar effect on mass transfer coefficients may exist. If mass transfer coefficients are not sufficiently high, then coal dissolution rates may be an important factor to consider in kinetic models. It is thought that supercritical fluids might act to rapidly solvate reactive intermediates and remove them from the coal matrix thus preventing retrogressive reactions. A delay may exist in removing these intermediates due to mass transfer limitations.

Papers and Publications

- The Kinetics of Coal Liquefaction Under Supercritical Conditions submitted to I&EC Process Design and Development, April, 1985.

- The Effect of Solvent Density on Coal Liquefaction Under Supercritical Conditions, paper to be presented at the ACS Meeting, Chicago, September 10, 1985; to be published in Division of Fuel Chemistry Proceedings.

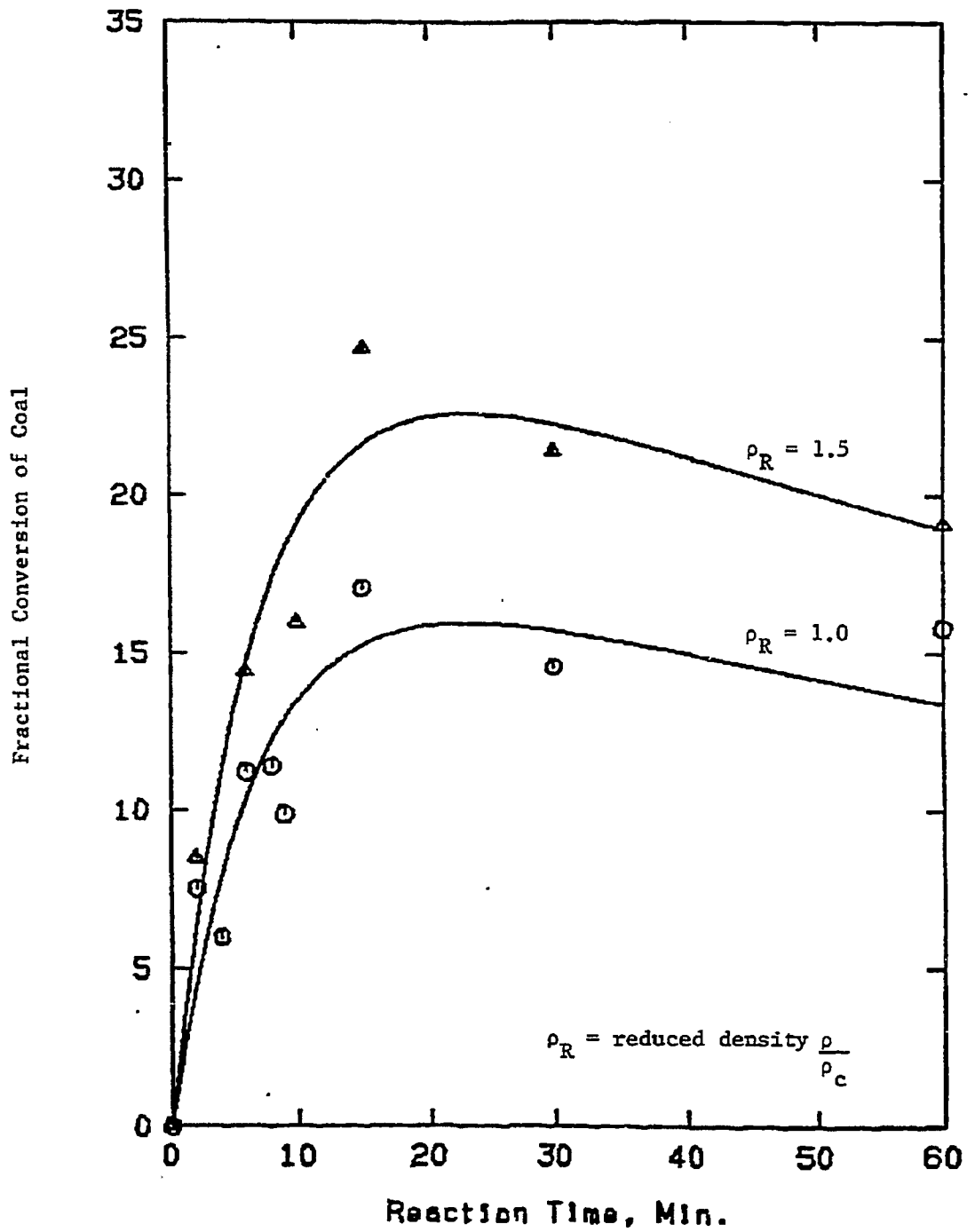
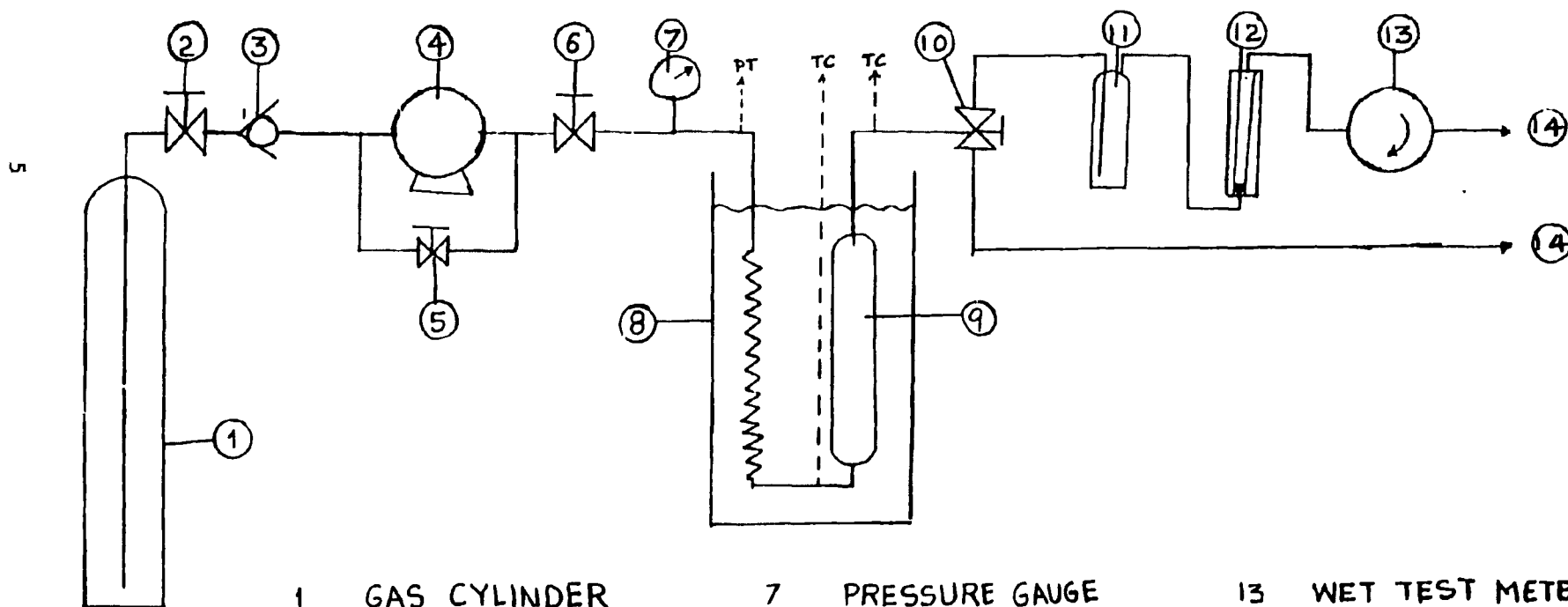


Figure 1: The Effect of Toluene Density on the Conversion of Coal to Liquids. Note that increasing density increases both the rate and the maximum conversion.

FIG: 2

SCHMATIC DIAGRAM OF EXPERIMENTAL SET UP

(MASS TRANSFER IN SUPERCRITICAL EXTRACTION)



- | | | | | | |
|---|-----------------|----|-----------------|------|----------------|
| 1 | GAS CYLINDER | 7 | PRESSURE GAUGE | 13 | WET TEST METER |
| 2 | REGULATOR | 8 | WATER BATH | 14 | VENT |
| 3 | CHECK VALVE | 9 | EXTRACTOR | TC | THERMOCOUPLE |
| 4 | PUMP | 10 | 3-WAY PRESSURE- | PT | PRESSURE - |
| 5 | BACK PRESSURE - | | -LET DOWN VALVE | | TRANSDUCER |
| 6 | METERING VALVE | 11 | SAMPLE BOTTLE | TC } | TO DATA LOGGER |
| | | 12 | ROTAMETER | PT } | |

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