**NOVEL REACTOR CONFIGURATION FOR SYNTHESIS GAS
CONVERSION TO ALCOHOLS**

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QUARTERLY REPORT

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I. Objectives for the Fourth Quarter, Year 1:

Our objective during this quarter was to complete Task IIIB, development of the algorithms for the dynamic response technique for parameter estimation; start Task IIIC, establishment of methodology for determination of the parameters of the trickle bed reactor in the microreactor assembly; and continue with Task IV, determination of the kinetics of the reaction in the slurry reactor.

II. Accomplishments, Fourth Quarter, Year 1:

We have completed the development of algorithms for data acquisition and data analysis for parameter estimation and have written the computer codes (Task IIIB). We have already started with Task IIIC, liquid fill studies in the microreactor assembly. For the liquid fill runs the parameters of interest are the mass transfer coefficient k_f , axial dispersion coefficient D_z , the effective diffusivity in the catalyst pores D_e , the adsorption equilibrium constant K_s , and the adsorption rate constant $k_s a_s$. We have shown that the tracer does not adsorb on this catalyst. Figure 1 shows change in k_f with Reynolds Numbers (superficial velocity), as expected k_f increases with Reynolds Number. Figures 2 shows that the effective diffusivity remains constant and does not change with Reynolds Number. This is a nice criterion to test the consistency of the data. Adsorption equilibrium (if there is adsorption of the tracer) and the diffusion are processes that take place within the pores of the catalyst and hence are independent of the hydrodynamics external to the catalyst particle. Therefore adsorption equilibrium constant and the effective diffusivity should be independent of the superficial velocity. Figure 3 shows how the Peclet Number changes with the Reynolds Number; again, as expected, the Peclet Number increases with Reynolds Number. These data were obtained

employing very narrow pore size distribution, specific diameter, chromatographic grade spherical alumina (Properties presented in the previous Quarterly). We are now in process of repeating the runs with regular catalytic alumina where there is adsorption of the tracer.

During this quarter we have also continued with measuring the kinetics of the reaction in the slurry CSTR reactor. We could not maintain the oil in the reactor as explained in the previous quarterly. Therefore we are now operating the reactor with continuous oil recirculation. There were some experimental problems involved in continuous oil recirculation. But we have solved these problems by maintaining a constant head in the oil reservoir and adjusting the oil recirculation rate accordingly. We are using porous metal filters at the reactor effluent to maintain the catalyst in the reactor. We still have some deactivation problems which we hope to tackle in the next quarterly.

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Heptane and Hexadecane

FIGURE 1

Heptane and Hexadecane

Figure 2

Heptane and Hexadecane

Figure 3

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