

APPENDIX

CONVERSION AND SELECTIVITY CALCULATIONS

CALCULATIONS USE ON LINE GAS ANALYSES

C = CONCENTRATION IN MOLE %

CONVERSIONS

$$\text{CONVERSION (CO)} = \frac{\left(\frac{C_{CO}}{C_{Ar}}\right)_{\text{Feed}} - \left(\frac{C_{CO}}{C_{Ar}}\right)_{\text{Prod}}}{\left(\frac{C_{CO}}{C_{Ar}}\right)_{\text{Feed}}}$$

$$\text{CONVERSION (H}_2\text{)} = \frac{\left(\frac{C_{H_2}}{C_{Ar}}\right)_{\text{Feed}} - \left(\frac{C_{H_2}}{C_{Ar}}\right)_{\text{Prod}}}{\left(\frac{C_{H_2}}{C_{Ar}}\right)_{\text{Feed}}}$$

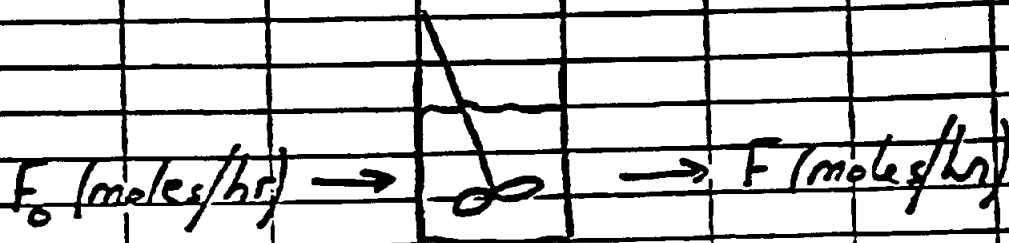
$$\text{CONVERSION (CO + H}_2\text{)} = \frac{\left(\frac{C_{CO} + C_{H_2}}{C_{Ar}}\right)_{\text{Feed}} - \left(\frac{C_{CO} + C_{H_2}}{C_{Ar}}\right)_{\text{Prod}}}{\left(\frac{C_{CO} + C_{H_2}}{C_{Ar}}\right)_{\text{Feed}}}$$

SELECTIVITIES

$$S_i = \frac{\left(\frac{C_N}{C_{Ar}}\right)_{Prod}}{\left(\frac{C_{Co}}{C_{Ar}}\right)_{Feed} - \left(\frac{C_{Co}}{C_{Ar}}\right)_{Prod}}$$

The equation above yields carbon-based selectivities. Before being used the selectivities were corrected for carbon dioxide formation in all cases except for that of carbon dioxide itself. Since carbon dioxide selectivities were usually about 50%, the corrected selectivities were about twice as high as they would have been if the carbon going to carbon dioxide had been taken into account in their calculation.

CALCULATION OF CONTACT TIME



\bar{V} is Volume of liquid in Autoclave

W is weight in grams of UO₂

material balance:

$$F_0 - F = \bar{r} \cdot W \cdot \bar{V}$$

$$F_0 - F_0(1-x) = \bar{r} \cdot W \cdot \bar{V}$$

$$F_0 x = \bar{r} \cdot W \cdot \bar{V}$$

$$\bar{r} = \frac{F_0 x}{W \bar{V}} = \frac{x}{\left(\frac{W \bar{V}}{F_0}\right)}$$

$$\frac{W \bar{V}}{F_0} = \text{CONTACT TIME (SPACE TIME)}$$