Table 1. Isosynthesis Characteristics of Different Catalysts

Item	Catalyst #1	Catalyst #2	J&E [1]
Isosynthesis Profile [2]	4.55±1.28	2.29±0.79	2.30
Branched/ Linear C_4	2.71±0.67	2.97±0.33	0.18
$i\text{-}C_4H_8$/ All C_4's	0.63±0.06	0.37±0.15	0.84

[1] N.B. Jackson and J.G. Ekerdt (1990). 425°C, 35 atm, 1:1 H_2/CO

[2] Defined as (total weight of C_4 hydrocarbons / total weight of C_2's and C_3's)

All the ratios are calculated on weight basis.

Table 2 Microkinetic Reaction Parameters

Reaction	E_A^f(kcal/mol)	E_A^r(kcal/mol)
(1)$H_2 + 2Zr \rightleftharpoons 2ZrH$	15	-7
(2)$ZrH + ZrO \rightleftharpoons ZrOH + Zr$	45	26
(3)$CO + Zr \rightleftharpoons ZrCO$	-32	
(4)$ZrCO + Zr \rightleftharpoons ZrC + ZrO$	25	-32
(5)$ZrC + ZrH \rightleftharpoons ZrCH + Zr$	39	5
(6)$ZrCH + ZrH \rightleftharpoons ZrCH_2 + Zr$	18	23
(7)$ZrCH_2 + ZrH \rightleftharpoons ZrCH_3 + Zr$	5	33
(8)$ZrCH_3 + ZrH \rightleftharpoons CH_4 + 2Zr$		
(9)$ZrCH_3 + ZrH \rightleftharpoons ZrCH_4 + Zr$	1	34
(10)$ZrCO + ZrH \rightleftharpoons ZrOCH + Zr$	13	19
(11)$ZrOCH + Zr \rightleftharpoons ZrCH + ZrO$	31	51
(12)$ZrOCH + ZrH \rightleftharpoons ZrOCH_2$	33	3
(13)$ZrOCH_2 + Zr \rightleftharpoons ZrCH_2 + ZrO$	4	-24
(14)$ZrOCH_2 + ZrH \rightleftharpoons ZrOCH_3 + Zr$	-4	23
(15)$ZrOCH_3 + ZrH \rightleftharpoons ZrCH_3OH + Zr$		
(16)$ZrCH_3OH + Zr \rightleftharpoons ZrCH_3 + ZrOH$		
(17)$ZrOCH_3 + ZrH \rightleftharpoons CH_3OH + 2Zr$		
(18)$ZrCH_3OH + Zr \rightleftharpoons ZrCH_3 + ZrOH$		
(19)$ZrCO + ZrOH \rightleftharpoons ZrOOCH + Zr$	17	18
(20)$ZrOOCH + Zr \rightleftharpoons ZrOCH + ZrO$	13	45
(21)$ZrOOCH + ZrH \rightleftharpoons ZrHCOOH + Zr$		
(22)$ZrOOCH + Zr \rightleftharpoons ZrO_2C + ZrH$	21	-13

XRD of Batch #1 - 4 Days after Preparation

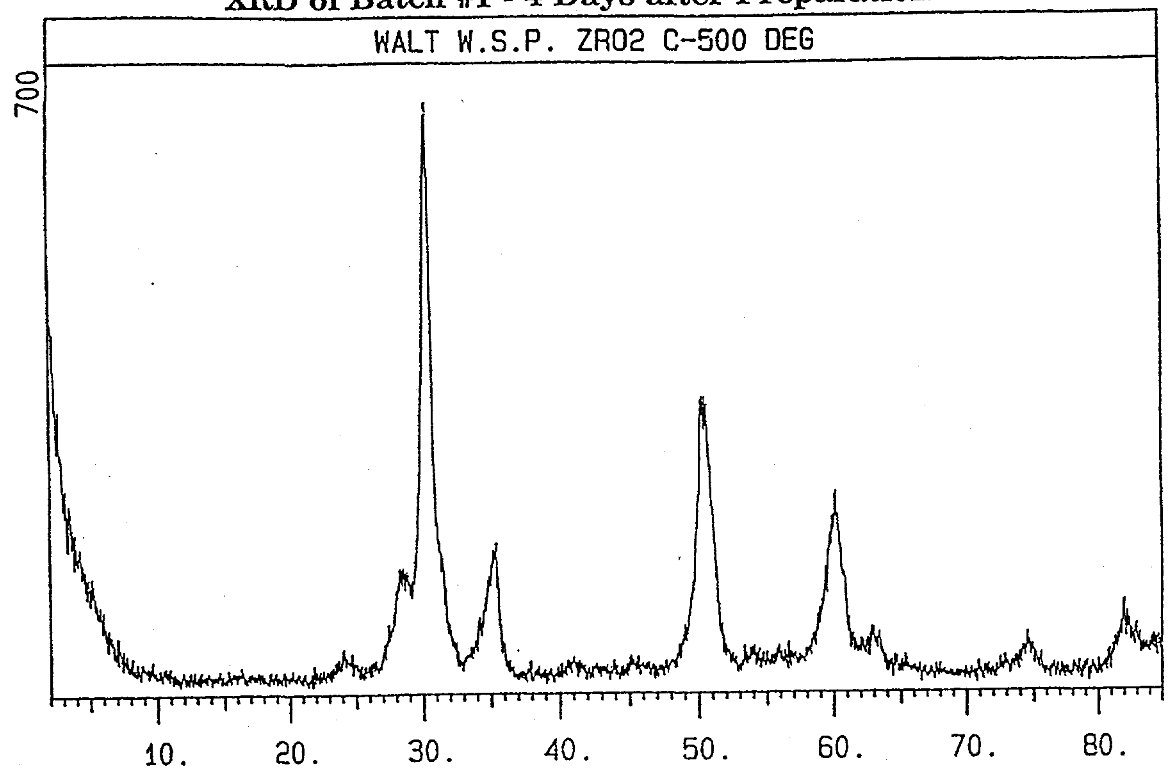

Figure 1. Catalyst #1, Batch #1 -- XRD Pattern Indicates Formation of Cubic or Tetragonal Zirconia.

XRD of Batch #1 - 6 Months after Preparation

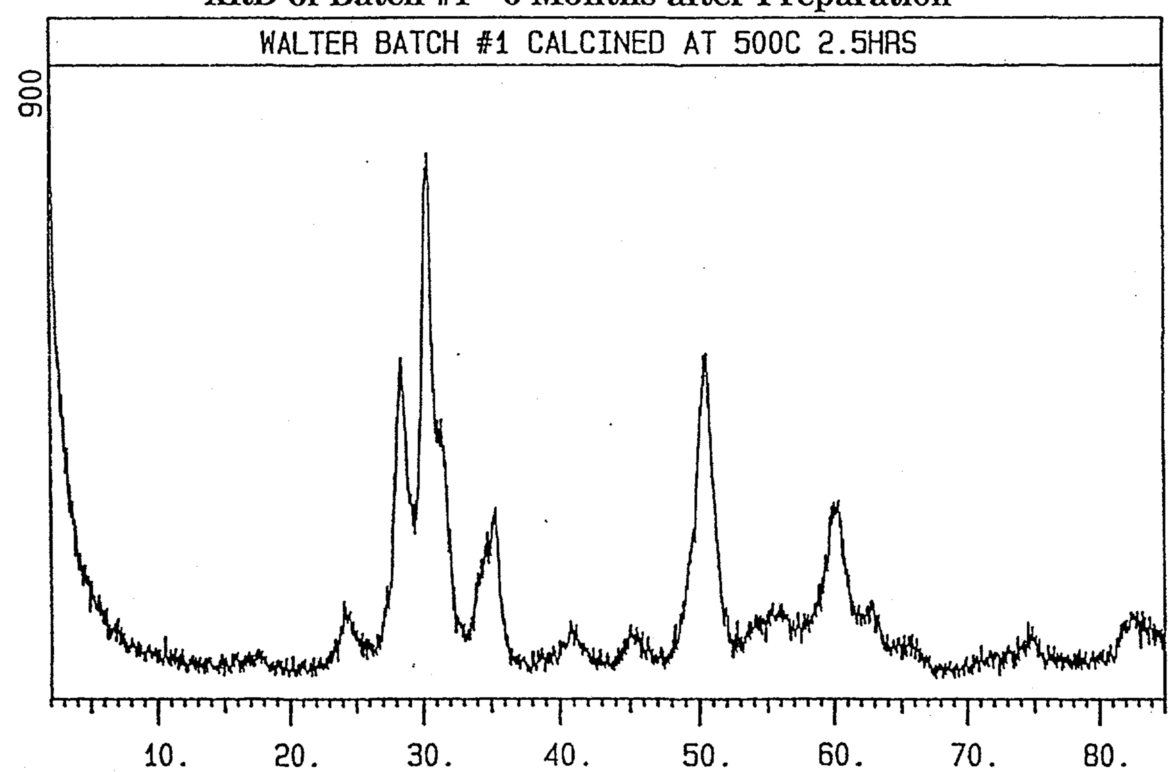

Figure 2. Catalyst #1, Batch #1 -- After Setting in Desiccator For Six Months.

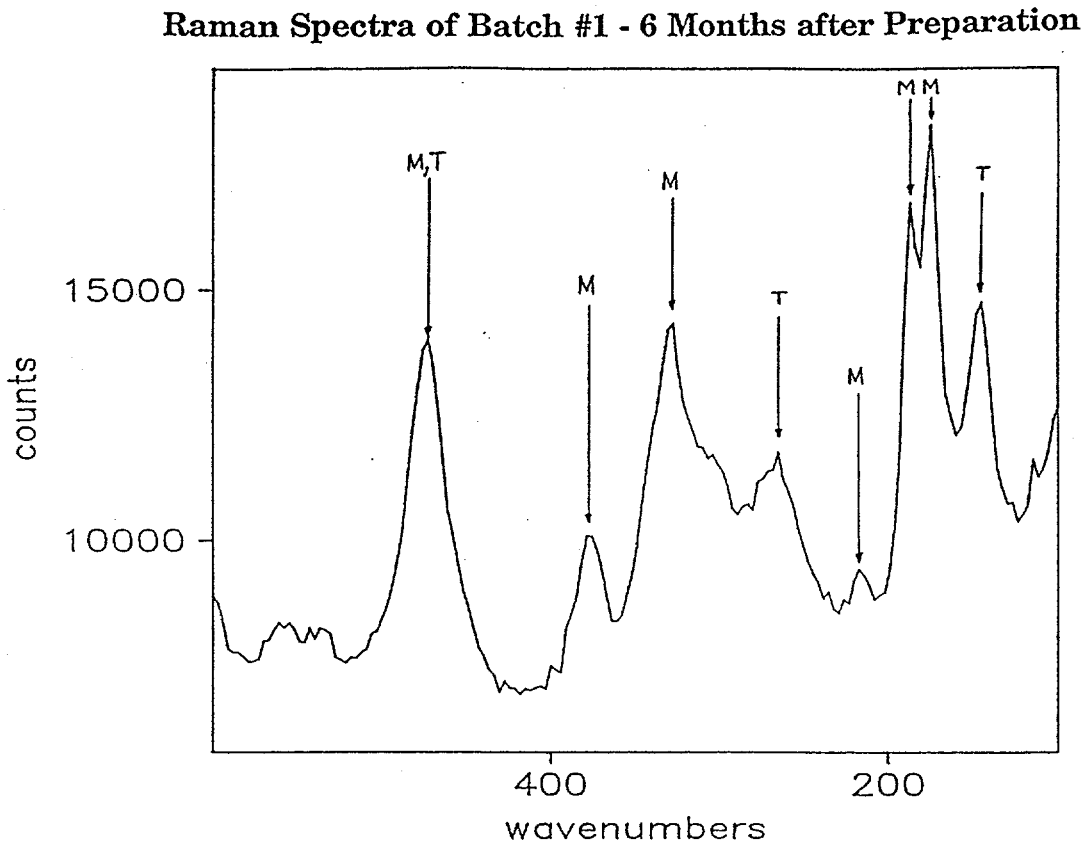

Figure 3. Catalyst #1, Batch #1 -- Raman Spectra Indicates Presence of Monoclinic and Tetragonal Zirconia.

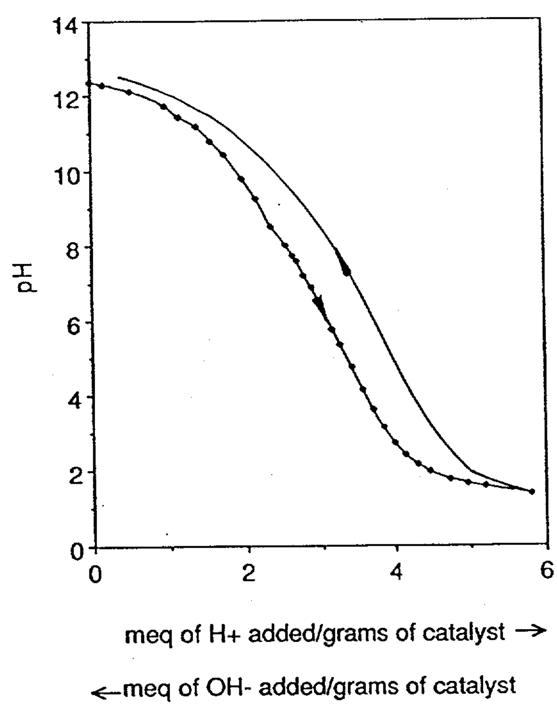

Figure 4. Titration Curve for Hydrous Sodium Zirconium Oxide.

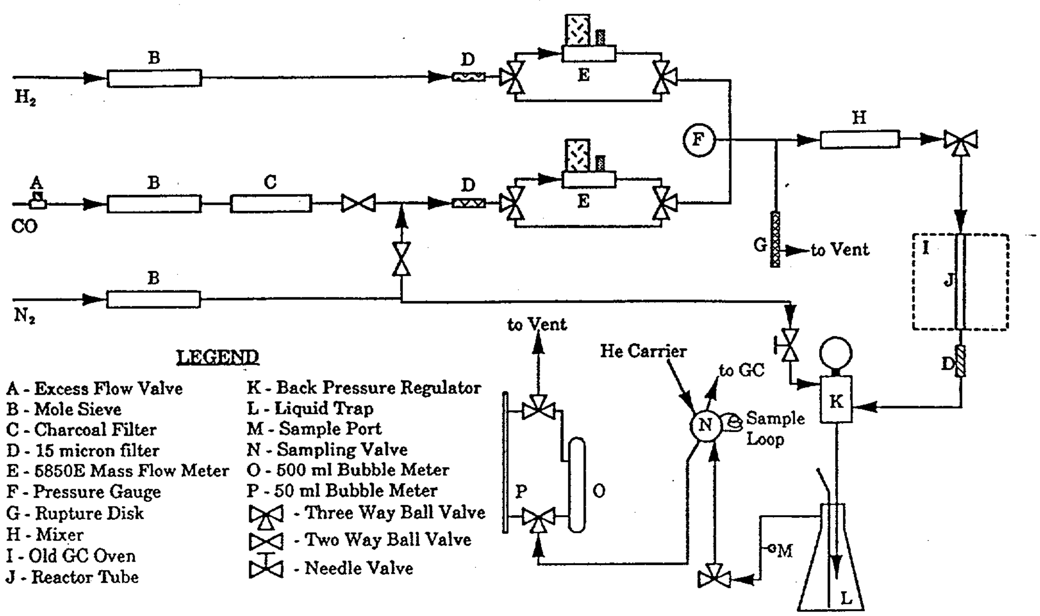

Figure 5. Schematic Diagram of Bench Top Reactor System #1.

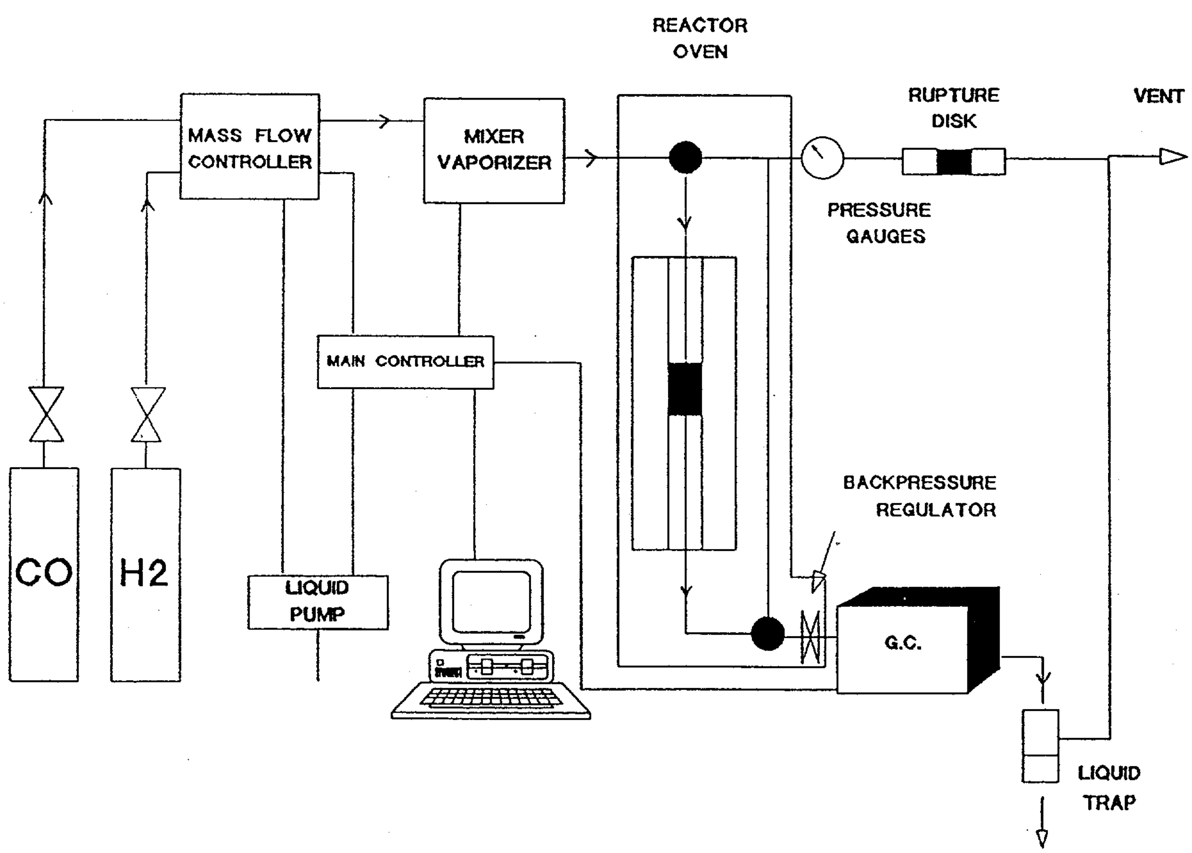

Figure 6. Schematic Diagram of AE MSBTR 900 (Formerly CDS 900) Reactor System

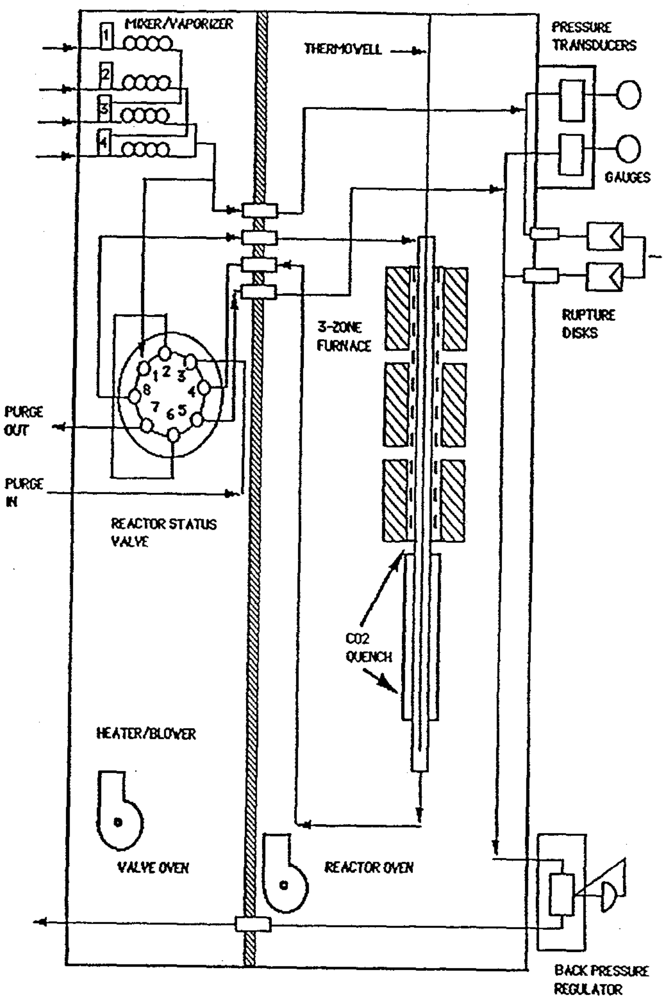

Figure 7. Reactor, Reactor Oven and Switching Valve Oven for AE MSBTR 900

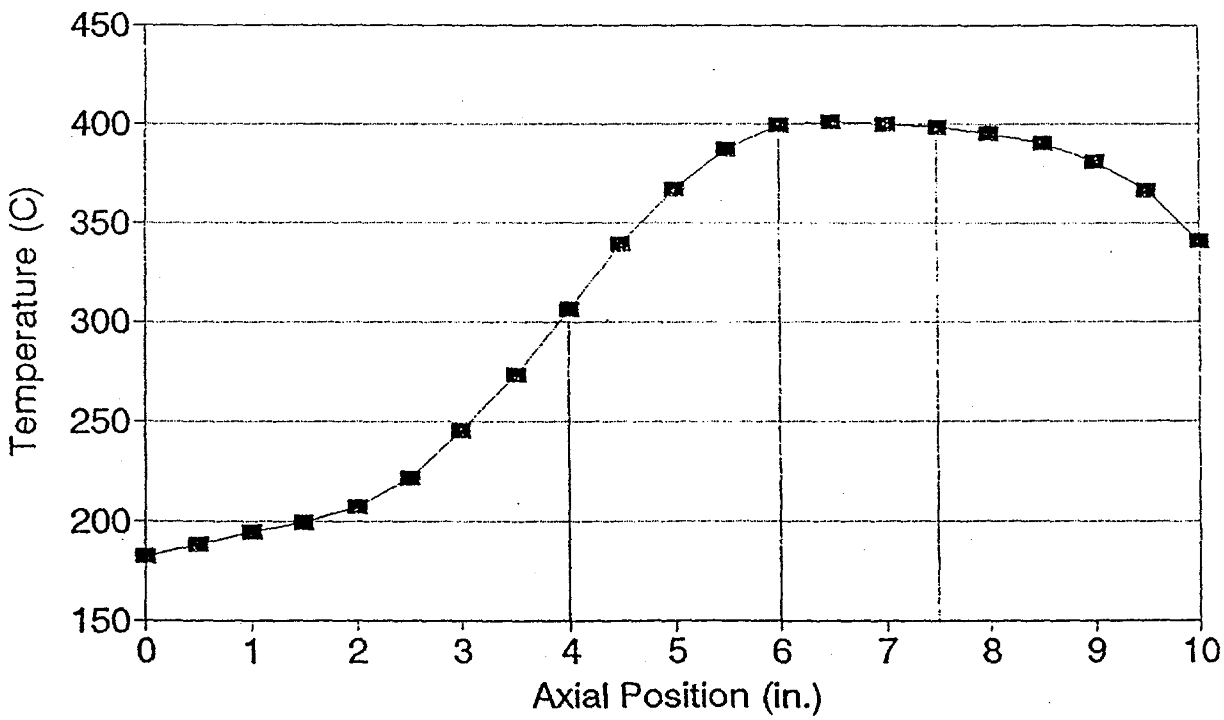

Figure 8. Typical Temperature Profile in the Reactor

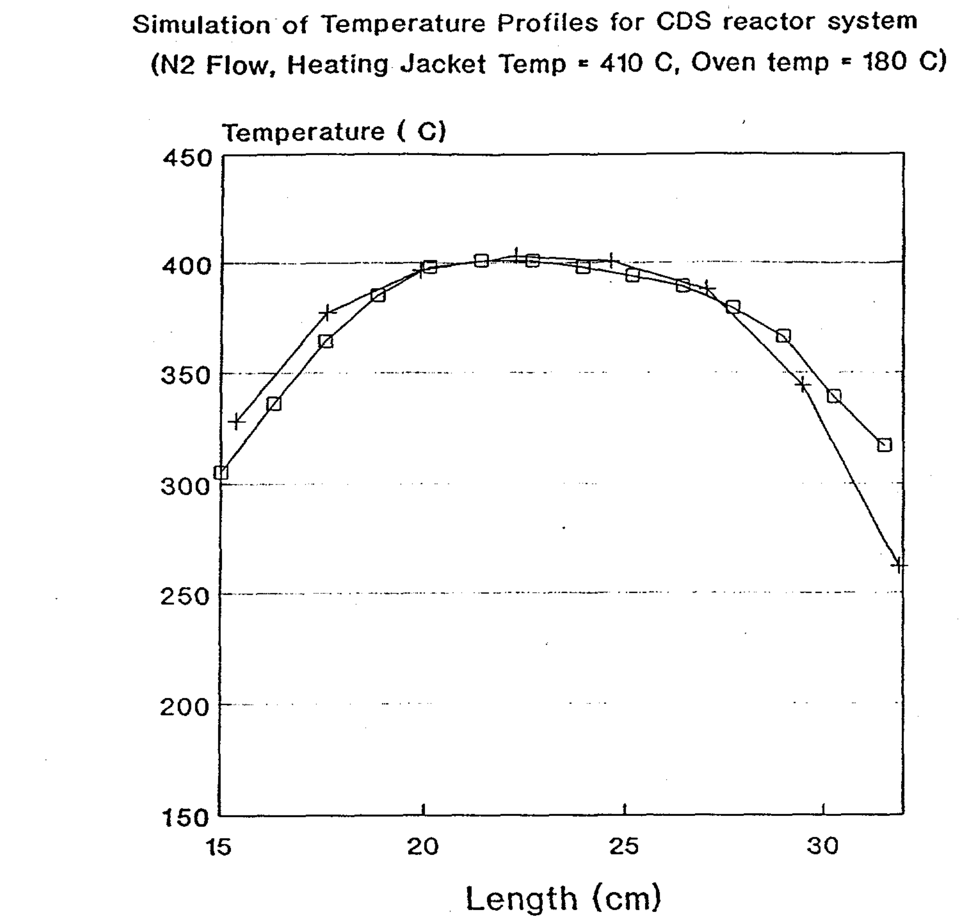

Figure 9. Actual and Calculated (Simulated) Reactor Profile for AE MSBTR 900

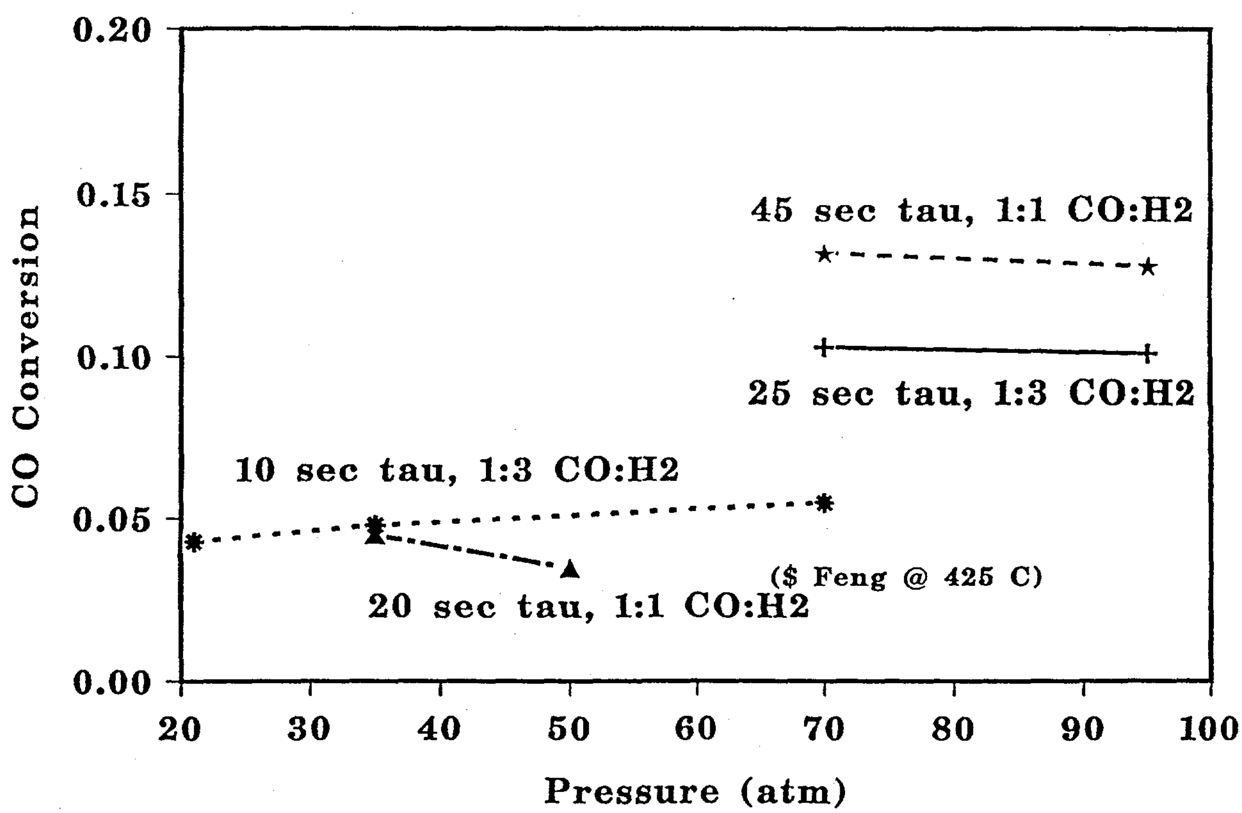

Figure 10. Activities and Effect of Pressure on Activity for Catalysts #1 and #2. (Cat. 2 is indicated by the ($ Feng @ 425 °C).).

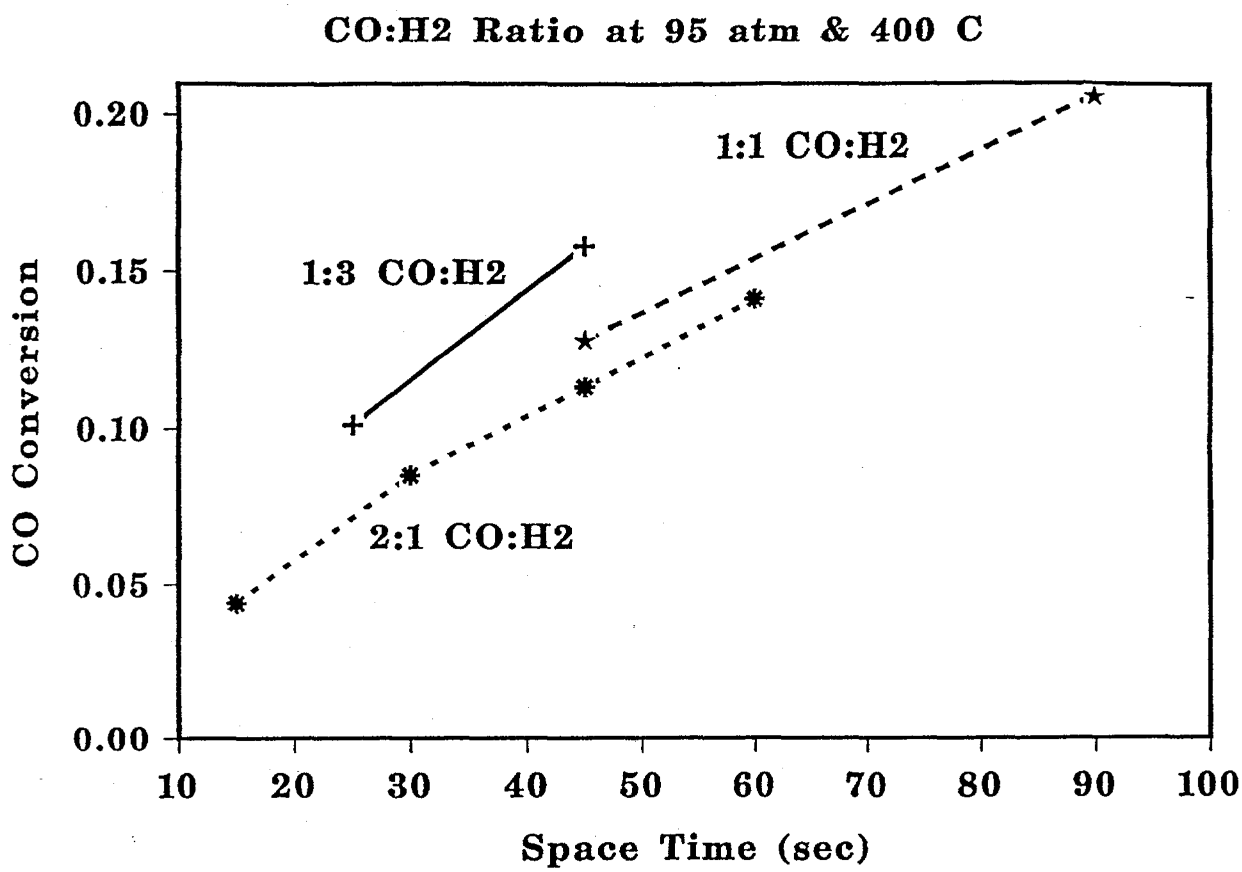

Figure 11. Activity as a Function of Space Time and Feed Ratios for Cat. #1.

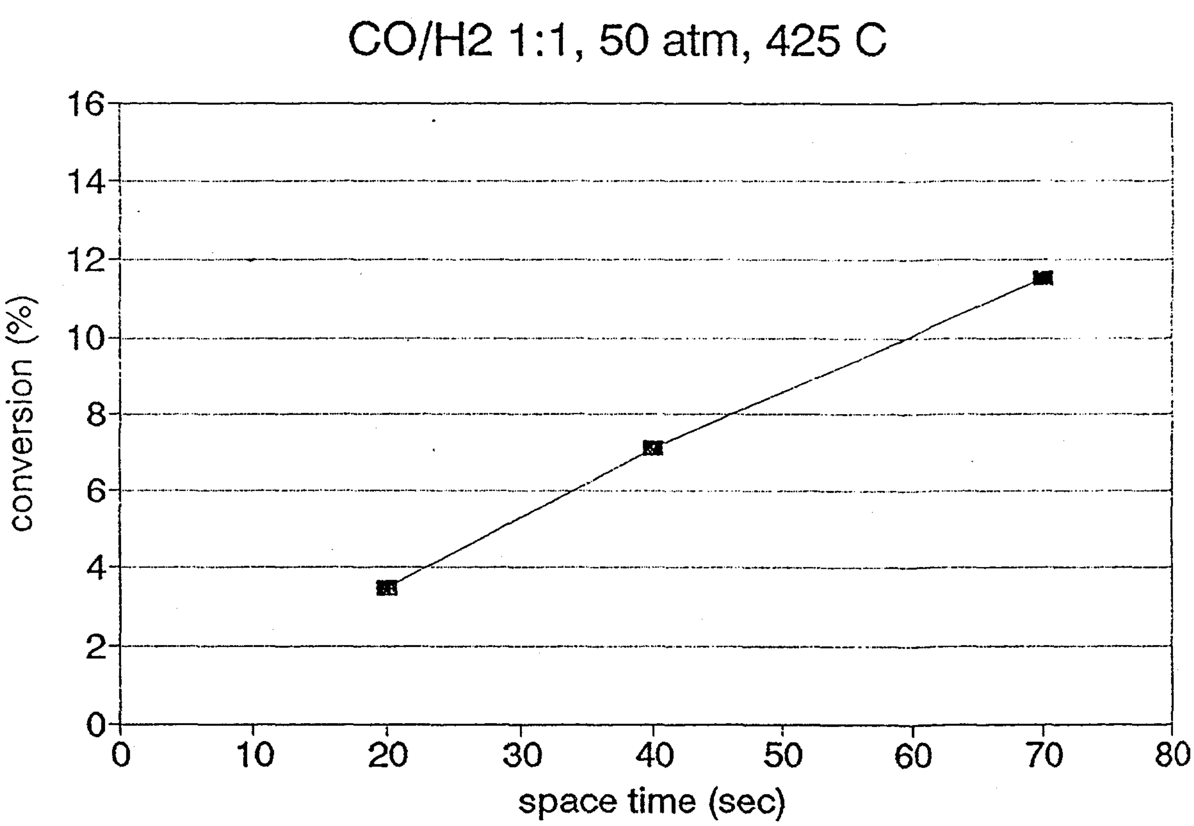

Figure 12. Activity of Catalyst #2.

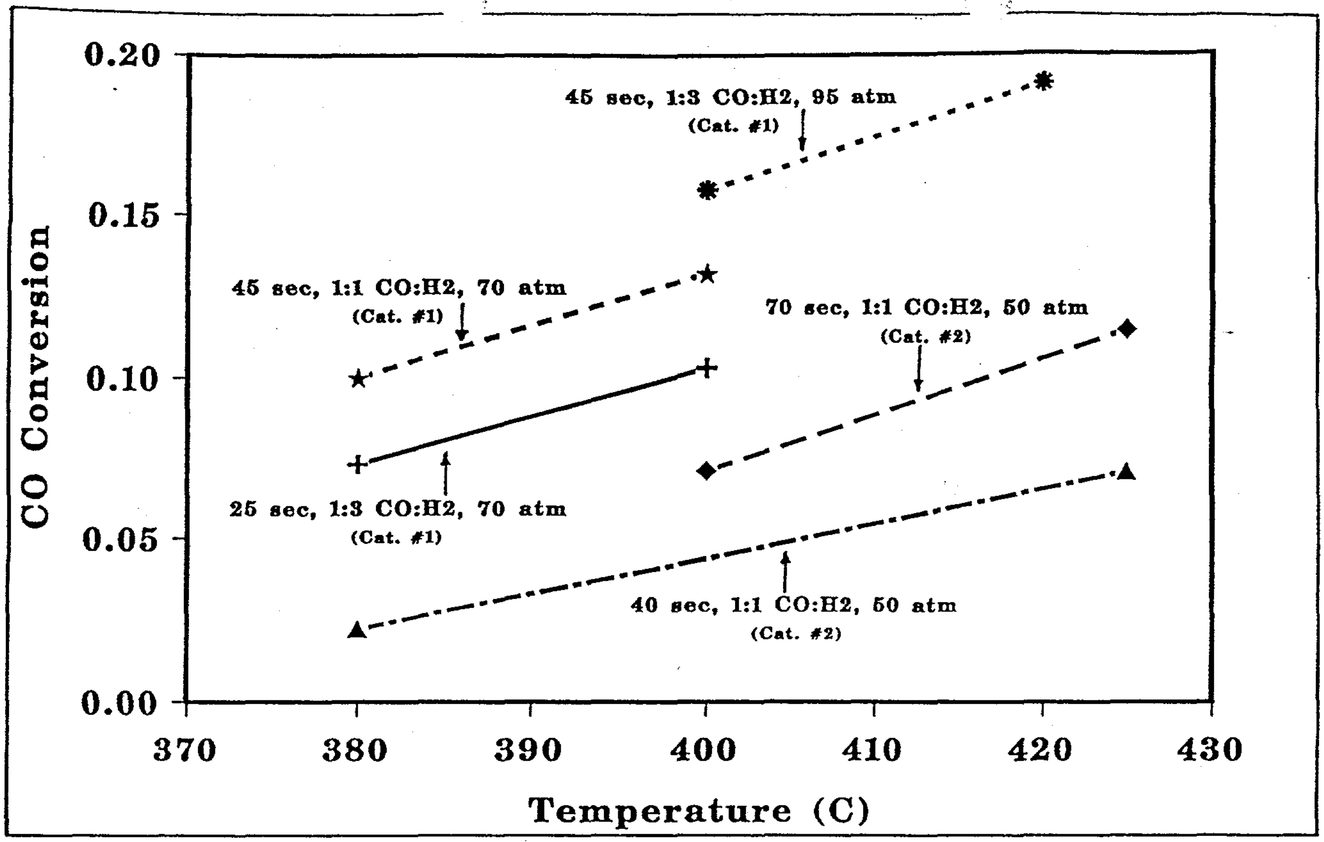

Figure 13. Comparison of Activities of Catalyst 1 and 2. Trends with respect to temperature are the same.

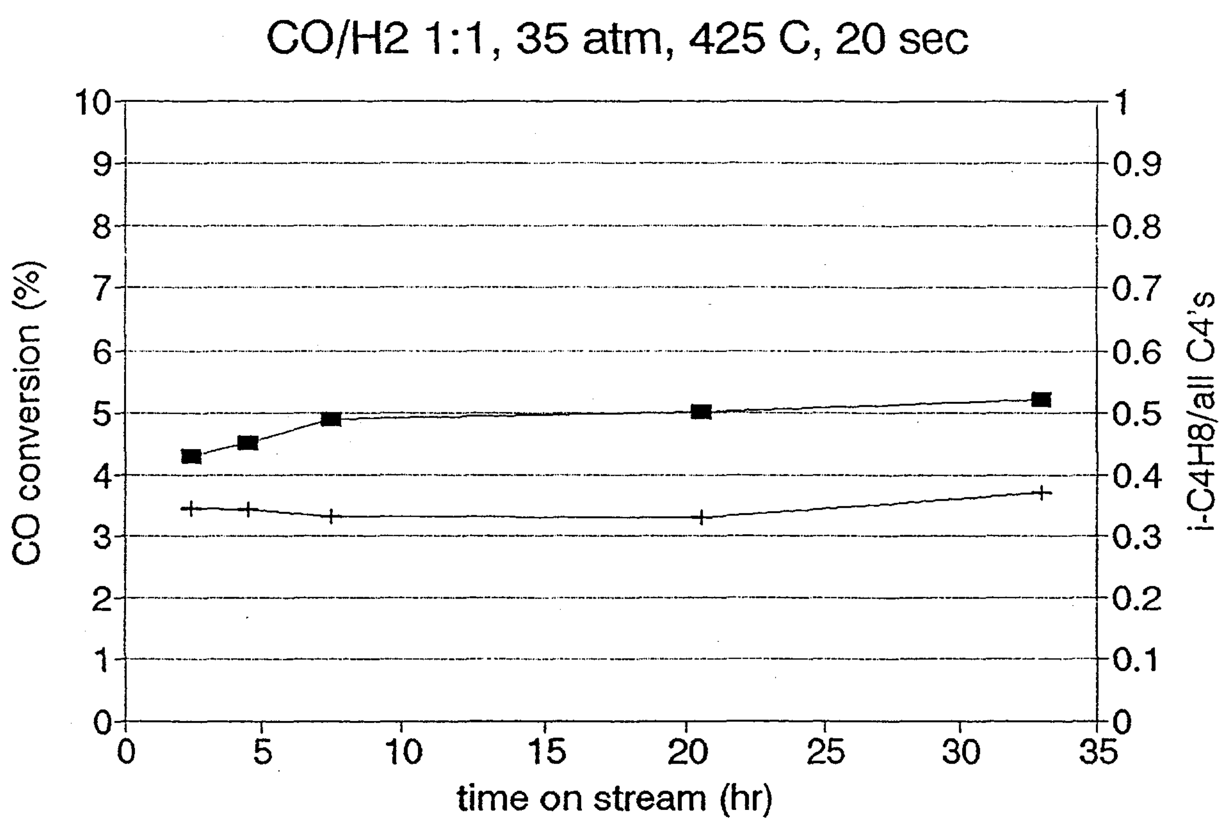

Figure 14. Selectivity and Conversions for Cat. 2 with Time on Stream.

ALKANES

$$CO + \{(n+1)/2n\}\ H_2 = \{1/2n\}\ C_nH_{2n+2} + 0.5\ CO_2$$

$$CO + \{(2+1/n\}\ H_2 = \{1/n\}\ C_nH_{2n+2} + H_2O$$

OLEFINS

$$CO + 0.5\ H_2 = \{1/2n\}\ C_nH_{2n} + 0.5\ CO_2 \qquad n > 1$$

$$CO + 2\ H_2 = \{1/n\}\ C_nH_{2n} + H_2O \qquad n > 1$$

Figure 15. Potential Reaction Stoichiometry For Formation of Hydrocarbons.

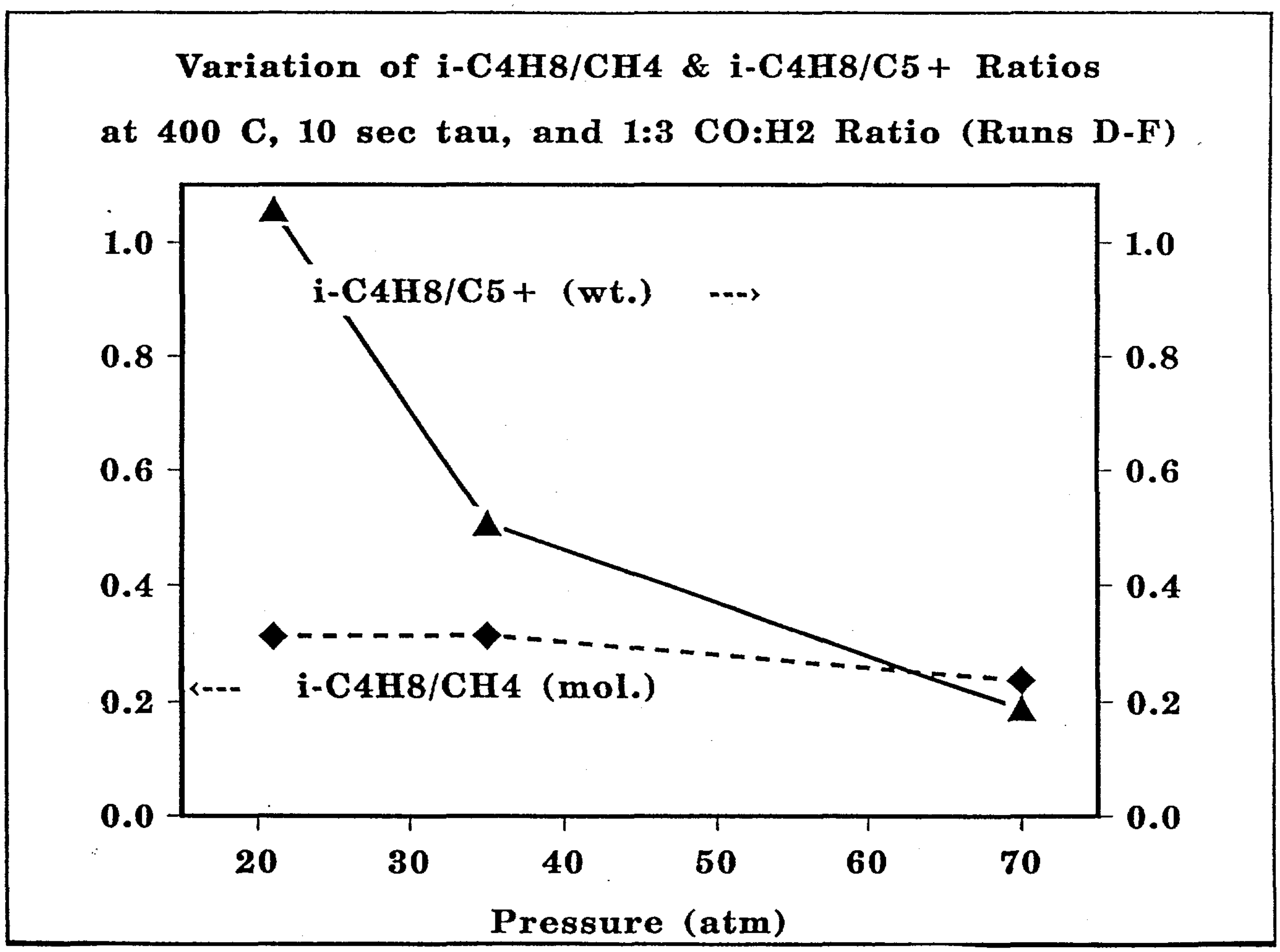

Figure 16. Effect of Pressure on Selectivities for Catalyst #1.

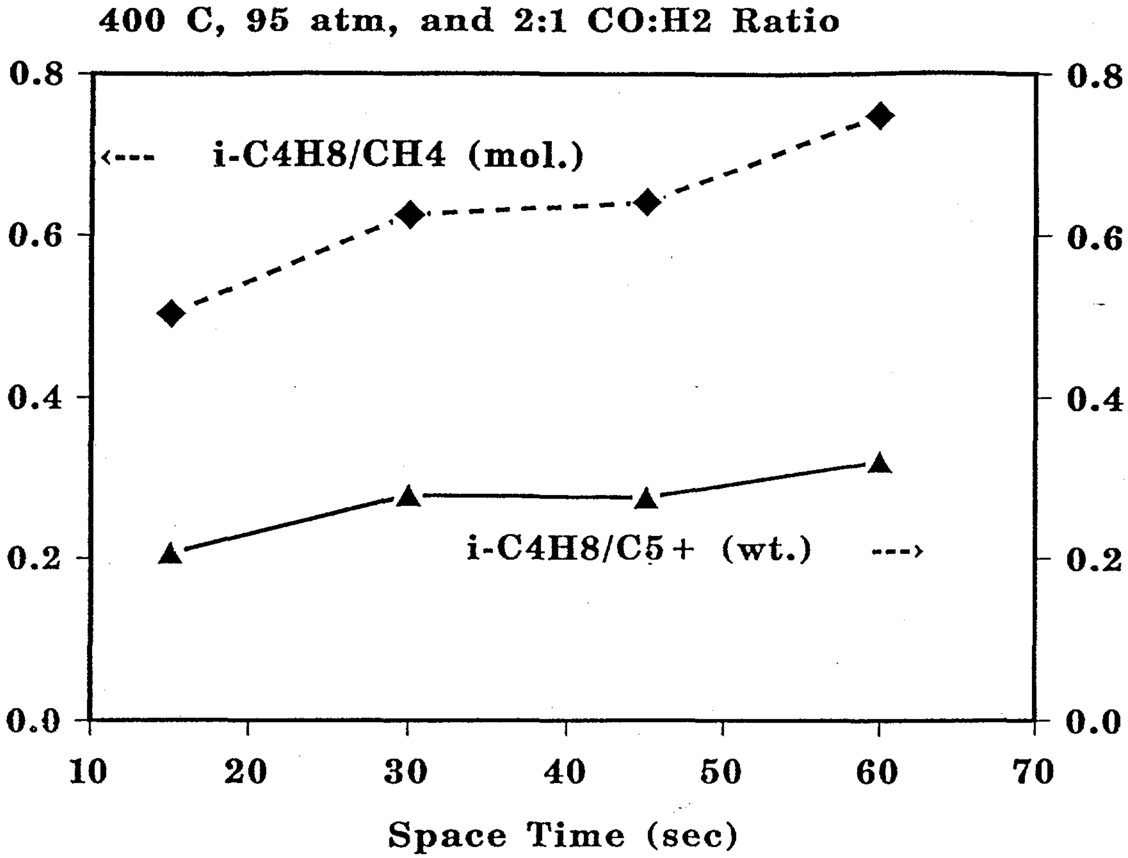

Figure 17. Selectivities For Catalyst #1.

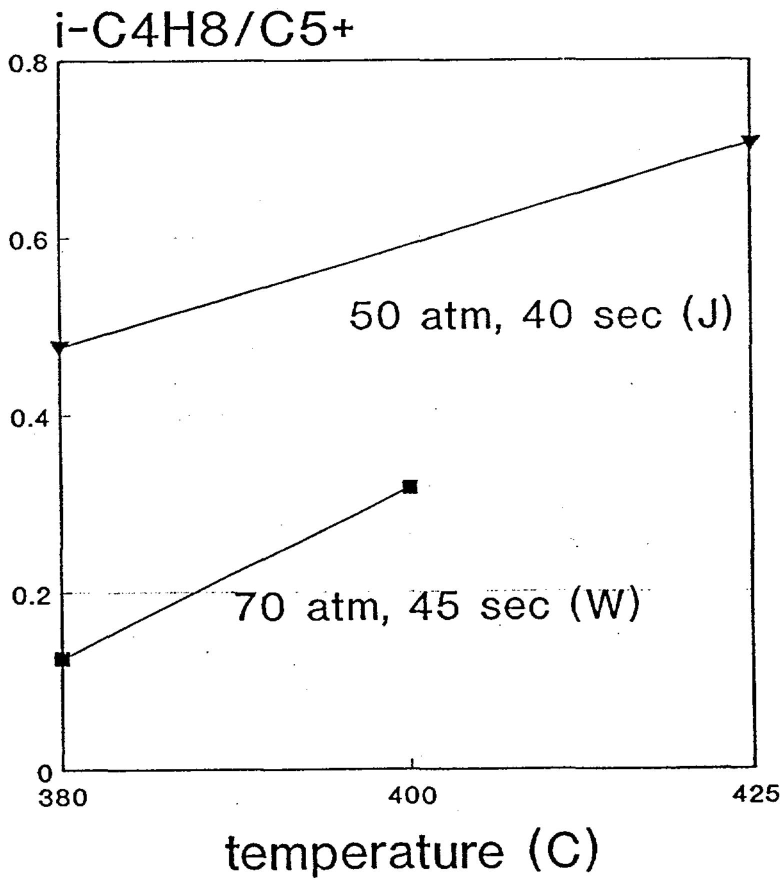

Figure 18. Weight Ratio of Isobutylene to C_5^+ Increases with Temperature For Cat. 1 and 2.

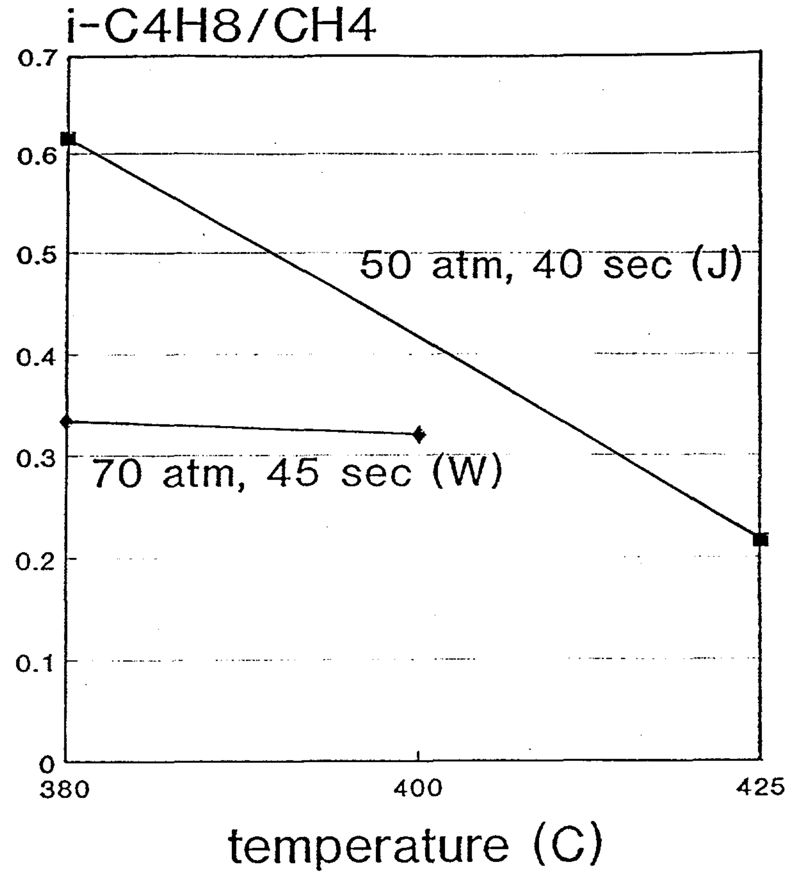

Figure 19. Weight Ratio of Isobutylene to Methane for Cat. 2 (J) and Cat. 1 (W).

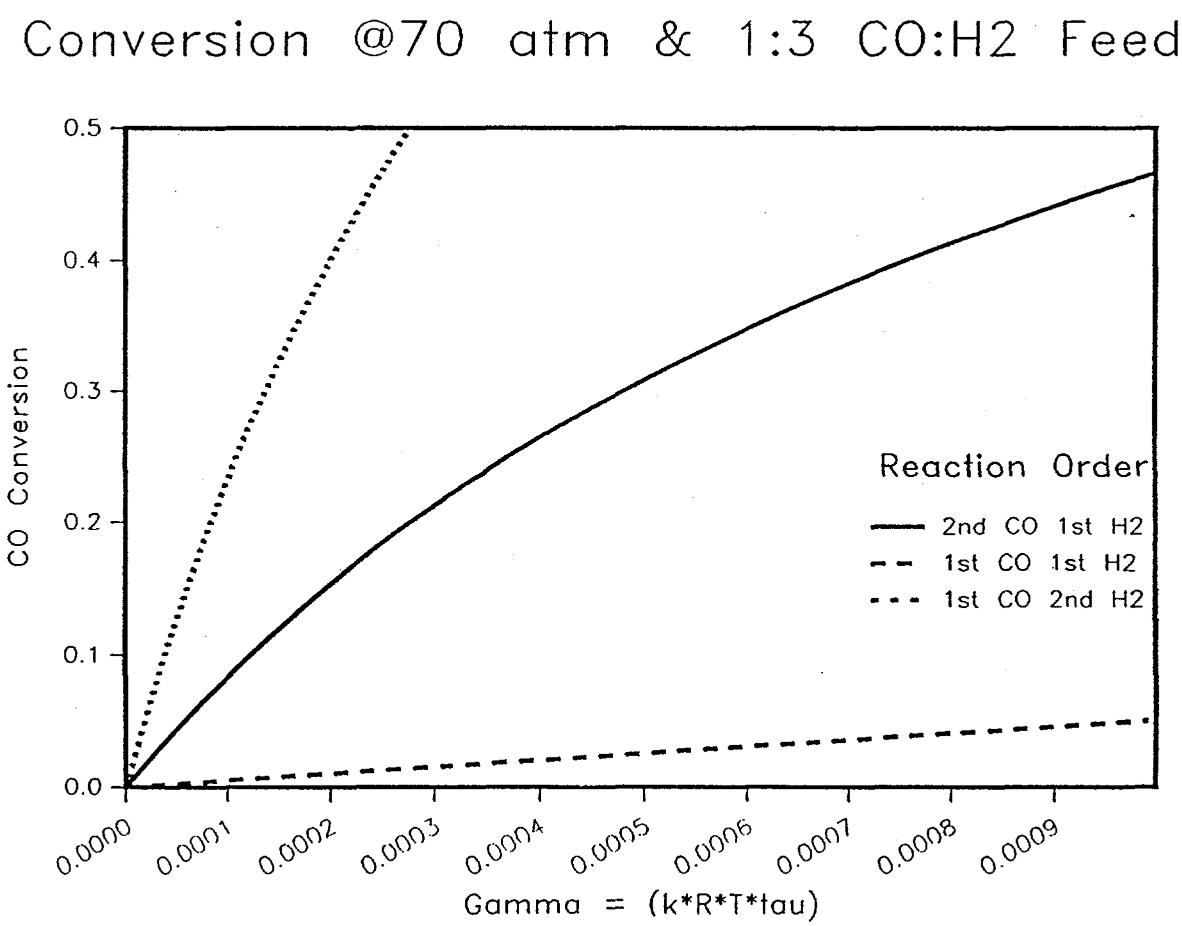

Figure 20. Calculated Conversions For Plug Flow Reactor With $CO{:}H_2$ Ratio of 1:3.

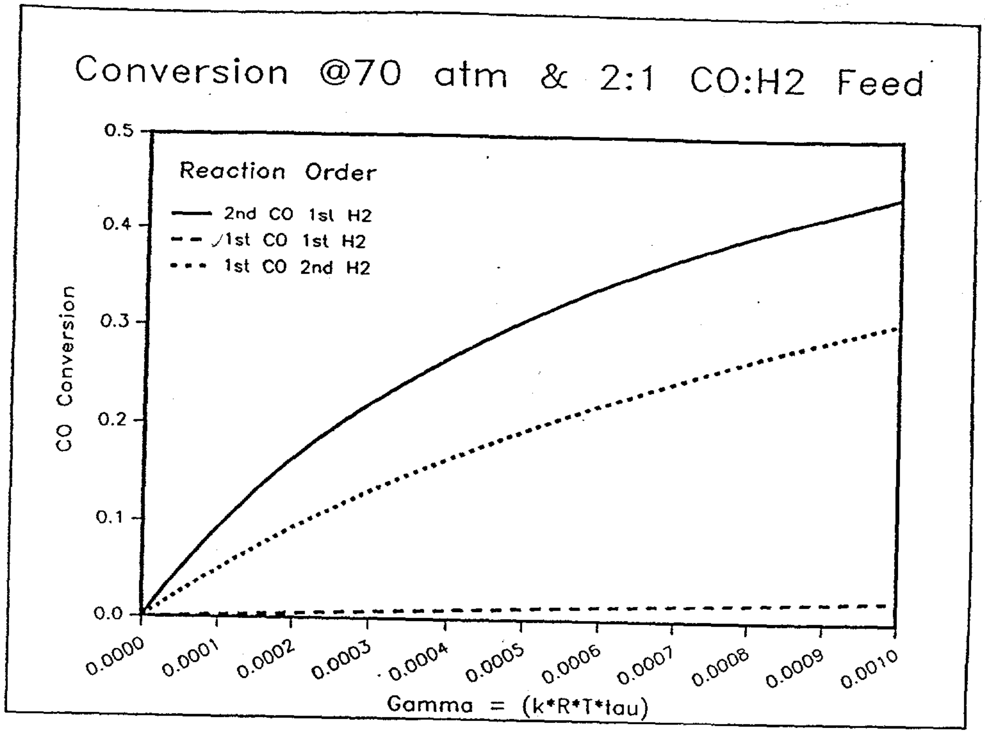

Figure 21. Calculated Conversions For Plug Flow Reactor With $CO:H_2$ Ratio of 2:1.

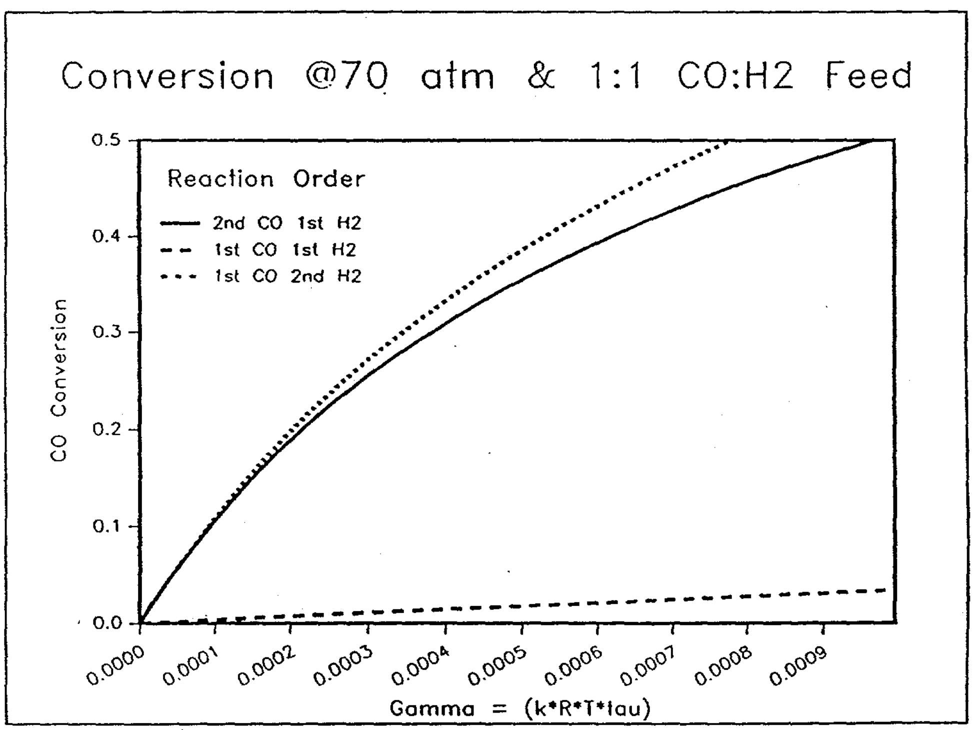

Figure 22. Calculated Conversions For Plug Flow Reactor With $CO:H_2$ Ratio of 1:1.

TRICKLE BED REACTOR MODEL

A two—dimensional three—phase isothermal trickle bed reactor with axial mixing, flux boundary conditions and a nonlinear reaction

$$A + B \rightleftharpoons C$$

The gas phase

$$\frac{\partial Y}{\partial Z} + F_L \cdot W^o \cdot \left(\frac{K}{H} \cdot Y - X\right) + (1-f) \cdot F_{gs} \cdot W^o \cdot \left(\frac{K}{H} \cdot Y - X_s\Big|_{U=1}\right) = 0$$

The liquid phase

$$\frac{\partial^2 X}{\partial Z^2} - P_{el} \cdot \frac{\partial X}{\partial Z} + P_{el} \cdot F_L \cdot \left(\frac{K}{H} \cdot Y - X\right) - f \cdot P_{el} \cdot F_{ls} \cdot \left(X - X_s\Big|_{U=1}\right) = 0$$

The solid phase

$$U \cdot \frac{\partial^2 X_s}{\partial U^2} + \frac{3}{2} \cdot \frac{\partial X_s}{\partial U} = \frac{1}{4} \cdot \mathcal{R}$$

with

$$\mathcal{R}_i = D_{f_i} \cdot \prod_i X_{s,i}^{a_i} - D_{bi} \cdot \prod_i X_{s,i}^{b_i}$$

Where
X and Y are dimensionless concentration vectors.
With boundary condition

$$Y_i\Big|_{Z=0^+} = Y_i\Big|_{Z=0^-}$$

$$X_i\Big|_{Z=0^+} = X_i\Big|_{Z=0^-} - \frac{1}{P_{el}} \cdot \frac{\partial X_i}{\partial Z}$$

$$\frac{\partial X_i}{\partial Z}\Big|_{Z=1} = 0$$

$$\frac{\partial X_{si}}{\partial U}\Big|_{U=0} = finite$$

$$\frac{\partial X_{si}}{\partial U}\Big|_{U=1} = \frac{1}{2} \cdot f \cdot Sh_{lsi} \cdot \left(X_i - X_{si}\Big|_{U=1}\right) + \frac{1}{2} \cdot (1-f) \cdot Sh_{gsi} \cdot \left(\frac{K}{H_i} \cdot Y_i - X_{si}\Big|_{U=1}\right)$$

Figure 23. Trickle Bed Reactor Model In Dimensionless Variables.

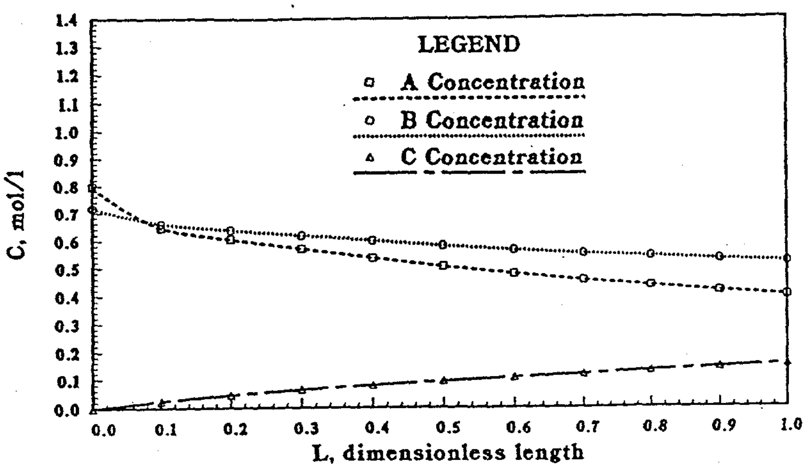

Figure 24. Calculated Gas Phase Profile For Model Presented in Figure 23.

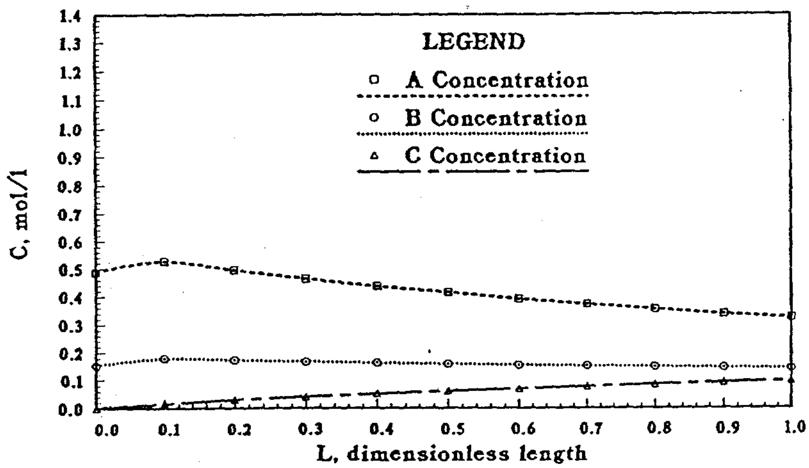

Figure 25. Calculated Liquid Phase Profile For Model Presented in Figure 23.

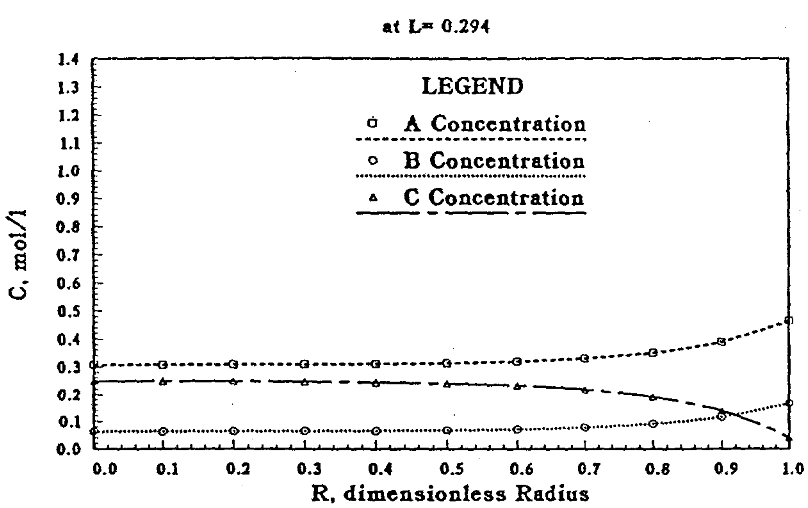

Figure 26. Calculated Solid Phase Profile For Model Presented in Figure 23 and Resistance to Pore Diffusion.