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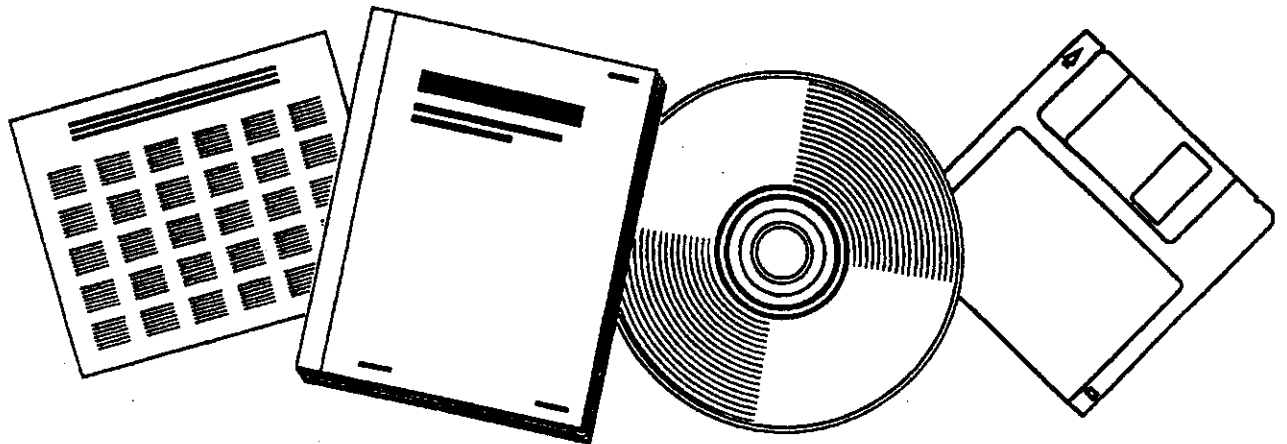
FISCHER-TROPSCH SLURRY PHASE PROCESS VARIATIONS TO UNDERSTAND WAX FORMATIONS: QUARTERLY REPORT, JANUARY 1, 1988-MARCH 31, 1988

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Fischer-Tropsch Slurry Phase

Process Variations to Understand

Wax Formations

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Summary

A method has been developed for calculating the three parameters needed to characterize the carbon number distribution of products of the Fischer-Tropsch synthesis. Using non-linear regression, experimental data are fit by a modified Schulz-Flory model which has two chain growth probabilities. Excellent fit is shown for data from precipitated and fused iron catalysts.

The model is used to calculate selectivity information of interest in catalyst comparison and reactor design. Advantages of this model over asymptotic regression methods are discussed in detail.

Introduction

The products of the Fischer-Tropsch synthesis are primarily linear hydrocarbons distributed over a wide range of carbon numbers. Herington (1946) reported that a model of stepwise addition of single-carbon units could predict the fraction of product at each carbon number. This and other early treatments discussed by Anderson, at al. (1951) are formulations of a condensation polymerization model developed independently and in another context by Schulz (1935) and Flory (1936). These matters are discussed in detail by Satterfield and Huff (1982). In its simpler forms, the model suggests that a semi-logarithmic plot of mole fraction of product as a function of carbon number should produce a straight line with a slope characteristic of the chain growth probability, α. Anderson, et al. (1951) developed a more detailed treatment which also considered isomer distributions.

In extensive studies of six iron catalysts in a German pilot plant in 1943, the "Schwarzheide tests", an increase or "break" in the slope of Schulz-Flory plots was observed at a carbon number of about 10. This phenomenon received little further attention until recently, when several investigators reported the same effect under a variety of conditions, suggesting it may be a rather general phenomenon. Two chain growth probabilities have been observed on iron catalysts by König and Gaube (1983), Huff and Satterfield (1984), Schliebs and Gaube (1985), Egiebor, et al. (1985), and Dictor and Bell (1986), on cobalt by Schulz et al. (1982), and on ruthenium by Inoue et al. (1987).

The causes of two probabilities for chain growth, frequently termed the "double-α", are unclear, but an understanding of these causes might provide insights into methods for altering the Fischer-Tropsch product distribution. König and Gaube suggest that two sites, one promoted by potassium and the other unpromoted, may cause such behavior. However, Dictor and Bell (1986) and recent data from this

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laboratory indicate that two chain growth probabilities exist even on catalysts not promoted by potassium.

It is not easy to determine the experimental product distribution accurately over a wide range of carbon numbers. Matsumoto and Satterfield (in prep.) discuss how calculated values of α may be affected by the selection of data used in calculations. Here, we develop and present a more general model for calculating the correct values of α from data which includes contributions by both chain growth probabilities. The model is not based on any assumptions about the cause of the double-α.

Previous attempts to model Fischer-Tropsch product distributions with multiple values of α have several limitations. Rice and Wojciechowski (1987) have presented a comprehensive analysis of such product distributions. By assuming that the products at each carbon number are of uniform molecular weight, they remove the difficulty of dealing with variations in alkene/alkane ratio with carbon number. We follow a similar assumption here. They develop an equation providing for contributions from two chain growth probabilities. By differentiating this equation, they establish relationships between the observed product distribution and α_1 and α_2. Their model, however. does not provide a tractable method for rigorously determining α_1 and α_2 from experimental data, because it depends on numerical or graphical differentiation to estimate "local alphas" at each carbon number.

König and Gaube (1983) and Schliebs and Gaube (1985) appear to use normalized weight fractions. rather than absolute mole fractions to determine the values of the chain growth probabilities. This may lead

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to errors in the values of α and, in some cases, failure to describe the distribution of heavier products correctly.

Stenger (1985) extended König and Gaube's theory that potassium causes multiple chain growth probabilities in a model that describes α as a function of local potassium loading, with a Gaussian-type distribution of potassium on the surface. Inoue et al. (1987) have shown that distributed-α and double-α models, each having three adjustable parameters, can only be distinguished if reliable data at high carbon numbers are available. Accurate data at high carbon numbers may be difficult to obtain (Huff, 1982; Matsumoto and Satterfield, in prep.).

Novak et al. (1981, 1984) develop several models for deviations from Schulz-Flory distributions. In particular, they present a model based on two active sites, one for hydrocarbon growth and the other for cracking. However, Schulz, et al. (1970) and Pichler and Schulz (1970) have reported that cracking is not significant on iron or cobalt catalysts under the usual conditions of Fischer-Tropsch synthesis. Novak's model requires four adjustable parameters as well as knowledge of surface rates and intermediates which is difficult to obtain experimentally.

The most straightforward method for determining α_1 and α_2 from experimental data would seem to be linear regression of the asymptotes of a Schulz-Flory plot. Figure 1 shows a typical Schulz-Flory diagram from a potassium promoted precipitated iron catalyst. The diagram shows two distinct slopes. However, even several carbon numbers away from the intersection of the two lines, the values of α_1 and α_2

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determined by linear regression are in error by 5 to 10%, demonstrating that simple linear regression is inappropriate.

The model presented in this paper offers a method for determining α_1 and α_2 from rigorous statistical techniques. The error produced in analyzing data by linear regression is discussed. In calculating α_1 and α_2, this method uses the entire experimental product distribution including those points between the asymptotes. Excellent agreement between the model and experimental data from iron catalysts is shown. For a precipitated iron catalyst, experimental data from an overhead product stream are fit by the model and the value of α_2 is shown to agree with that calculated from a slurry wax sample. In addition, product stream data from a fused iron catalyst are fit.

The regression technique assumes no mechanistic explanation for the double-α. For the purposes of this model, α is considered to be the probability that a C_n species will go on to become a C_{n+1} species. In the simplest case, with no products re-adsorbing and incorporating into growing chains and with no branching, this definition of α reduces to the traditional definition of $r_p/(r_p+r_t)$, where r_p and r_t are the rates of chain propagation and termination, respectively.

Development of the Model

As discussed above, the hydrocarbon products of Fischer-Tropsch are generally taken to follow the Schulz-Flory distribution. For carbon number n, the mole fraction of product M_n, as determined by a single chain growth probability, is given by:

$$M_n = (1-\alpha) \, \alpha^{(n-1)} \tag{1}$$

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Normally, product mole fractions are plotted on a semi-logarithmic scale since the chain-growth probability α can be calculated from the slope of such a plot. Again, for a single-α:

$$\ln(M_n) = n \ln(\alpha) + \ln[(1-\alpha)/\alpha)] \tag{2}$$

If two chain growth probabilities contribute to the total product distribution, the appropriate equation is:

$$M_n = A \alpha_1^{(n-1)} + B \alpha_2^{(n-1)} \tag{3}$$

The values of A and B must be known to characterize the product distribution. First, the ratio of A to B is found by noting that at the break point on the Schulz-Flory diagram the contributions of each term in equation (3) are equal.

$$A \alpha_1^{(n-1)} = B \alpha_2^{(n-1)} \tag{4}$$

If ξ is designated as the break point, then:

$$B = A (\alpha_1/\alpha_2)^{(\xi-1)} \tag{5}$$

ξ is not necessarily an integral carbon number. This is a somewhat different approach than has been taken previously by Schliebs and Gaube (1985) and by Huff (1982). In their models, A and B were assumed to correspond directly to the fractions of products produced from α_1 and α_2 respectively. Instead it is noted that, since the sum of the mole fractions over all carbon numbers is unity,

$$\sum_{n=1}^{\infty} M_n = \sum_{n=1}^{\infty} [A \alpha_1^{(n-1)} + B \alpha_2^{(n-1)}] = 1 \tag{6}$$

Evaluating the geometric series, this equation can be expressed as:

$$A [1/(1-\alpha_1)] + B [1/(1-\alpha_2)] = 1 \tag{7}$$

Equations (5) and (7) are two linearly independent equations which are used to solve explicitly for the values of A and B:

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$$A = \frac{1}{1/(1-\alpha_1) + (\alpha_1/\alpha_2)^{(\xi \cdot 1)}[1/(1-\alpha_2)]} \qquad (8)$$

B is then calculated from equation (5). This method places no artificial constraints on the system. The equations presented above allow computation of theoretical product distributions based on chosen values of α_1, α_2, and ξ.

Differentiating the logarithm of equation (3) with respect to carbon number, it is possible to obtain a "local alpha", α_{loc}, which is the slope of the Schulz-Flory curve and is a function of carbon number. This slope accounts for contributions by both chain-growth probabilities.

$$\alpha_{loc}(n) = \exp\left[\frac{d}{dn}[\ln(M_n)]\right] = \exp\left[\frac{\ln(\alpha_1) + (\alpha_2/\alpha_1)^{(n-\xi)}\ln(\alpha_2)}{1 + (\alpha_2/\alpha_1)^{(n-\xi)}}\right] \qquad (9)$$

At low carbon numbers, the local alpha approaches α_1 and, at high carbon numbers, it approaches α_2. The differences between local alphas and the true values of α_1 and α_2 in the region near the break point cannot be eliminated experimentally. Figure 2 shows how the ratios α_{loc}/α_1 and α_{loc}/α_2 vary with distance from the break point, $(n-\xi)$, for values of $\alpha_1/\alpha_2=0.5$ and $\alpha_1/\alpha_2=0.7$.

By iteratively calculating distributions based on different combinations of α_1, α_2 and ξ and comparing them to experimental data, the best fit theoretical distribution can be determined. The method used here is minimization of the sum of square errors as recommended for this type of regression by Churchill (1979) and given below:

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$$\Phi = \sum_{n=3}^{N} [\ln(M_n) - \ln(m_n)]^2 \qquad (10)$$

Here, M_n is the theoretical mole fraction of product at C_n and m_n is the experimental value. The summation is taken from C_3 to C_N, where N is the highest carbon number at which reliable data are available. The sum begins at C_3, since experimentally obtained C_1 and C_2 products frequently do not obey a Schulz-Flory model (König and Gaube, 1983; Rice and Wojciechowski, 1987).

At higher carbon numbers, experimental uncertainties may be introduced in continuous-flow slurry and fixed-bed reactor systems. In fixed beds, less volatile products accumulate throughout the bed and, specifically, in catalyst pores. Huff and Satterfield (1985) give theoretical analyses regarding the time-on-stream necessary for the exit stream to be truly representative of the products being synthesized.

In slurry reactors, non-volatile products are retained in the slurry liquid. Volatile products are flashed overhead, but a significant fraction, particularly in the range C_{15} to C_{25}, is distributed between the two phases in a manner that changes with time-on-stream (Huff and Satterfield, 1984). Experimental data are usually based on volatile overhead products, occasionally supplemented by analysis of slurry liquid. Higher molecular weight products require longer time-on-stream to reach vapor-liquid equilibrium. Thus, N is the carbon number above which product distributions are observed to change with time-on-stream. This point can be affected by such variables as catalyst activity, catalyst loading, and reaction

temperature. Huff (1982) indicates that for representative experimental conditions, apparent deviations from the Schulz-Flory diagram may be expected for products above roughly C_{15}.

Removing C_1 and C_2 products to fit theoretical distributions to data leads to the following modifications to equations (6) and (8):

$$\sum_{n=3}^{\infty} M_n = \sum_{n=1}^{\infty} [A \, \alpha_1^{(n-1)} + B \, \alpha_2^{(n-1)}] - A(1+\alpha_1) - B(1+\alpha_2) \qquad (6a)$$

or

$$\sum_{n=3}^{\infty} M_n = 1 - m_1 - m_2 \qquad (6b)$$

and

$$A = \frac{1 - m_1 - m_2}{[1/(1-\alpha_1) - (1+\alpha_1) + (\alpha_1/\alpha_2)^{(\zeta-1)}[1/(1-\alpha_2) - (1+\alpha_2)]} \qquad (8a)$$

B is still calculated from equation (5).

There are at least two distinct advantages of this type of model over those presented previously. First, the model provides a deterministic method of calculating α_1 and α_2 from experimental data. An alternative method, presented by Rice and Wojciechowski (1987) involves first fitting the asymptotic tail of the data, then subtracting the α_2 contribution from the total product distribution; however, their method depends on having reliable data at high carbon numbers to determine the value of α_2, and as discussed above, such data may be difficult to obtain. In addition, their method involves graphical differentiation, which makes calculations very sensitive to any scatter in the experimental data.

A second advantage of our model is that it allows inclusion of all

reliable product distribution data, including that near ξ, which cannot be used in asymptotic fitting methods (König and Gaube, 1983; Inoue, et al., 1987). As mentioned, when volatile products of the synthesis are used to determine product distributions, vapor-liquid equilibrium effects cause the Schulz-Flory model to deviate from data at carbon numbers greater than roughly C_{15} (Huff, 1982). Inclusion of, for example, C_7 to C_{14} mole fractions effectively doubles the quantity of data which can be used to calculate chain growth probabilities. Three parameters are needed to characterize the system (König and Gaube, 1983; Schliebs and Gaube, 1985; Stenger, 1985; Rice and Wojciechowski, 1987). Additional points in the analysis greatly improve the statistical significance of the regression.

The regression routine allows selective exclusion of individual data points within a given carbon number range. There are at least two instances in which this feature is useful. First, if hydrocarbons of a given carbon number are deliberately added to the synthesis gas feed, the data from that carbon number may be excluded from the fitting routine. Second, if an impurity of some sort is known to occur at a given carbon number, the data from that carbon number need not be regressed.

Results

I. Comparison with Experimental Data

The ability of this model to describe product distributions correctly on potassium promoted fused iron and unpromoted precipitated iron catalysts is shown in Figure 3. The data were collected in a

slurry reactor system described elsewhere (Huff and Satterfield, 1982, 1983; Matsumoto, 1987). The fused iron catalyst is a United Catalysts C-73 ammonia synthesis catalyst and the precipitated catalyst was prepared for this laboratory by the Pittsburgh Energy Technology Center (PETC). The compositions of the catalysts are given in Table 1. Both catalysts exhibit two chain growth probabilities. For this set of data on the fused iron catalyst, $\alpha_1-0.59$, $\alpha_2-0.90$ and ξ is about 7, and for the precipitated catalyst $\alpha_1-0.62$, $\alpha_2-0.88$ and ξ is near 7. The parameters have been optimized using C_3 to C_{16} data for the fused iron catalyst and C_3 to C_{14} data for the precipitated catalyst. The value calculated for α_2 on the precipitated catalyst matches the value determined by linear regression of the Schulz-Flory plot from a slurry wax sample. C_{30} to C_{40} data from the wax sample shown in Figure 4 indicate $\alpha_*0.88$ for this catalyst. This shows that the non-linear regression routine matches the asymptotic linear regression at high carbon numbers. The model is able to correctly fit the curve of the precipitated and fused catalysts, even though the data begin to fall off at higher carbon numbers due to vapor-liquid equilibrium effects.

II. Parametric Study on Theoretical Product Distributions

Representative values of α_1, α_2, and ξ can be used to generate theoretical product distributions, which can be used to determine selectivity to different product cuts. Generally, the product cuts of interest are methane (C_1), light gases (C_2 to C_4), gasoline (C_5 to C_{12}), diesel fuel (C_{13} to C_{20}), and wax (C_{21}^*). Figure 5a shows the yields of product cuts as functions of α_1, with α_2 and ξ held constant

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at typical values (α_2=0.90, ξ=10). The selectivity to gasoline is maximized when α_1 = 0.75. Similarly, Figure 5b shows the yields of product cuts as functions of α_2, with α_1 and ξ held constant at 0.65 and 10, respectively. The fraction of diesel fuel goes through a maximum when α_2 is near 0.93; however, the variation of the diesel cut is small, while the wax fraction increases dramatically with α_2, so the total yield of heavy products (C_{13}^*) can be increased by increasing α_2. In a practical process, diesel fuel selectivity could be maximized by maximizing α_2 and cracking waxes back to diesel range in a second stage. Similar plots have been generated for a range of values of α_1 (0.55 to 0.70), α_2 (0.80 to 0.95), and ξ (5.5 to 13), but are not shown here.

Discussion

There are several limitations to the applicability of this model. C_1 products may be synthesized by an independent mechanism and are, therefore, not subject to this model. In addition, C_2 products usually fall below the predicted Schulz-Flory value, possibly because of the high reactivity of ethene relative to other 1-alkenes. No three parameter model currently available can account for these factors. Further work is needed to describe fully Fischer-Tropsch product distributions.

This model was developed primarily for two reasons. First, no good explanation has yet been provided for the cause of the double-α, and part of the problem has been inadequate data analysis. Schliebs and Gaube (1983) have proposed a two-site mechanism in which unpromoted and potassium-promoted sites are responsible for α_1 and α_2

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respectively, but this hypothesis is not supported by their experimental evidence. Schliebs's methodology is to determine α_2 from C_{20} to C_{40} products, then to subtract the α_2 contribution from data at lower carbon numbers to determine α_1.

Schliebs and Gaube (1983) report studies on precipitated iron catalysts both with and without potassium. A catalyst without potassium appears to show a single-α distribution from carbon number data from C_3 to C_{18}, as reported in their Figure 6a for their Run 4. A catalyst containing potassium exhibited a double-α distribution as shown in their Figure 6b for their Run 14, but data for this run were available to C_{40}. However, Schliebs's thesis reports five other runs for a catalyst without potassium, in which carbon numbers up to C_{23} or C_{24} are available. Using this broader carbon number distribution, our model shows that two α values are needed to correlate the results for all five additional runs. For example, Schliebs's Run 2 is well fitted by the double-α model with $\alpha_1=0.66$ and $\alpha_2=0.83$. Figure 7 is a Schulz-Flory plot of the same data, with the values of α_1 and α_2 as given above. Deviation from a single-α begins to appear at about C_{14} and a single-α model is inadequate.

Data from our laboratory using a precipitated iron catalyst without potassium, similar to Schliebs's catalyst, also reveal a double-α (see Figures 3a and 4). Dictor and Bell (1986) and Huff and Satterfield (1984) have also previously reported two chain growth probabilities on iron and iron/manganese catalysts, neither containing potassium. This indicates clearly that the second chain growth probability is not caused by the presence of potassium on these

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catalysts. While improved mathematical treatment of data cannot explain the cause of the double-α, it can prevent some misinterpretation of data. The application of this model to data from potassium-promoted and unpromoted precipitated iron catalysts will be the subject of a subsequent paper (Donnelly and Satterfield, in prep.).

Second, and perhaps more importantly, this model presents a deterministic method for calculating the parameters needed to characterize product distributions. Values of chain growth probabilities reported previously in the literature suffer from inconsistencies in the carbon number ranges chosen for analysis and the methods used to regress the data. This model allows easy and consistent regression of experimental data. Use of points between the asymptotes on the Schulz-Flory diagram significantly increases the data available for regression and removes the sensitivity of calculated values of α_1 and α_2 to local scatter of data. This modified Schulz-Flory model thus provides a rigorous and accurate method for predicting and analyzing Fischer-Tropsch product distributions.

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Nomenclature

A	coefficient of α_1 in double-α model
B	coefficient of α_2 in double-α model
C_n	n^{th} carbon number
m_n	experimental mole fraction of products at carbon number n
M_n	theoretical mole fraction of products at carbon number n
n	carbon number
N	carbon number of termination of reliable experimental data
r_p	rate of chain propagation
r_τ	rate of chain termination
α	single chain growth probability
α_1	first chain growth probability
α_2	second chain growth probability
$\alpha_{loc}(n)$	local chain growth probability
ξ	carbon number of break point
Φ	sum of squared errors of log arithmetic differences

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Figure 1:   Schulz-Flory Diagram from a Potassium-Promoted
Precipitated Iron Catalyst

Figure 2:   Effect of Carbon Number from Break on α_{loc}/α_1 or α_{loc}/α_2

Figure 3a: Schulz-Flory Distribution from
Precipitated Iron Catalyst without Potassium
Model versus Data

Figure 3b: Schulz-Flory Distribution from
Potassium-Promoted Fused Iron Catalyst
Model versus Data

Figure 4:   Products in Slurry Wax from
Precipitated Iron Catalyst without Potassium
Linear Regression

Figure 5a: Dependence of Selectivity on α_1
$\alpha_2 = 0.90$; $\zeta = 10$

Figure 5b: Dependence of Selectivity on α_2
$\alpha_2 = 0.90$; $\zeta = 10$

Figure 6:   Schulz-Flory Distribution from
Precipitated Iron Catalyst without Potassium
Model versus Data from Schliebs (1984) Run 2

Product Distribution
from Potassium-Promoted Precipitated Iron Catalyst
with Asymptotic Regression Lines
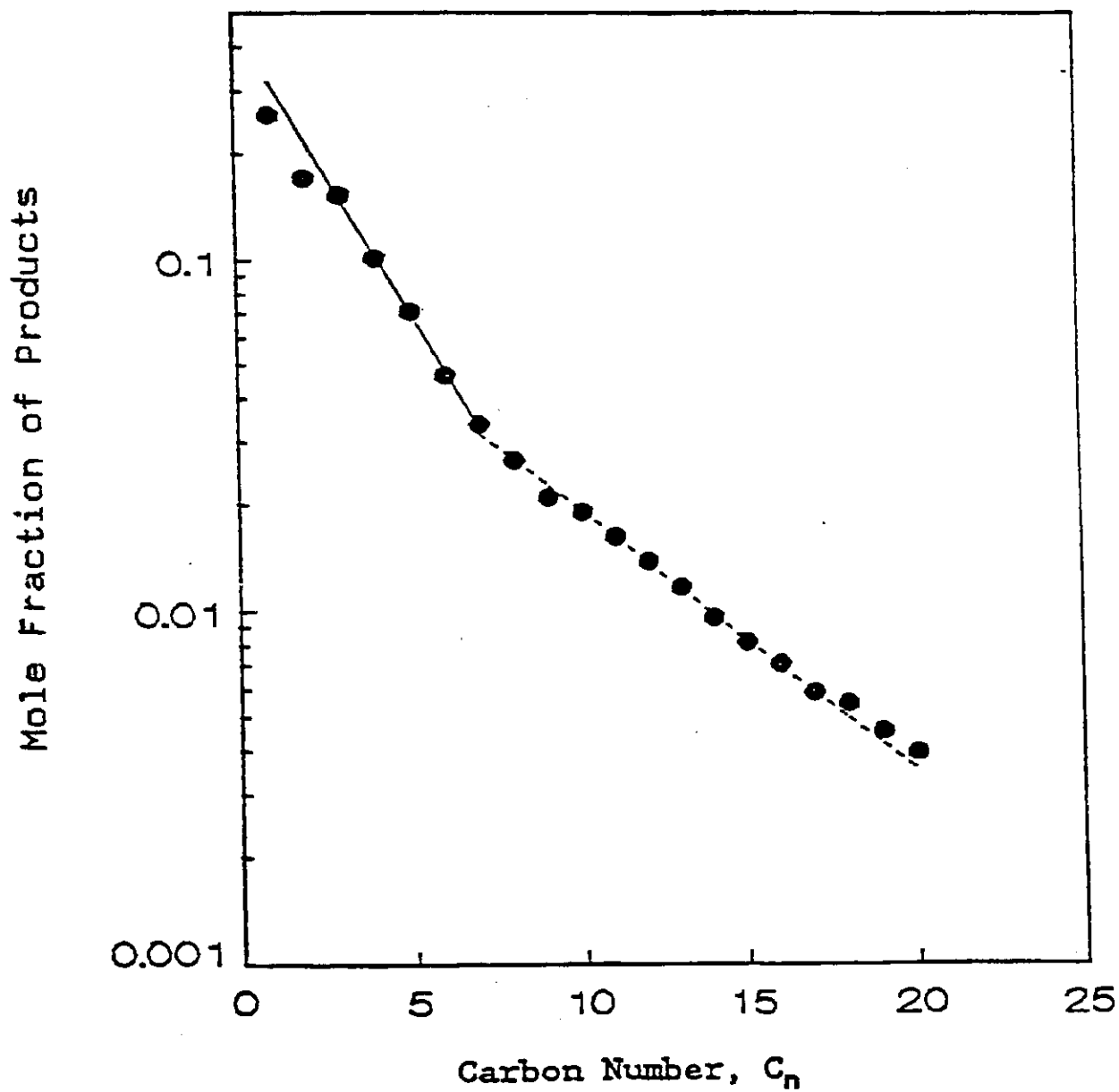
Figure 1

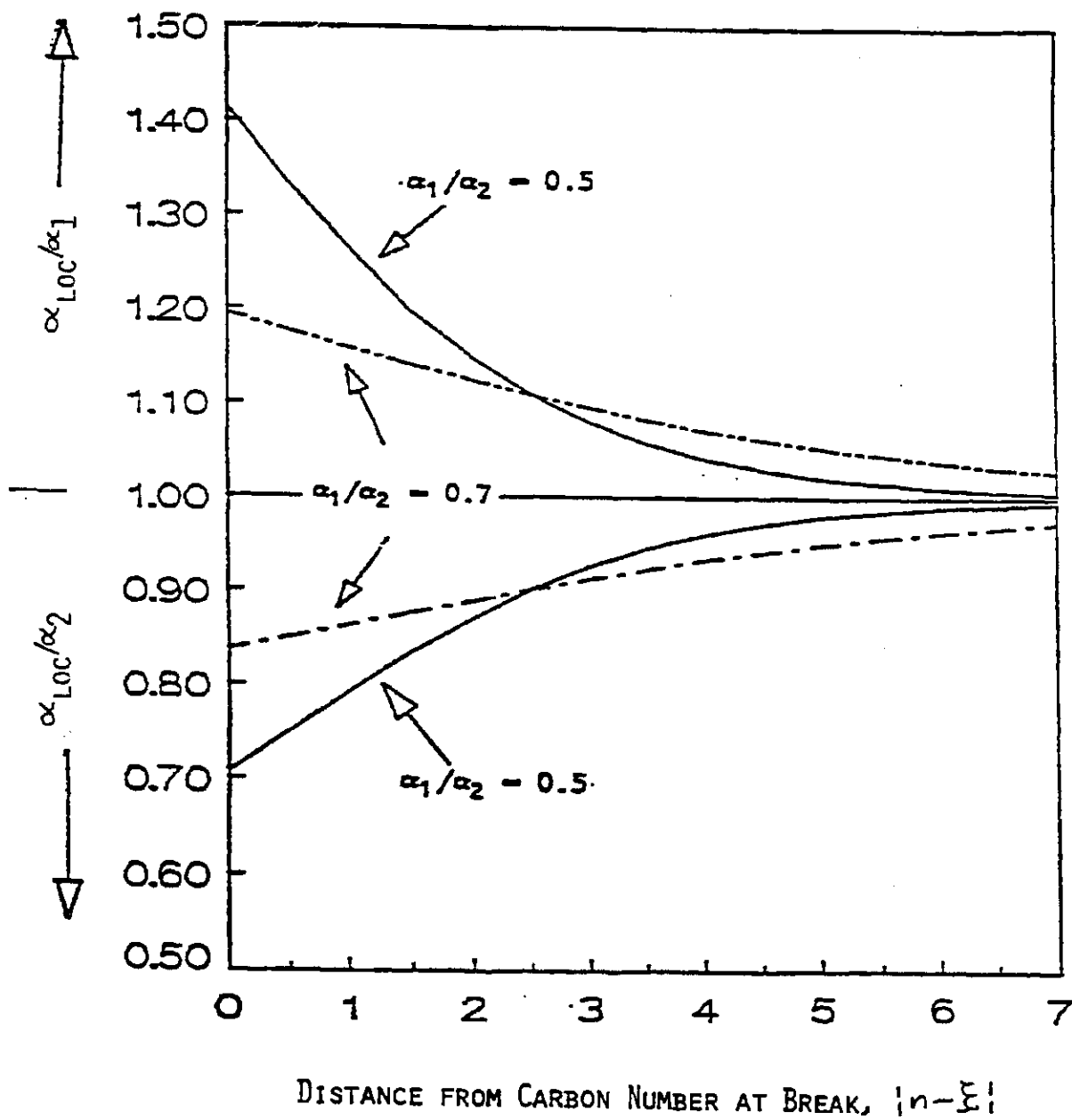EFFECT OF CARBON NUMBER ON α_{Loc}/α_1 OR α_{Loc}/α_2

DISTANCE FROM CARBON NUMBER AT BREAK, $|n-\Sigma|$

FIGURE 2

PRODUCT DISTRIBUTION
FROM UNPROMOTED PRECIPITATED IRON CATALYST
MODEL VERSUS DATA

$\alpha_1 = 0.62$

$\alpha_2 = 0.88$

T = 260°C
P = 1.46 MPa
$H_2/CO = 1.0$
$CO+H_2$ conv. = 44.8%

Carbon Number, C_n

● Data   —— Model
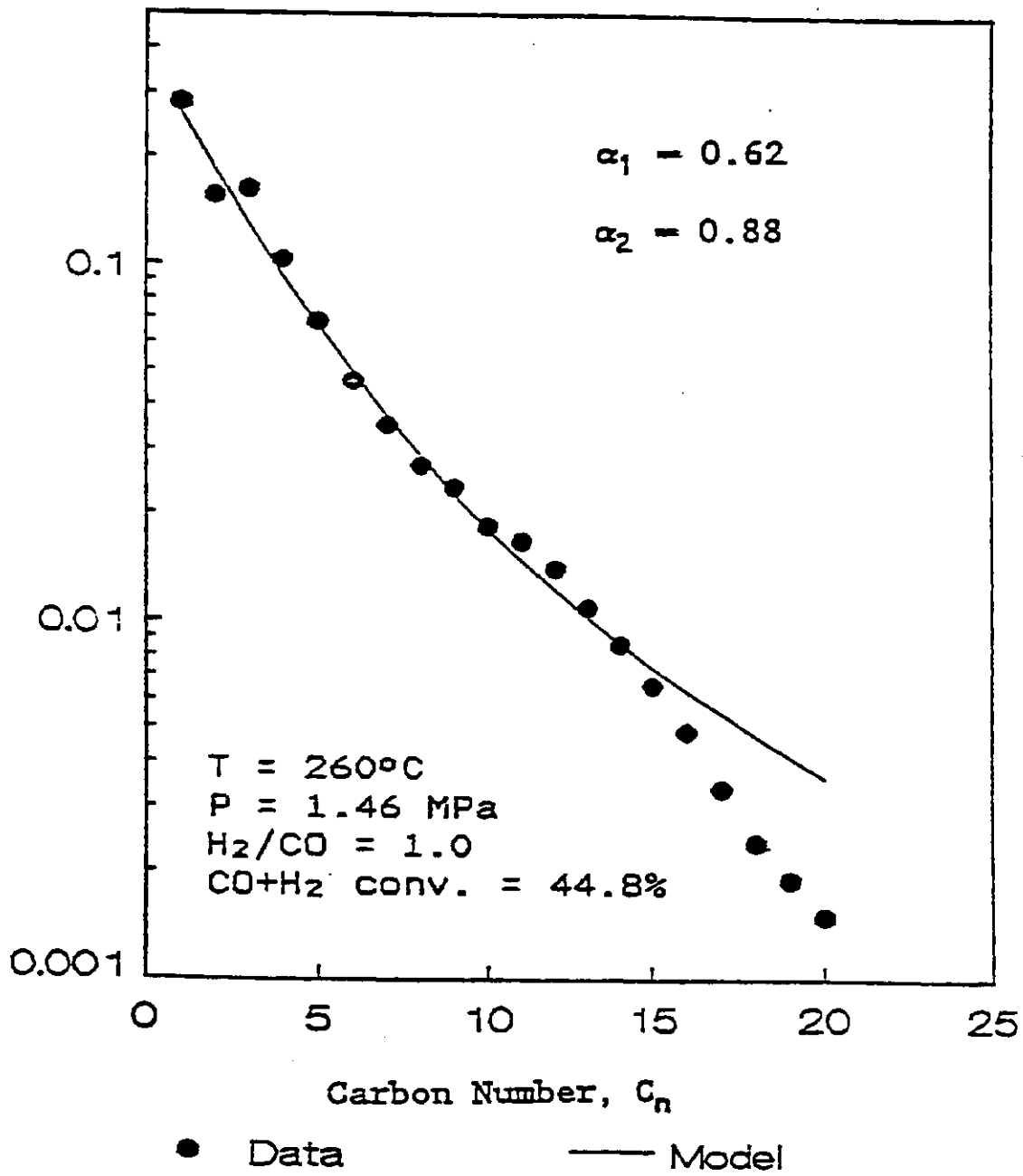
Figure 3a

Fused Iron Catalyst Product Distribution
Model versus Data

$\alpha_1 = 0.59$

$\alpha_2 = 0.90$

Carbon number, Cn

Mole Fraction of Products

● Data ——— Model
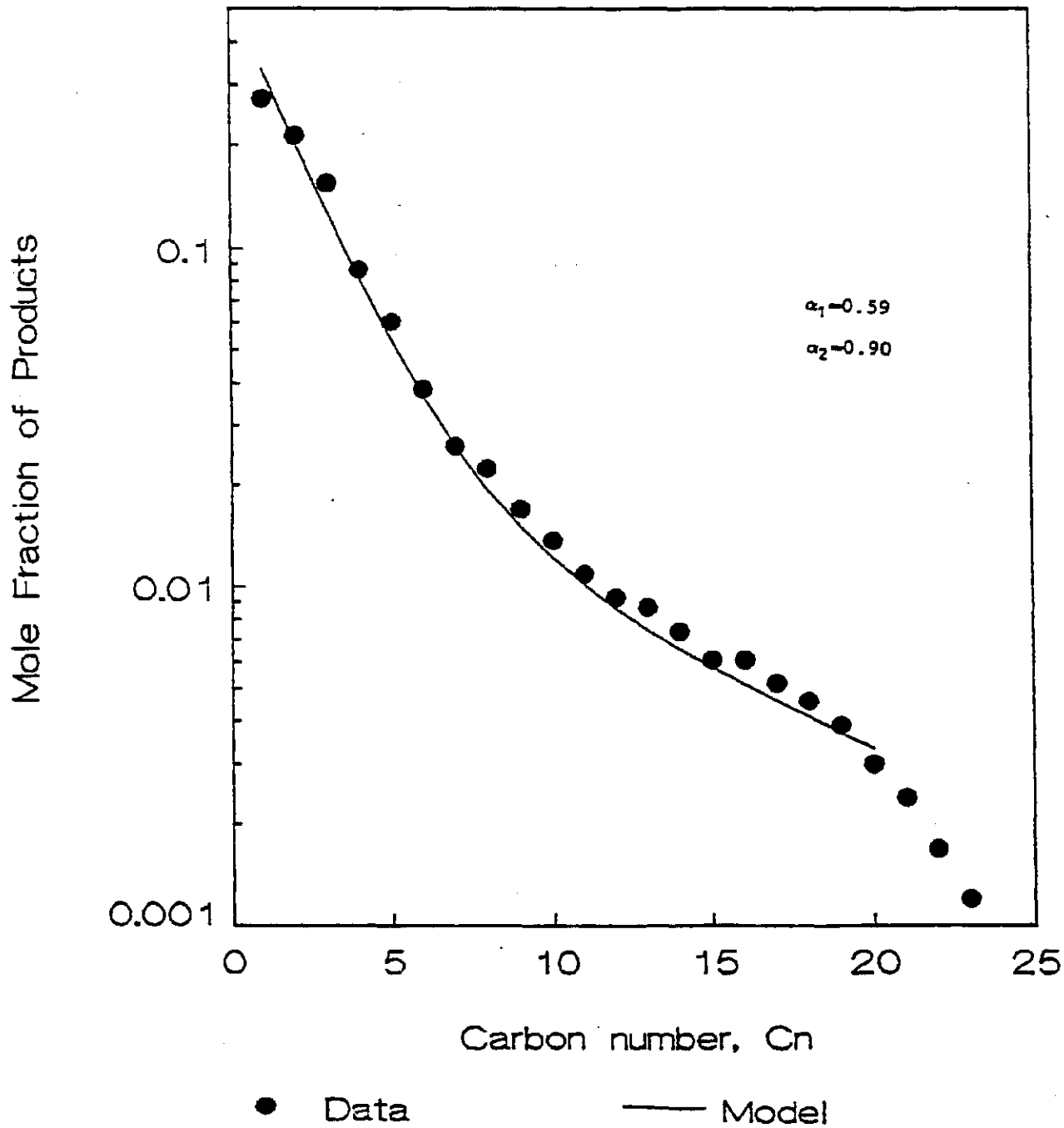
FIGURE 3B

Slurry Wax Analysis of Products
from Unpromoted Precipitated Iron Catalyst
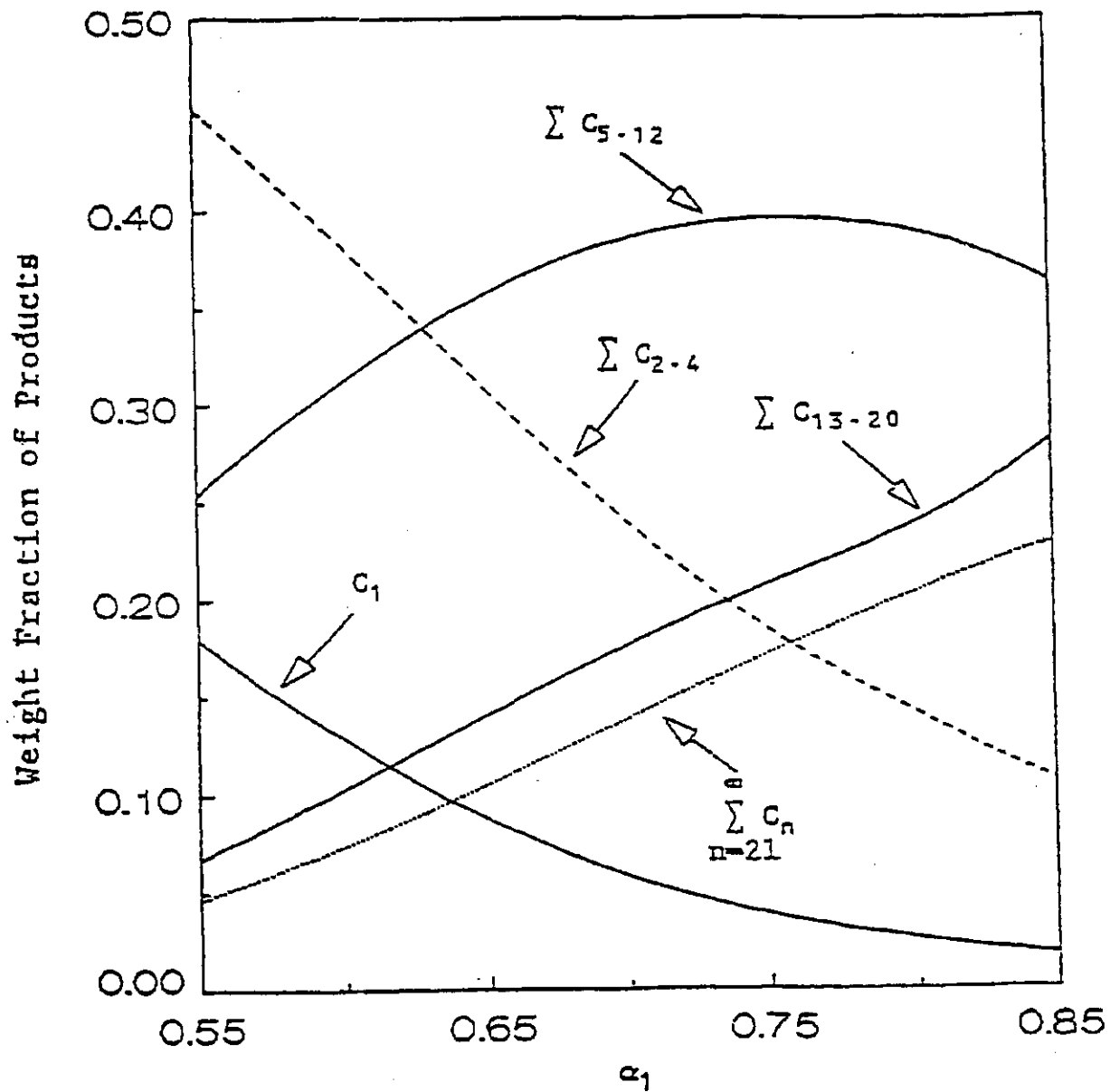Linear Regression
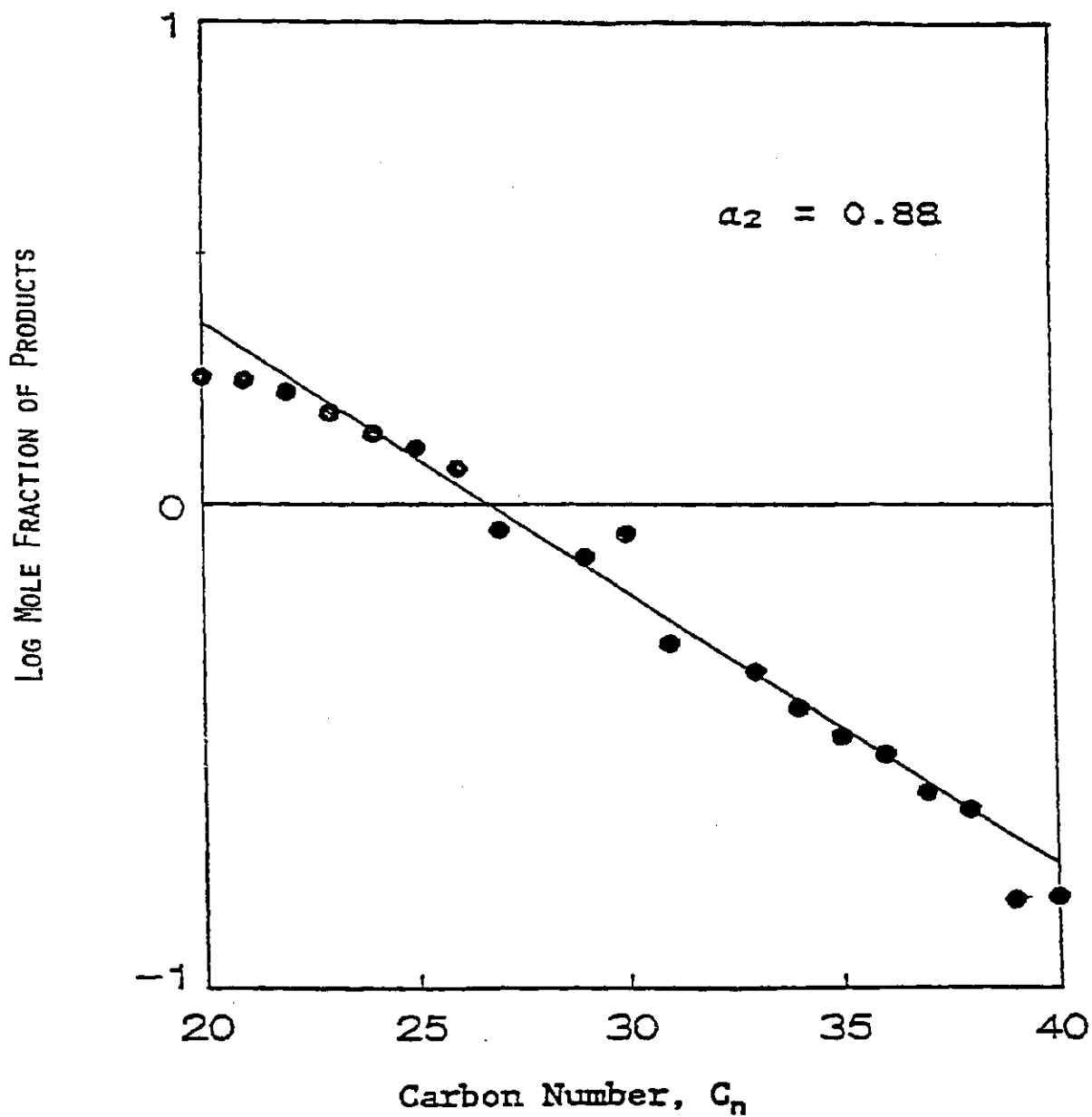
$a_2 = 0.88$

Figure 4

Figure 5a

Dependence of Selectivity on α_2

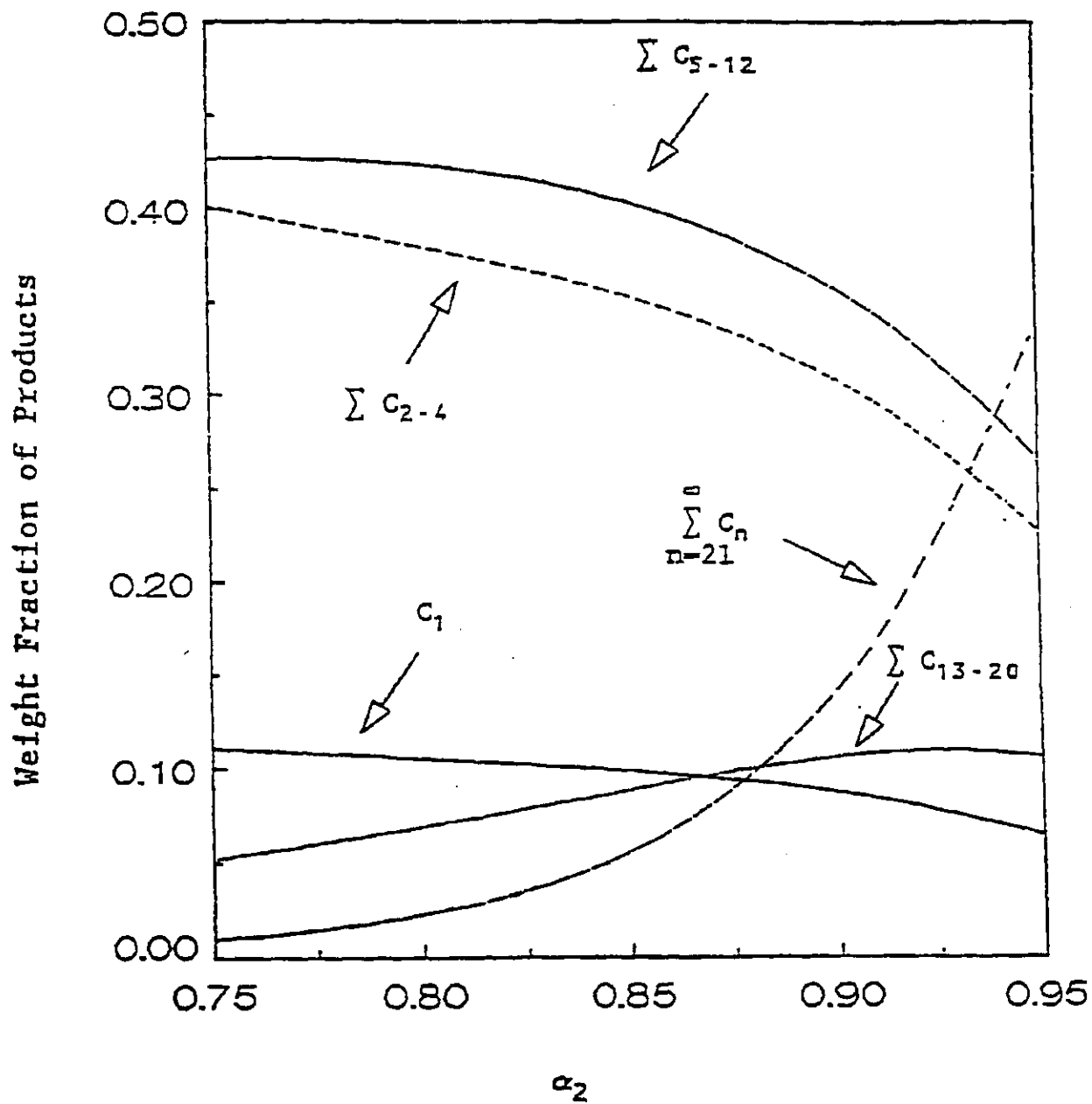$\alpha_1 = 0.65; \xi = 10$

Figure 5b

PRODUCT DISTRIBUTION
FROM UNPROMOTED PRECIPITATED IRON CATALYST
MODEL VERSUS EXPERIMENTAL DATA FROM SCHLIEBS RUN 2 (1984)
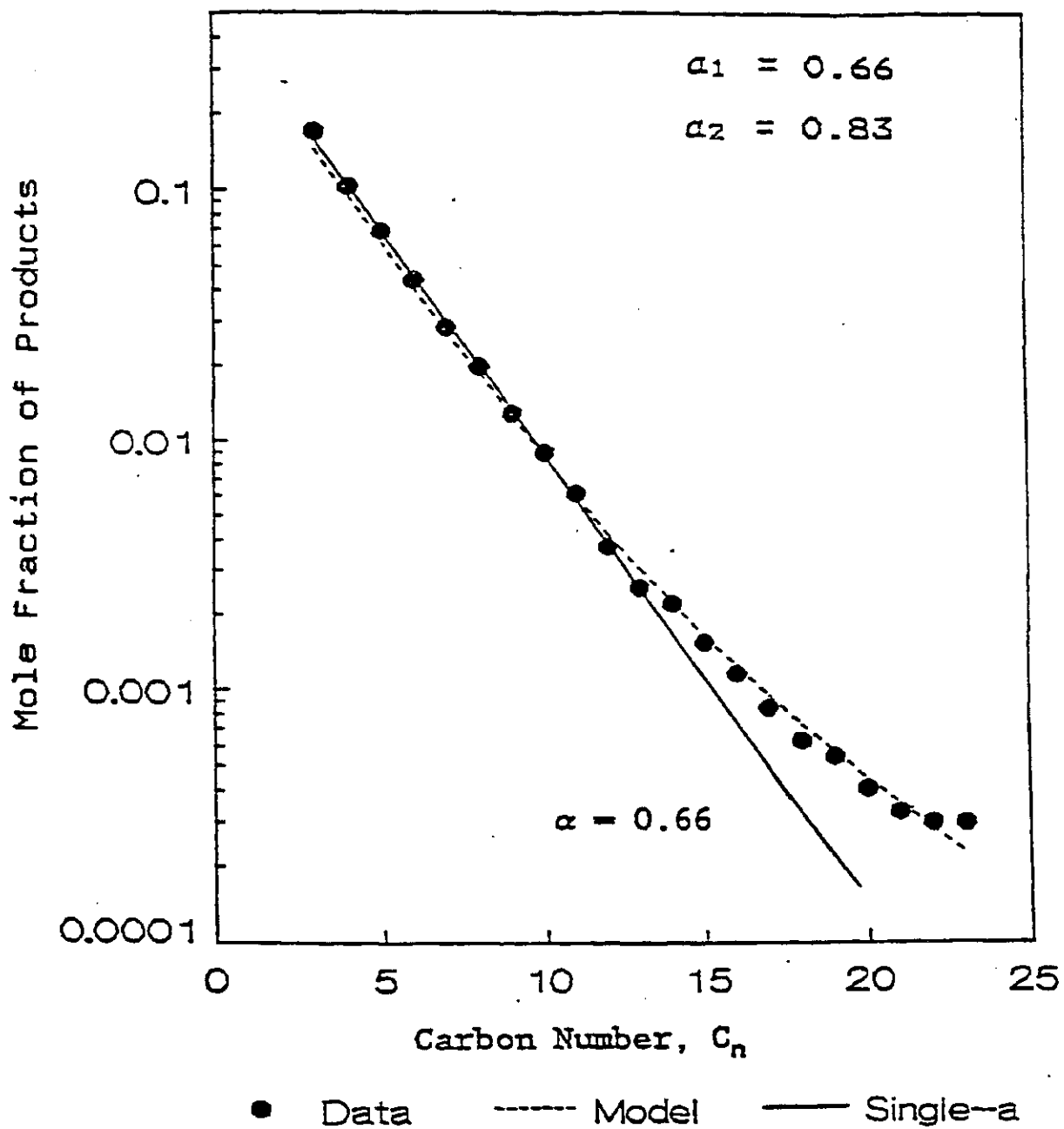
FIGURE 6