THE EFFECT OF ULTRASONIC VIBRATIONS AND CATALYST PARTICLE SIZE ON THE DECOMPOSITION OF CUMENE

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Abstract

The effect of ultrasonic vibrations on the vapor phase decomposition of cumene to benzene and proplyene was investigated using silica-aluminum as the cracking catalyst.

The system consists of a tubular reactor with a 4 inch long catalyst chamber made from 1 cm. diameter stainless steel tubing. The catalyst bed was irradiated from above by means of an ultrasonic horn.

The reactor was run at temperatures of 850 to 950°F., frequencies of 26,000 and 39,000 Hz, with a power input of 0.30 watts/cm.^{2} . Feed rates of 100 to 300 gms./hr. and catalyst particle sizes of 0.0209 to 0.358 cm. were used.

Using the reactor design equation and the data obtained from this research it can be shown that in the area where surface reaction controlled, the surface reaction rate constant was not increased by the addition of ultrasound.

Therefore it is postulated that ultrasonic vibrations do not cause localized heating within the catalyst bed, but that ultrasound causes acoustic streaming within the catalyst pores, resulting on higher diffusion rates.

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INTRODUCTION

Research has been performed in the field of gas-solid catalysis using high frequency vibrations directed on to the catalyst bed. Recent work has shown that the addition of these ultrasonic vibrations to a catalytic cracking reaction increases the overall rate constant of the reaction. This thereby increases the conversion of feed to product over the conversion obtained in the absence of ultrasound. The pure kinetic rate constant, however, is obscured by the effects of pore diffusion. The elimination of this effect is necessary for the determination of the result of ultrasonic vibrations on the Arrehenius activation energy.

LITERATURE SURVEY

Work was done by Garver (1955) who developed and determined the actual reaction mechanism for the vapor phase decomposition of cumene on silica-alumina catalyst, the system to be studied in this paper.

For the continuous reaction model it was assumed that the reaction mechanism consisted of seven distinct processes and that the rate of the reaction was controlled by the slowest process. These processes are:

1. Gas film diffusion of reactants
2. Pore diffusion of reactants
3. Adsorption of reactants
4. Surface reaction of reactants
5. Desorption of products
6. Pore diffusion of products
7. Gas film diffusion of products

By experimentation at temperatures of 850, 950 and 1050°F, Garver discovered that the reaction was single site with surface rate of reaction controlling and proplyene not adsorbed.

The design equations Garver developed for pore diffussion and surface reaction controlling, steps two, four and six are Equations 1 and 2. Both are also inclusive of the adsorption and desorption effects. For the reversible reaction equation 1 is valid.

$$W/Fao = \gamma\left[\left[\frac{1}{2}\delta - \frac{1}{2\delta^3}\right] \ln \frac{(1 + X_A\delta)}{(1 - X_A\delta)} + \frac{X_{A_2}}{\delta^2}\right]$$

$$+ \beta\left[\frac{1}{2\delta^3} \ln \frac{(1 + X_A\delta)}{(1 - X_A\delta)} - \frac{1}{2\delta^2} \ln(1 - \delta^2 X_A^2 - \frac{X_{A_2}}{\delta^2}\right]$$

Where,

$$\gamma = \frac{1}{\epsilon L k_2 K_A \pi} + \frac{1}{\epsilon L k_2}$$

$$\beta = \frac{2}{\epsilon L k_2 K_A \pi} + \frac{K_R}{\epsilon L k_2 K_A} \qquad (1)$$

$$\delta = (1 + \frac{\pi}{K})^{\frac{1}{2}}$$

For the irreversible reaction equation 2 can be used.

$$W/Fao = \gamma X_A + \beta\left[-\ln(1-X_A) - X_A\right] \qquad (2)$$

Values for K, K_a and K_r can be found using the data in Appendix I, while ϵLk_2 will be discussed within this paper. The derivations for both equations are contained in Appendix II.

Work by Lintner (1973) gives us the design equation for gas film diffusion of products and reactant controlling. By experimentation Lintner has shown that at low flow rates equation 3 holds:

$$W/Fao = \frac{X_{AF}\ RT}{P_T K_g \alpha \ln(1+Y_{ALm})} \qquad (3)$$

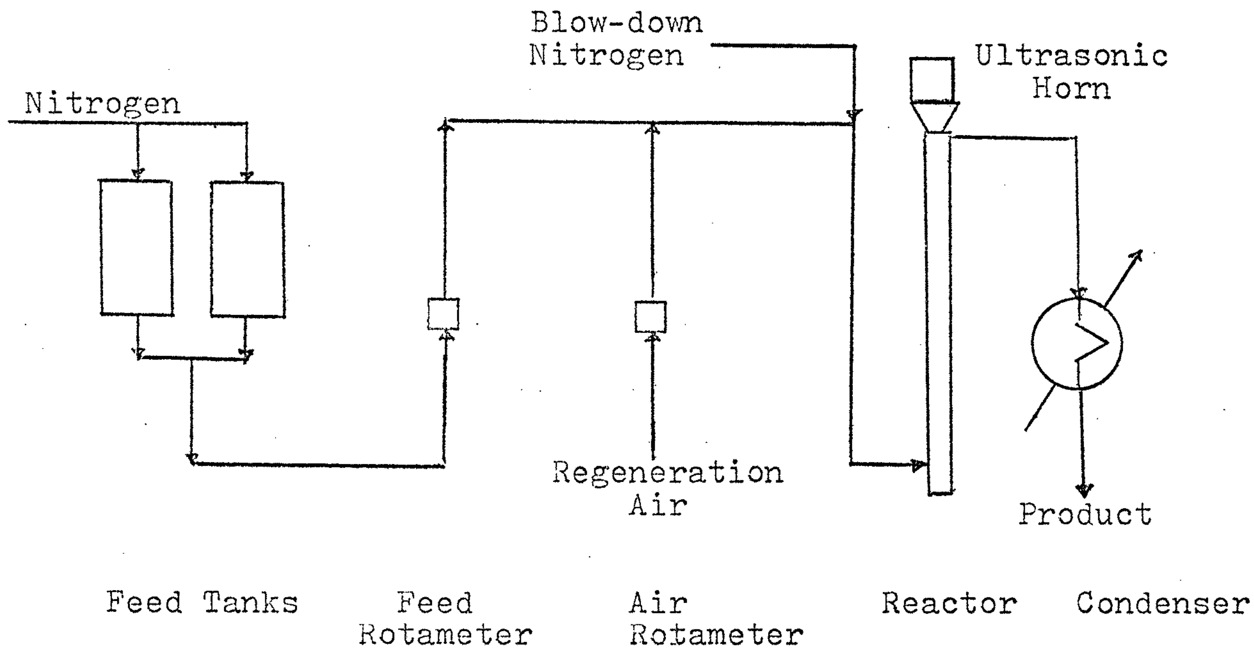
Example calculations for determining K_g and Y_{ALm} are in Appendix II, while the determination of α is shown in Appendix I.

One of the first studies done with the application of ultrasound to the vapor phase decomposition of cumene was done by Zhorov (1967). In Zhorov's work, cumene was fed into a continuous reactor at a reciprocial space velocity of W/Fao = 9468 gm. cat - sec/gmole. An increase of 20% conversion was obtained when ultrasonic energy was introduced for a half hour at a frequency of 20,000 Hz.

Extensive work was done by Lintner (1973) using ultrasonic vibrations on the cumene/silicia-alumina system. His system, Figure 1, consists of two feed tanks to which cumene is stored, a feed rotometer, a reactor on top of which rests

FIGURE NO. 1

FLOW CHART FOR
EXPERIMENTAL SYSTEM USED



an ultrasonic horn. A heat exchanger is included to condense the product. Detailed specifications of all equipment have been described by Lintner and are contained in his Doctoral dissertation (1973). Lintner's work showed that:

1. The relationship between conversion and the reciprocal space velocity (W/Fao)gave second order polynomials for all temperatures and frequency of ultrasounds.
2. The mass transfer coefficient, K_g, therefore the rate of reaction when external bulks diffusion controls, Equation 3, increases with increasing frequency.
3. The surface reaction/pore diffusion coefficient, therefore the rate of reaction when pore diffusion and surface reaction controls, Equation 1, increases with increasing frequency.
4. The kinetic rate constant $\epsilon L k_2$ increases with increasing frequency.
5. The apparent activation energy calculated from the data decreases with increasing frequency.

Scope

In order to determine the seperate effects of ultrasonic vibrations on the parameters contained in the kinetic rate constant, ϵLk_2 , the scope must be established for which this study will follow. This range must make a strong attempt to eliminate as many influencing factors as possible. Then, by studying the change in ϵLk_2 with the addition of ultrasonic vibrations, the effects on each can be determined.

One important factor is the mass transfer of cumene from the gas stream to the catalyst surface. In order to study the term ϵLk_2 effectively it must be made certain that the mass transfer coefficient is as large as possible so that its effect on the total reaction rate is small.

If it is assumed that a combination of resistences, gas film diffusion and chemical surface reaction/pore diffusion , exists, then when both resistences exist, a mean reaction rate constant k_{obs} is used in accordance with the equation :

$$-\frac{1}{S_{ex}}\frac{dN_b}{dt} = b\, k_{obs}\, C_A \qquad (4)$$

The combination of resistences can be treated in a manner analogous to series resistences in heat transfer by the equation:

$$k_{obs}\, C_A = \frac{1}{1/K_g + 1/\epsilon L k_2}\, C_A \qquad (5)$$

where:

k_g = rate due to gas film diffusion.

$\epsilon L k_2$ = rate from other factors than gas film diffusion.

ϵ = catalyst effectiveness factor. Defined as the actual rate of reaction with pore diffusion present divided by the rate of reaction if resistence due to pore diffusion were absent.

L = the total concentration of active sites.

k_2 = the forward Arrehenius reaction rate constant for surface reaction.

It follows that by allowing k_g to get as large as possible, the term $1/k_g$ will get proportioally smaller. The contribution then of the gas film constant in equation 5 becomes slight. If:

$$1/k_g \lll 1/\epsilon L k_2 \qquad (6)$$

then equation 5 reduces to:

$$k_{obs}\, C_A = \frac{1}{1/\epsilon L k_2}\, C_A \qquad (7)$$

which gives

$$K_{obs} = \epsilon L k_2 \qquad (8)$$

The studying of k_{obs} then will result in the studying of ϵLk_2 or the rate term other than gas film diffusion that being surface reaction and pore diffusion.

Another important factor is the effect of temperature on the rate of reaction. By studying ϵLk_2 it is not possible to study the effect of ultrasound on ϵ if the term Lk_2 is the controlling factor.

Figure 2 is a plot of the mass transfer coefficient versus the reciprocal space velocity at various temperatures for the particle size used by Lintner. It is apparent from the graph that at very low flow rates, $W/Fao > 40,000$, the effect of low temperature, $T < 750^{o}F$ is still the influencing factor. This is shown by very little change in k_g over the flow range.

At high temperatures, $T > 750^{o}F$, the influencing factor is the flow rate as shown by the large change in the mass transfer coefficient over the range of reciprocal space velocities at any of the three temperatures, Figure 3 is a plot of ϵLk_2 versus temperature at various space velocities. From the graph it can be seen that at high temperatures $T > 750^{o}F$, the flow rate starts to begin to effect the term Lk_2. A difference of 33.2% is observed from the plot.

TABLE NO. 1

MASS TRANSFER COEFFICIENT AT VARIOUS FLOW RATES AND TEMPERATURES

(Lintner, 1973)

K_g, cm./sec.

Temperature, deg. F.

W/Fao x 10^{-3}	650	750	850	950
20	.0068	.0397	.0635	.0680
30	.0067	.0384	.0571	.0624
40	.0063	.0369	.0523	.0589
50	.0061	.0367	.0502	.0574
60	.0053	.0329	.0422	.0510
70	.0047	.0304	.0368	.0467
80	.0046	.0304	.0357	.0463
90	.0040	[illegible]	.0305	.0420
100	.0034	.0250	.0251	.0375

TABLE NO. 2

ϵLk_2 AT VARIOUS TEMPERATURES AND W/Fao
(Lintner, 1973)

Particle Diameter = 0.358 cm.

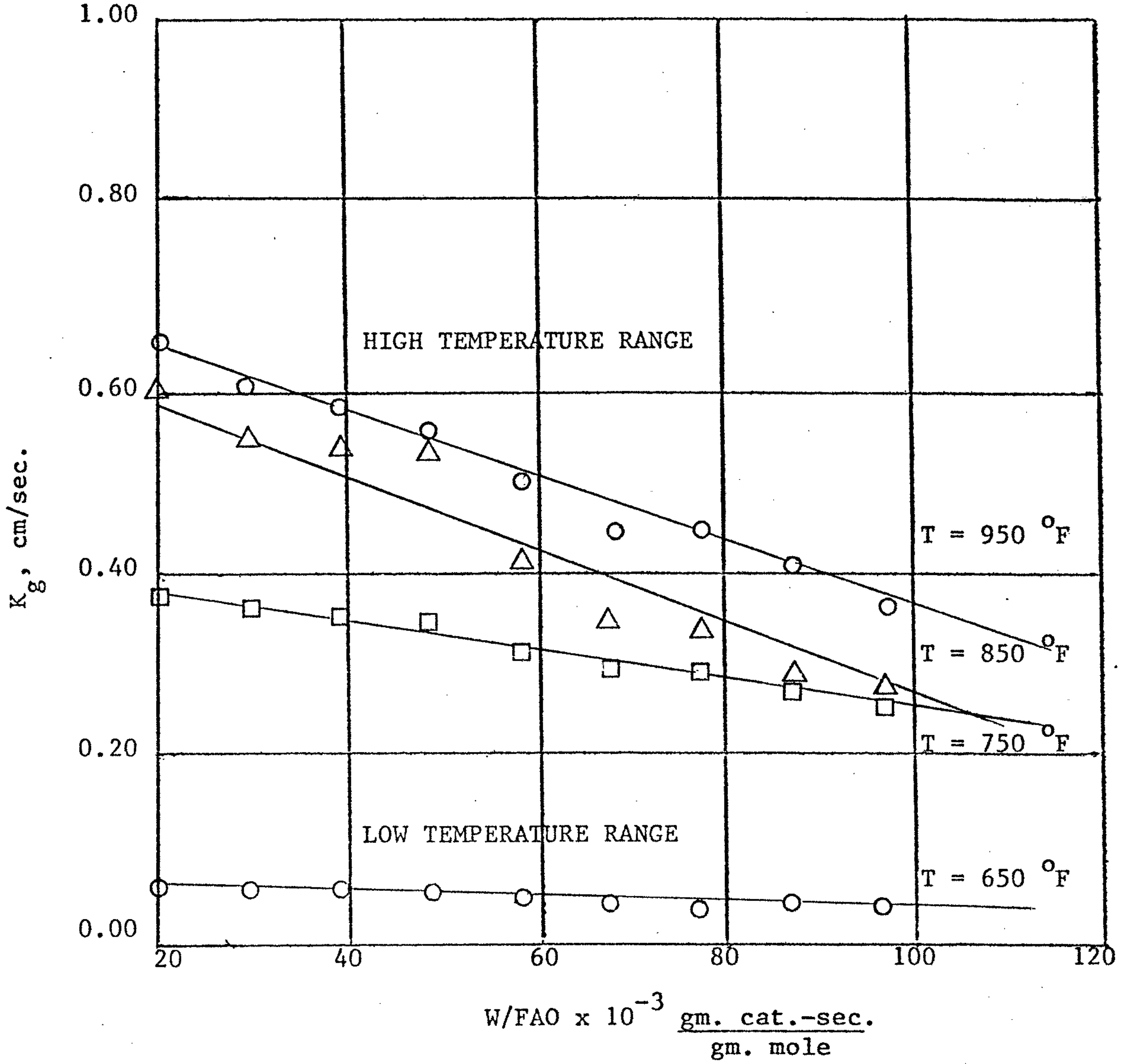
$Lk_2 \times 10^5$

W/Fao $\times 10^{-3}$

Temperature	20	40	60	80
650	0.199	0.194	0.169	0.135
700	0.415	0.347	0.347	0.369
750	1.478	1.431	1.331	[illegible]
800	1.794	1.593	[illegible]	[illegible]
850	2.960	2.500	2.096	1.641
900	3.399	2.663	[illegible]	1.969
950	3.440	[illegible]	[illegible]	[illegible]

FIGURE NO. 2

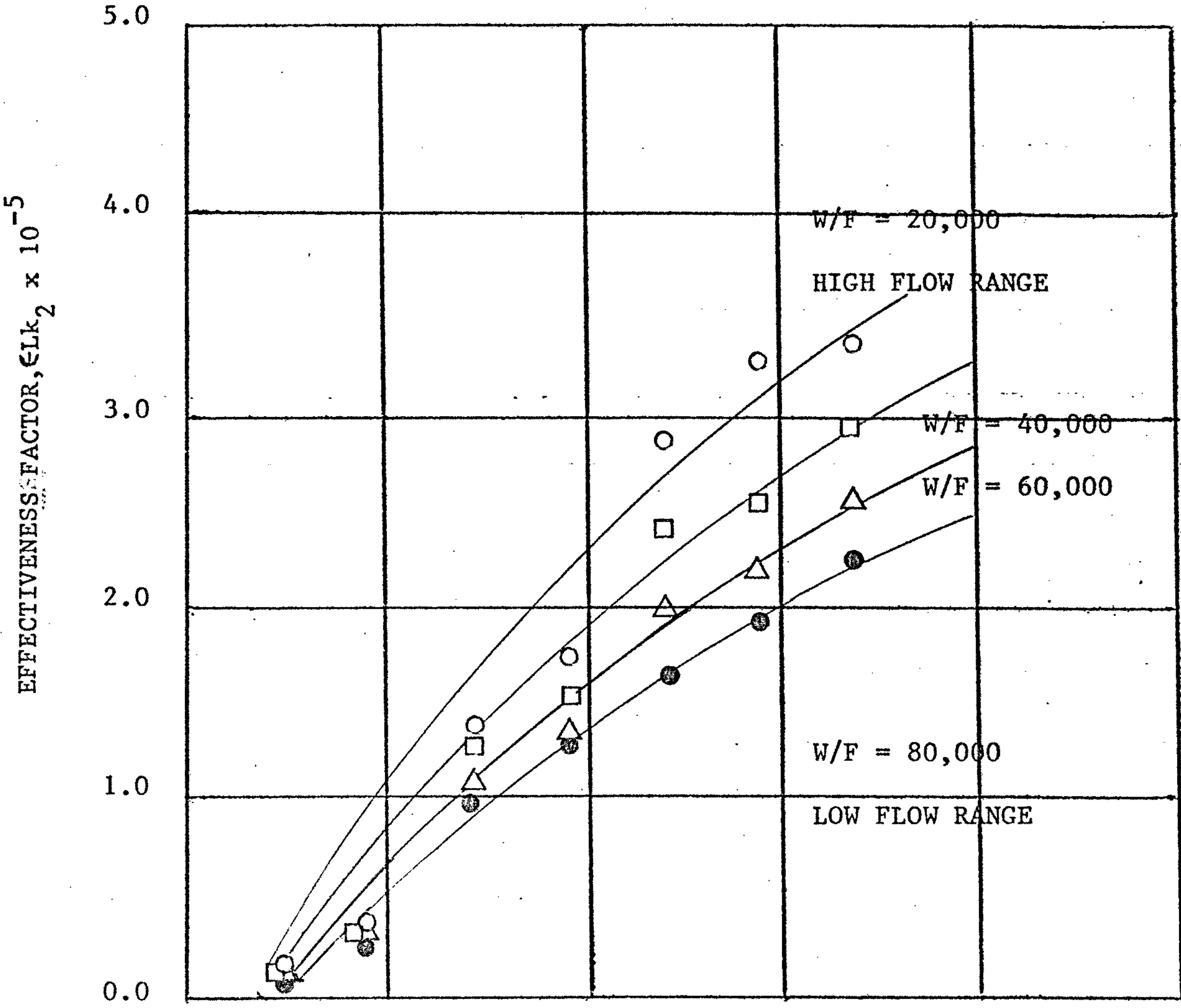
MASS TRANSFER COEFFICIENT VERSUS W/FAO



PARTICLE DIAMETER = 0.358 cm.

FIGURE NO. 3

EFFECTIVENESS FACTOR VERSUS TEMPERATURE



TEMPERATURE, DEG. K.

PARTICLE DIAMETER = 0.358 cm.

After reviewing these graphs with the rest of Lintner's study, a matrix showing the rate limiting steps for variations in feed flow and temperature can be developed.

	High Flow	Low Flow
High Temp.	External Diffusion Pore Diffusion	External Diffusion Pore Diffusion
Low Temp.	Surface Reaction Pore Diffusion	External Diffusion Surface Reaction Pore Diffusion

where : High Temperature $>$ 750 ^{o}F.
Low Temperature $<$ 750 ^{o}F.
High Flow $>$ 50 gm./hr.
low Flow $<$ 50 gm./hr.

From the previous discussion it can be seen that a high flow rate, or low space velocity, is necessary to keep the effects of the mass transfer coefficient out of the term $\epsilon L k_2$. Also it has been shown that a high temperature is needed so that the surface reaction rate does not overshadow any effects of the term ϵ, the effectiveness factor. This combination of high temperature and high flow places this study in the first quadrant of the matrix. Here the rate controlling mechanisms are :

1. External diffusion from the gas stream to the catalyst surface.

2. Pore diffusion.

The temperature range for this study will be taken greater than 750 ^{o}F so as to be far enough out of the region of surface reaction controlling. The range will be from 850^{o}F to 950^{o}F at intervals of 25 deg. F.. This will allow for data, five points , to develop a plot of rate versus temperature to determine the apparent activation energy.

The flow regime called for is high flow. Even in the matrix we see that external diffusion effects are still present, therefore flows will be much greater that the limit of 50 gm./hr. , 100, 200, and 300 gm./hr. flows will be used.

The effect of pore diffusion and its behavior will be handled in the theory.

Theory

With the scope of this study choosen where pore diffusion controls the observed reaction rate, this research will try to eliminate this factor and study the effects of ultrasonic vibrations on the activation energy, E. To reduce the effect of pore diffusion examination of the term ϵ and what effects it must be done.

Satterfield developed the mathematical model which represents the effectiveness factor as a function of the Thiele modulus. In a spherical catalyst for a first order irreversible reaction the relationship becomes:

$$\epsilon = \left[\frac{3}{h_s} \quad \frac{1}{\tanh h_s} \quad - \quad \frac{1}{h_s} \right] \qquad (9)$$

where:

$$\tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

where:

$$h_s = \text{Thiele modulus} \tag{10}$$

$$h_s = R \left[\frac{S_V \; k'_s \; C_S^{m-1}}{D_E} \right]^{\frac{1}{2}} \tag{11}$$

where:

m = order of reaction

S_V = pore surfacr, $cm.^2/cm.^3$

R = radius of catalyst, cm.

D_E = effective diffusivity, $cm.^2/sec.$

k'_s = intrinsic reaction rate constant.
$(cm.^3 \text{ fluid})^m/cm.^2$ cat. surface $(g.mole)^{m-1}$-sec.

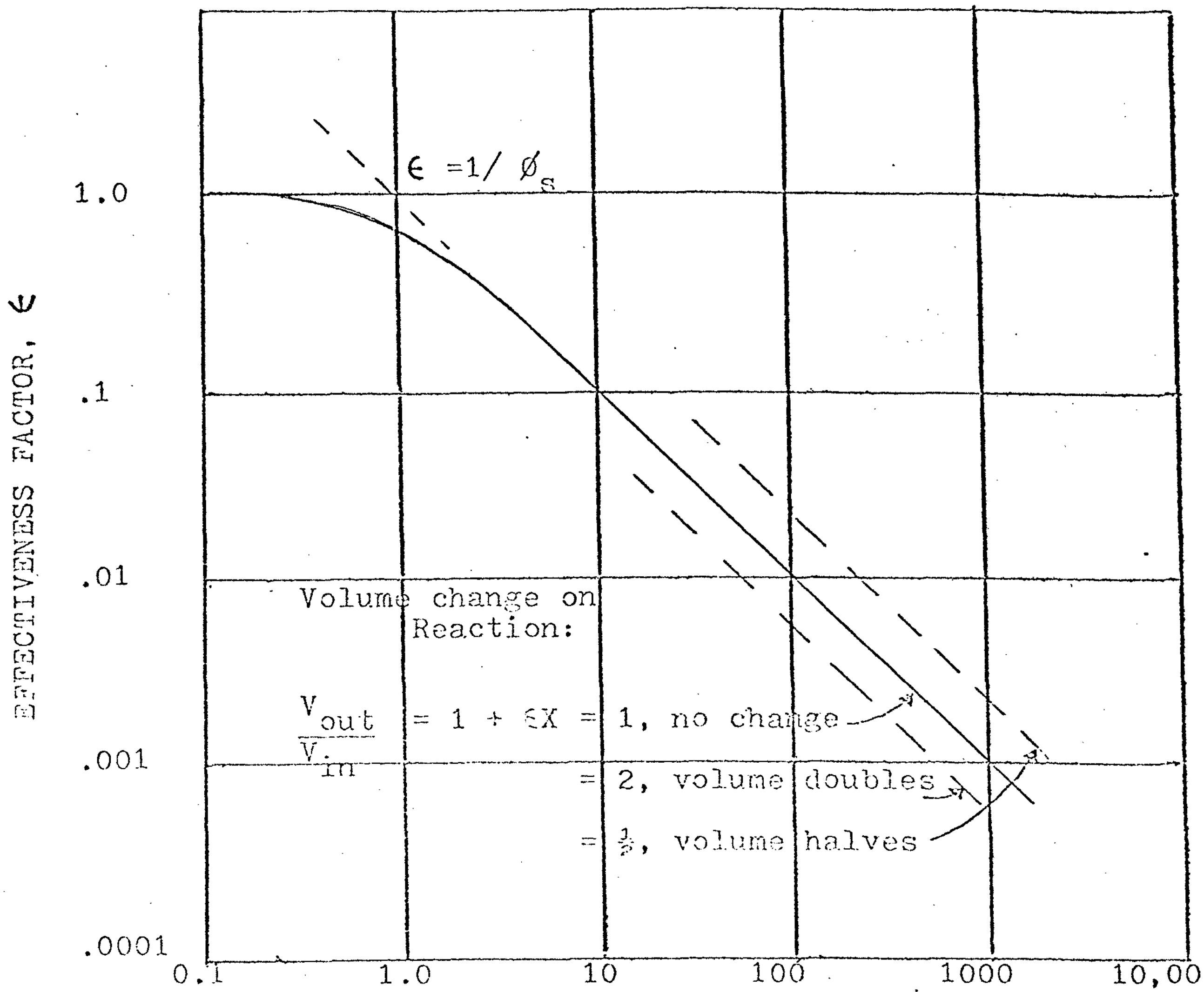
At fixed temperature with order equal to one and a specified catalyst type equation 11 reduces to:

$$h_s = (\text{constant})\, R \tag{12}$$

The effect of particle size on the effectiveness factor is shown in Figure 4. It is evident that at very small particle sizes, corresponding to a value of the Thiele modulus that is also small, the effectiveness factor approaches unity. This study will then use small catalyst diameters in an attempt to eliminate the effectiveness factor from the kinetic rate constant. Then the term ϵLk_2 can be analyzed in the presence of ultrasonic vibrations to determine an effect, if any.

FIGURE NO. 4

EFFECTIVENESS FACTOR, ϵ , VERSUS THIELE MODULUS



ϕ , Thiele Modulus

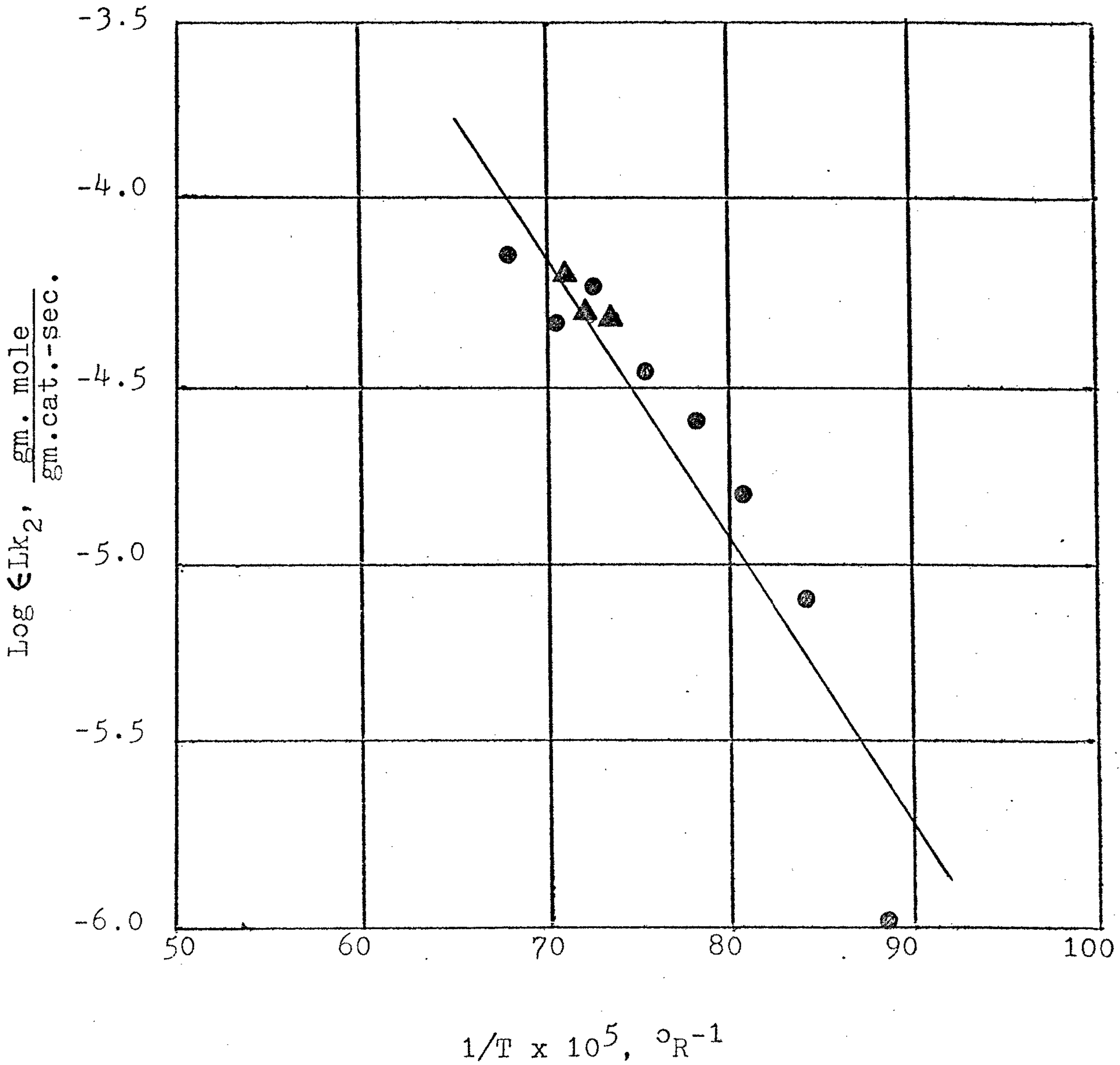
Defined as ϕ_s, $L(k'_s C_s^{m-1}/D_E)^{\frac{1}{2}}$

where :

L = pore length

FIGURE NO. 5

EFFECTIVENESS FACTOR, ϵLk_2, VERSUS TEMPERATURE



● Lintner's Data

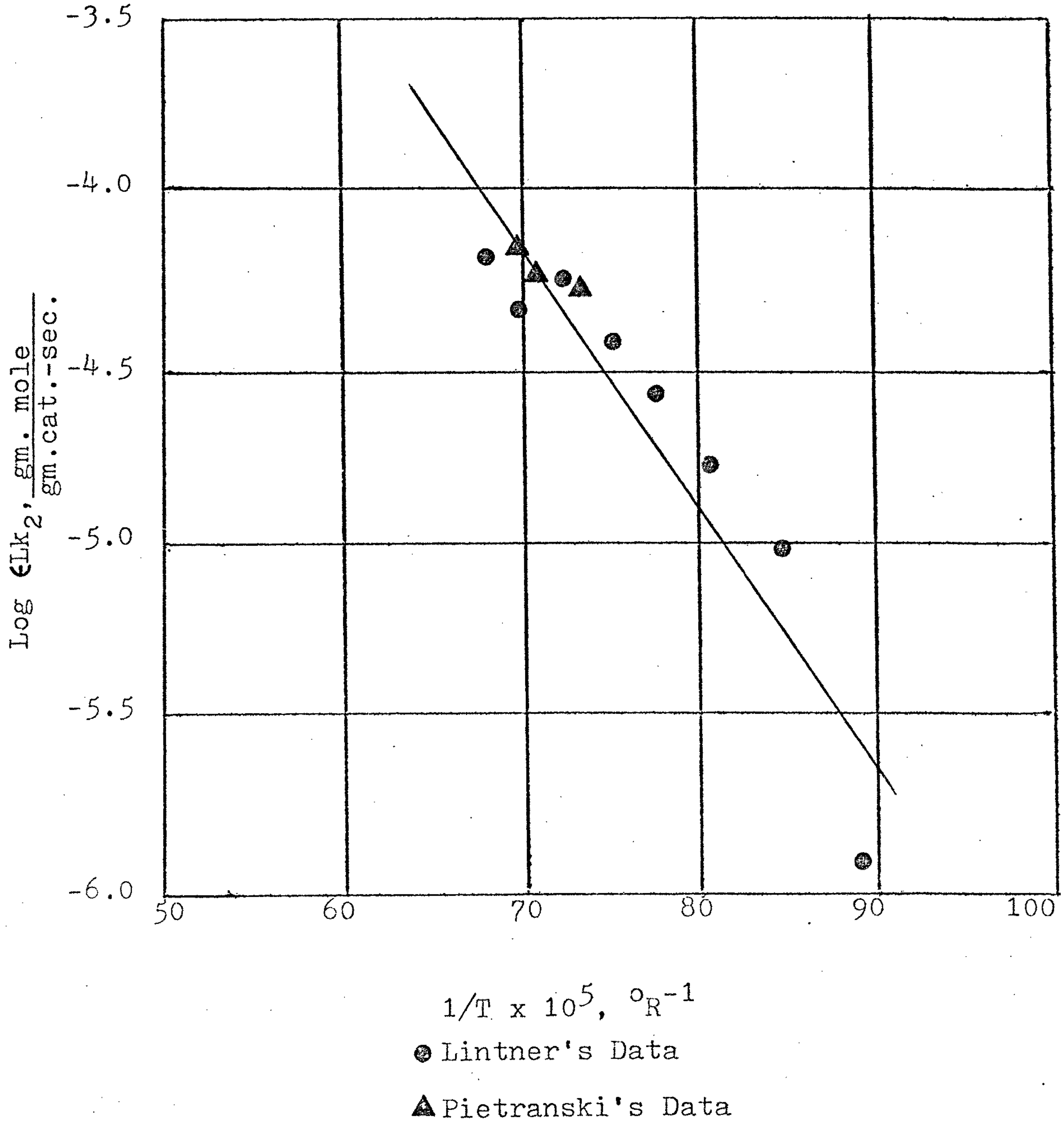
▲ Pietranski's Data

Ultrasound = 0 cps

Particle Diameter = 0.358 cm.

FIGURE NO. 6

EFFECTIVENESS FACTOR, ϵLk_2, VERSUS TEMPERATURE

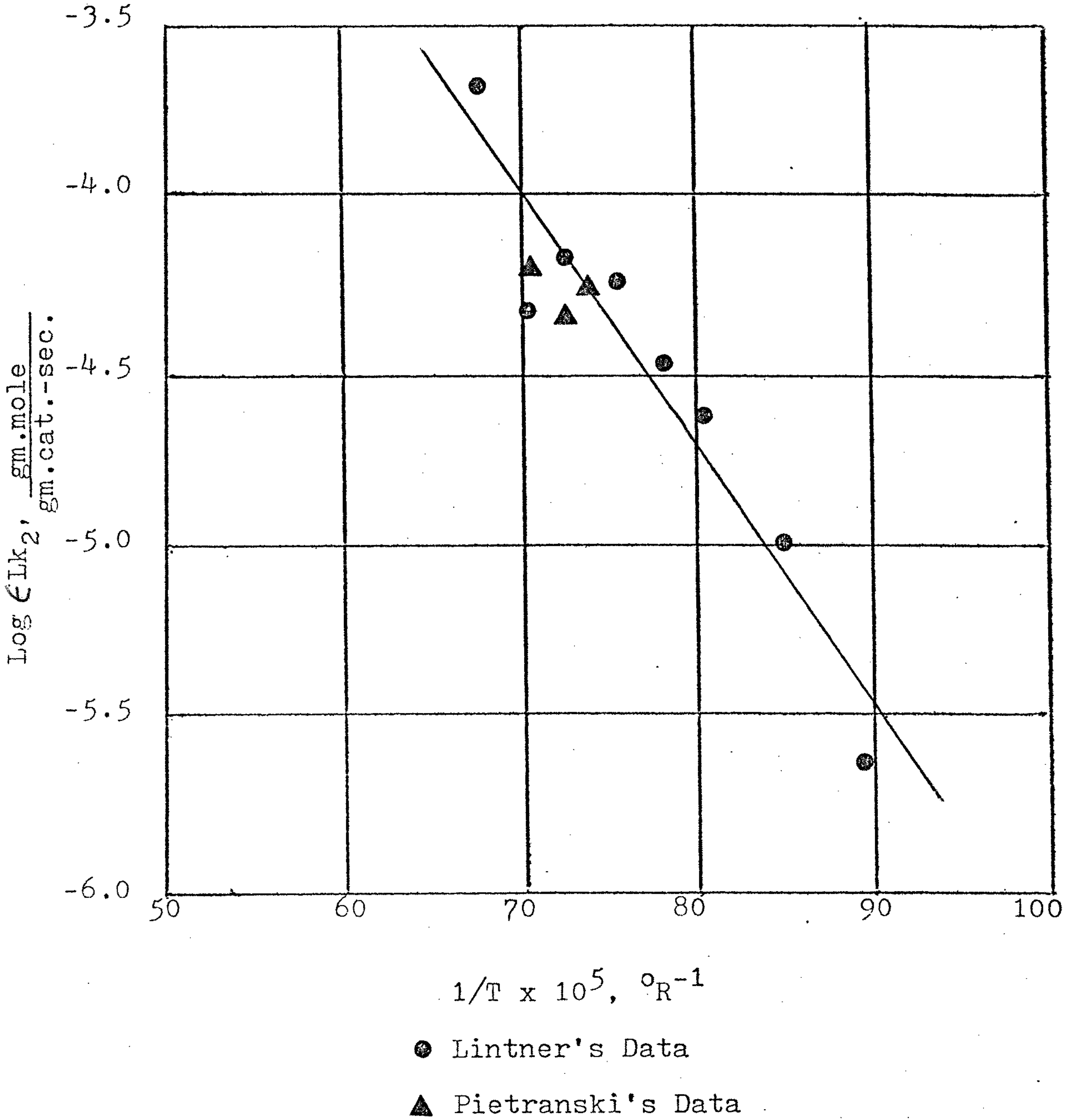


Ultrasound = 26,000 cps

Particle Diameter = 0.358 cm.

FIGURE NO. 7

EFFECTIVENESS FACTOR VERSUS TEMPERATURE



Ultrasound = 39,000 cps

Particle Diameter = 0.358 cm.

Experimental Procedure

Operating Conditions

The operating conditions used in this investigation were temperatures of 850 °F. to 950 °F., feed rates of 100, 200, and 300 grams per hour and catalyst loadings of 2.10 to 3.65 grams. The ultrasonic frequencies used were 26,000 and 39,000 cycles per second at power output of approximately 0.30 watts per square centimeter. Catalyst diameters of 0.358, 0.200, 0.0841, 0.0419, and 0.0209 cm. were used

Detailed Procedure

The details of the experimental procedure for a typical run are as follows:

1. Set the reactor air purge rate at 6.0 scfh employing the air rotameter.

2. Adjust the heater controls to obtain the desired reactor temperature.

3. Adjust the automatic temperature controller set point to the desired reactor temperature.

4. Allow approximately 24 hours for the reactor to equilibrate at the desired temperature.

5. Turn on the hot oil recirculation pump and adjust the heater control to maintain the oil at 155-160 deg. Centigrade.

6. Turn off the air purge and purge the reactor with nitrogen for 20 minutes.

7. Shut down the nitrogen purge and pressurize the cumene feed tank to 10 psig with nitrogen.

8. Feed cumene to the reactor at the desired rate employing the feed flow rotameter to monitor that rate.

9. Record the feed tank level and time.

10. While maintaining all other operating conditions constant, activate the ultrasonic generator and adjust it to the desired frequency.

11. The first product will appear in 5 to 10 minutes. Collect for 30 seconds the product every two minutes for the required time.

12. Record the feed tank level and time.

13. Shut off the feed and purge the reactor with nitrogen for 20 minutes.

14. Shut down the power to the ultrasonic generator, and the hot oil heater along with the power to the recirculation pump

15. Shut down the nitrogen purge and set the air purge rate at 6 scfh.

16. Air purge the reactor for about 12 hours at the reaction temperature prior to starting the next run.

17. After blending each sample thoroughly, inject a portion of the sample three times into the gas chromatograph and calculate the conversion.

Verification of Equipment

Before any new data can be added to the work done by Lintner, the technique used in the present research must be validated. The following steps are then required:

1. Reassemble Lintner system.

2. Obtain data using the particle size used by Lintner

at:

a. Temperatures of 875, 900, and 925°F.

b. Ultrasounds of 0, 26,000 and 39,000 cps.

3. Develop equations of conversion versus reciprocal space velocity.

4. Using the design equation derived by Garver along with the computer program 'Cumene' obtain values of the kinetic rate constant, ϵLk_2

5. Compare to the previously published values of Lintner to verify the technique used in this research.

The data obtained from this procedure is contained in Appendix V. Table 4 summarizes the results of this research with those of Lintner's. Figures 5 through 7 graphically verify the technique.

Table 3 contains the steps used for developing the data to a suitable form. Runs made with catalyst diameters of 0.358 and 0.200 cm. were performed using Lintner's technique.

1. The first product will appear in 5 to 10 minutes. Discard the product collected during the first 10 minutes. Collect, blend and sample the product obtained during the second 10 minutes.

2. While maintaining all other operating conditions constant, activate the ultrasonic generator and adjust it to the desired frequency.

3. Repeat step 1 for the first ultrasound.

4. Repeat steps 2 and 3 for the second ultrasound.

When the third particle size was initially used a large drop in conversion was encountered using Lintner's

TABLE NO. 3

CALCULATIONAL PROCEDURS FOR REGRESSION OF DATA

1. If needed obtain conversion versus time data and develop exponential equations of the form:

$$Xa = Ae^{Bt}$$

2. Determine an average conversion over the time period studied using the formula:

$$\overline{Xa} = \int_{t_0}^{t_f} \frac{Xa(t)\ dt}{t_{total}}$$

3. Obtain conversion versus reciprocal space velocity as a second order polynomial.

$$Xa = A + B(W/Fao) + C(W/Fao)^2$$

4. Using the design equation developed by Garver obtain an average value of ϵLk_2 in the range of W/Fao for which data was taken.

5. Take the logarithms of these averages from step 4. and plot versus reciprocal temperature and determine the constants for the linear equation which results.

$$Log(\epsilon Lk_2) = A + B(1/T)$$

6. Using the smooth curve from step 5. obtain and plot the data as $Log(\epsilon Lk_2)$ against Log(Particle Diameter) on constant temperature lines.

7. Where the resulting curve from step 6. flattens out to suggest $\epsilon \to 1$, or $\epsilon Lk_2 \approx Lk_2$, take data and plot $Log(Lk_2)$ versus reciprocal temperature for the various ultrasounds.

By comparing the activation energy obtained from the slopes of the lines we can observe the effect of ultrasonic vibrations on the surface rate of reaction.

TABLE NO. 4

ϵLk_2 AT VARIOUS TEMPERATURES AND ULTRASOUNDS

Particle Diameter = 0.358 cm.

Temperature deg. F.	1/T, $^oR^{-1}$ x 10^5	Ultrasound cps x 10^{-3}	ϵLk_2 x 10^5	Log ϵLk_2
650*	90.1	0	0.0991	-6.0038
		26	0.1165	-5.9337
		39	0.2448	-5.6112
700*	86.2	0	0.8115	-5.0907
		26	0.9537	-5.0206
		39	1.2269	-4.9112
750*	82.6	0	1.3737	-4.8621
		26	1.6932	-4.7713
		39	2.5829	-4.5879
800*	79.4	0	2.4592	-4.6092
		26	2.8048	-4.5521
		39	3.6459	-4.4382
850*	76.3	0	3.8887	-4.4102
		26	4.0804	-4.3893
		39	4.5541	-4.3416
875	74.9	0	5.3162	-4.2744
		26	5.4714	-4.2619
		39	5.8898	-4.2299
900	73.5	0	5.2881	-4.2767
		26	5.0664	-4.2953
		39	4.8073	-4.3181
900*	73.5	0	5.8803	-4.2306
		26	5.9416	-4.2261
		39	6.8945	-4.1615
925	72.2	0	6.9279	-4.1594
		26	7.0567	-4.1514
		39	7.0016	-4.1548
950*	70.9	0	4.4957	-4.3472
		26	4.7775	-4.3208
		39	5.0315	-4.2983
1000*	68.5	0	6.7499	-4.1707
		26	6.7375	-4.1715
		39	22.5110	-3.6476

*Values obtained from Linter's data.

TABLE NO. 5

EFFECTIVENESS FACTOR VERSUS PARTICLE DIAMETER

Ultrasound = 39,000 cycles/sec.

Temperature	Log d_p -1.3778	-1.0757	-0.6990	-0.4461
	Log εLk2			
850	-4.2793	-4.1751	-4.0578	-4.2639
875	-4.0943	-3.9971	-4.0308	-4.2476
900	-3.9161	-3.8256	-4.0048	-4.2320
925	-3.7443	-3.6604	-3.9797	-4.2169
950	-3.5786	-3.5010	-3.9556	-4.2024

Ultrasound = 26,000 cycles/sec.

Temperature				
850	-4.2819	-4.1378	-4.0791	-4.3122
875	-4.0967	-3.9709	-4.0468	-4.2790
900	-3.9114	-3.8041	-4.0145	-4.2458
925	-3.7395	-3.6492	-3.9845	-4.2150
950	-3.5675	-3.4943	-3.9545	-4.1841

Ultrasound = 0 cycles/sec.

Temperature				
850	-4.1849	-4.2031	-4.0989	-4.3053
875	-4.0212	-3.9971	-4.0557	-4.2754
900	-3.8575	-3.7910	-4.0125	-4.2456
925	-3.7055	-3.5997	-3.9723	-4.2179
950	-3.5534	-3.4084	-3.9322	-4.1902

technique. This led to the need for obtaining conversion versus time data. This method was used for particle sizes 0.0841, 0.0419 and 0.0209 cm. and is explained in the detailed procedure.

Regeneration of the Catalyst

The reactor was purged with air at the reaction temperature after each run for a period of approximately 12 hours to burn off any carbon deposit enabling the catalyst to be reused. Calculations indicate (Appendix VII) that 10 minutes should be sufficient to burn off any carbon. Visual inspection by Lintner, of the reactor, after regeneration for 30 minutes showed that the reactor was carbon free. Comparisions of conversions in the absence of ultrasound between runs employing the same catalyst at the same conditions indicated complete reactivation.

EXPERIMENTAL RESULTS AND DISCUSSION

The regression of the experimental data at step #6 is shown in table 5. It is prepared by using the equations in Appendix IV to obtain Log ϵLk_2 at various temperatures and ultrasounds. This data is plotted versus log d_p in Figures 8 through 10. It can be seen from these graphs that there is a leveling off of the effectiveness factor as the particle size decreases. It is from this region where data will be taken, as Lk_2, and plotted against reciprocal temperature to obtain the activation energy for each ultrasound.

The data from Figures 8 through 10 will be linearized and extrapolated to a particle size of 0.0032 cm. corresponding to a log d_p = -2.5. This can be done by:

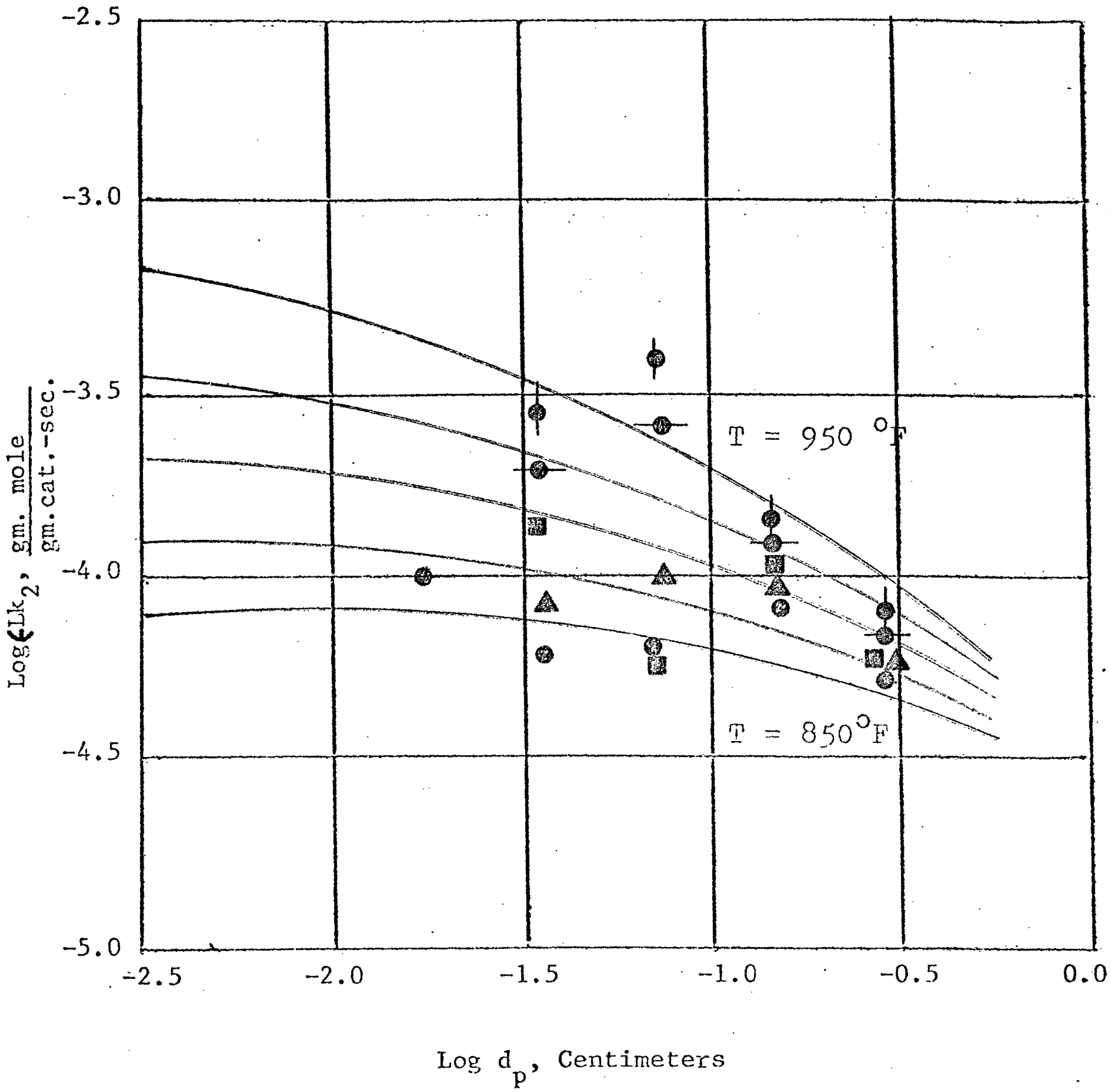
1. making the terms Log ϵLk_2 and Log d_p positive therefore allowing the logarithms to be taken again.

2. This becomes a linear plot and by using a least squares analysis, the slope and intercept values can be found.

Table 6. contains the values of Log ϵLk_2 and Log d_p. Figures 11 through 13 contain the plots from least squares analysis. Table 7 contains the slope and intercept values. The extrapolated values are found in Table 8 and plotted in Figure 14. The activation energies, E, are found in Table 9. E, is calculated by multiplying the slope found in Table 9 by the ideal gas constant = 1.987 gm.-cal/gmole-^{o}k.

FIGURE NO. 8

EFFECTIVENESS FACTOR, ϵLk_2, VERSUS PARTICLE DIAMETER



ULTRASOUND = 0 cycles/sec.

TEMPERATURE = 950. Deg. F.

925. Deg. F.

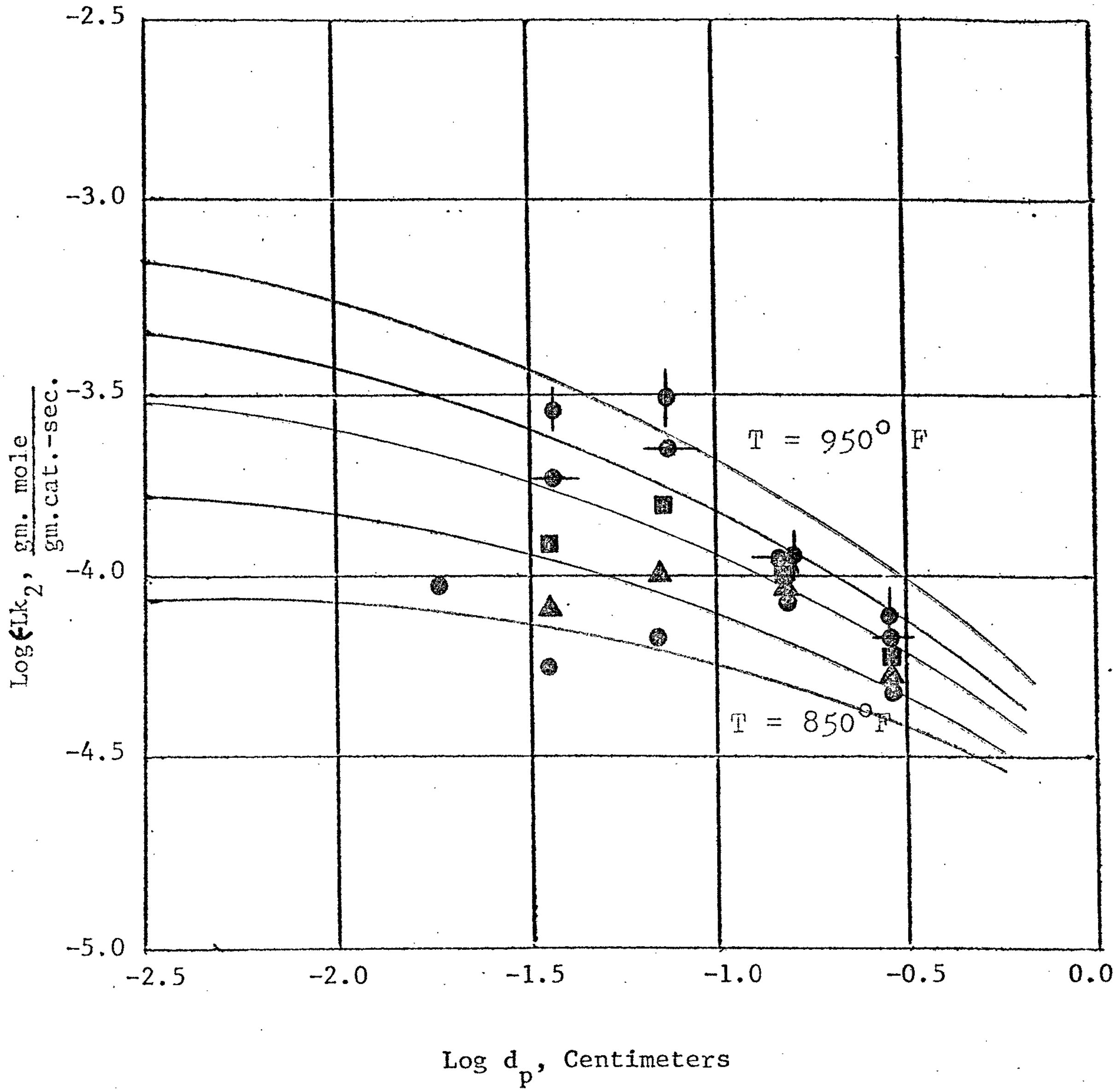
900. Deg. F.

875. Deg. F.

850. Deg. F.

FIGURE NO. 9

EFFECTIVENESS FACTOR, ϵLk_2, VERSUS PARTICLE DIAMETER

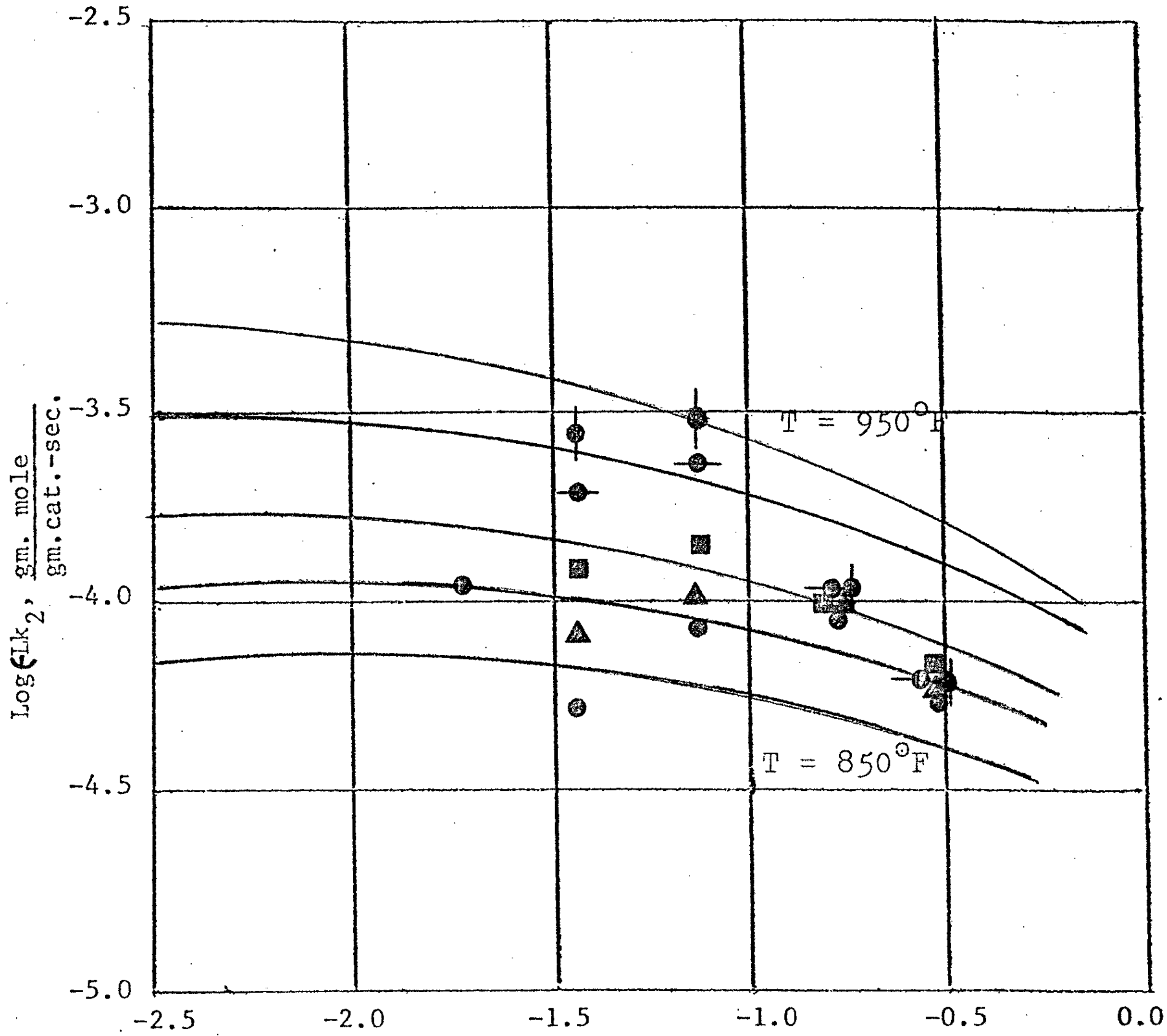


ULTRASOUND = 26,000 cycles/sec.

TEMPERATURE = 950. Deg. F.
925. Deg. F.
900. Deg. F.
875. Deg. F.
850. Deg. F.

FIGURE NO. 10

EFFECTIVENESS FACTOR, ϵLk_2, VERSUS PARTICLE DIAMETER



Log d_p, Centimeters

ULTRASOUND = 39,000 cycles/sec.

TEMPERATURE = ● 950. Deg. F.

● 925. Deg. F.

■ 900. Deg. F.

▲ 875. Deg. F.

● 850. Deg. F.

TABLE NO. 6

EFFECTIVENESS FACTOR VERSUS LOG PARTICLE DIAMETER

Ultrasound = 39,000 cycles/sec.

Temperature	Log(-Log(d_p)) .1392	.0317	-.1555	-.3506
	Log(-Log(Lk2)			
850	.6314	.6207	.6083	.6298
875	.6122	.6017	.6054	.6281
900	.5929	.5827	.6026	.6265
925	.5734	.5635	.5999	.6250
950	.5537	.5442	.5972	.6235

Ultrasound = 26,000 cycles/sec.

Temperature				
850	.6316	.6168	.6106	.6347
875	.6124	.5989	.6071	.6313
900	.5923	.5803	.6036	.6280
925	.5728	.5622	.6004	.6248
950	.5524	.5434	.5971	.6216

Ultrasound = 0 cycles/sec.

Temperature				
850	.6217	.6236	.6127	.6340
875	.6044	.6017	.6081	.6340
900	.5863	.5788	.6034	.6279
925	.5688	.5563	.5990	.6251
950	.5506	.5326	.5946	.6222

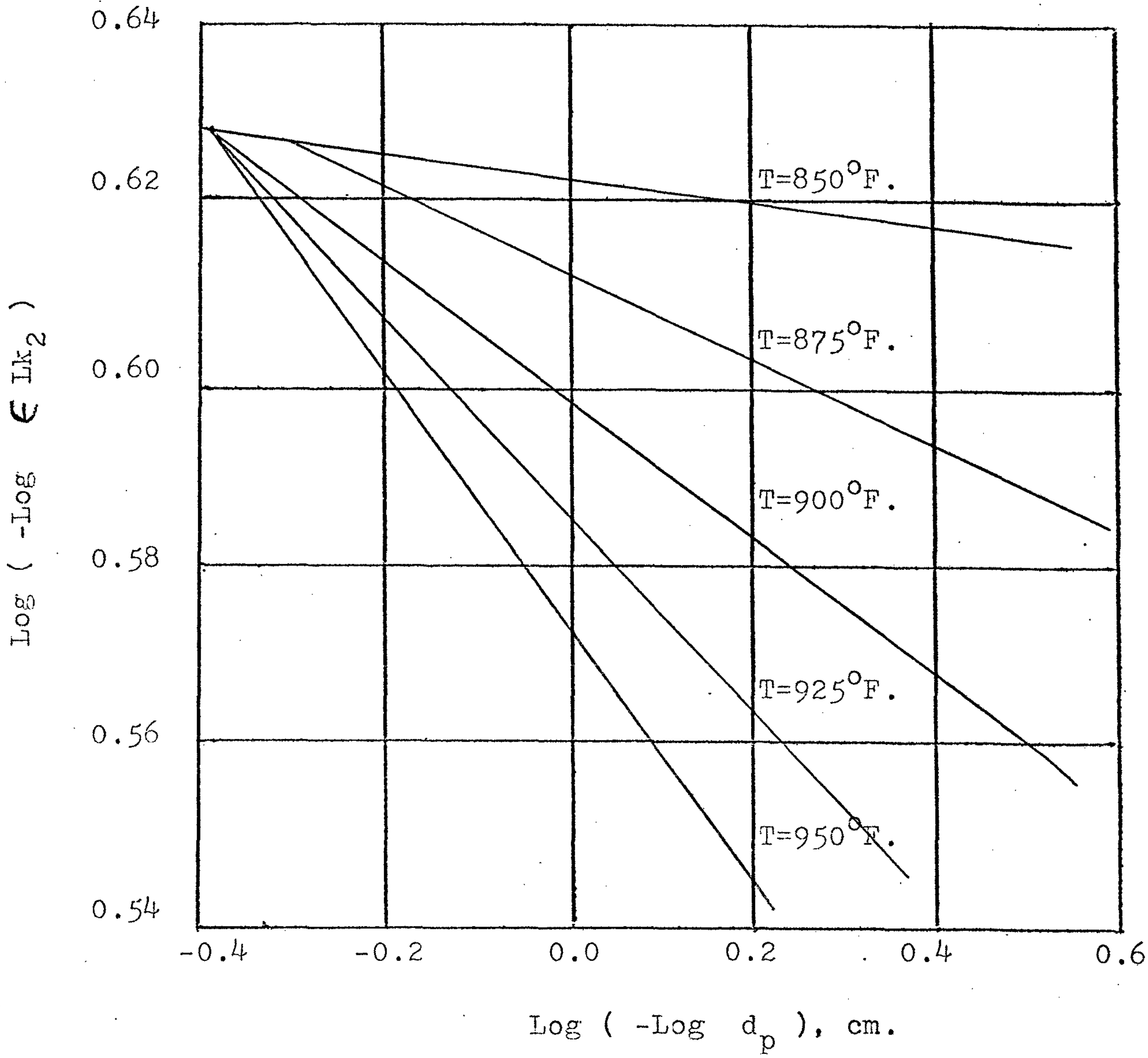
TABLE NO. 7

COEFFICIENTS FOR $\mathrm{Log}(-\mathrm{Log}\ \epsilon L k_2) = A + \mathrm{Log}(-\mathrm{Log}\ d_p)\ B$

Temperature deg. F.	Ultrasound cps x 10^{-3}	A	B
850	39	.6231	.00608
875		.6089	-.03564
900		.5947	-.07775
925		.5803	-.12060
950		.5659	-.16385
850	26	.6228	-.00739
875		.6087	-.04464
900		.5940	-.08409
925		.5798	-.12251
950		.5646	-.16491
850	0	.6215	-.01734
875		.6070	-.06080
900		.5911	-.09464
925		.5761	-.13365
950		.5604	-.17459

FIGURE NO. 11

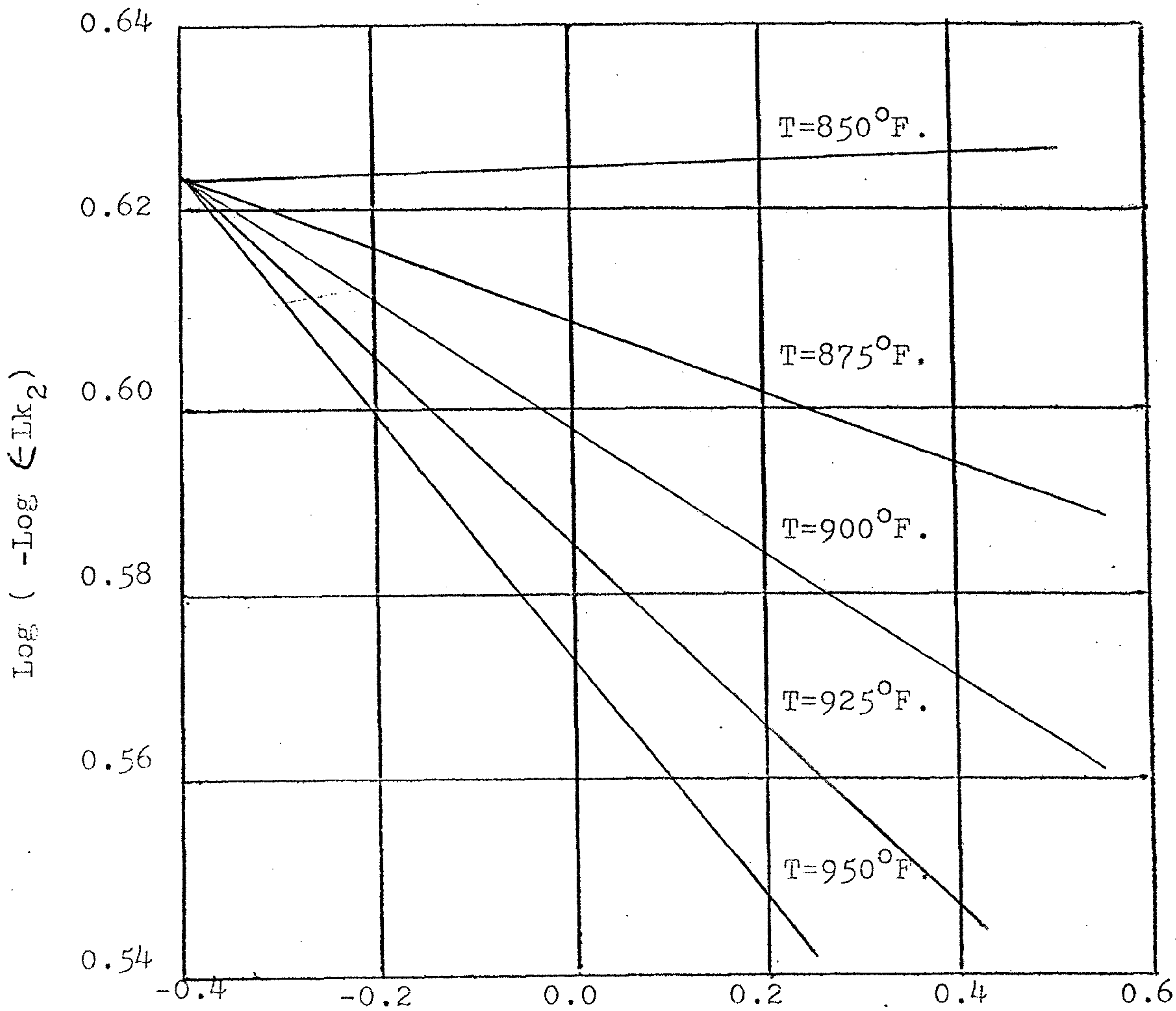
EFFECTIVENESS FACTOR VERSUS Log(-Log d_p)



Ultrasound = 0 cps

FIGURE NO. 12

EFFECTIVENESS FACTOR VERSUS Log(-Log d_p)

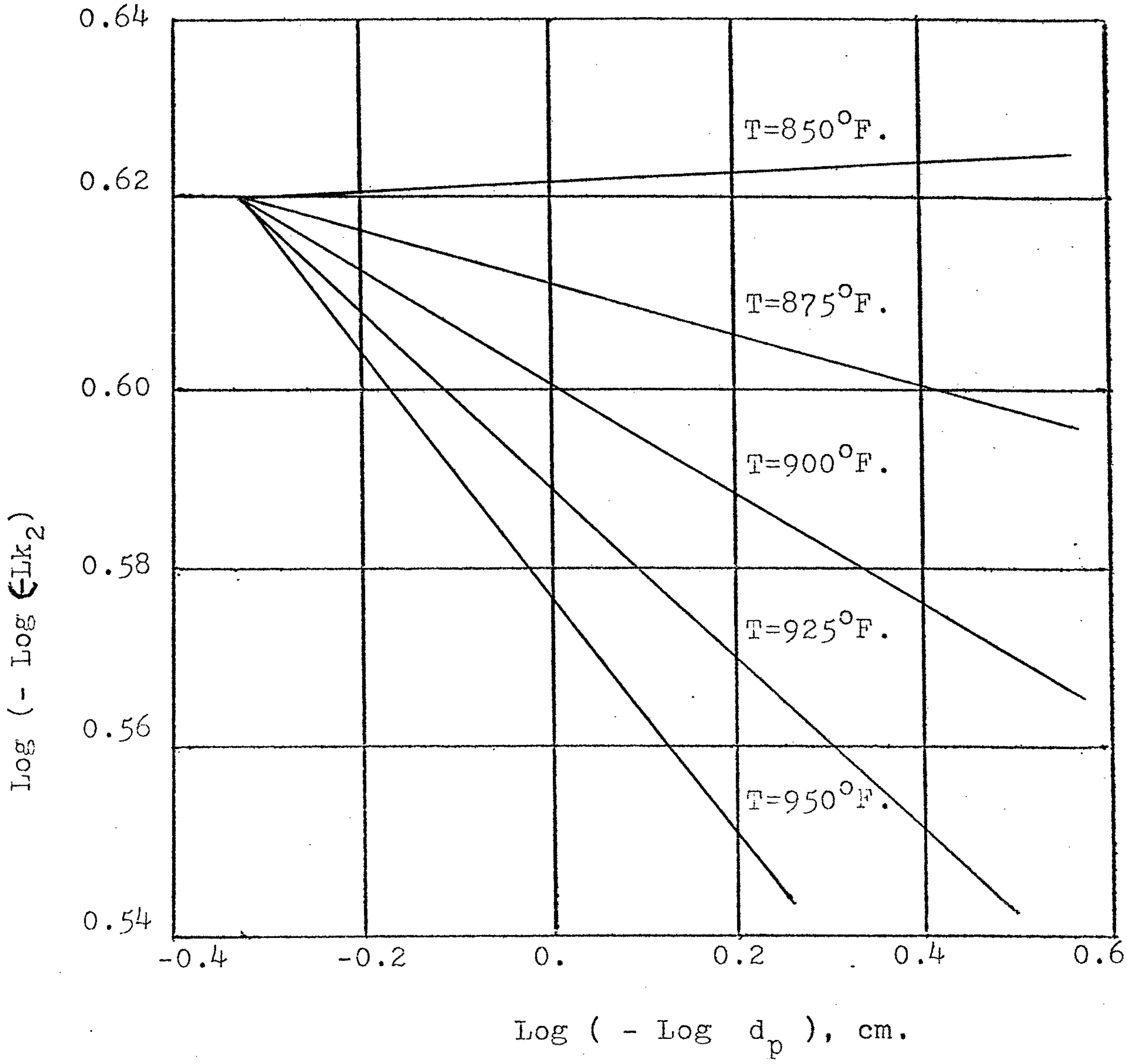


Log (- Log d_p), cm.

Ultrasound = 26,000 cps

FIGURE NO. 13

EFFECTIVENESS FACTOR VERSUS Log(-Log d_p)



Ultrasound = 39,000 cps

TABLE NO. 8

EFFECTIVENESS FACTOR, LOG Lk_2, VERSUS TEMPERATURE

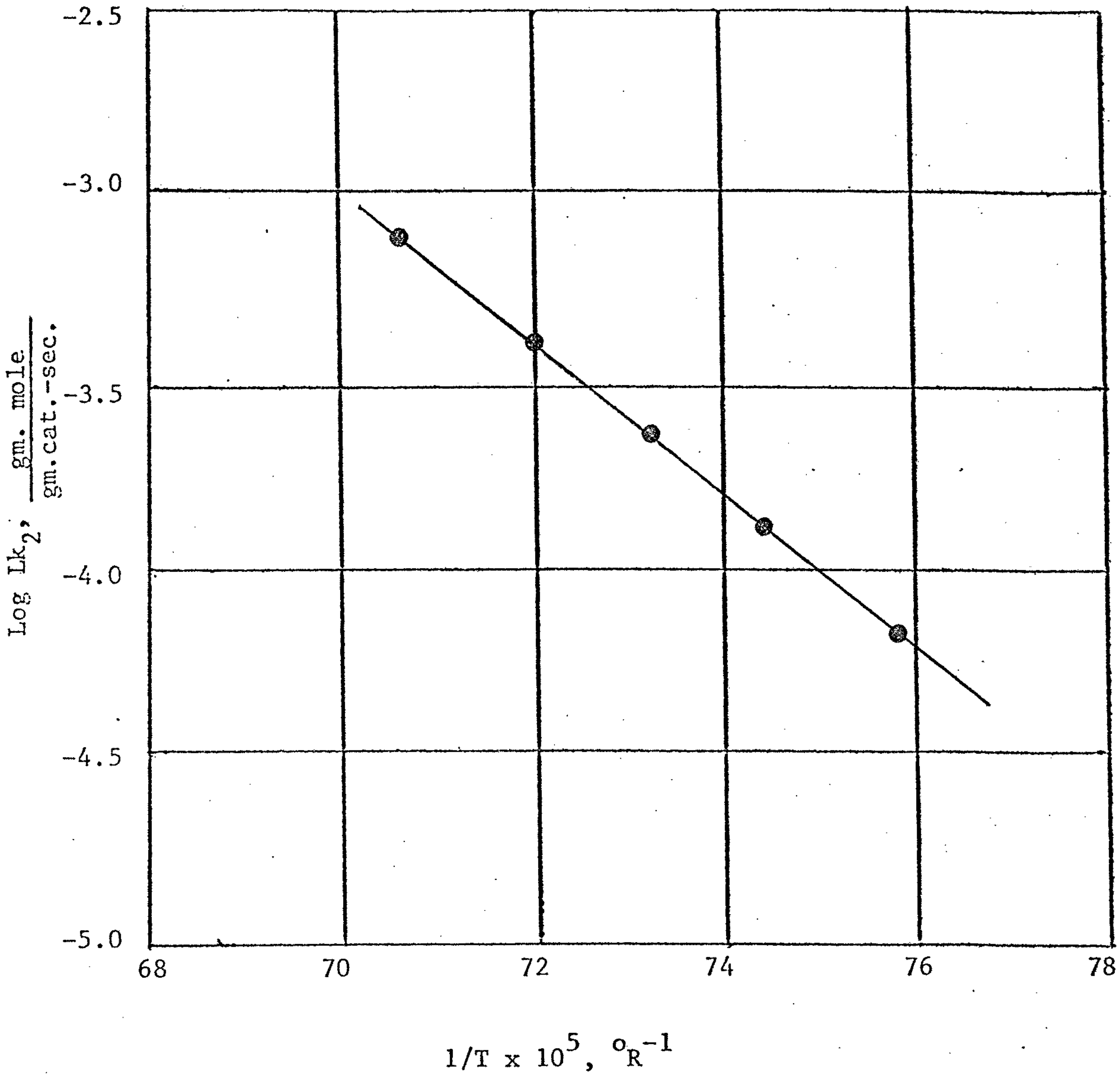
Data extrapolated to Log d_p = -2.5

d_p = 0.0032 cm.

Temperature deg. F.	1/T, $^oR^{-1}$ x 10^5	Ultrasound cps x 10^{-3}	Log Lk_2
850	76.3	0	-4.1172
		26	-4.1677
		39	-4.1745
875	74.9	0	-3.8247
		26	-3.8976
		39	-3.9319
900	73.5	0	-3.5752
		26	-3.6341
		39	-3.6610
925	72.2	0	-3.3312
		26	-3.3947
		39	-3.4049
950	70.9	0	-3.0930
		26	-3.1521
		39	-3.1652

FIGURE NO. 14

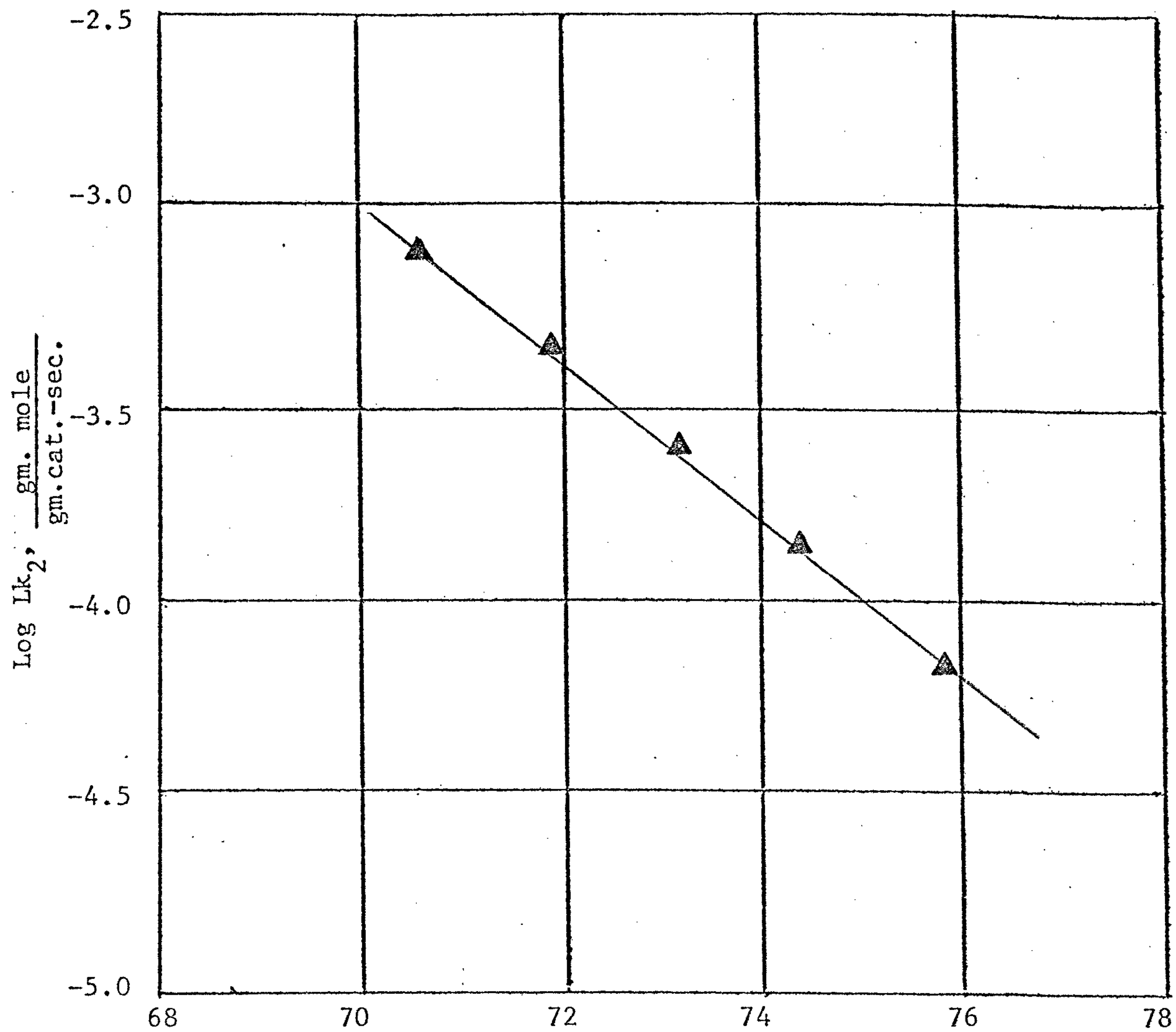
EFFECTIVENESS FACTOR, Lk_2, VERSUS TEMPERATURE



Ultrasound = 0 cps

FIGURE NO. 15

EFFECTIVENESS FACTOR, Lk_2, VERSUS TEMPERATURE

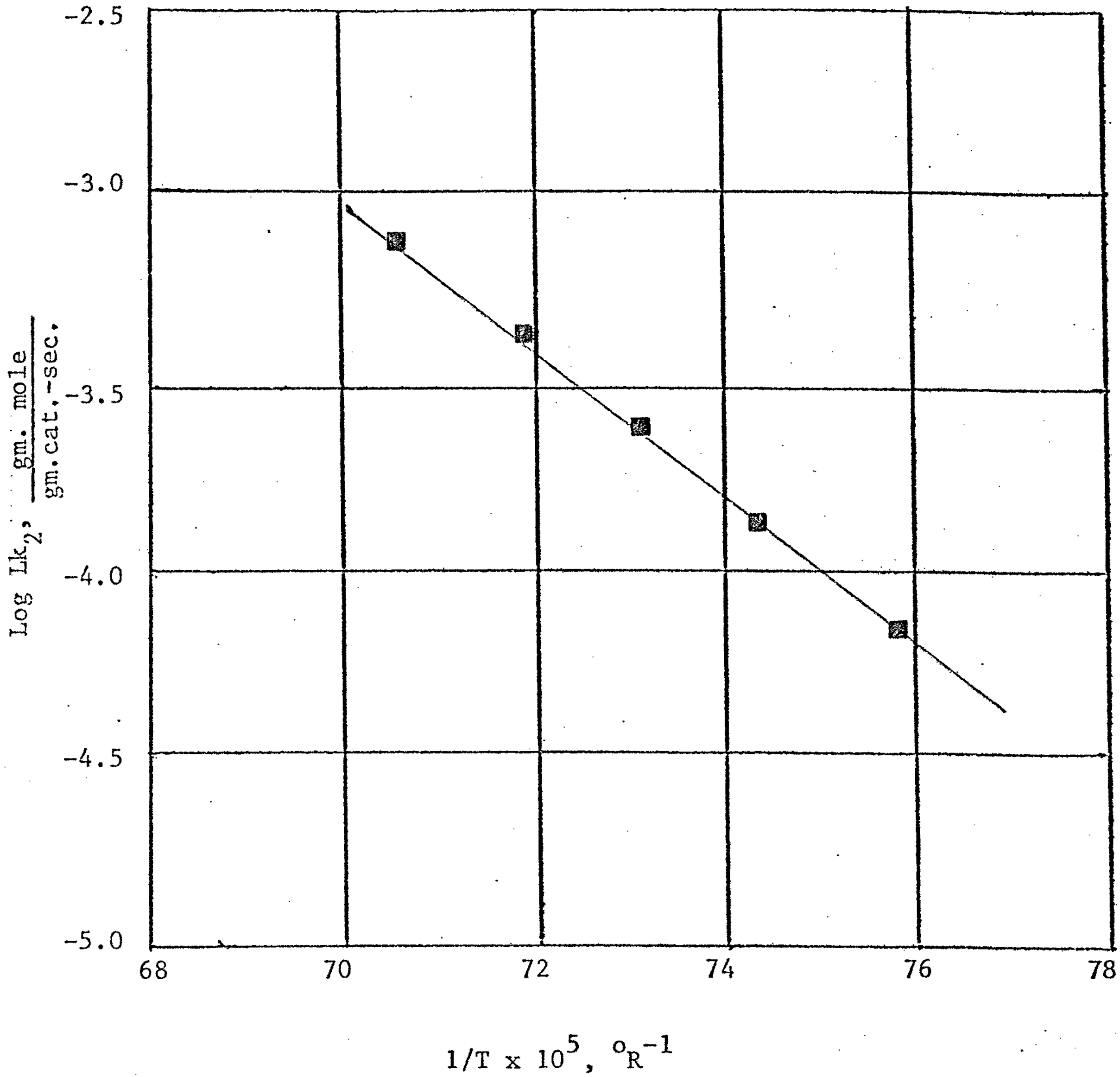


$1/T \times 10^5$, $^oR^{-1}$

Ultrasound = 26,000 cps

FIGURE NO. 16

EFFECTIVENESS FACTOR, Lk_2, VERSUS TEMPERATURE



Ultrasound = 39,000 cps

TABLE NO. 9

$$\text{Log } Lk_2 = A + B/T$$

Ultrasound	Activation Energy E, cal./gmole	A	B
0	37,445.6	10.274	-18845.3
26,000	37,360.2	10.182	-18802.3
39,000	37,514.8	10.274	-18880.1

The assumption that the effectiveness factor has leveled off to a value of unity must now be checked. The procedure used for this test was taken from Lintner and Satterfield:

1. First calculated the forward intrinsic rate constant for surface reaction, k_s, by equation 13.

$$k_s = \epsilon L k_2 \frac{K_A \pi}{(1 + K_A \pi) \; C_{A_o} \; S_g} \qquad (13)$$

2. Calculate the Thiele modulus, h_s, knowing the rate constant and catalyst specfifications.

$$h_s = r_p \left[\frac{S_v \, k'_s}{D_e} \right]^{\frac{1}{2}} \qquad (14)$$

3. Calculate ϵ, using equation 15.

$$\epsilon = \frac{3}{h_s} \left[\frac{1}{\tanh h_s} - \frac{1}{h_s} \right] \qquad (15)$$

4. Compare the calcuated ϵ, to the assumed ϵ value of one.

Table 10 contains the calculations from this check and it should be pointed out that by assuming ϵ to be unity gives a maximum calculated ϵ differing by 1.40%.

The apparent activation energies obtained in this study were therefore derived without pore diffusion effects. The use of ultrasonic vibrations in this region of small

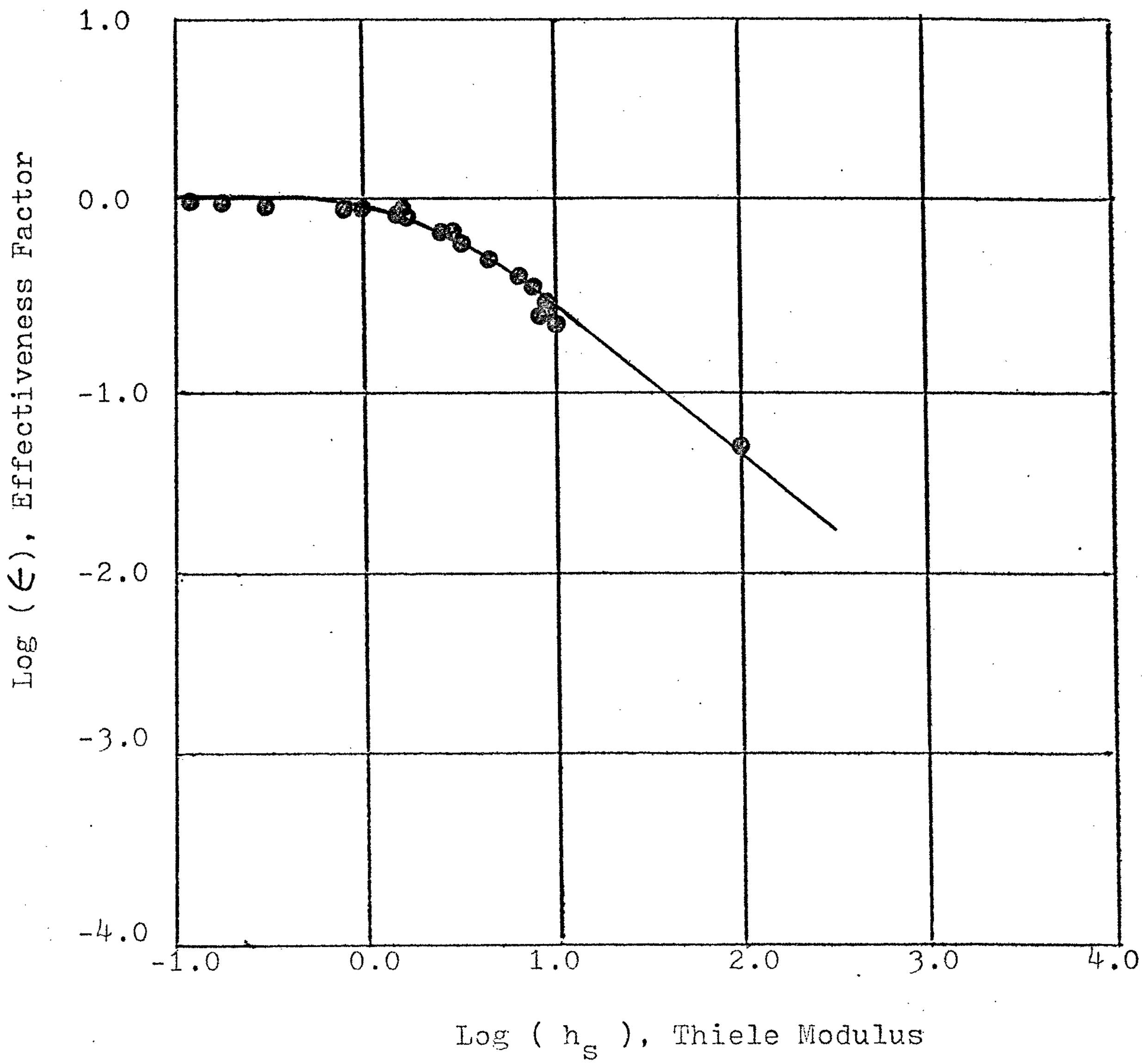
TABLE NO. 10

Calculated Effectiveness Factors From Equations - using measured Data.

Temperature Deg. F.	Lk_2 x 10^4 = 1	k_s x 10^6	h_s	tanh h_s	
850	0.7635	1.2502	.1412	.1402	.9987
875	1.4973	2.5050	.1990	.1964	.9974
900	2.6593	4.5093	.2655	.2594	.9953
925	4.6644	7.9783	.3515	.3377	.9919
950	8.0724	13.9354	.4624	.4320	.9860

FIGURE NO. 17

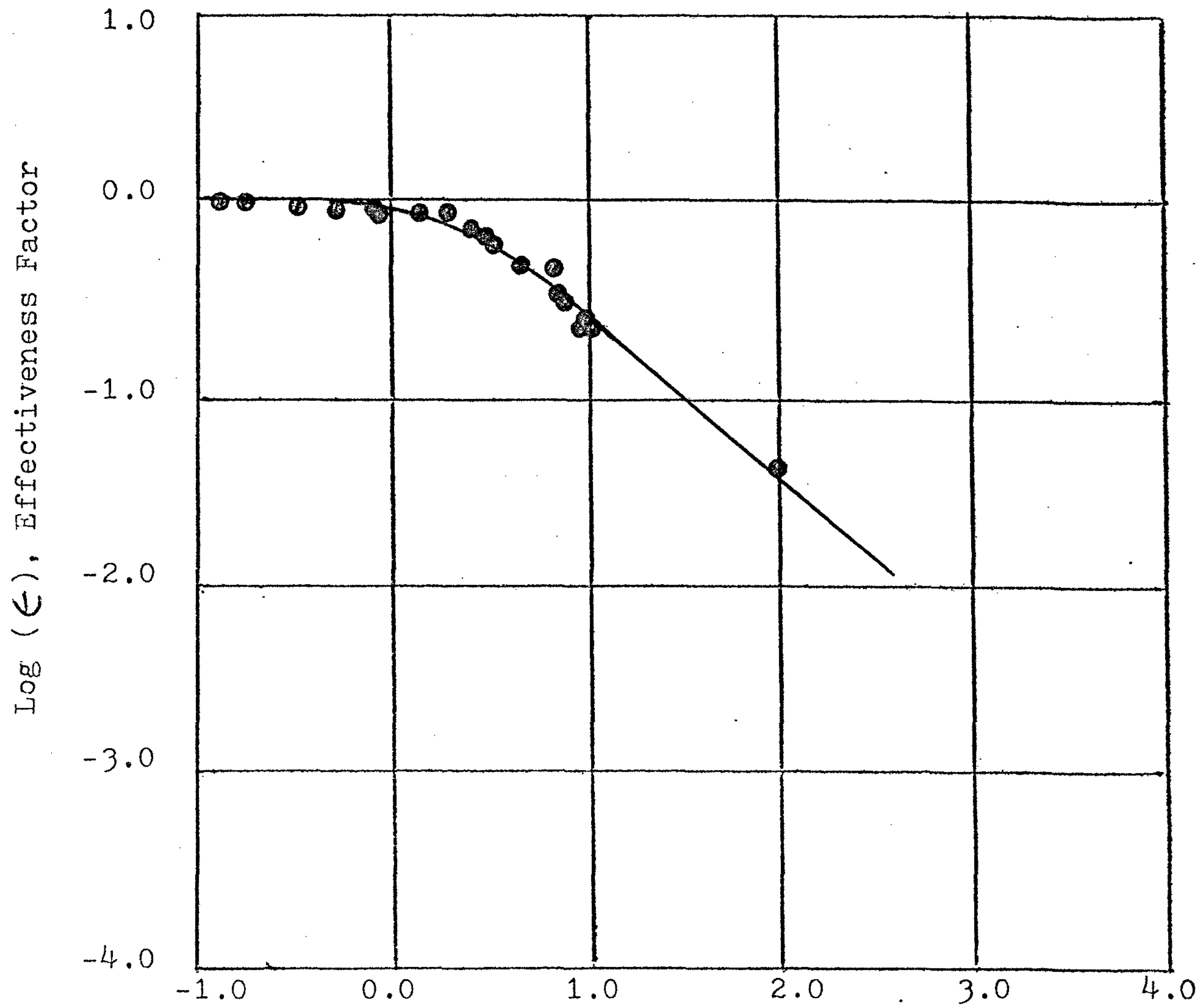
EFFECTIVENESS FACTOR VERSUS THIELE MODULUS



Ultrasound = 39,000 cps

FIGURE NO. 18

EFFECTIVENESS FACTOR VERSUS THIELE MODULUS

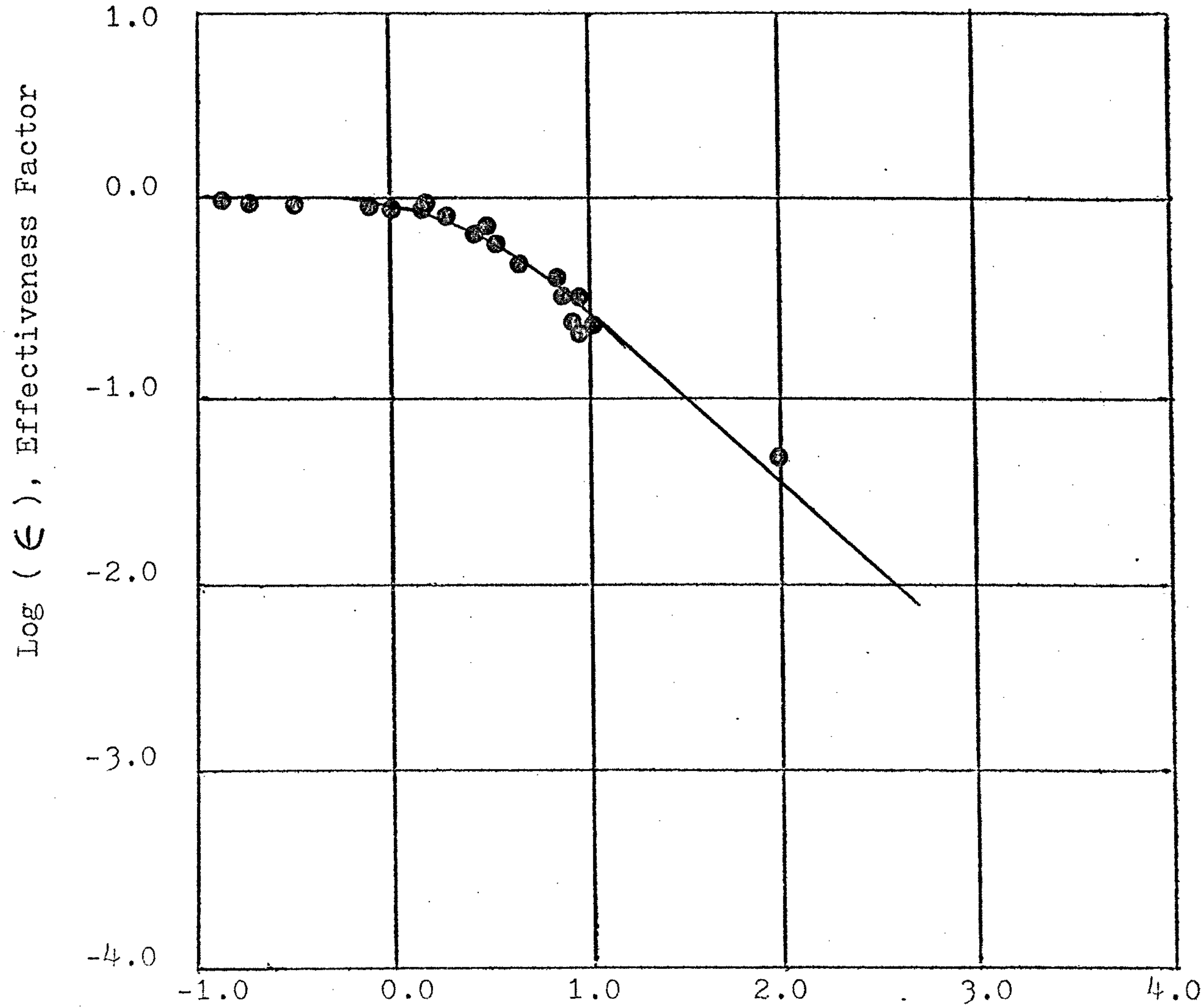


Log (h_s), Thiele Modulus

Ultrasound = 26,000 cps

FIGURE NO. 19

EFFECTIVENESS FACTOR VERSUS THIELE MODULUS



Log (h_s), Thiele Modulus

Ultrasound = 0 cps

particle sizes demonstrates a negligible effect on the apparent activation energy, or the concentration of active sites for the temperature range studied.

Therefore, it is concluded that the ultrasonic differences noted by Lintner for values of ϵLk_2 are the result of pore diffusion effects affecting rather than the term Lk_2.

The following plots of Log effectiveness factor versus Log thiele modulus, Figures 17 through 19 were obtained by methods described in Appendix VIII. A difference of a few percent were calculated between the curves with and without ultrasound.

It is this researchers opinion that the curves developed for conversion versus W/Fao, Appendix V, need more data points than those obtained in this research. With more concise curves the addition of ultrasound could possibly be analyzed more readily.

Conclusions

1. Ultrasonic vibrations at all temperature and frequencies studied appears to not effect:
   a. L, the concentration of active sites.
   b. k_2, the forward reaction rate constant for surface reaction.
   c. E, the apparent activation energy.

2. Therefore ultrasonic vibrations do not cause localized heating within the catalyst bed as suggested by Lintner.(1973)

3. It is then suggested that the noticable increases from Lintner's use of ultrasound are the result of an increase in the effectiveness factor being caused by an increase in the pore diffusion rate.

Recommendations

This research demonstrates that the effects of ultrasonic vibrations on the surface reaction rate constant Lk_2 is negligible. It is thought then that pore diffusion might be effected by ultrasound.

Further research would be recommended as follows:

1. Add more data to this research to quantify the effects of ultrasonic vibrations on pore diffusion.
2. Study a range of frequencies to show whether a relationship between them exists and if there is an optimum frequency.
3. Study the effects of Ultrasonic Vibrations on systems other than the cumene and silica-alumina cracking reaction.

APPENDIX I

PHYSICAL PROPERTIES

FIGURE NO. 20

REACTION CONSTANTS VERSUS TEMPERATURE

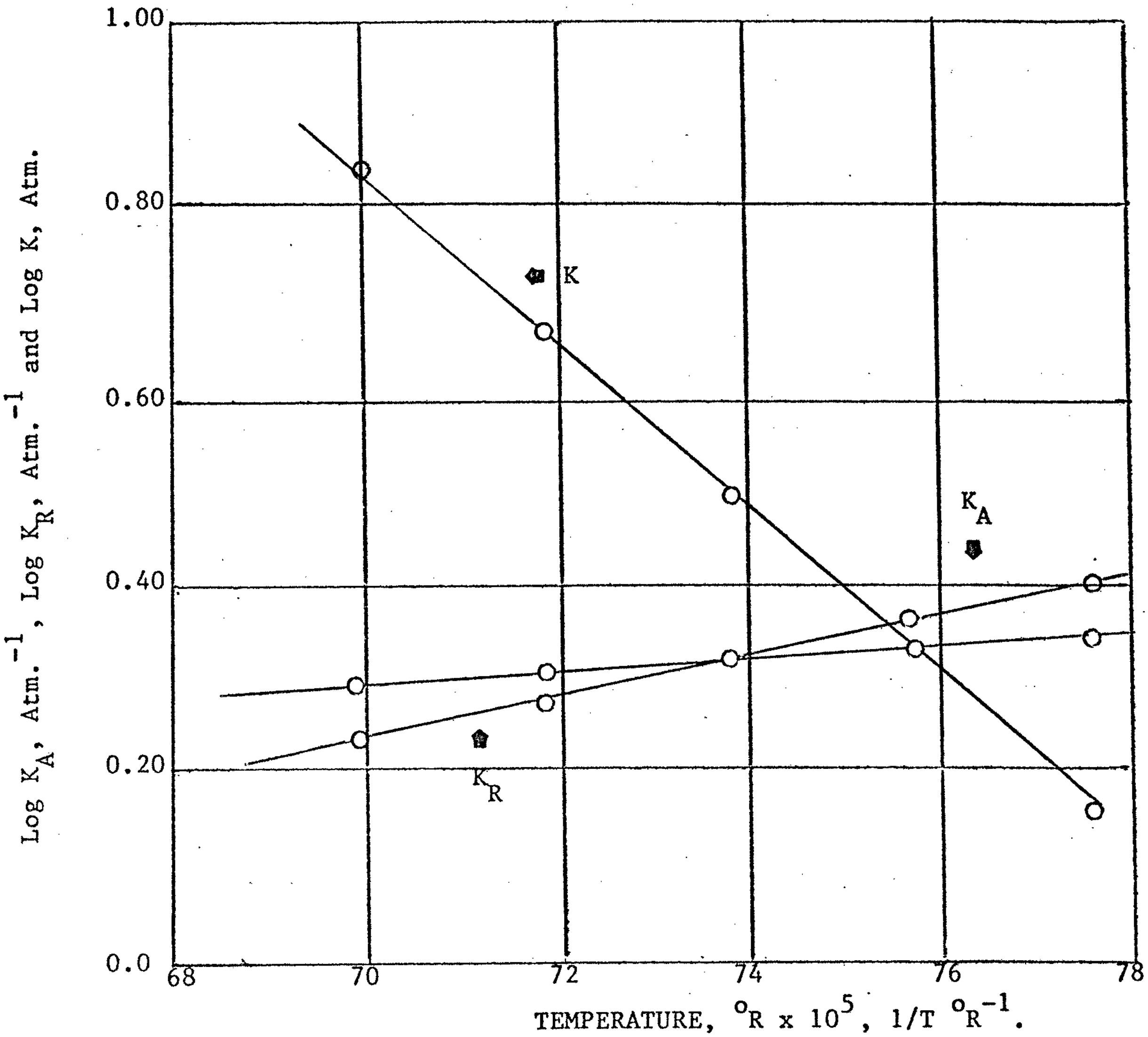


TABLE NO. 11

REACTION CONSTANTS VERSUS TEMPERATURE

Temperature $°R^{-1}$	Log K_A	Log K_R	Log K
0.00070	.3110	.2505	.8771
0.00072	.3250	.2944	.6985
0.00074	.3390	.3383	.5200
0.00076	.3530	.3822	.3415
0.00078	.3670	.4261	.1629

$$\text{Log } K = -8927(1/T) + 7.126$$

$$\text{Log } K_A = 700(1/T) - 0.179$$

$$\text{Log } K_R = 2195(1/T) - 1.286$$

T is in deg. R.

PHYSICAL PROPERTIES OF SILICA-ALUMINA CATALYST

The catalyst employed in this study was TCC (thermofor Catalytic Cracking) Silica-Alumina Cracking Catalyst, supplied by the Mobil Chemical Company, Paulsboro Catalyst Plant, Paulsboro, New Jersey. The Catalyst is designated as "Durabead 1" by Mobil.

The physical properties and Tyler screen data for the catalyst are as follows:

Loose bulk density	ρ_L = 0.74 gms./cm.^{3}
Packed bulk density	ρ_B = 0.82 gms./cm.^{3}
Particle density	ρ_P = 1.28 gms./cm.^{3}
Solid density	ρ_T = 2.32 gms./cm.^{3}
Average diameter	d_P = 0.358 cm.
Surface area	S_g = 250 x 10^{4}cm.^{2}/gm.
Average pore diameter	P_d = 72 x 10^{-8}cm.
Effective pore diffusivity	D_e = 0.015 cm.^{2}/sec.
Pore volume	V_g = 0.35 cm.^{3}/gm.
Internal void fraction	θ = 0.448
External void fraction	ϵ = 0.32
Superficial surface area	α = 13.1 cm.^{2}/gm.
Equivalent pore radius	r_e = 2.8 x 10^{-7} cm.
Tortuosity factor	τ = 5.6
Total surface of porous catalyst	S_V = 320 x 10^4 cm.^{2}/cm.^{3}

Tyler Screen Analysis	Wt.%
on 4 mesh	2.5
on 5 mesh	27.0
on 6 mesh	43.4
on 7 mesh	22.2
on 8 mesh	3.9
on 10 mesh	0.6
Through 10 mesh	0.3
	99.9

Calculation of Superficial Area of Catalyst Surface, α

Catalyst area/pellet = $4 \ \ r_p^2$ cm.^{2}/pellet

Catalyst wt./pellet $= (\frac{4}{3} \ r_p^3$ cm.^{3}/pellet)*($\ _p$gms./cm.^{3})

$$= \frac{4}{3} \ r_p^3 \ \ _p \text{ gms./pellet}$$

$$\alpha = \frac{4 \ \ r_p^2 \text{cm.}^2\text{/pellet}}{\frac{4}{3} \ r_p^3 \ \ _p \text{ gms./pellet}} = \frac{3}{r_p \ \ _p} \text{ cm.}^2\text{/gm.}$$

r_p = 0.179 cm.

$\ _p$ = 1.28 gms./cm.^{3}

$$\alpha = \frac{3}{(0.179)(1.28)} = 13.10 \text{ cm.}^2\text{/gm.}$$

TABLE NO. 12

SUPERFICIAL AREAS OF VARIOUS CATALYST SIZES

Tyler Screen Size	radius of particle, r_p cm.	α cm.^{2}/gm.
6	0.179	13.10
10	0.100	23.44
20	0.04205	55.72
40	0.02095	111.87
70	0.01045	224.28
140	0.00520	450.72

Calculation of Effective Diffusivity, D_e

$$D_e = \underline{D_s \qquad}$$

$$= D_s \frac{(0.448)}{5.6}$$

$$= 0.080\ D_s$$

Calculation of Combined Diffusivity, D_s

$$1/D_s = 1/D_{AB} + 1/D_K$$

Knudsen Diffusivity, $D_K = 2.478 \times 10^{-4}\ (T)^{\frac{1}{2}} \quad T = {}^oK$

Molecular Diffusivity, $D_{AB} = -0.00633 + 0.1008 \times 10^{-5}(T)^{1.82}$

$T = {}^oK$

TABLE NO. 13

DIFFUSIVITIES AT VARIOUS TEMPERATURES

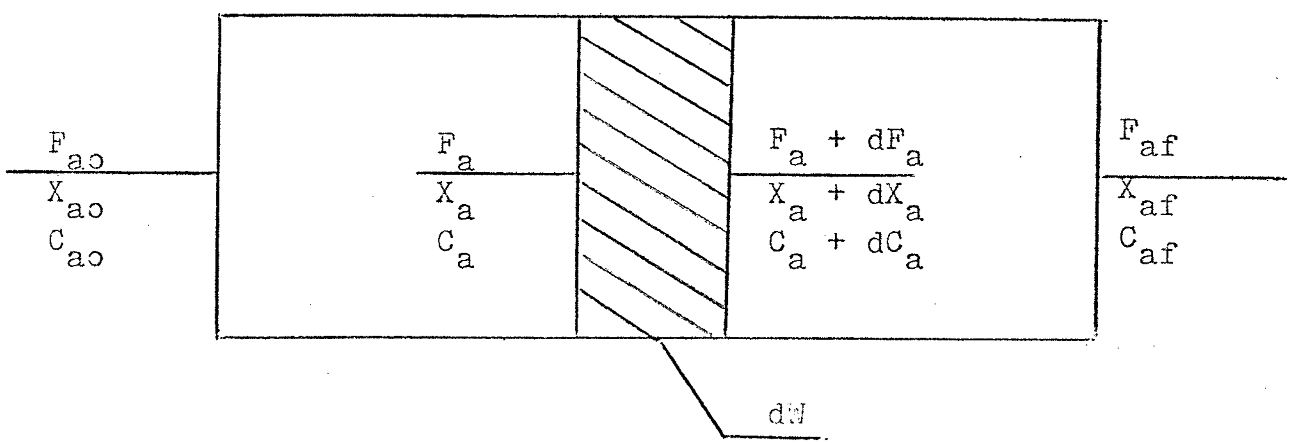
Temperature deg. F.	deg. K.	D_{AB} cm^2/sec	D_K cm^2/sec	D_S cm^2/sec	D_e cm^2/sec
850	727.8	.1568	.00669	.00642	.000514
875	741.7	.1624	.00675	.00648	.000518
900	755.6	.1684	.00681	.00655	.000524
925	769.4	.1741	.00687	.00661	.000529
950	783.3	.1799	.00693	.00677	.000534

APPENDIX II

REACTOR DESIGN EQUATION

FIGURE NO. 21

CROSS SECTION OF PLUG FLOW REACTOR SHOWING DIFFERENTIAL ELEMENT



REACTOR DESIGN EQUATION

(Lintner, 1973)

The reaction design equation is derived by substituting the rate equation for the single site mechanism, S (propylene) not absorbed, with surface reaction controlling into the plug flow reactor design equation. The derivation is as follows:

Derivation of Design Equation for Plug Flow Reactor Flow Chart (Figure 20).

Material Balance

Input - Output + Generation = Accumulation

Input

F_A gm. moles A/ sec.

Output

$(F_A + dF_A)$ gm.moles A/ sec.

Generation

$$(+r_A \frac{\text{gm.moles A}}{\text{gm.cat-sec.}})(dW \text{ gm.cat.}) = (+r_A)dW \frac{\text{gm.moles A}}{\text{sec.}}$$

Accumulation

= 0 (steady state)

Material Balance

$$F_A - F_A - dF_A = r_A dW = 0$$

$$-dF_A = (-r_A)dW$$

$$F_A = F_{A_o} - X_A F_{A_o}$$

$$dF_A = -F_{A_o} dX_A$$

$$F_{A_o} dX_A = (-r_A) dW$$

$$\frac{dW}{F_{A_o}} = \frac{dX_A}{(-r_A)}$$

Intergrate

$$\int_0^W \frac{dW}{F_{A_o}} = \int_{X_{A_o}}^{X_{A_f}} \frac{dX_A}{(-r_A)}$$

$$\frac{W}{F_{A_o}} = \int_{X_{A_o}}^{X_{A_f}} \frac{dX_A}{(-r_A)}$$

Calculation of Reaction Design Equation, Surface Reactions Controlling.

Rate Equation for Single Site Mechanism, S (Proplyene) Not Adsorbed, and Surface Reaction Controlling.

$$(-r_A) = \frac{\epsilon L k_2 K_A \left[p_A - \frac{p_R p_S}{K} \right]}{1 + K_A p_A + K_R p_R}$$

Substitute Rate Equation Into Plug Flow Reactor Design Equation

$$\frac{W}{F_{A_o}} = \int_{X_{A_o}}^{X_{A_f}} \frac{dX_A}{\dfrac{\epsilon L k_2 K_A\left[-\dfrac{p_R p_S}{K} + p_A\right]}{1 + K_A p_A + K_R p_R}}$$

Solve for Partial Pressures in Terms of Conversion and Total Pressure

Material Balance

	Inlet	Reactor	Outlet
A	$N_{A_o}=N_{A_o}$	$N_A=N_{A_o}-X_AN_{A_o}$	$N_{A_f}=N_{A_o}-X_{A_f}N_{A_o}$
R	$N_{R_o}=N_{R_o}$	$N_R=N_{R_o}+X_AN_{A_o}$	$N_R=N_{R_o}+X_{A_f}N_{A_o}$
S	$N_{S_o}=N_{S_o}$	$N_S=N_{S_o}+X_AN_{A_o}$	$N_S=N_{S_o}+X_{A_f}N_{A_o}$
Total	$N_{A_o}+N_{R_o}+N_{S_o}$	$N_{A_o}+N_{R_o}+N_{S_o}+X_AN_{A_o}$	$N_{A_o}+N_{R_o}+N_{S_o}+X_{A_f}N_{A_o}$

$$p_A = \frac{N_A \pi}{N_T} = \frac{(N_{A_o}-X_AN_{A_o})\,\pi}{(N_{A_o}+N_{R_o}+N_{S_o}+X_AN_{A_o})}$$

$$p_R = \frac{N_R \pi}{N_T} = \frac{(N_{R_o}+X_AN_{A_o})\,\pi}{(N_{A_o}+N_{R_o}+N_{S_o}+X_AN_{A_o})}$$

$$p_S = \frac{N_S \pi}{N_T} = \frac{(N_{S_o}+X_AN_{A_o})\,\pi}{(N_{A_o}+N_{R_o}+N_{S_o}+X_AN_{A_o})}$$

However, $N_{R_o} = N_{S_o} = 0$

$$p_A = \frac{N_{A_o}(1 - X_A)\pi}{N_{A_o}(1 + X_A)} = \frac{(1 - X_A)\pi}{(1 + X_A)}$$

$$p_R = \frac{X_A N_{A_o}\pi}{N_{A_o}(1 + X_A)} = \frac{(X_A \pi)}{(1 + X_A)}$$

$$p_S = \frac{X_A N_{A_o}\pi}{N_{A_o}(1 + X_A)} = \frac{X_A \pi}{(1 + X_A)}$$

<u>Substitute for Partial Pressures in Rate Equation</u>

$$(-r_A) = \frac{\epsilon L k_2 K_A \left[p_A - \frac{p_S p_R}{K}\right]}{1 + K_A p_A + K_R p_R}$$

$$= \frac{\epsilon L k_2 K_A \left[\frac{(1-X_A)\pi}{(1+X_A)} - \frac{X_A^2 \pi^2}{(1+X_A)^2 K}\right]}{1 + \frac{K_A(1-X_A)\pi}{(1+X_A)} + \frac{K_A X_A \pi}{(1+X_A)}}$$

$$\frac{1}{(-r_A)} = \frac{(1 + K_A \pi)}{\epsilon L k_2 K_A \pi (1 - (1 + \frac{\pi}{K})\, X^2)}$$

$$+ \frac{(2 + K_R \pi) X_A}{\epsilon L k_2 K_A \pi (1 - (1 + \frac{\pi}{K})\, X_A^2)}$$

$$+ \frac{(1 - K_A \pi + K_R \pi)\, X_A^2}{\epsilon L k_2 K_A \pi (1 - (1 + \frac{\pi}{K})\, X_A^2}$$

$$\frac{(1 + K_A \pi)}{\epsilon L k_2 K_A \pi \left(1 - (1+\frac{\pi}{K}) X_A^{\,2}\right)}$$

$$= \left[\frac{1}{\epsilon L k_2 K_A \pi} + \frac{K_A \pi}{\epsilon L k_2 K_A \pi} \right] \left[\frac{1}{1 - (1+\frac{\pi}{K}) X_A^{\,2}} \right]$$

$$= \gamma \left[\frac{1}{1 - \delta^2 X_A^{\,2}} \right]$$

$$\gamma = \frac{1}{\epsilon L k_2 K_A \pi} + \frac{1}{\epsilon L k_2}$$

$$\delta = \left[1 + \frac{\pi}{K} \right]^{\frac{1}{2}}$$

$$\frac{(2 + K_R \pi) X_A}{\epsilon L k_2 K_A \pi \left(1 - (1+\frac{\pi}{K}) X_A^{\,2}\right)}$$

$$= \left[\frac{2}{\epsilon L k_2 K_A \pi} + \frac{K_R \pi}{\epsilon L k_2 K_A \pi} \right] \left[\frac{X_A}{1 - (1+\frac{\pi}{K}) X_A^{\,2}} \right]$$

$$= \beta \left[\frac{X_A}{1 - \delta^2 X_A^{\,2}} \right]$$

$$\beta = \frac{2}{\epsilon L k_2 K_A \pi} + \frac{K_R}{\epsilon L k_2 K_A}$$

$$\frac{(1 - K_A\pi + K_R\pi)X_A^2}{\epsilon Lk_2K_A\pi(1 - (1+\frac{\pi}{K})X_A^2)}$$

$$= \left[\frac{1}{\epsilon Lk_2K_A\pi} - \frac{K_A\pi}{\epsilon Lk_2K_A\pi} + \frac{K_R\pi}{\epsilon Lk_2K_A\pi}\right]\left[\frac{X_A^2}{1 - (1+\frac{\pi}{K})X_A^2}\right]$$

$$= \left[\frac{1}{\epsilon Lk_2K_A\pi} - \frac{1}{\epsilon Lk_2} + \frac{K_R}{\epsilon Lk_2K_A}\right]\left[\frac{X_A^2}{1 - (1+\frac{\pi}{K})X_A^2}\right]$$

$$= \left[\beta - \gamma\right]\left[\frac{X_A^2}{1 - \delta^2X_A^2}\right] = \left[\frac{(\beta - \gamma)X_A^2}{1 - \delta^2X_A^2}\right]$$

$$\beta - \gamma = \frac{2}{\epsilon Lk_2K_A\pi} + \frac{K_R}{\epsilon Lk_2K_A} - \frac{1}{\epsilon Lk_2K_A\pi} - \frac{1}{\epsilon Lk_2}$$

$$= \frac{1}{\epsilon Lk_2K_A\pi} - \frac{1}{\epsilon Lk_2} + \frac{K_R}{\epsilon Lk_2K_A}$$

$$\frac{1}{(-r_A)} = \frac{\gamma}{1 - \delta^2X_A^2} + \frac{\beta X_A}{1 - \delta^2X_A^2} + \frac{(\beta - \gamma)X_A^2}{1 - \delta^2X_A^2}$$

<u>Substitute Rate Equation Into Plug Flow Reactor Design Equation and Intergrate</u>

$$\frac{W}{F_{A_o}} = \int_{X_{A_o}}^{X_{A_f}} \frac{\gamma\, dX_A}{1 - \delta^2X_A^2} + \int_{X_{A_o}}^{X_{A_f}} \frac{\beta X_A\, dX_A}{1 - \delta^2X_A^2} + \int_{X_{A_o}}^{X_{A_f}} \frac{(\beta - \gamma)X_A\, dX_A}{1 - \delta^2X_A^2}$$

$$= \gamma \int_0^{X_A} \frac{dX_A}{-\delta^2 X_A^{\,2}+1} = \frac{\gamma}{2\delta} \ln \left[\frac{1+X_A\delta}{1+X_A\delta}\right]_0^{X_A} = \frac{\gamma}{2\delta} \ln \frac{1+X_A\delta}{1+X_A\delta}$$

$$+ \beta \int_0^{X_A} \frac{X_A dX_A}{-\delta^2 X_A+1} = \frac{\beta}{-2\delta^2} \ln \left[-\delta^2 X_A^{\,2}+1\right]_0^{X_A} = \frac{-\beta}{2\delta^2} \ln(-\delta^2 X_A^{\,2}+1)$$

$$+(\beta-\gamma) \int_0^{X_A} \frac{X_A^{\,2} dX_A^{\,2}}{-\delta^2 X_A^{\,2}+1} = \frac{(\beta-\gamma)X_A}{-\delta^2} - \frac{(\beta-\gamma)}{-\delta^2} \int_0^{X_A} \frac{dX_A}{-\delta^2 X_A^{\,2}+1}$$

$$= \frac{-(\beta-\gamma)\,X_A}{\delta^2} + \frac{(\beta-\gamma)}{2} \left[\frac{1}{2\delta} \ln \frac{(1+X_A\delta)}{(1-X_A\delta)}\right]$$

$$\frac{W}{F_{A_o}} = \frac{\gamma}{2\delta} \ln \frac{(1+X_A\delta)}{(1-X_A\delta)} - \frac{\beta}{2\delta^2} \ln(-\delta^2 X_A^{\,2}+1) - \frac{(\beta-\gamma)X_A}{\delta^2}$$

$$+ \frac{(\beta-\gamma)}{\delta^2} \left[\frac{1}{2\delta} \ln \frac{(1+X_A\delta)}{(1+X_A\delta)}\right]$$

$$\frac{W}{F_{A_o}} = \gamma \left[\left[\frac{1}{2\delta} - \frac{1}{2\delta^3} \right] \ln \frac{(1+X_A\delta)}{(1-X_A\delta)} + \frac{X_A}{\delta^2} \right]$$

$$+ \quad \frac{1}{2\delta^3} \ln \frac{(1+X_A\delta)}{(1-X_A\delta)} - \frac{1}{2\delta^2} \ln (1-\delta^2 X_A{}^2) - \frac{X_A}{\delta^2}$$

$$\gamma = \frac{1}{\epsilon L k_2 K_A \pi} + \frac{1}{\epsilon L k_2}$$

$$\beta = \frac{2}{\epsilon L k_2 K_A \pi} \quad \frac{K_R}{\epsilon L k_2 K_A}$$

$$\delta = \left[1 + \frac{\pi}{K} \right]^{\frac{1}{2}}$$

<u>Calculation of Reaction Design Equation, External Diffusion Controlling</u>

<u>Rate Equation for External Diffusion Controlling</u>

$$r_A = \frac{p_T k_g \alpha}{RT} \ln \frac{1+Y_{A_b}}{!+Y_{A_s}}$$

Substitute into Plug Flow Reactor Equation

$$\frac{W}{F_{A_o}} = \int_{X_{A_o}}^{X_{A_f}} \frac{dX_A}{\frac{p_T kg\,\alpha}{RT} \ln \frac{1+Y_{A_b}}{1+Y_{A_s}}}$$

$$\frac{W}{F_{A_o}} = \frac{X_{A_f}\ RT}{p_T k_g \alpha \ln \dfrac{1+Y_{A_b}}{1+Y_{A_s}}}$$

Calculation of Mass Transfer Coefficient, k_g

$$k_g = \frac{X_{A_f} RT}{(W/Fao)\, p_T \alpha \ln \dfrac{1+Yab}{1+Yas}}$$

Y_{A_s} = 0 (mole fraction cumene at catalyst surface)

R = 82.03 cm.^{3}-atm./gm.mole-^{o}K

T = ^{o}K

Fao = gm.moles cumene/sec.

W = gms. catalyst

p_T = 1.0 atm.

α = 13.1 cm.^{2}/gm.

k_g = cm./sec.

X_{A_f} = conversion

$Y_{A_b} = \dfrac{Yai-Yao}{\ln \dfrac{Yai}{Yao}} = Y_{A_{lm}}$ (mole fraction of cumene in bulk gas stream)

Yai = 1.0 (mole fraction cumene at reactor inlet)

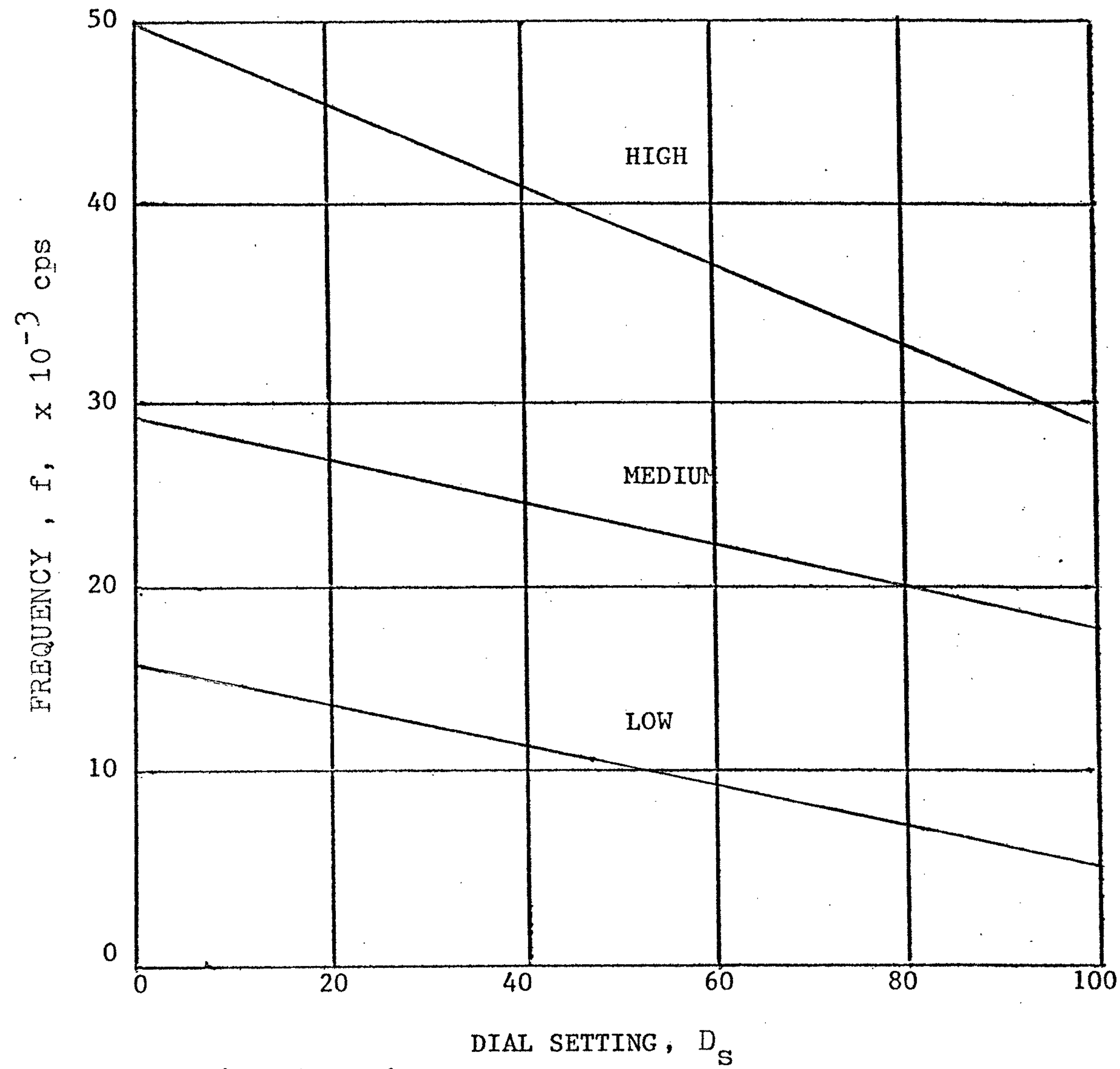
$Yao = \dfrac{1 - X_{Af}}{1 + X_{Af}}$ (mole fraction cumene at reactor outlet)

APPENDIX III

ROTAMETER CALIBRATIONS

FIGURE NO. 22

ULTRASONIC GENERATOR FRQUENCY CALIBRATION



Working Equations:

Low $f = 16.25 - 0.1125\ D_s$

Medium $f = 29.0 - 0.12\ D_s$

High $f = 50.0 - 0.21\ D_s$

FIGURE NO. 23

FEED ROTAMETER CALIBRATION CURVE

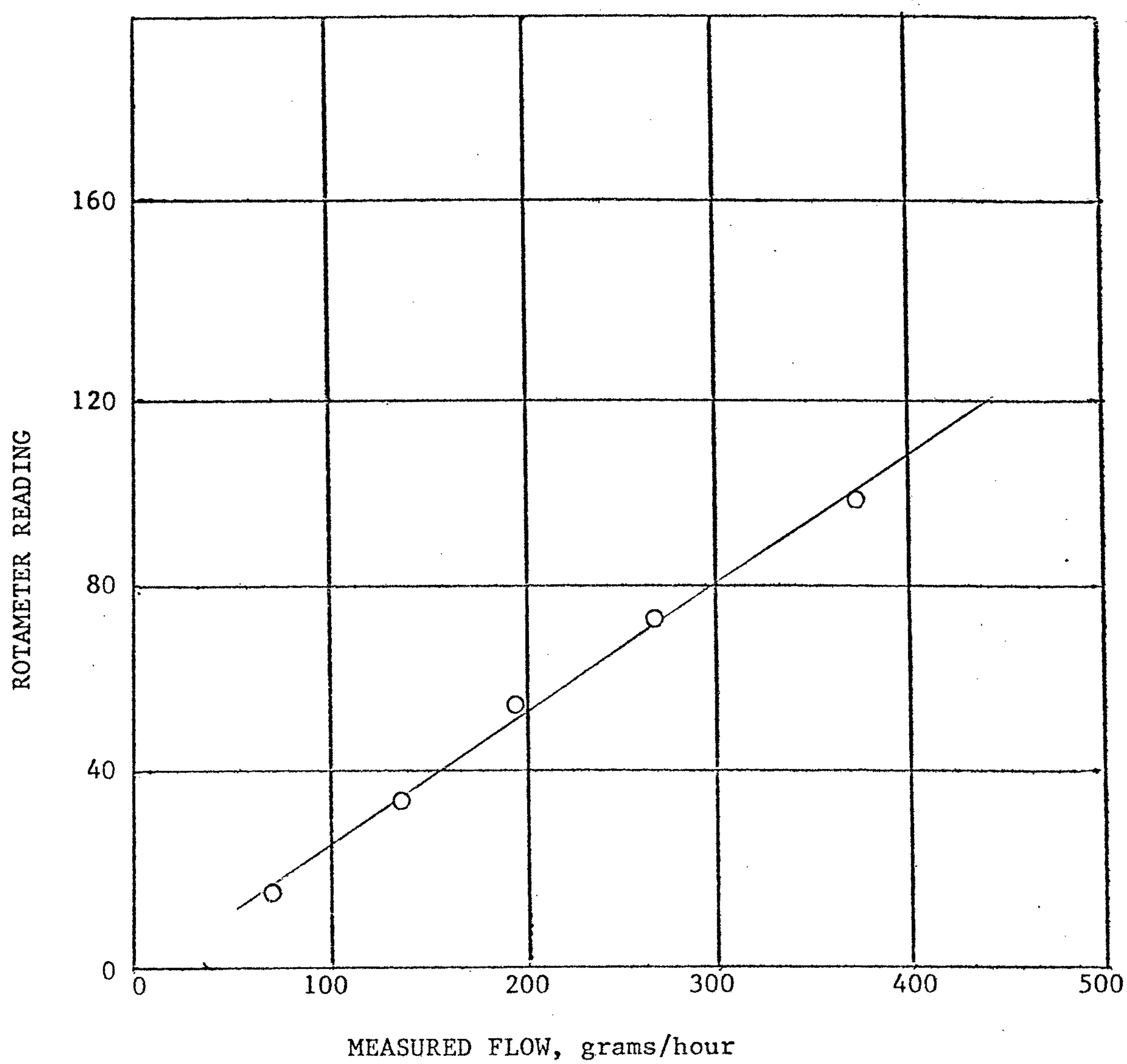


TABLE NO. 14

ROTATMETER CALIBRATION

Trial No.	Rotameter Reading	Measured Flow gm./hr.
	Y	X
1	18.75	71.03
2	37.50	144.80
3	57.25	206.27
4	76.50	286.86
5	100.50	389.31

Working Equation : $Y = 0.630 + 0.260(X)$

CALCULATION OF MEASURED FLOW RATE

L = Length of feed tank, inches.
D = Diameter of feed tank, inches.
= Density of feed, gm./cu.ft.

<u>Basis:</u> 1 inch long section of tank No. 1.

$$\text{Volume} = D^2L/4$$

$$= \frac{3.14 \quad *(1/12)^2(1/12)}{4}$$

$$= 4.5451 \times 10^{-4} \text{ cu.ft./inch}$$

Density = 62.38 lb./cu.ft x sp.gr. x 454 gm./lb.

24413.5 gm./cu.ft.

Flow rate per inch = Volume x Density

= 11.1 gm./inch

Flow in gm./hr. = gm./inch x inch/min. x 60 min./hr.

= 665.8 x in./min.

Where inches/min. can be measured. by height drop over a measured time.

APPENDIX IV

EFFECTIVENESS FACTOR VERSUS TEMPERATURE DATA

The data that appears in this Appendix was obtained using the coefficients of the quadratic expression for conversion found in Appendix V, and the computer program Cumene. Program Cumene calculates an average value for ϵLk_2 over a range of W/Fao.

It should be noted that this range was not the same for each instance because the upper limit for W/Fao varied for each run. However the effect of this difference is of the order of 2% or less and can be neglected.

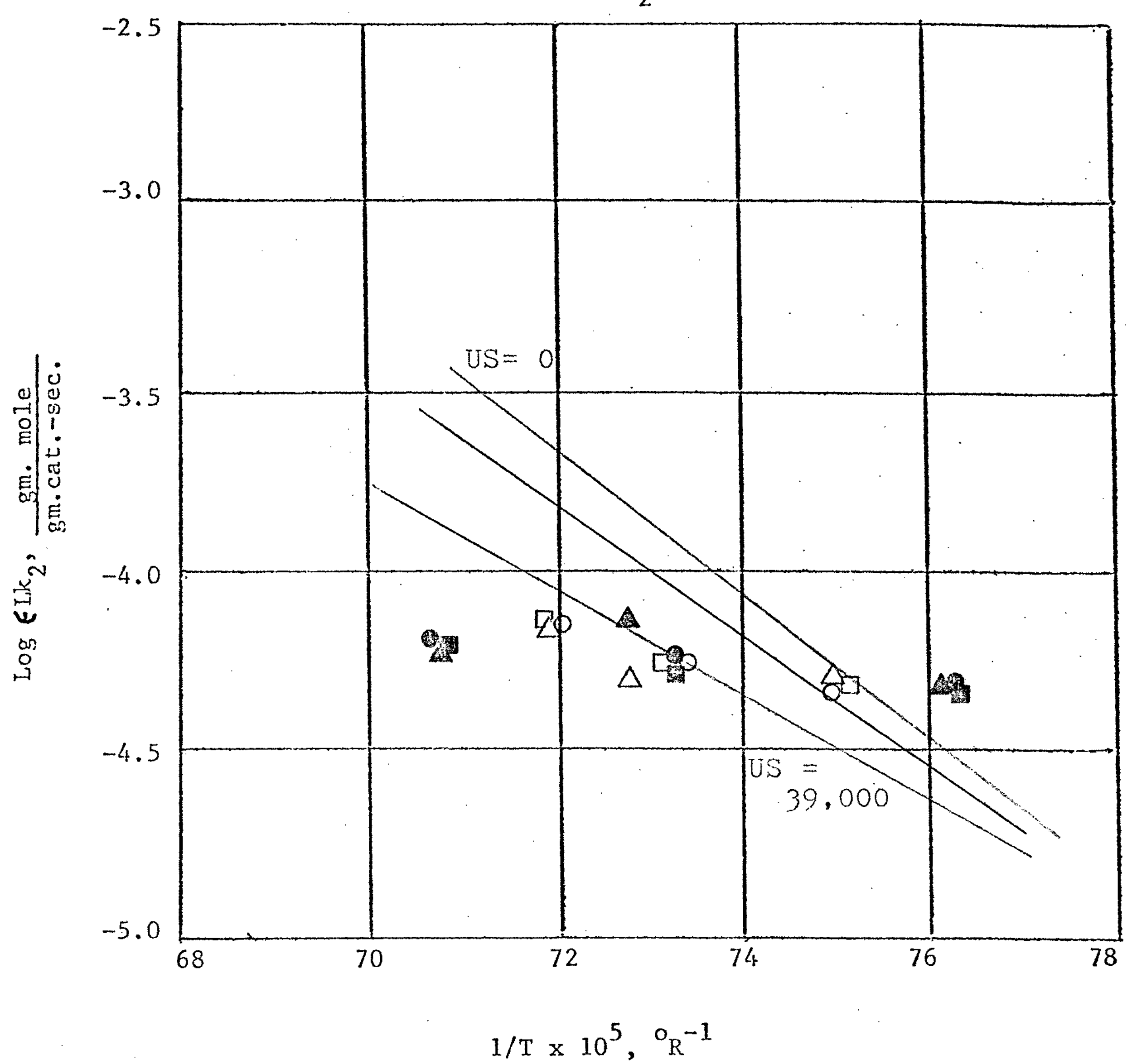
TABLE NO. 15

$$\mathrm{LOG}\ \epsilon L k_2 = A + B(1/T) \quad T,\ {}^{o}R^{-1}$$

Particle Diameter cm.	Ultrasound cps x 10^{-3}	A	B
0.358	0	-2.6788	-2131.6
	26	-2.5021	-2372.3
	39	-3.3966	-1136.2
0.200	0	-1.7433	-3087.3
	26	-2.3182	-2307.8
	39	-2.6163	-1888.4
0.0841	0	7.0251	-14715.8
	26	4.9542	-11916.0
	39	5.3306	-12452.5
0.0419	0	4.7377	-11694.1
	26	5.8127	-13210.1
	39	5.6011	-12943.4

FIGURE NO. 27

EFFECTIVENESS FACTOR, ϵLk_2, VERSUS TEMPERATURE



PARTICLE DIAMETER = 0.358 cm.

ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

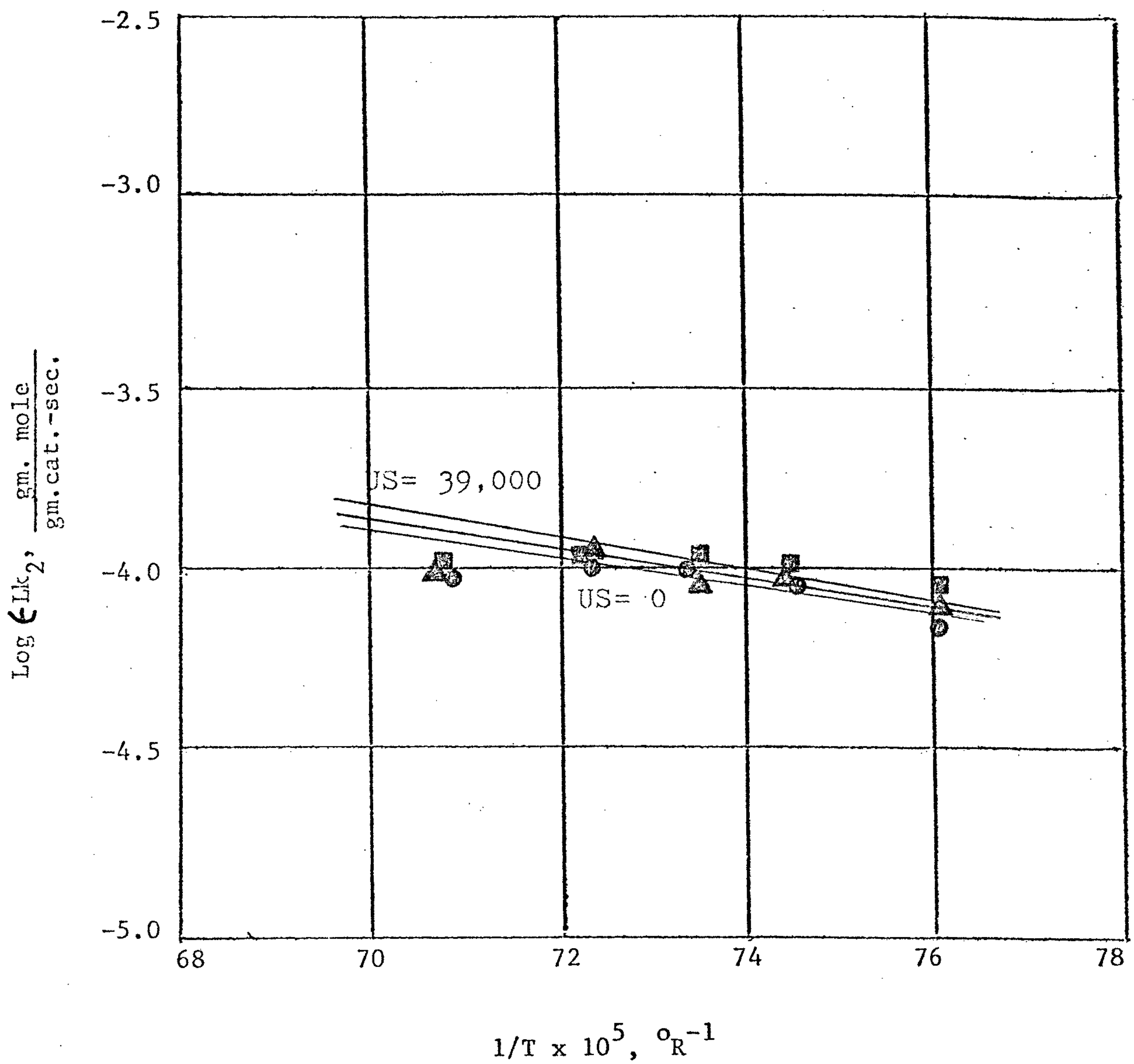
■ = 39000 cycles/second

● Represents Linter's Data

○ Represents Pietranski's Data

FIGURE NO. 26

EFFECTIVENESS FACTOR ϵLk_2, VERSUS TEMPERATURE



PARTICLE DIAMETER = 0.200 cm.

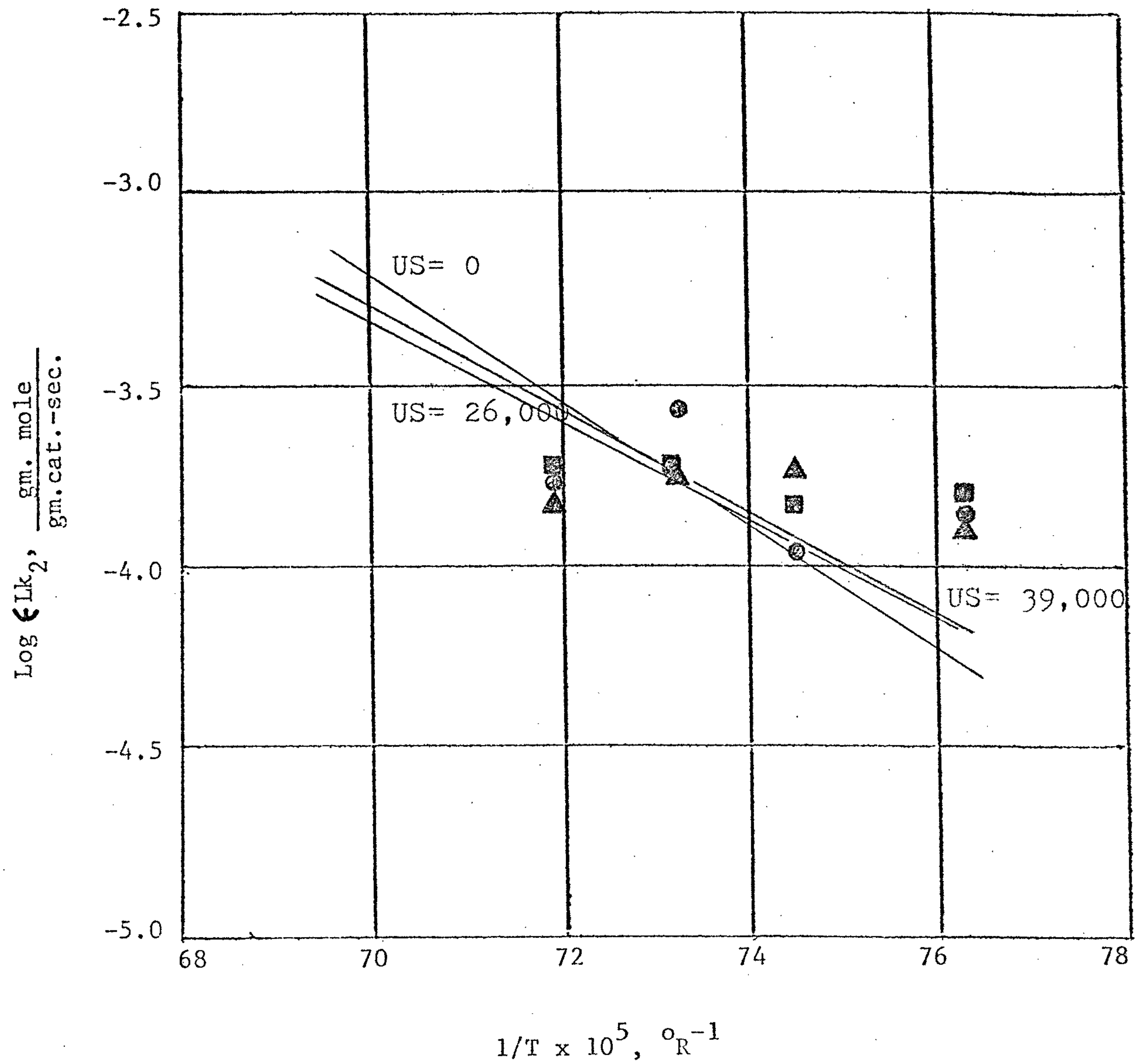
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 25

EFFECTIVENESS FACTOR, ϵLk_2, VERSUS TEMPERATURE



PARTICLE DIAMETER = 0.0841 cm.

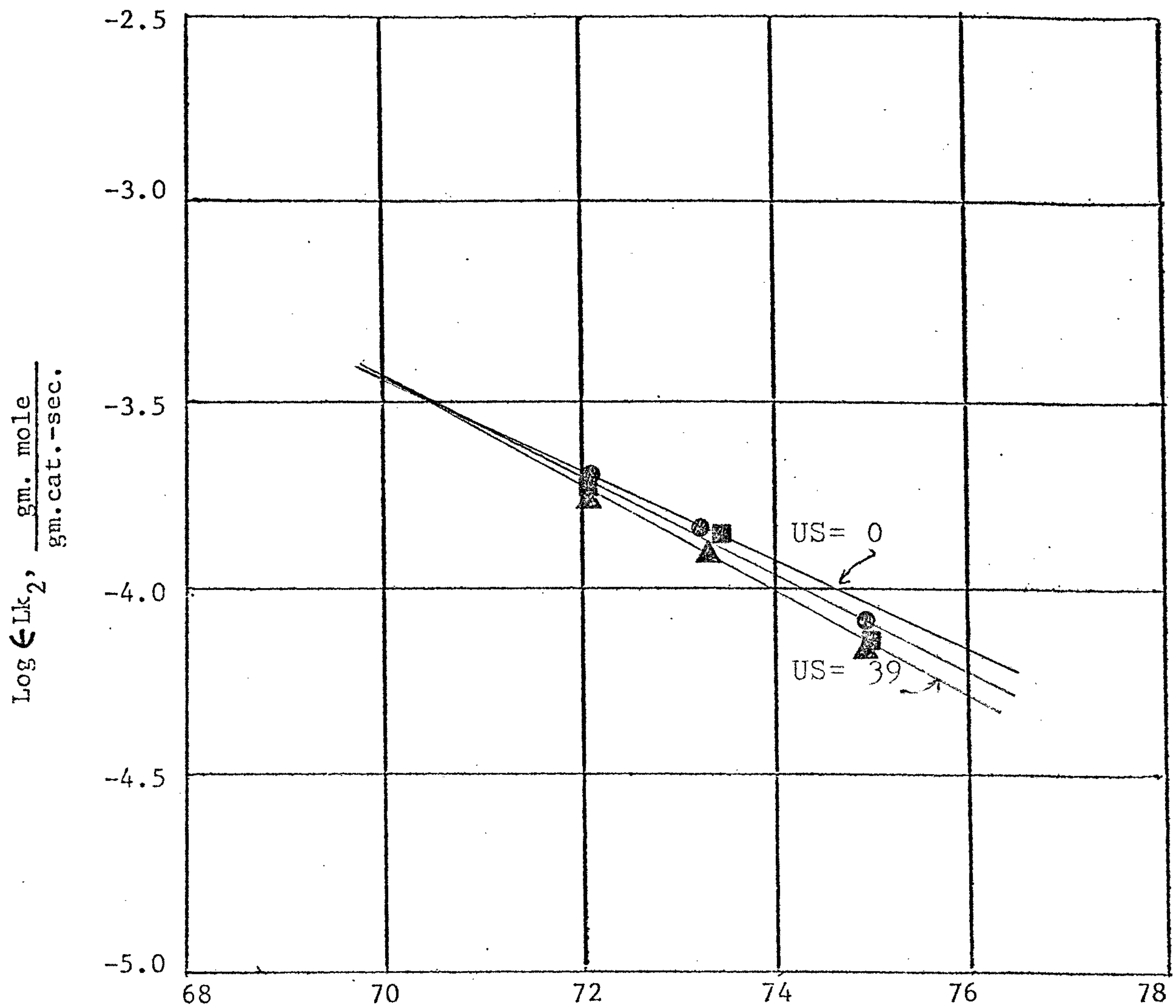
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 24

EFFECTIVENESS FACTOR, ϵLk_2, VERSUS TEMPERATURE



$1/T \times 10^5$, $^oR^{-1}$

PARTICLE DIAMETER = 0.0419 cm.

ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

TABLE NO. 16

ϵLk_2 AT VARIOUS TEMPERATURES AND ULTRASOUNDS

Particle Diameter = 0.358 cm.

Temperature deg. F.	1/T, $^{o}R^{-1}$ x 10^5	Ultrasound cps x 10^{-3}	ϵLk_2 x 10^5	Log ϵLk_2
850*	76.3	0	5.1867	-4.2851
		26	5.0218	-4.2992
		39	5.2356	-4.2816
875	74.9	0	5.3161	-4.2744
		26	5.4716	-4.2619
		39	5.8892	-4.2299
900*	73.5	0	5.1673	-4.2867
		26	5.2354	-4.2811
		39	6.8177	-4.1664
900	73.5	0	5.2885	-4.2767
		26	5.0663	-4.2953
		39	4.8077	-4.3181
925	72.2	0	6.9281	-4.1594
		26	7.0563	-4.1514
		39	7.0020	-4.1548
950*	70.9	0	6.3429	-4.1977
		26	6.4118	-4.1930
		39	5.7128	-4.2432

*Values obtained by re-regressing Linter's work using data for which W/Fao ≤ 25,000.

TABLE NO. 17

ϵLk_2 AT VARIOUS TEMPERATURES AND ULTRASOUNDS

Particle Diameter = 0.200 cm.

Temperature deg. F.	1/T, $^oR^{-1}$ x 10^5	Ultrasound cps x 10^{-3}	ϵLk_2 x 10^5	Log ϵLk_2
850	76.3	0	7.3614	-4.1330
		26	8.4052	-4.0755
		39	8.7242	-4.0593
875	74.9	0	9.5844	-4.0184
		26	8.7984	-4.0556
		39	9.1709	-4.0376
900	73.5	0	10.0911	-3.9961
		26	9.6763	-4.0143
		39	10.3178	-3.9864
925	72.2	0	10.5692	-3.9670
		26	10.6851	-3.9712
		39	10.3603	-3.9846
950	70.9	0	11.2682	-3.9481
		26	10.8962	-3.9627
		39	10.9906	-3.9590

TABLE NO. 18

ϵLk_2 AT VARIOUS TEMPERATURES AND ULTRASOUNDS

Particle Diameter = 0.0841 cm.

Temperature deg. F.	1/T, $^oR^{-1}$ x 10^5	Ultrasound cps x 10^{-3}	ϵLk_2 x 10^5	Log ϵLk_2
850	76.3	0	4.8219	-4.3168
		26	5.5233	-4.2578
		39	4.2392	-4.3727
875	74.9	0	11.2430	-3.9491
		26	15.1628	-3.8192
		39	18.3962	-3.7353
900	73.5	0	27.5555	-3.5598
		26	17.3914	-3.5797
		39	17.9625	-3.7456
925	72.2	0	16.7083	-3.7771
		26	18.4172	-3.7348
		39	15.6583	-3.8053

TABLE NO. 19

ϵLk_2 AT VARIOUS TEMPERATURES AND ULTRASOUNDS

Particle Diameter = 0.0419 cm.

Temperature deg. F.	1/T, $^oR^{-1}$ x 10^5	Ultrasound cps x 10^{-3}	ϵLk_s x 10^5	Log ϵLk_2
875	74.9	0	9.0161	-4.0450
		26	7.2496	-4.1397
		39	7.1802	-4.1439
900	73.5	0	15.5698	-3.8077
		26	15.0876	-3.8214
		39	15.6055	-3.8067
925	72.2	0	18.5621	-3.7314
		26	16.3542	-3.7864
		39	15.8815	-3.7991

TABLE NO. 20

ϵLk_2 AT VARIOUS TEMPERATURES AND ULTRASOUNDS

Particle Diameter = 0.0209 cm.

Temperature deg. F.	1/T, $^{o}R^{-1}$ x 10^5	Ultrasound cps x 10^{-3}	ϵLk_2 x 10^5	Log ϵLk_2
850	76.3	0	10.5776	-3.9756
		26	9.9580	-4.0018
		39	10.9558	-3.9604

APPENDIX V

CONVERSION VERSUS W/FAO DATA

The data that appears in this Appendix was obtained by taking the coefficients of the exponential equations derived in Appendix VI. An average conversion was calculated using the equation:

$$\overline{Xa} = \int_{t_1}^{t_2} \frac{Xa(t)\ dt}{t_{total}}$$

To establish uniformity all conversions were averaged using:

1. t_2 = 20 minutes
2. t_1 = 0 minutes
3. t_{total} = 20 minutes

The average conversion is plotted against reciprocal space velocity in Figures 27 through 42. A least squares analysis was used to determine the coefficients of the quadratic:

$$\overline{Xa} = a + b(W/Fao) = C(W/Fao)^2$$

It should be noted that the origin was included in the regression analysis.

TABLE NO. 21

QUADRATIC EQUATION CONSTANTS

$$Xa = a + b(W/Fao) + c(W/Fao)^2$$

Particle Diameter = 0.358 cm.

Temperature deg. F.	Ultrasound cps x 10^{-3}	a x 10^{2}	b x 10^{4}	c x 10^{9}
850*	0	-2.4441	.2252	-.4643
	26	-1.6063	.2104	-.4464
	39	-1.2151	.2002	-.3345
875	0	.3082	.1997	-.6882
	26	.1798	.2134	-.7760
	39	.1425	.2343	-.8854
900	0	-.2134	.1720	-.3029
	26	-.1795	.1613	-.2580
	39	.0792	.1475	-.2135
900*	0	-.7006	.2122	-.6372
	26	-.6456	.2120	-.6612
	39	-.1477	.2605	-.8210
925	0	-.0323	.2651	-1.0490
	26	.2149	.2519	-.9139
	39	.0722	.2522	-.8967
950*	0	-1.1170	.1992	-.2794
	26	-.8406	.2084	-.3934
	39	-.7340	.1901	-.3877

*Values obtained by re-regressing Linter's work using data for which W/Fao ≤ 25,000.

TABLE NO. 22

QUADRATIC EQUATION CONSTANTS

$$Xa = a + b(W/Fao) + c(W/Fao)^2$$

Particle Diameter = 0.200 cm.

Temperature deg. F.	Ultrasound cps x 10^{-3}	a x 10^2	b x 10^4	c x 10^9
850	0	-.2780	.2596	-.4976
	26	-.2736	.3106	-.7816
	39	-.2715	.3197	-.7895
875	0	-.0125	.3241	-.9162
	26	.1076	.3042	-.8168
	39	.9815	.3033	-.7900
900	0	.0385	.3348	-.9118
	26	-.1571	.3407	-1.0500
	39	.0946	.3498	-1.0420
925	0	-.1719	.3490	-.9961
	26	-.0893	.3504	-1.0020
	39	-.2107	.3473	-1.0220
950	0	.0001	.3707	-1.1900
	26	.0002	.3645	-1.2120
	39	.0000	.3407	-.9044

TABLE NO. 23

QUADRATIC EQUATION CONSTANTS

$$Xa = a + b(W/Fao) + c(W/Fao)^2$$

Particle Diameter = 0.0841 cm.

Temperature deg. F.	Ultrasound cps x 10^{-3}	a x 10^2	b x 10^4	c x 10^8
850	0	0.4811	.1098	-.0321
	26	-.6844	.2334	-.0740
	39	-.3108	.1476	-.0178
875	0	0.1696	.4395	-.1658
	26	1.0050	.5310	-.2196
	39	1.9720	.6710	-.3421
900	0	10.34	.5530	-.2371
	26	0.1039	.6077	-.2404
	39	0.3449	.6455	-.2935
925	0	-.1505	.6175	-.2775
	26	-.0175	.6135	-.2956
	39	-.0887	.5730	-.2279

TABLE NO. 24

QUADRATIC EQUATION CONSTANTS

$$Xa = a + b(W/Fao) + c(W/Fao)^2$$

Particle Diameter = 0.0419 cm.

Temperature deg. F.	Ultrasound cps $\times 10^{-3}$	$a \times 10^2$	$b \times 10^4$	$c \times 10^8$
875	0	0.0609	.2902	-.0891
	26	0.0373	.2818	-.0558
	39	0.1270	.2690	-.2526
900	0	-.0227	.5826	-.2526
	26	0.1012	.6402	-.3631
	39	-.0099	.6396	-.3658
925	0	-.6191	.6646	-.3058
	26	-.6296	.5079	-.1457
	39	0.1491	.2502	+.1690

TABLE NO. 25

QUADRATIC EQUATION CONSTANTS

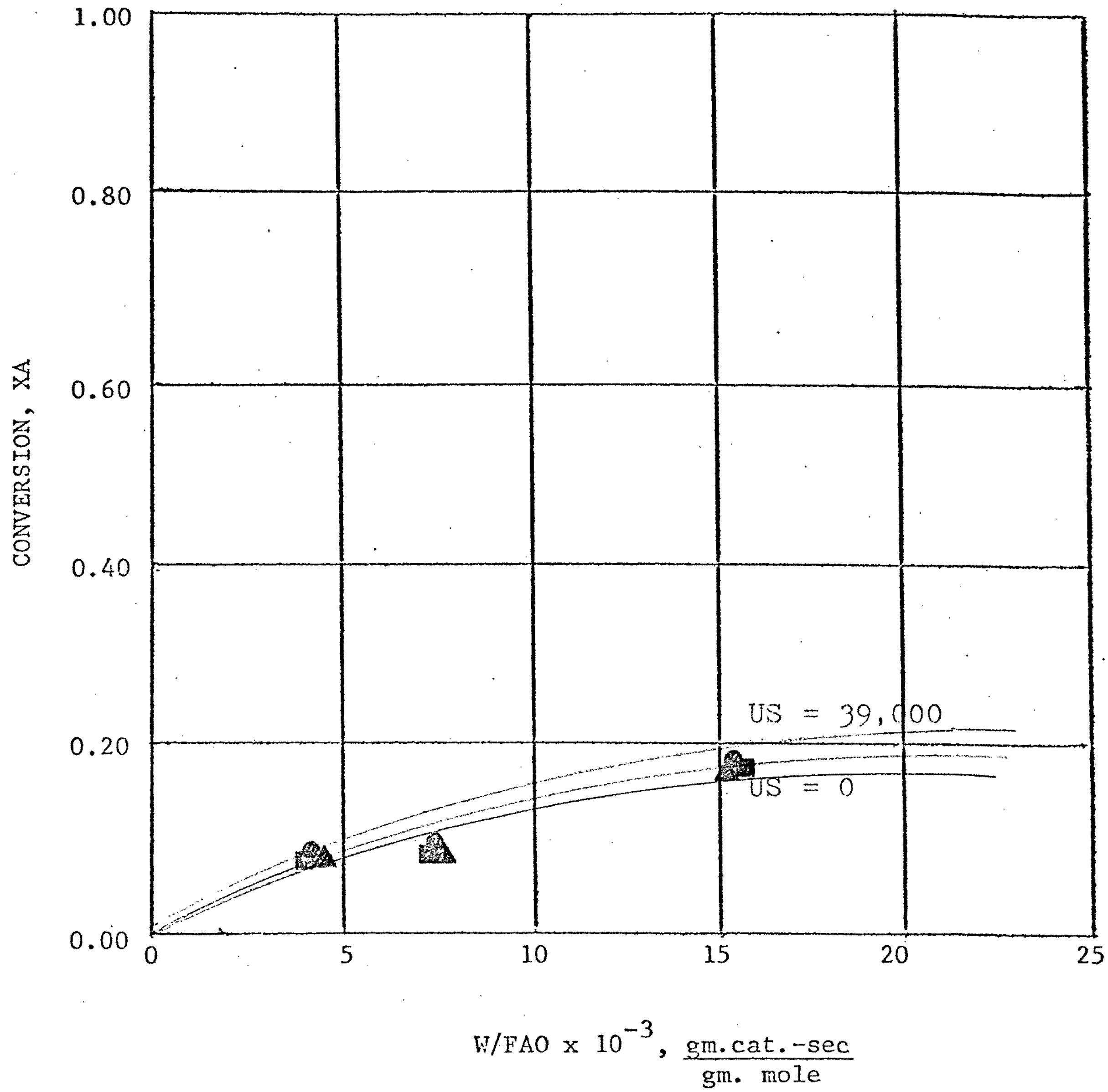
$$Xa = a + b(W/Fao) + c(W/Fao)^2$$

Particle Diameter = 0.0209 cm.

Temperature deg. F.	Ultrasound cps x 10^{-3}	a x 10^2	b x 10^4	c x 10^8
850	0	-0.0075	.4704	-.3456
	26	1.0356	.3578	-.2128
	39	0.7766	.4513	-.3372

FIGURE NO. 28

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.358 cm.

TEMPERATURE = 925 deg. F.

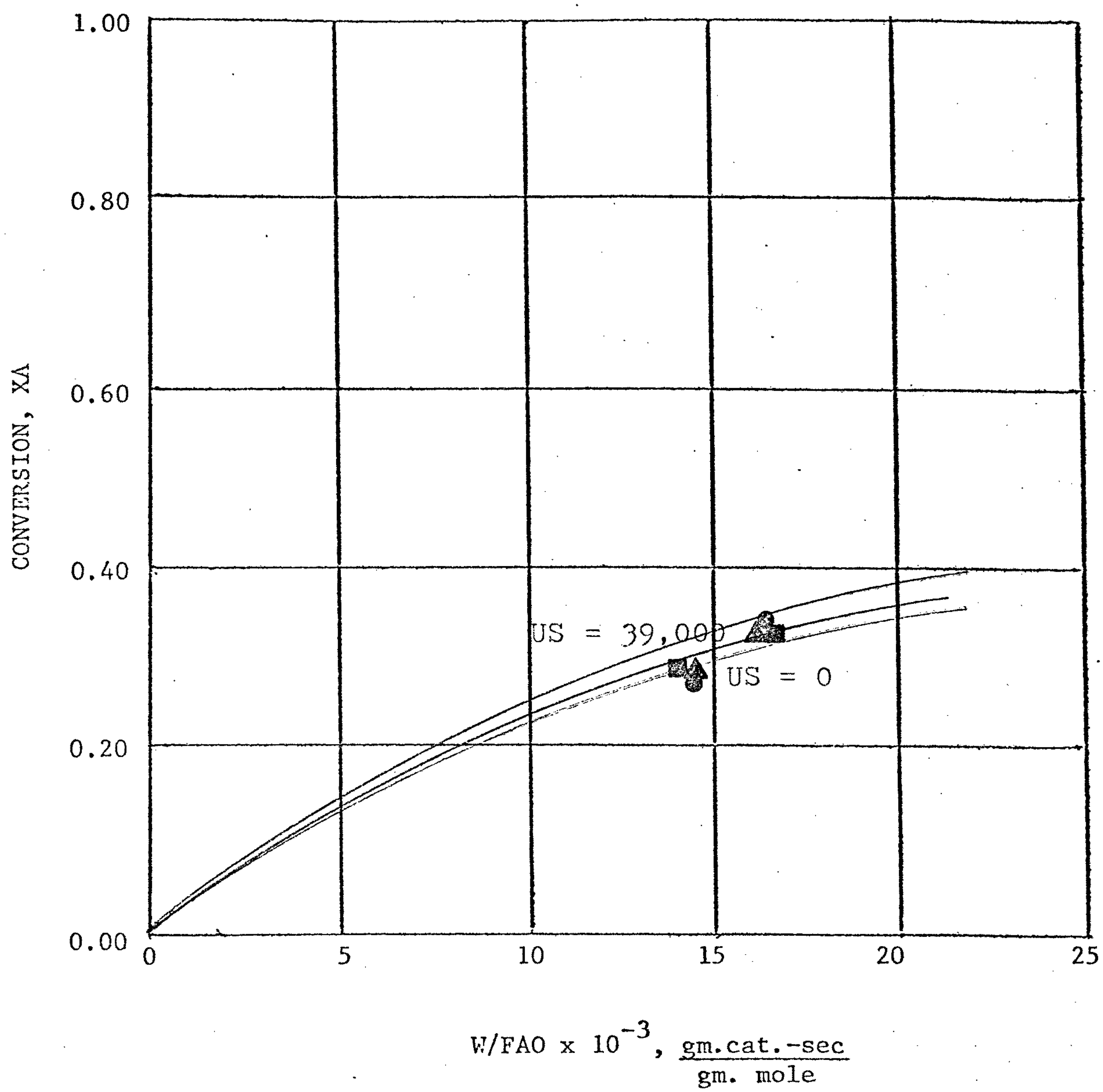
ULTRASOUND ⊕ = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 29

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.358 cm.

TEMPERATURE = 900 deg. F.

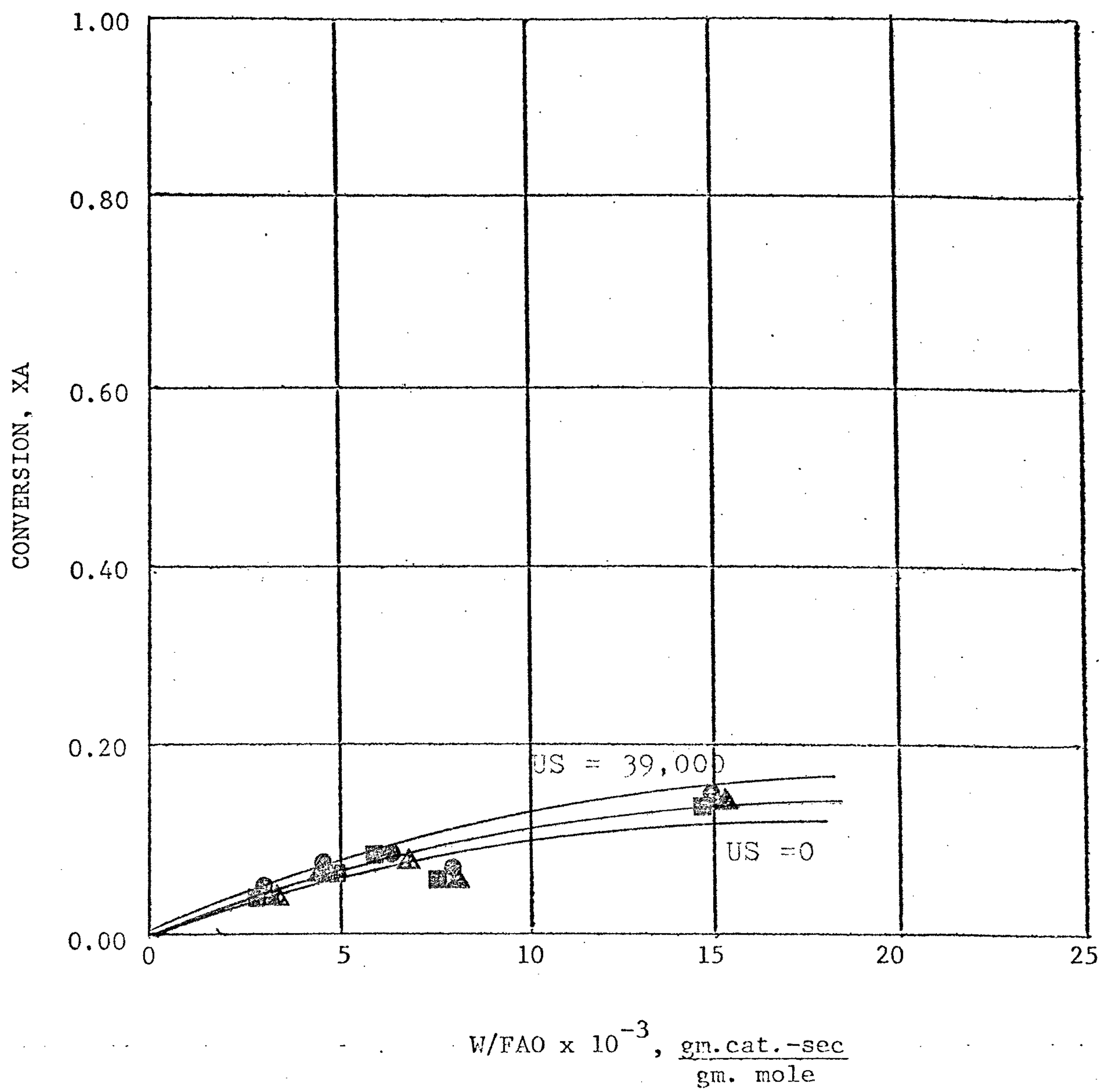
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 30

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.358 cm.

TEMPERATURE = 875 deg. F.

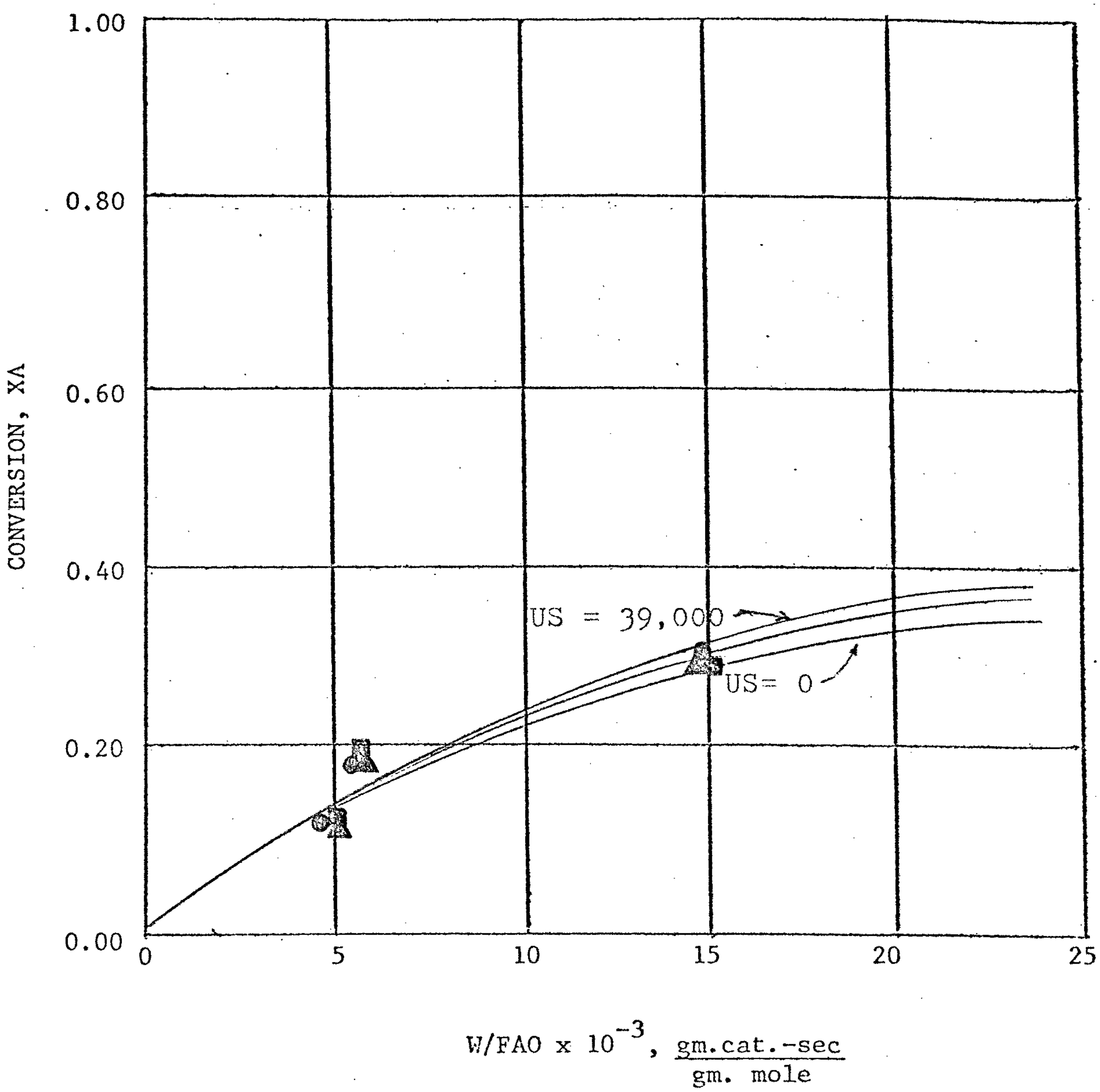
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 31

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.200 cm.

TEMPERATURE = 850 deg. F.

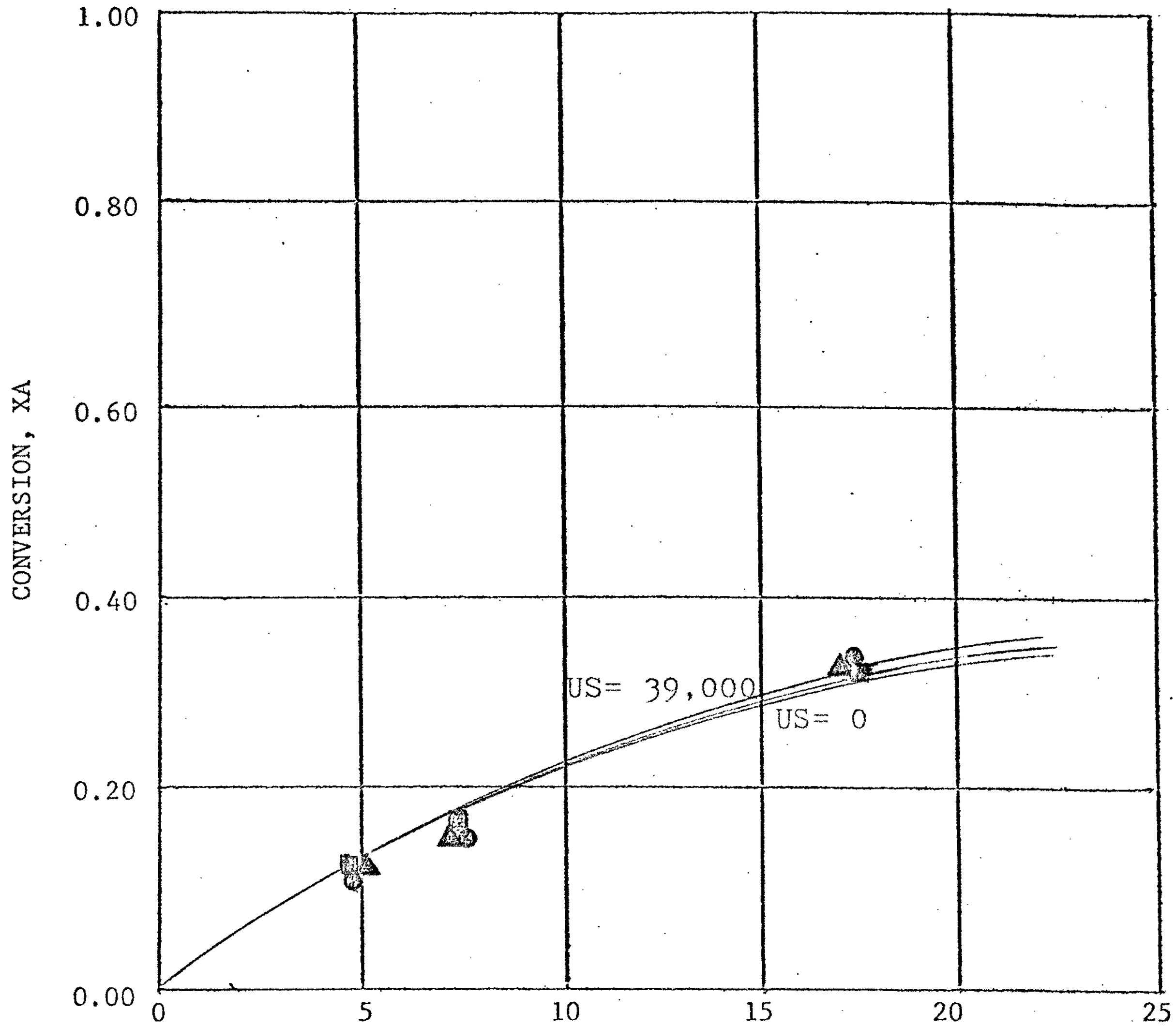
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 32

CONVERSION, XA, VERSUS W/FAO



W/FAO x 10^{-3}, $\frac{\text{gm.cat.-sec}}{\text{gm. mole}}$

PARTICLE DIAMETER = 0.200 cm.

TEMPERATURE = 875 deg. F.

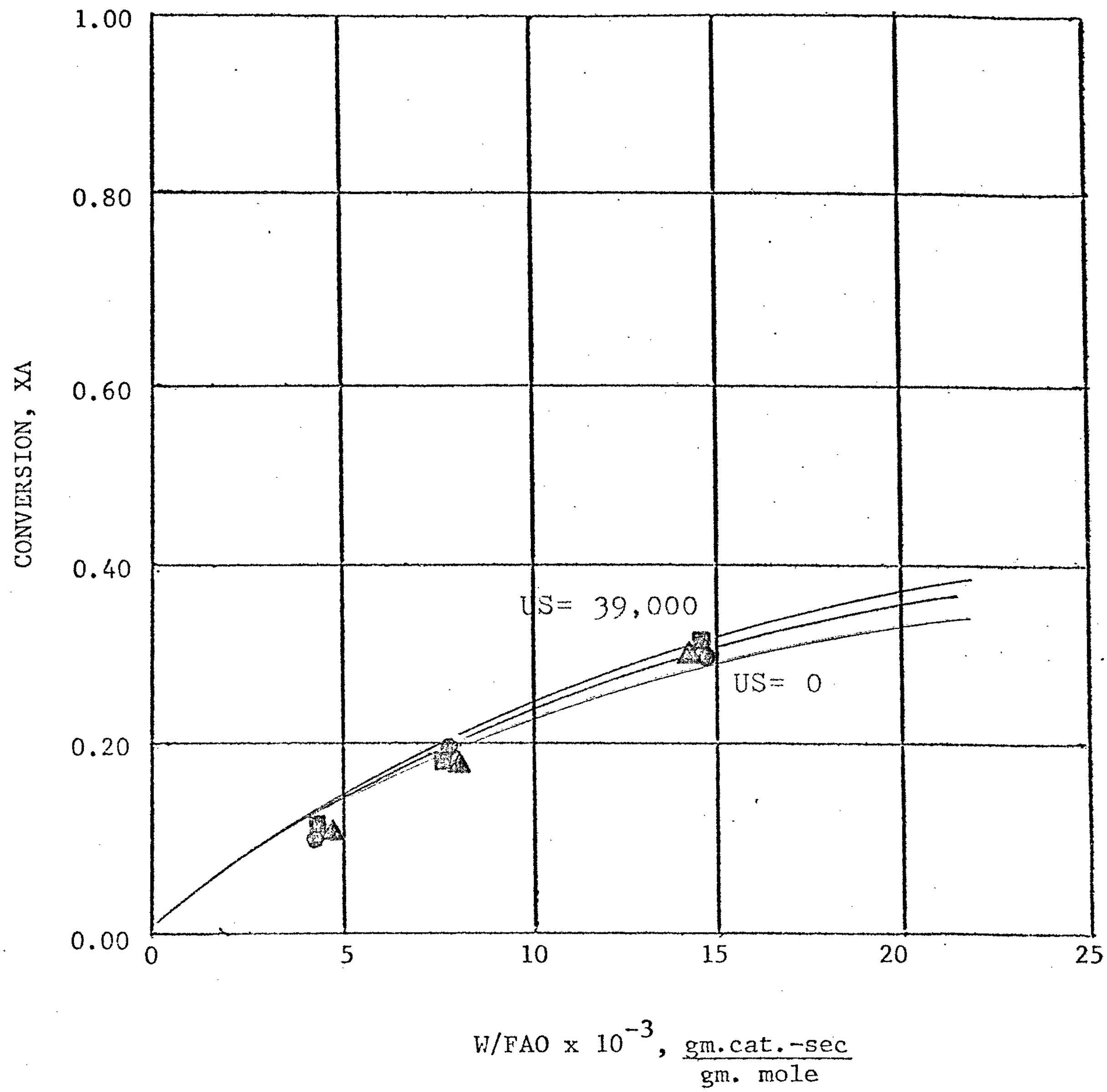
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 33

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.200 cm.

TEMPERATURE = 900 deg. F.

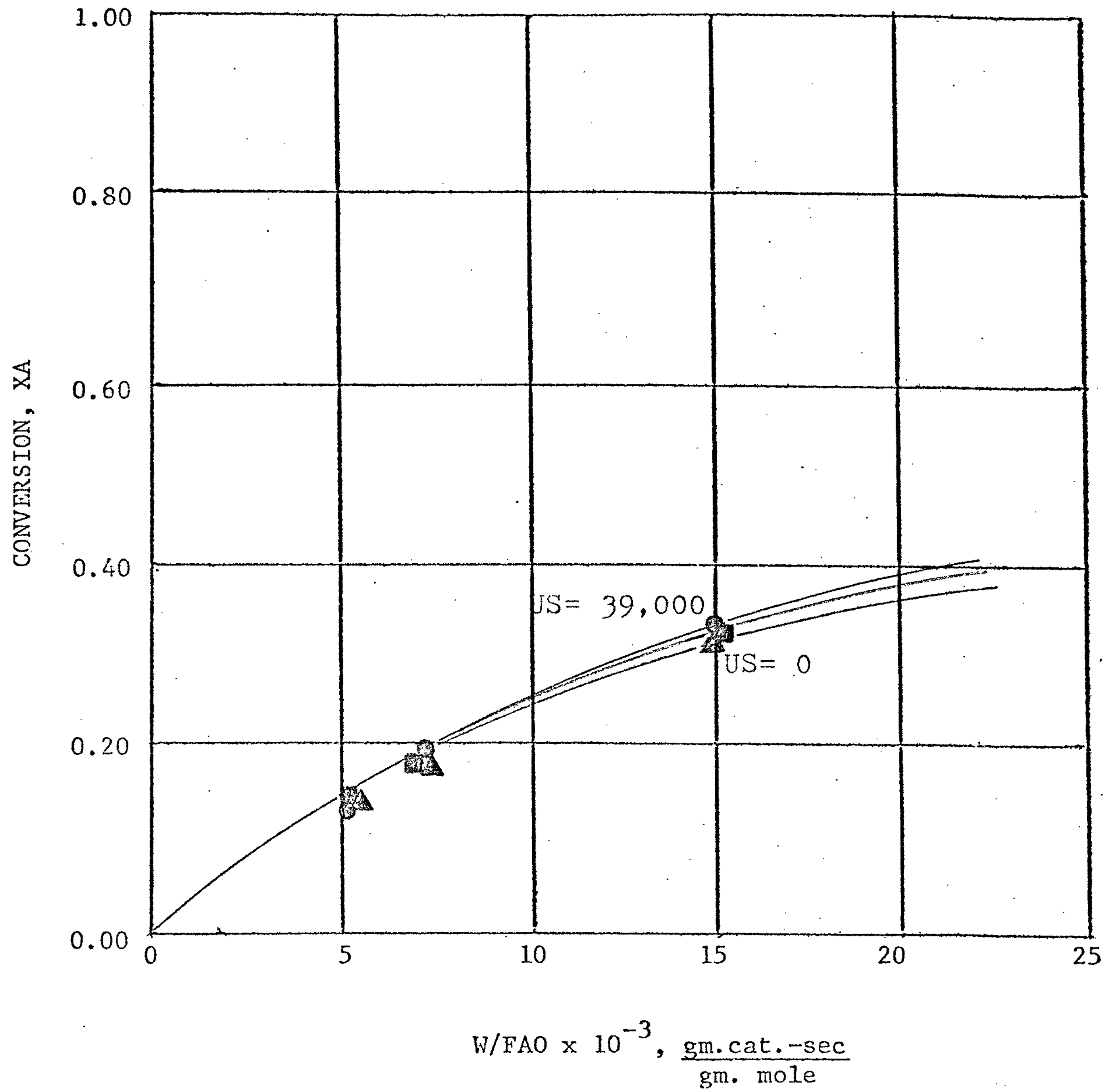
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 34

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.200 cm.

TEMPERATURE = 925 deg. F.

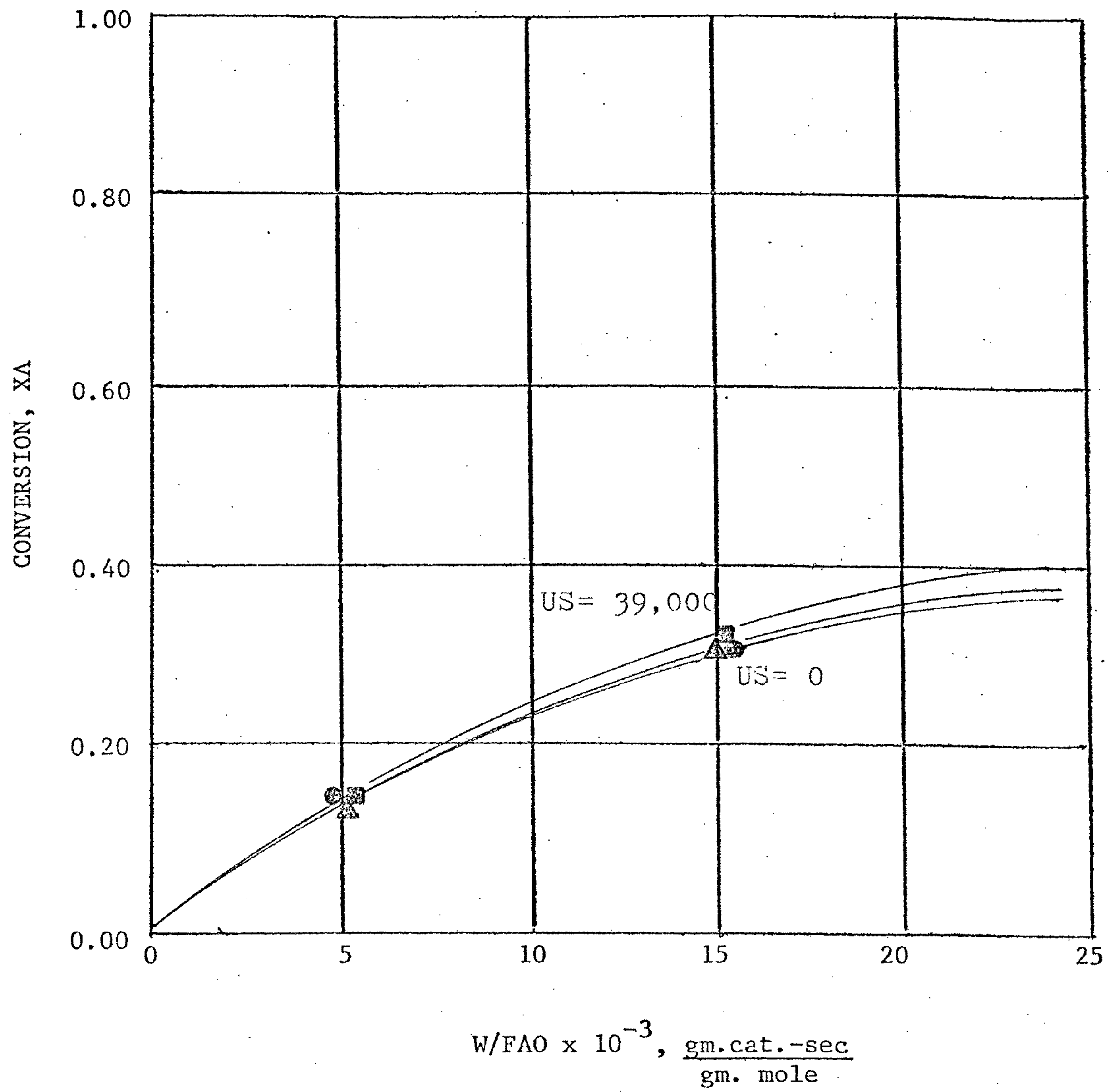
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 35

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.200 cm.

TEMPERATURE = 950 deg. F.

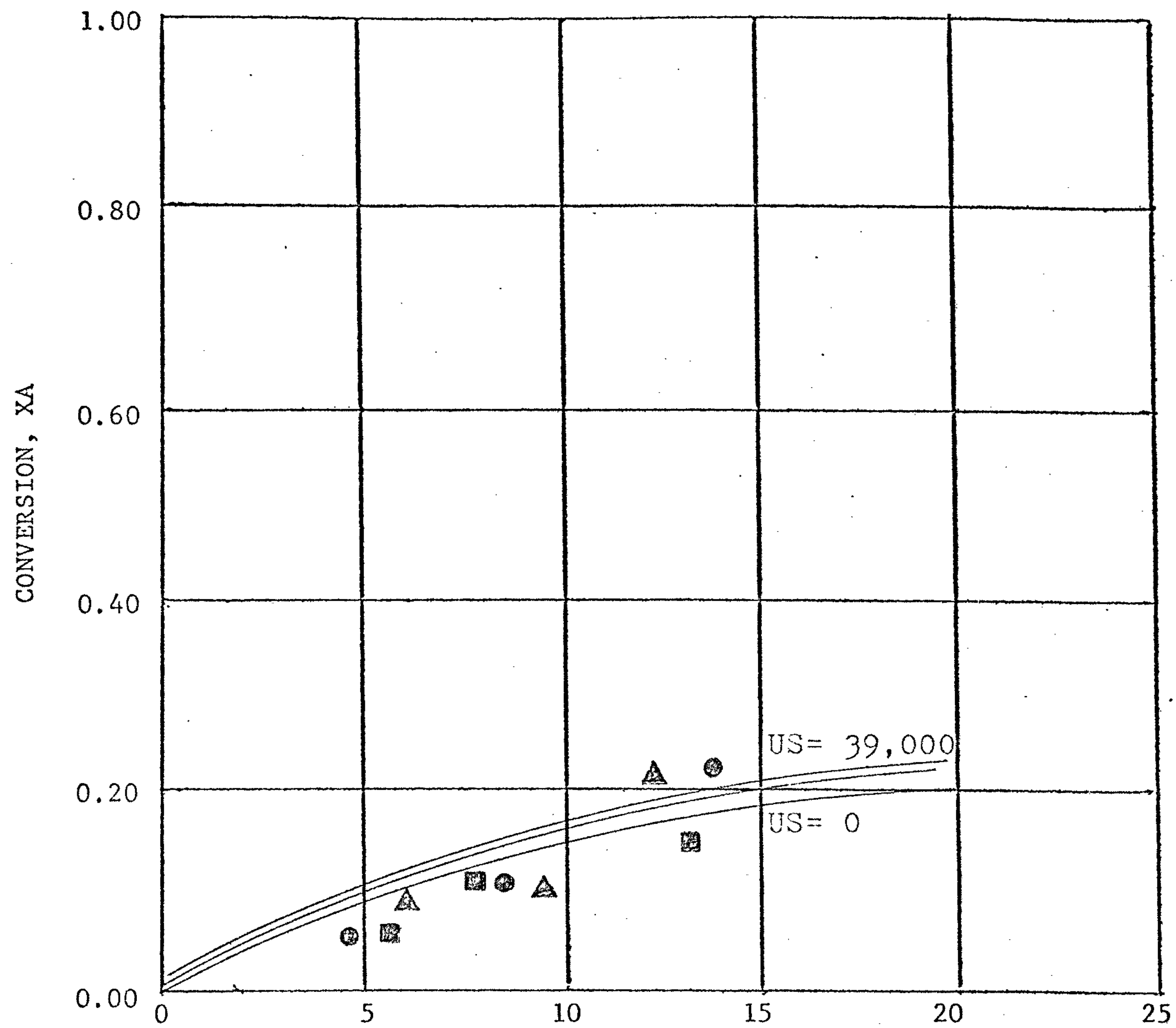
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 36

CONVERSION, XA, VERSUS W/FAO



W/FAO x 10^{-3}, $\frac{\text{gm.cat.-sec}}{\text{gm. mole}}$

PARTICLE DIAMETER = 0.0841 cm.

TEMPERATURE = 850 deg. F.

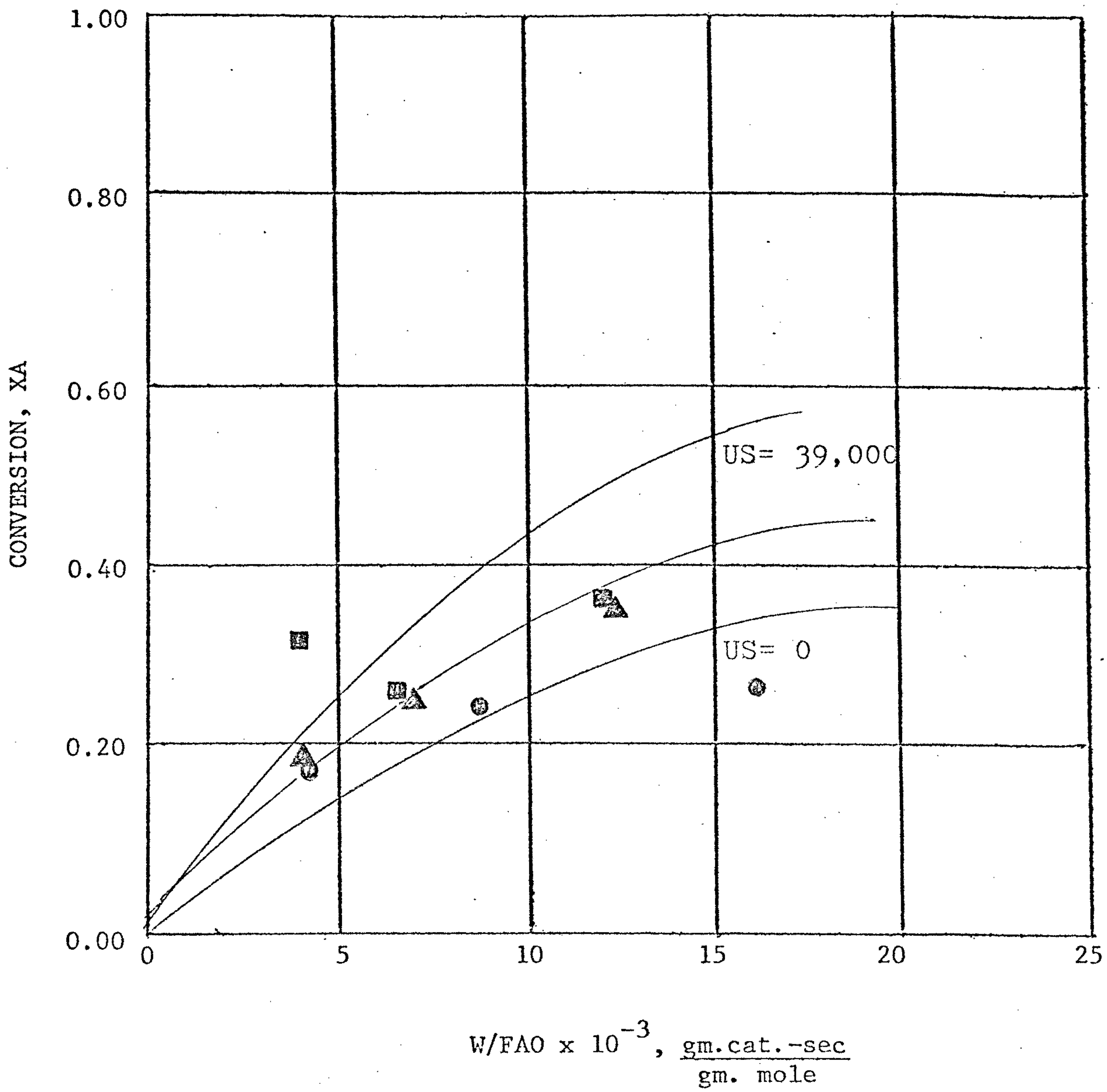
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 37

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.0841 cm.

TEMPERATURE = 875 deg. F.

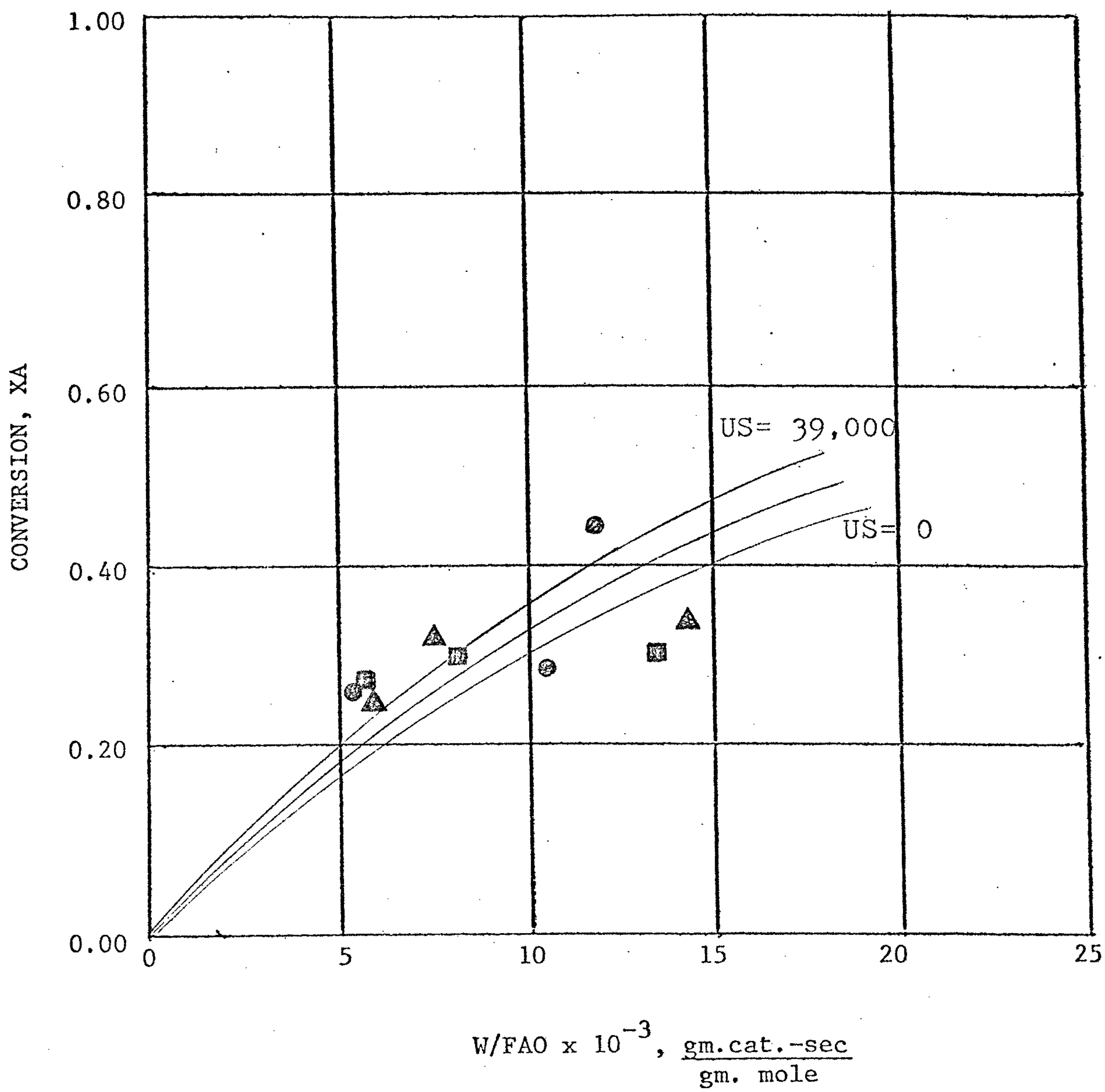
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 38

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.0841 cm.

TEMPERATURE = 900 deg. F.

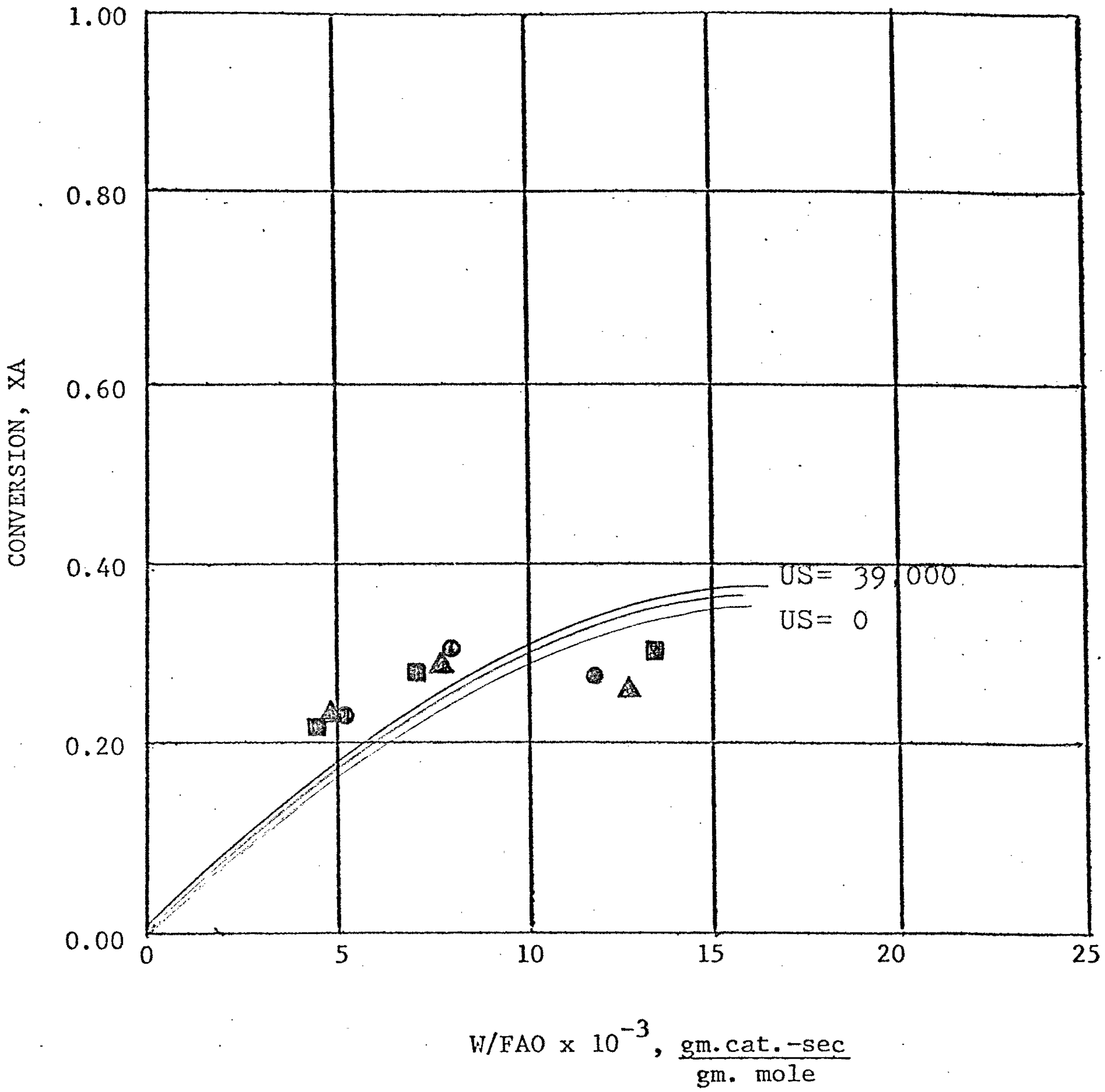
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 39

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.0841 cm.

TEMPERATURE = 925 deg. F.

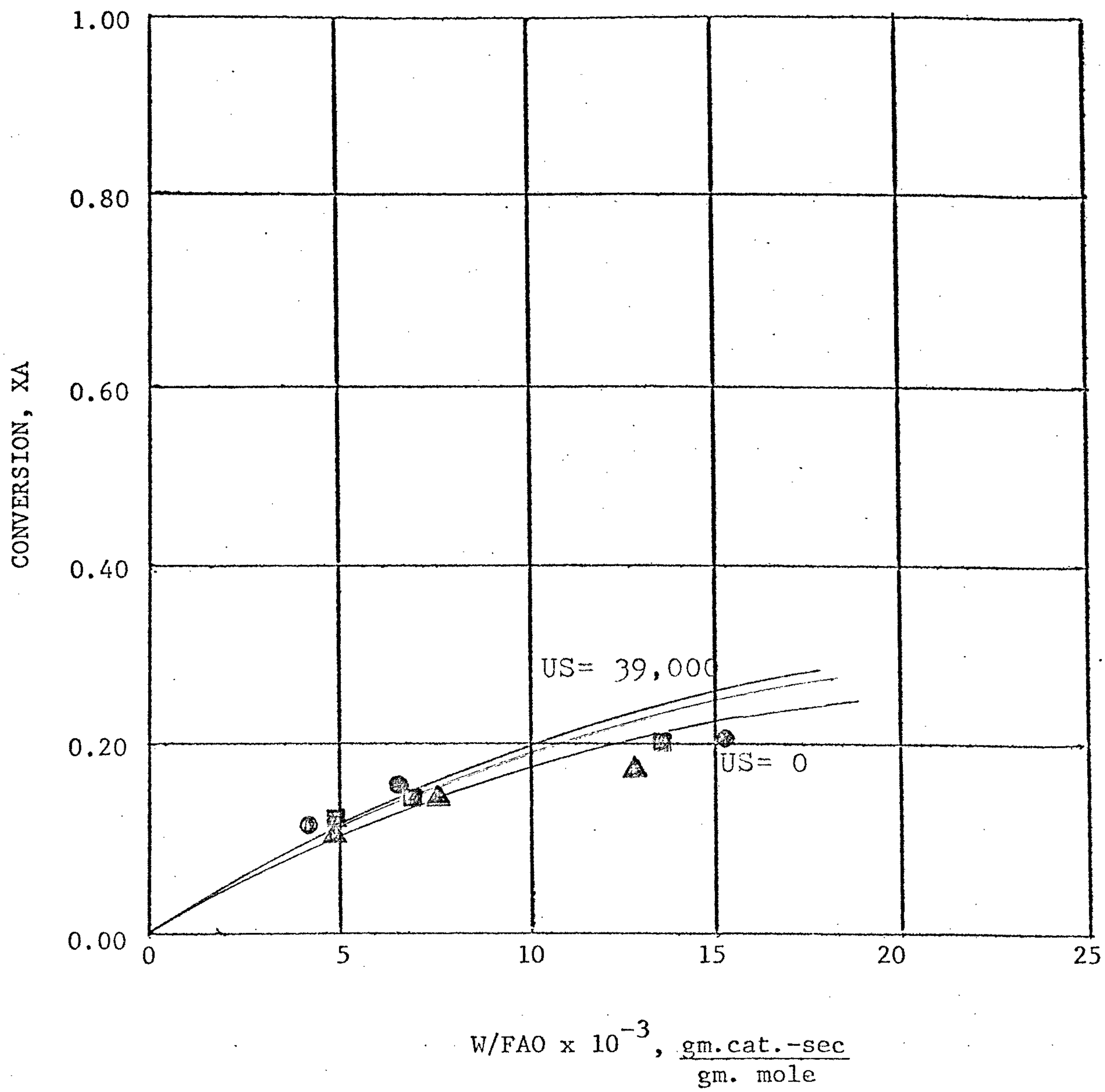
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 40

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.0419 cm.

TEMPERATURE = 875 deg. F.

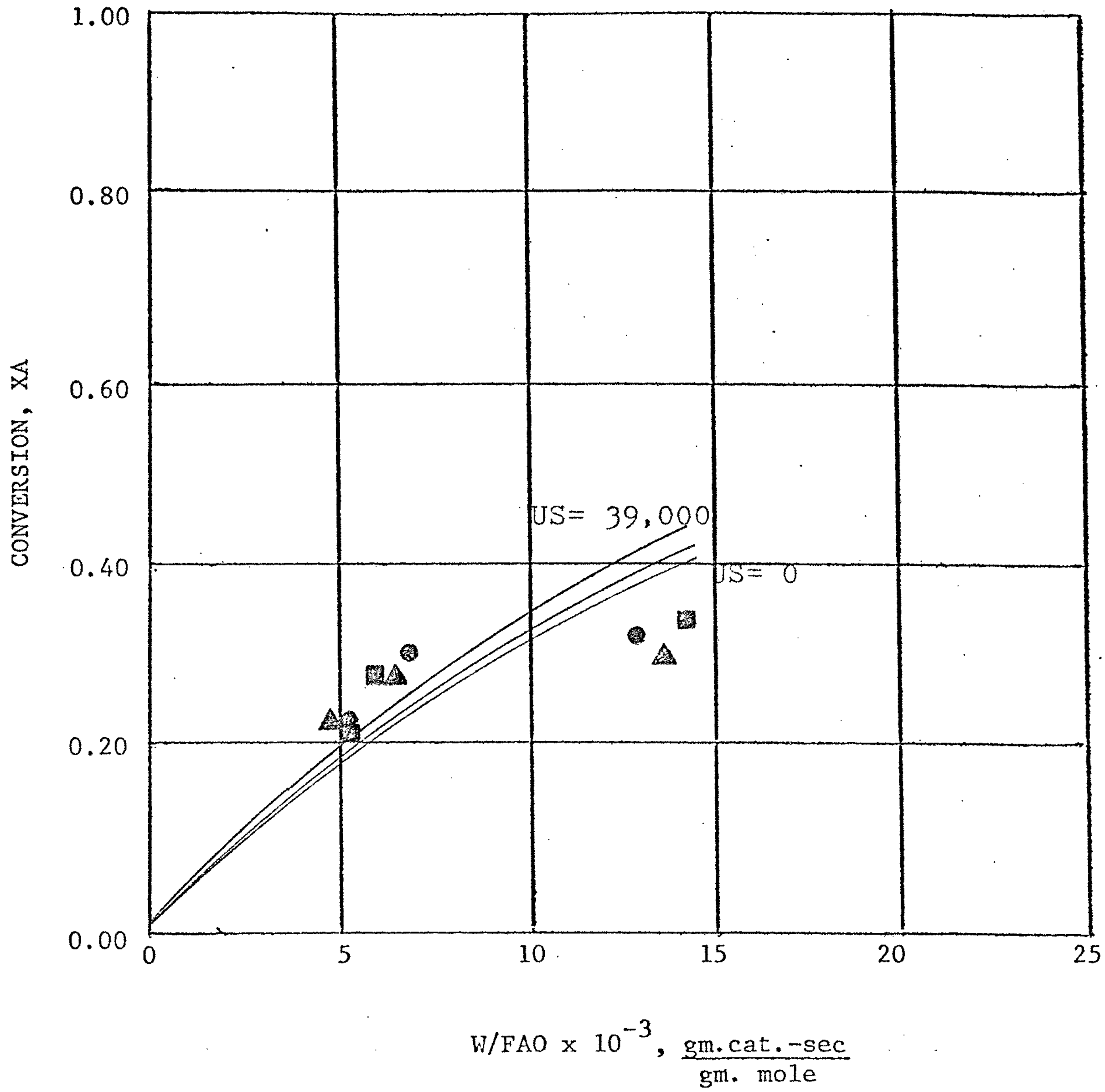
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 41

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.0419 cm.

TEMPERATURE = 900 deg. F.

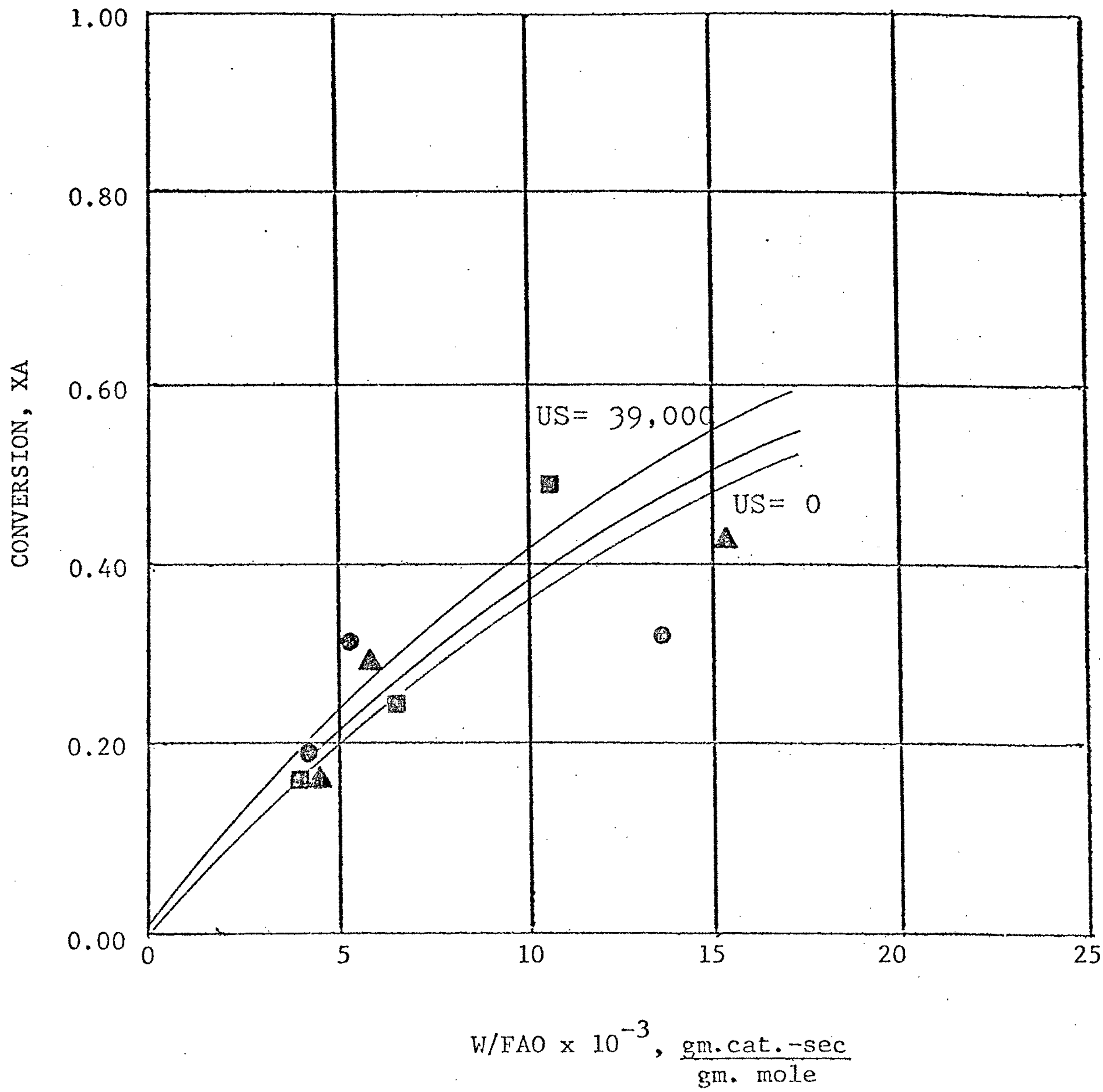
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 42

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.0419 cm.

TEMPERATURE = 925 deg. F.

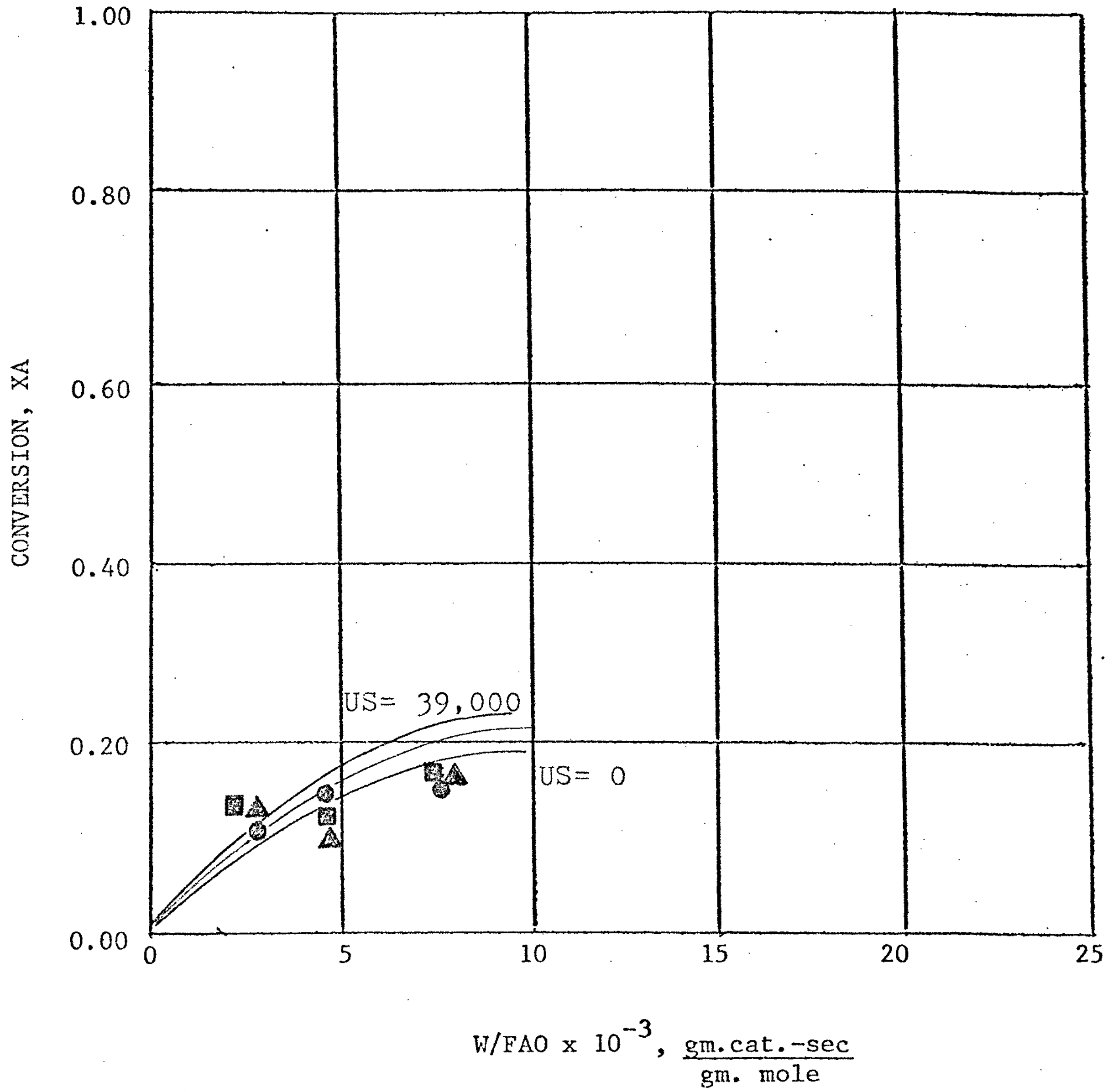
ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

FIGURE NO. 43

CONVERSION, XA, VERSUS W/FAO



PARTICLE DIAMETER = 0.0209 cm.

TEMPERATURE = 850 deg. F.

ULTRASOUND ● = 0 cycles/second

▲ = 26000 cycles/second

■ = 39000 cycles/second

TABLE NO. 26

CONVERSION AT VARIOUS W/FAO AND ULTRASOUNDS

Particle Diameter = 0.358 cm.
Weight of Catalyst = 3.650 gm.

Temperature deg. F.	Flow Rate gms./hr.	W/Fao $\frac{\text{gm.cat.-sec.}}{\text{gmole}}$	Ultrasound cps x 10^{-3}	$\overline{Xa}$
875	202.0	7812	0	.1185
875	202.0	7812	26	.1154
875	202.0	7812	39	.1142
875	106.5	14820	0	.1664
875	106.5	14820	26	.1482
875	106.5	14820	39	.1552
875	450.1	3507	0	.0729
875	450.1	3507	26	.0695
875	450.1	3507	39	.0765
875	327.0	4827	0	.0920
875	327.0	4827	26	.0887
875	327.0	4827	39	.0877
875	233.0	6773	0	.1299
875	233.0	6773	26	.1127
875	233.0	6773	39	.1382
900	93.6	16867	0	.2218
900	93.6	16867	26	.2147
900	93.6	16867	39	.1877
900	42.7	36997	0	.2705
900	42.7	36997	26	.2429
900	42.7	36997	39	.2537
900	111.7	14125	0	.1592
900	111.7	14125	26	.1576
900	111.7	14125	39	.1664
925	102.5	15406	0	.1782
925	102.5	15406	26	.1743
925	102.5	15406	39	.1767
925	211.1	7477	0	.1397
925	211.1	7477	26	.1334
925	211.1	7477	39	.1373
925	350.0	4509	0	.1074
925	350.0	4509	26	.1046
925	350.0	4509	39	.0986

TABLE NO. 27

CONVERSION AT VARIOUS W/FAO AND ULTRASOUNDS

Particle Diameter = 0.200 cm.
Weight of Catalyst = 3.640 gm.

Temperature deg. F.	Flow Rate gms./hr.	W/Fao gm.cat.-sec./gmole	Ultrasound cps x 10^{-3}	$\overline{Xa}$
850	104.0	15134	0	.2960
850	104.0	15134	26	.2868
850	104.0	15134	39	.2983
850	231.0	6816	0	.1856
850	231.0	6816	26	.1899
850	231.0	6816	39	.1954
850	294.8	5340	0	.1241
850	294.8	5340	26	.1208
850	294.8	5340	39	.1254
875	91.9	17128	0	.2889
875	91.9	17128	26	.2827
875	91.9	17128	39	.2862
875	218.0	7219	0	.1749
875	218.0	7219	26	.1739
875	218.0	7219	39	.1862
875	324.0	4852	0	.1337
875	324.0	4852	26	.1340
875	324.0	4852	39	.1350
900	109.0	14442	0	.2936
900	109.0	14442	26	.2705
900	109.0	14442	39	.2892
900	216.0	7278	0	.1946
900	216.0	7278	26	.1977
900	216.0	7278	39	.1969
900	322.0	4889	0	.1443
900	322.0	4889	26	.1329
900	322.0	4889	39	.1517
925	107.0	14690	0	.2951
925	107.0	14690	26	.2972
925	107.0	14690	39	.2864
925	225.0	7003	0	.2069
925	225.0	7003	26	.2021
925	225.0	7003	39	.2070
925	281.0	5614	0	.1486
925	281.0	5614	26	.1567
925	281.0	5614	39	.1433
950	104.5	15059	0	.2884
950	104.5	15059	26	.2739
950	104.5	15059	39	.3079
950	305.0	5152	0	.1594
950	305.0	5152	26	.1556
950	305.0	5152	39	.1515

TABLE NO. 28

CONVERSION AT VARIOUS W/FAO AND ULTRASOUNDS

Particle Diameter = 0.0841 cm.
Weight of Catalyst = 3.670 gm.

Temperature deg. F.	Flow Rate gms./hr.	W/Fao gm.cat.-sec. / gmole	Ultrasound cps x 10^{-3}	$\overline{Xa}$
850	115.6	13730	0	.2206
850	175.6	9039	0	.1162
850	351.0	4518	0	.0753
850	130.5	12165	26	.2196
850	156.0	10166	26	.1188
850	268.0	5922	26	.0929
850	120.9	13130	39	.1564
850	198.8	7982	39	.1224
850	281.7	5633	39	.0559
875	98.3	16158	0	.2797
875	171.0	9242	0	.2624
875	350.5	4528	0	.1713
875	217.2	7308	26	.2433
875	127.2	12465	26	.3386
875	357.8	4436	26	.2421
875	131.0	12129	39	.3455
875	224.4	7077	39	.2499
875	369.1	4302	39	.3230
900	136.6	11626	0	.4341
900	313.4	5068	0	.2721
900	145.6	10907	0	.3068
900	113.4	14000	26	.3814
900	216.3	7343	26	.3113
900	290.6	5464	26	.2680
900	118.1	13449	39	.3434
900	212.4	7476	39	.3054
900	311.7	5096	39	.2736
925	115.2	13789	0	.3214
925	221.4	7174	0	.3071
925	304.1	5222	0	.2364
925	112.9	14072	26	.2848
925	232.6	6829	26	.2853
925	317.5	5001	26	.2342
925	101.9	15587	39	.3382
925	257.9	6157	39	.2728
925	309.8	5127	39	.2251

TABLE NO. 29

CONVERSION AT VARIOUS W/FAO AND ULTRASOUNDS

Particle Diameter = 0.0419 cm.
Weight of Catalyst = 3.70 gm.
= 3.52 gm.*

Temperature deg. F.	Flow Rate gms./hr.	W/Fao $\frac{\text{gm.cat.-sec.}}{\text{gmole}}$	Ultrasound cps x 10^{-3}	$\overline{Xa}$
875	95.6	16608	0	.2049
875	213.0	7156	0	.1479
875	331.7	4826	0	.1259
875	118.1	13561	26	.1761
875	195.5	8191	26	.1541
875	307.4	5209	26	.1183
875	109.9	14570	39	.2049
875	210.9	7590	39	.1479
875	300.8	5322	39	.1259
900	126.9	12616	0	.2245
900	215.5	7429	0	.2740
900	282.6	5666	0	.2441
900	116.4	13761	26	.1951
900	220.9	7148	26	.2671
900	302.5	5293	26	.2445
900	111.9	14309	39	.3168
900	259.5	6169	39	.2625
900	359.4	4455	39	.2108
925	117.1	13573	0	.3267
925	256.6	5936*	0	.3238
925	321.2	4742*	0	.1932
925	100.4	15177*	26	.4268
925	241.7	6303*	26	.2947
925	308.8	4932*	26	.1659
925	135.2	11263*	39	.4995
925	219.3	6947*	39	.2483
925	318.5	4782*	39	.1681

TABLE NO. 30

CONVERSION AT VARIOUS W/FAO AND ULTRASOUNDS

Particle Daimeter = 0.0209 cm.
Weight of Catalyst = 2.100 gm.

Temperature Deg. F.	Flow Rate gms./hr.	W/Fao $\frac{gm.cat.-sec.}{gmole}$	Ultrasound cps x 10^{-3}	$\overline{Xa}$
850	113.1	8034	0	.1547
850	192.6	4719	0	.1452
850	321.0	2831	0	.1051
850	112.4	8087	26	.1695
850	183.2	4961	26	.0990
850	317.8	2860	26	.1331
850	116.7	7788	39	.1621
850	182.3	4984	39	.1232
850	335.1	2712	39	.1315

APPENDIX VI

CONVERSION VERSUS TIME DATA

The data that appears in this Appendix was obtained by setting up a run at:

1. Fixed catalyst loading.
2. Fixed catalyst diameter.

With set operating conditions:

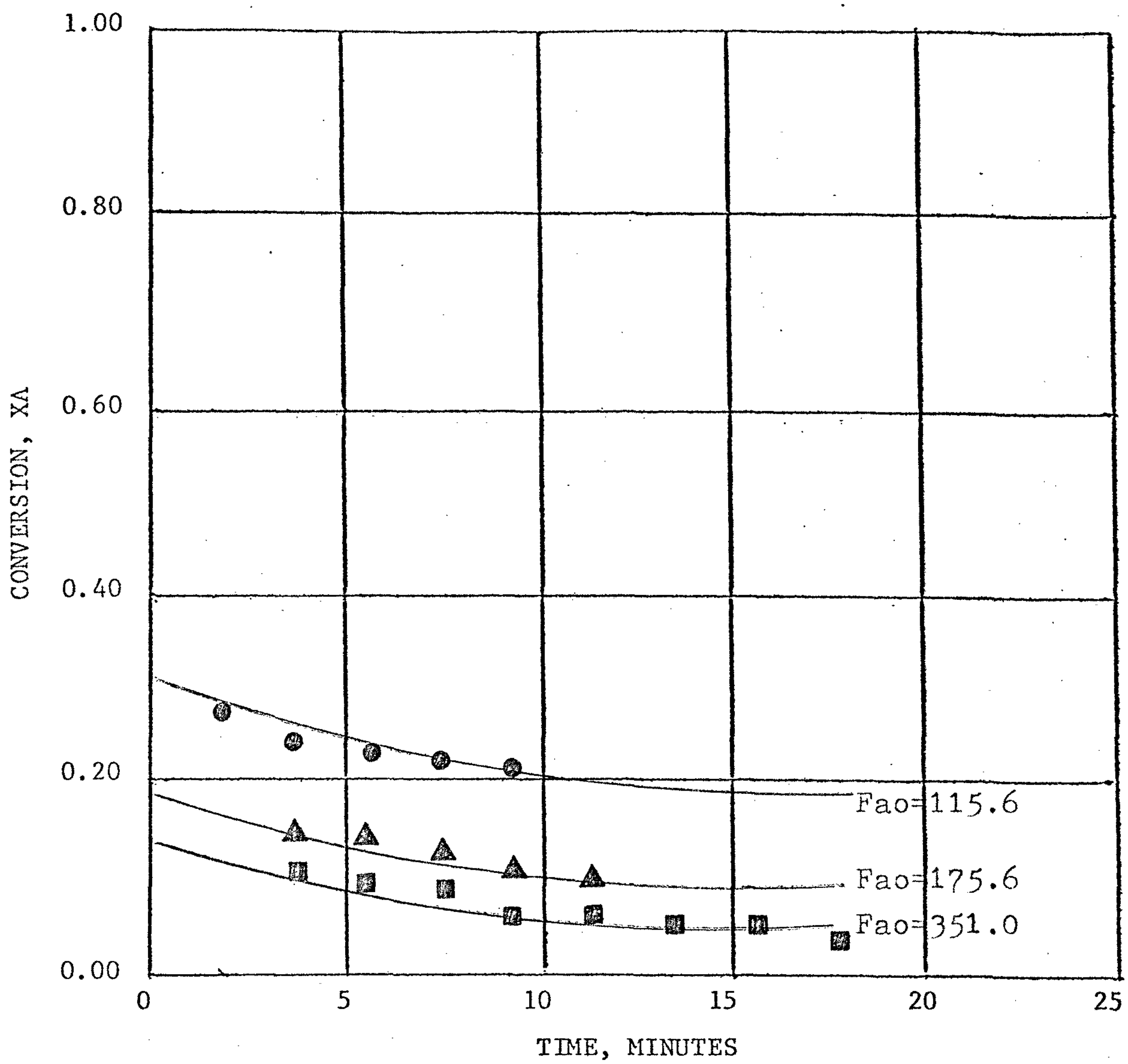
1. Specified temperature.
2. Specified ultrasonics.
3. Set flow rate.

Samples were taken for 30 seconds at 2 minute intervals. The data lent itself to a least squares analysis using the exponential equation as a fit to the conversion versus time data.

$$Xa = Ae^{Bt}$$

FIGURE NO. 44

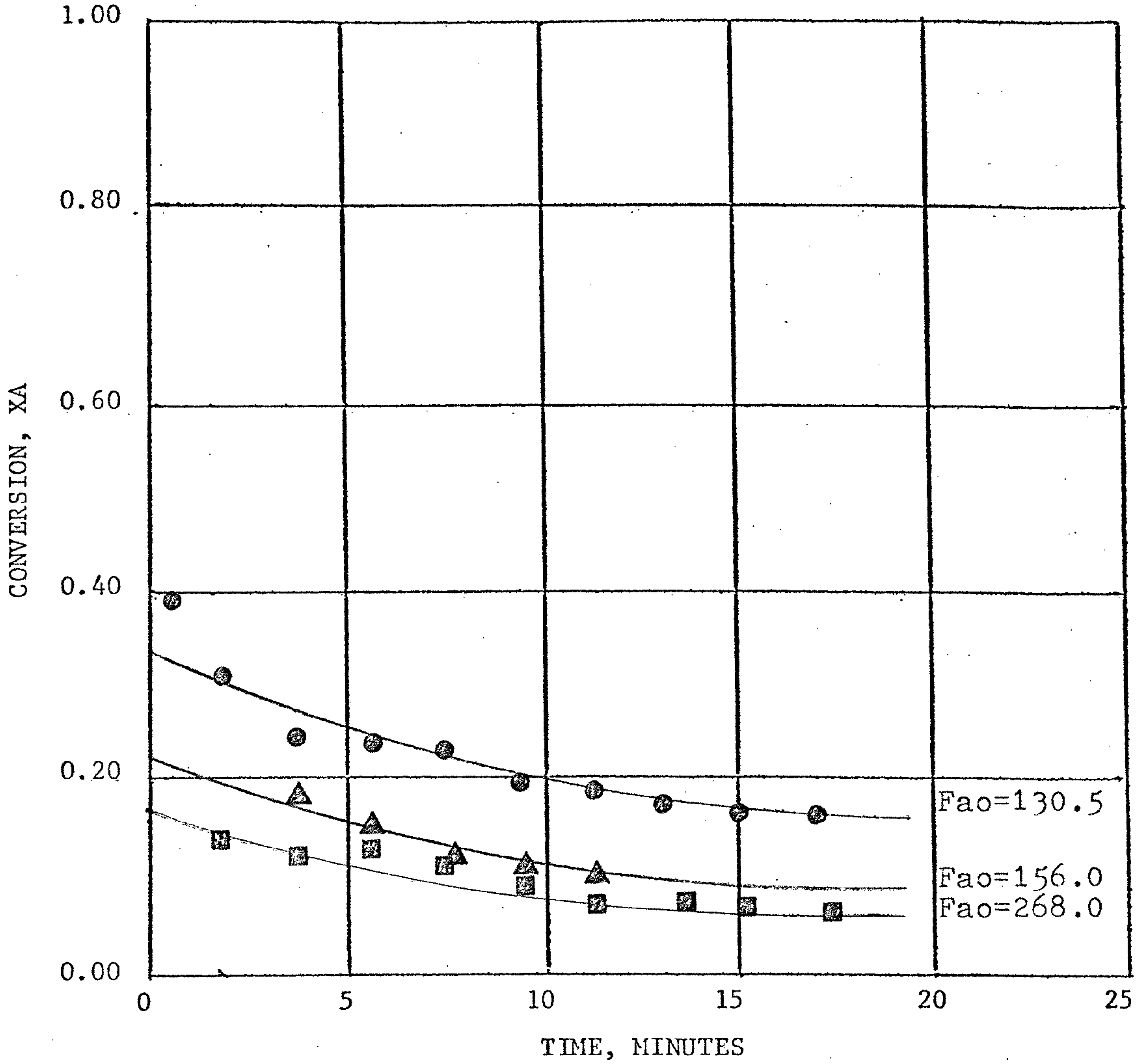
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	850	deg. F.
	ULTRASOUND	=	0	cycles/sec.
● Represents	W/FAO	=	13730	g.cat-sec/gmole
	FAO	=	115.6	gm./hr.
▲ Represents	W/Fao	=	9039	g.cat-sec/gmole
	Fao	=	175.6	gm./hr.
■ Represents	W/Fao	=	4518	g.cat-sec/gmole
	Fao	=	351.0	gm./hr.

FIGURE NO. 45

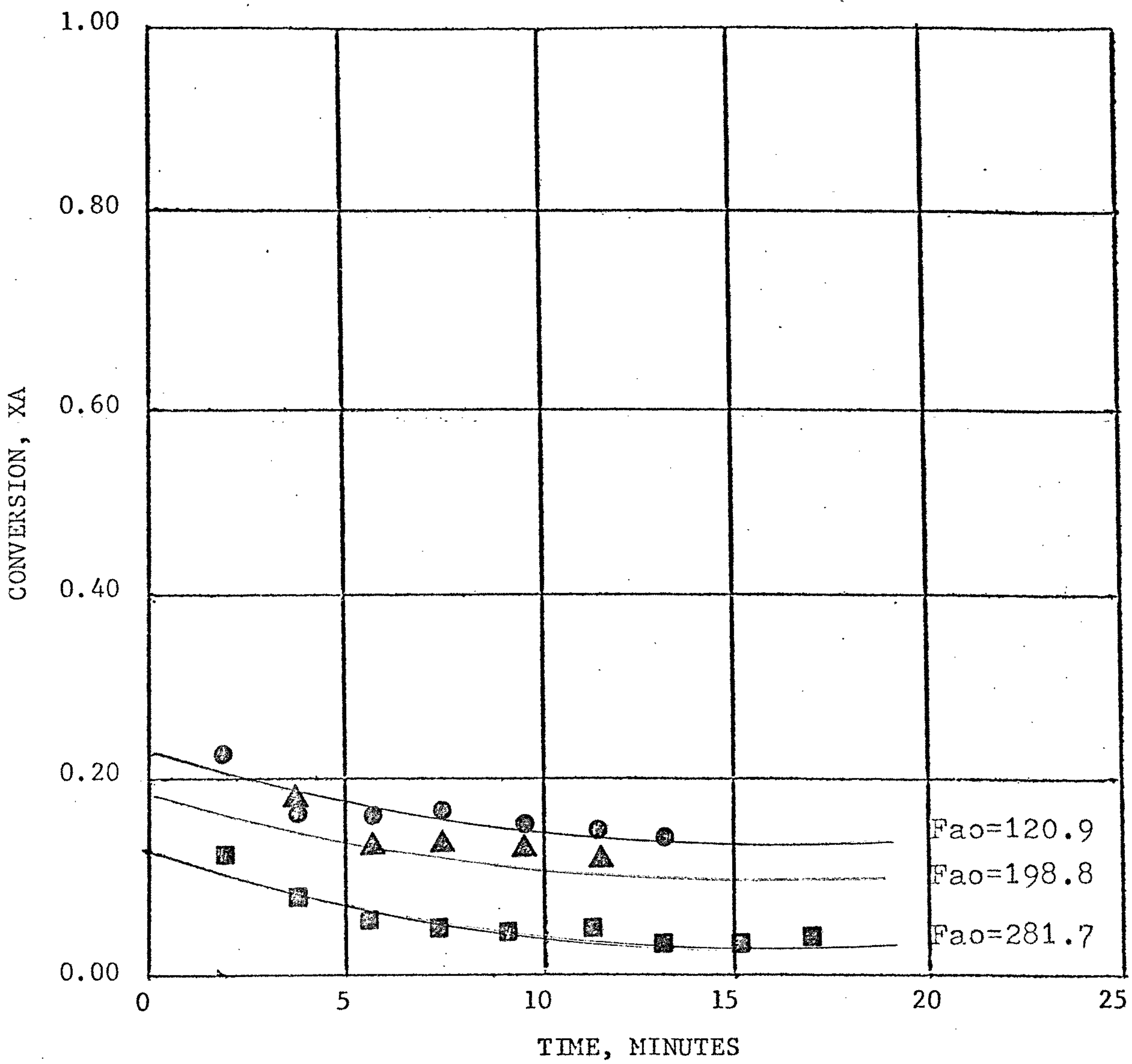
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	850	deg. F.
	ULTRASOUND	=	26,000	cycles/sec.
● Represents	W/FAO	=	12165	g.cat-sec/gmole
	FAO	=	130.5	gm./hr.
▲ Represents	W/Fao	=	10166	g.cat-sec/gmole
	Fao	=	156.0	gm./hr.
■ Represents	W/Fao	=	5922	g.cat-sec/gmole
	Fao	=	268.0	gm./hr.

FIGURE NO. 46

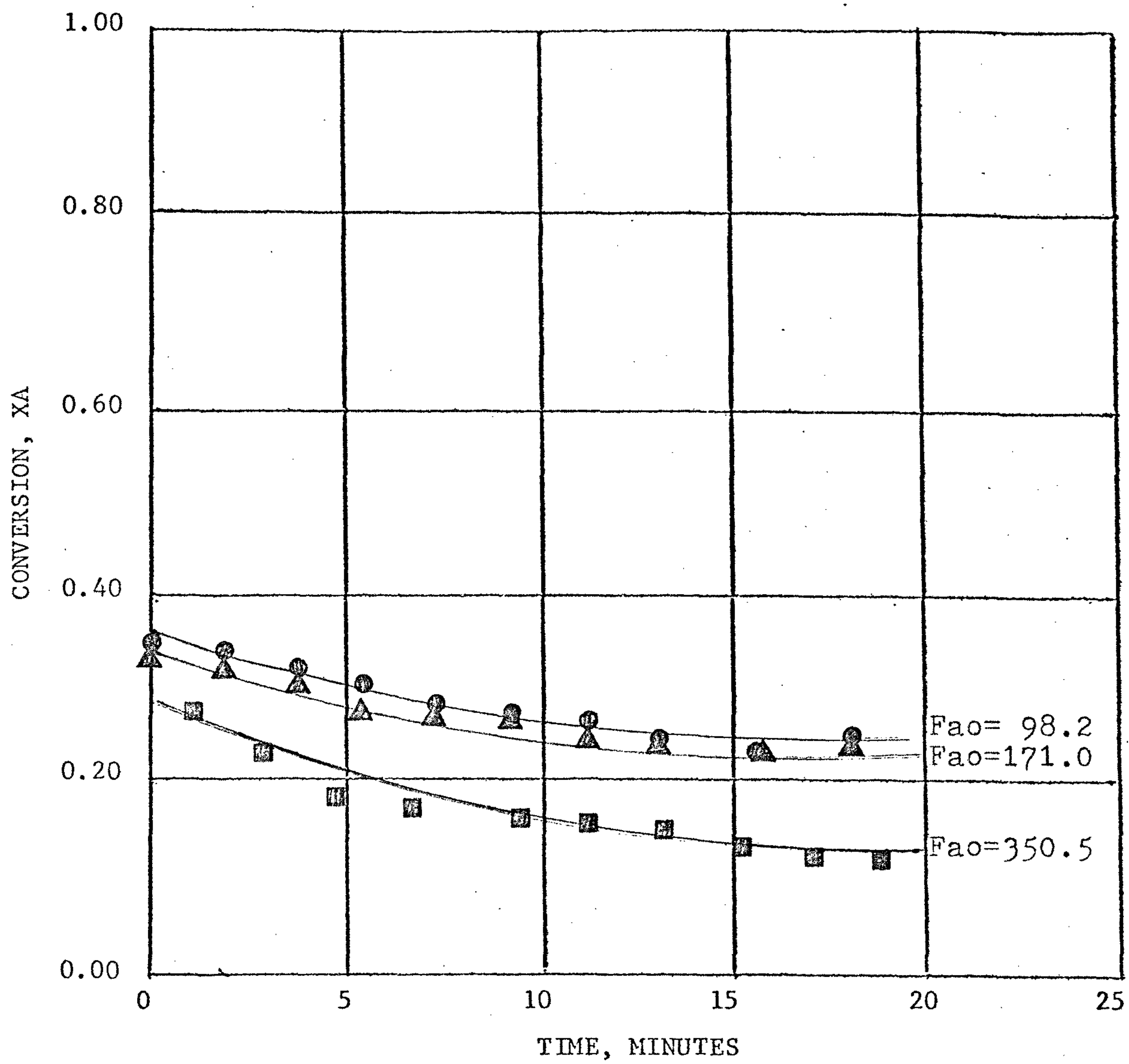
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	850	deg. F.
	ULTRASOUND	=	39,000	cycles/sec.
● Represents	W/FAO	=	13130	gm.cat.-sec./gmole
	FAO	=	120.9	gm./hr.
▲ Represents	W/Fao	=	9782	g.cat-sec/gmole
	Fao	=	198.8	gm./hr.
■ Represents	W/Fao	=	5633	g.cat-sec/gmole
	Fao	=	281.7	gm./hr.

FIGURE NO. 47

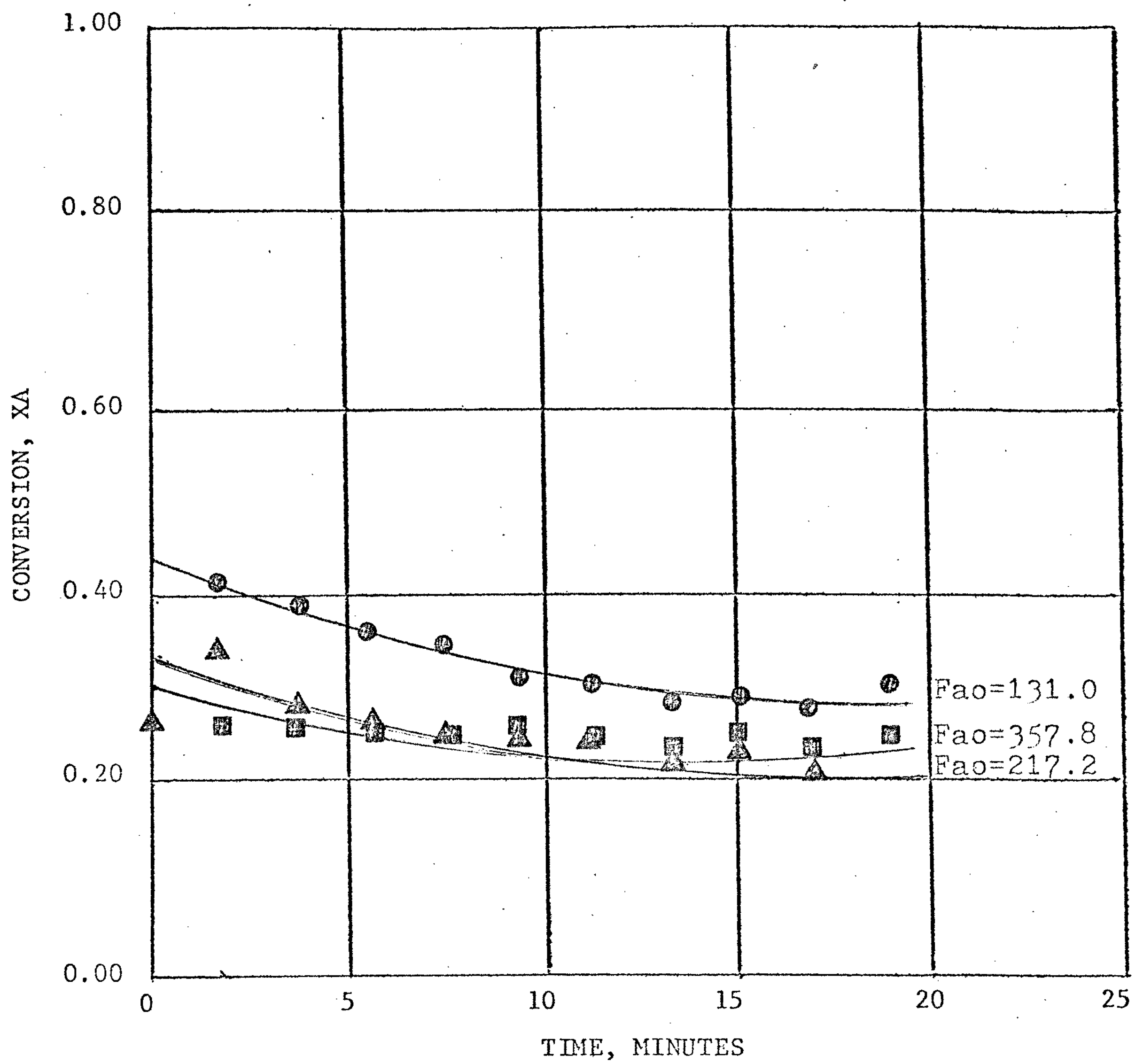
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	875	deg. F.
	ULTRASOUND	=	0	cycles/sec.
⊗ Represents	W/FAO	=	16158	g.cat-sec/gmole
	FAO	=	98.2	gm./hr.
▲ Represents	W/Fao	=	9242	g.cat-sec/gmole
	Fao	=	171.0	gm./hr.
■ Represents	W/Fao	=	4528	g.cat-sec/gmole
	Fao	=	350.5	gm./hr.

FIGURE NO. 48

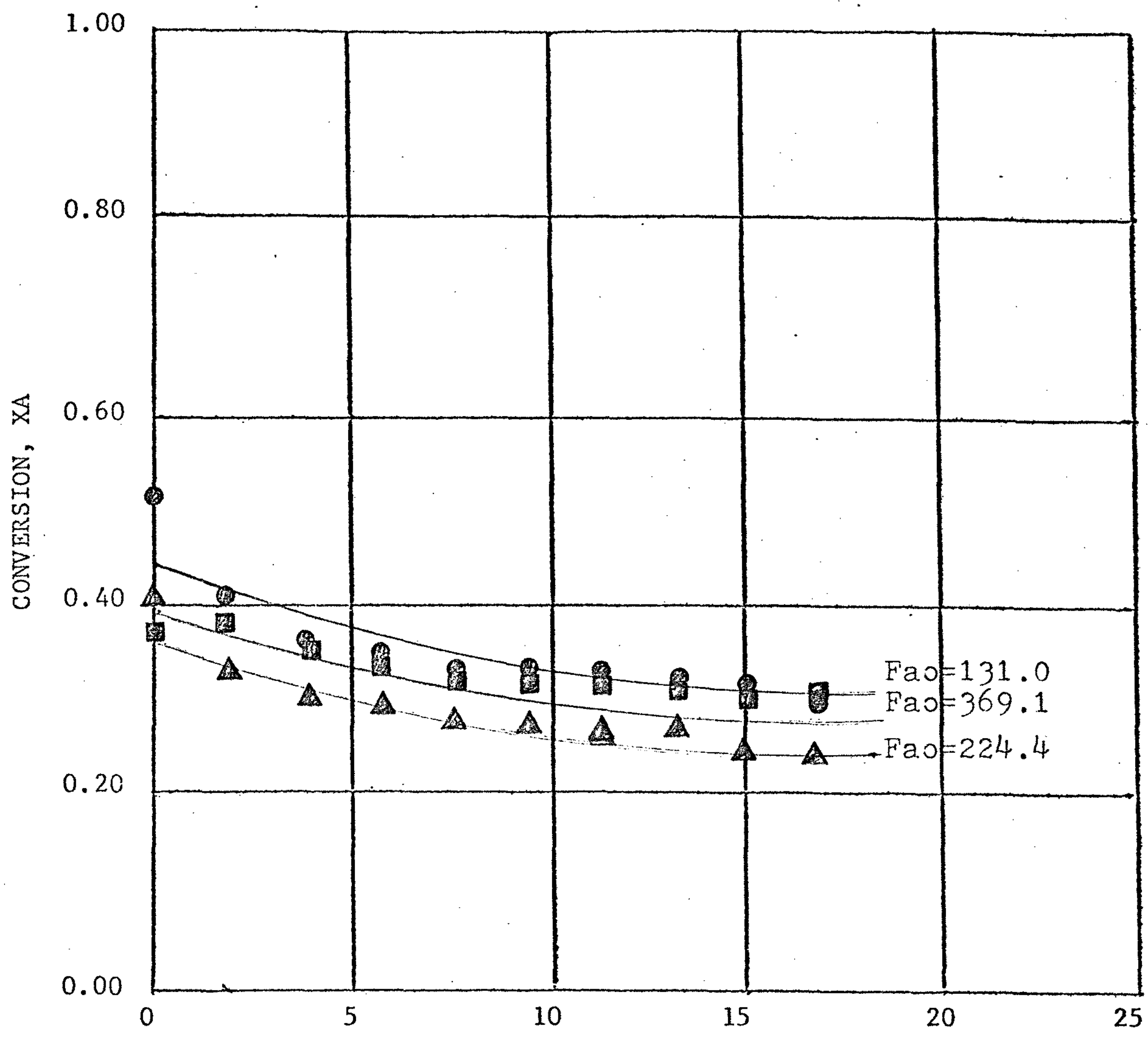
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	875	deg. F.
	ULTRASOUND	=	26,000	cycles/sec.
● Represents	W/FAO	=	12465	g.cat-sec/gmole
	FAO	=	127.2	gm./hr.
▲ Represents	W/Fao	=	7308	g.cat-sec/gmole
	Fao	=	217.2	gm./hr.
■ Represents	W/Fao	=	4436	g.cat-sec/gmole
	Fao	=	357.8	gm./hr.

FIGURE NO. 49

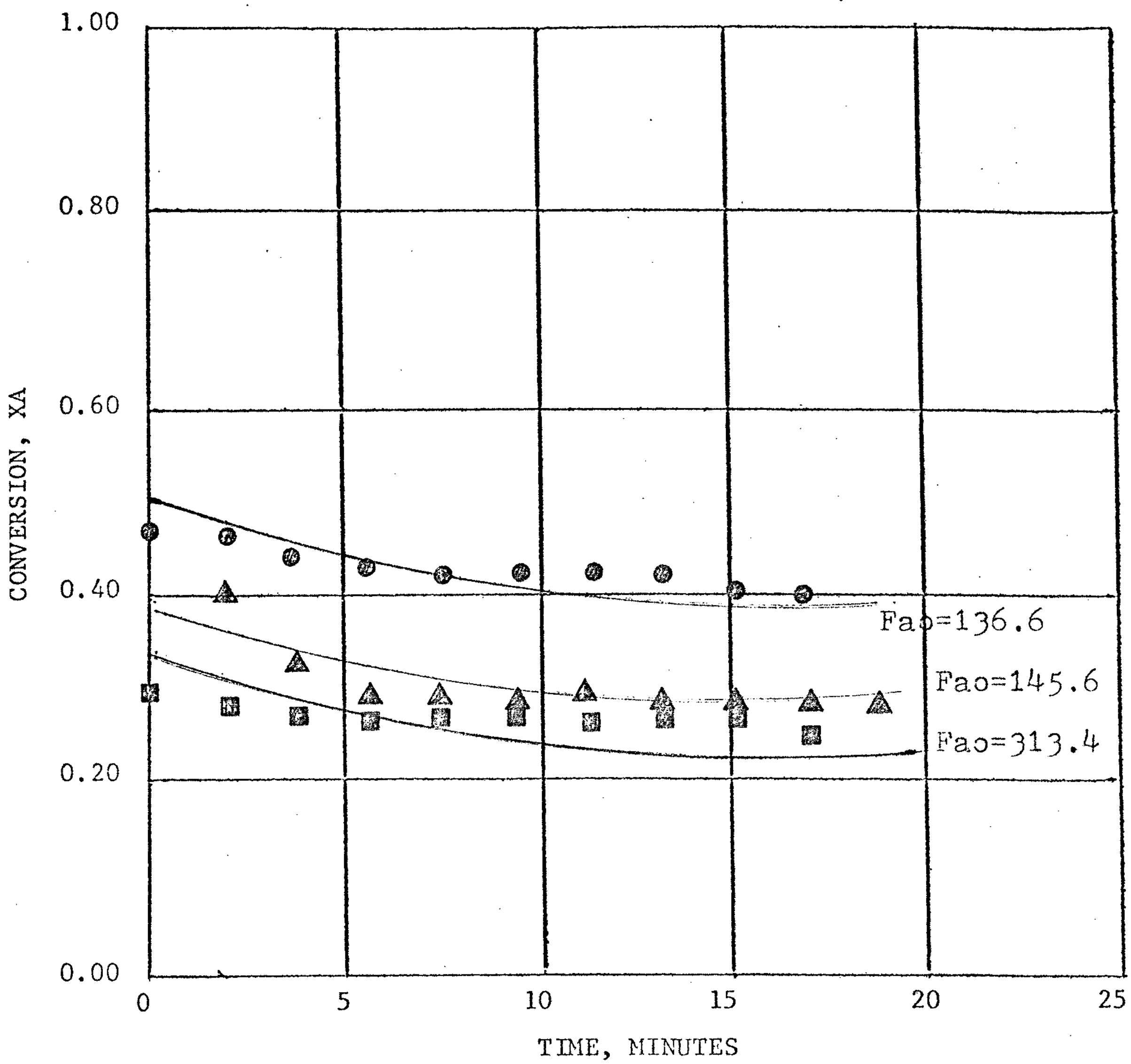
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	875	deg. F.
	ULTRASOUND	=	39,000	cycles/sec.
● Represents	W/FAO	=	12129	g.cat-sec/gmole
	FAO	=	131.0	gm./hr.
▲ Represents	W/Fao	=	7077	g.cat-sec/gmole
	Fao	=	224.4	gm./hr.
■ Represents	W/Fao	=	4302	g.cat-sec/gmole
	Fao	=	369.1	gm./hr.

FIGURE NO. 50

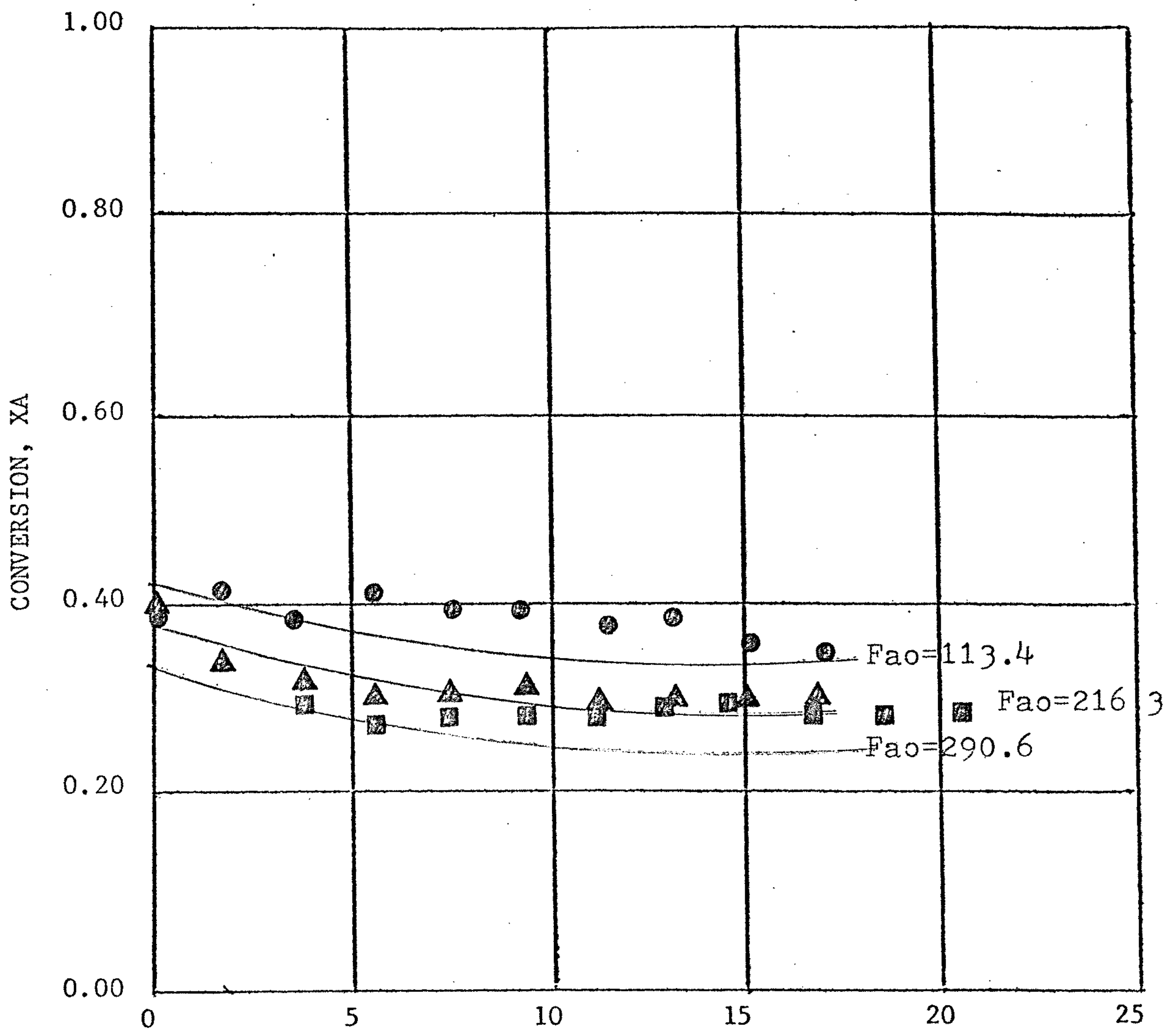
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	900	deg. F.
	ULTRASOUND	=	0	cycles/sec.
● Represents	W/FAO	=	11626	g.cat-sec/gmole
	FAO	=	136.6	gm./hr.
▲ Represents	W/Fao	=	5068	g.cat-sec/gmole
	Fao	=	313.4	gm./hr.
■ Represents	W/Fao	=	10907	g.cat-sec/gmole
	Fao	=	145.6	gm./hr.

FIGURE NO. 51

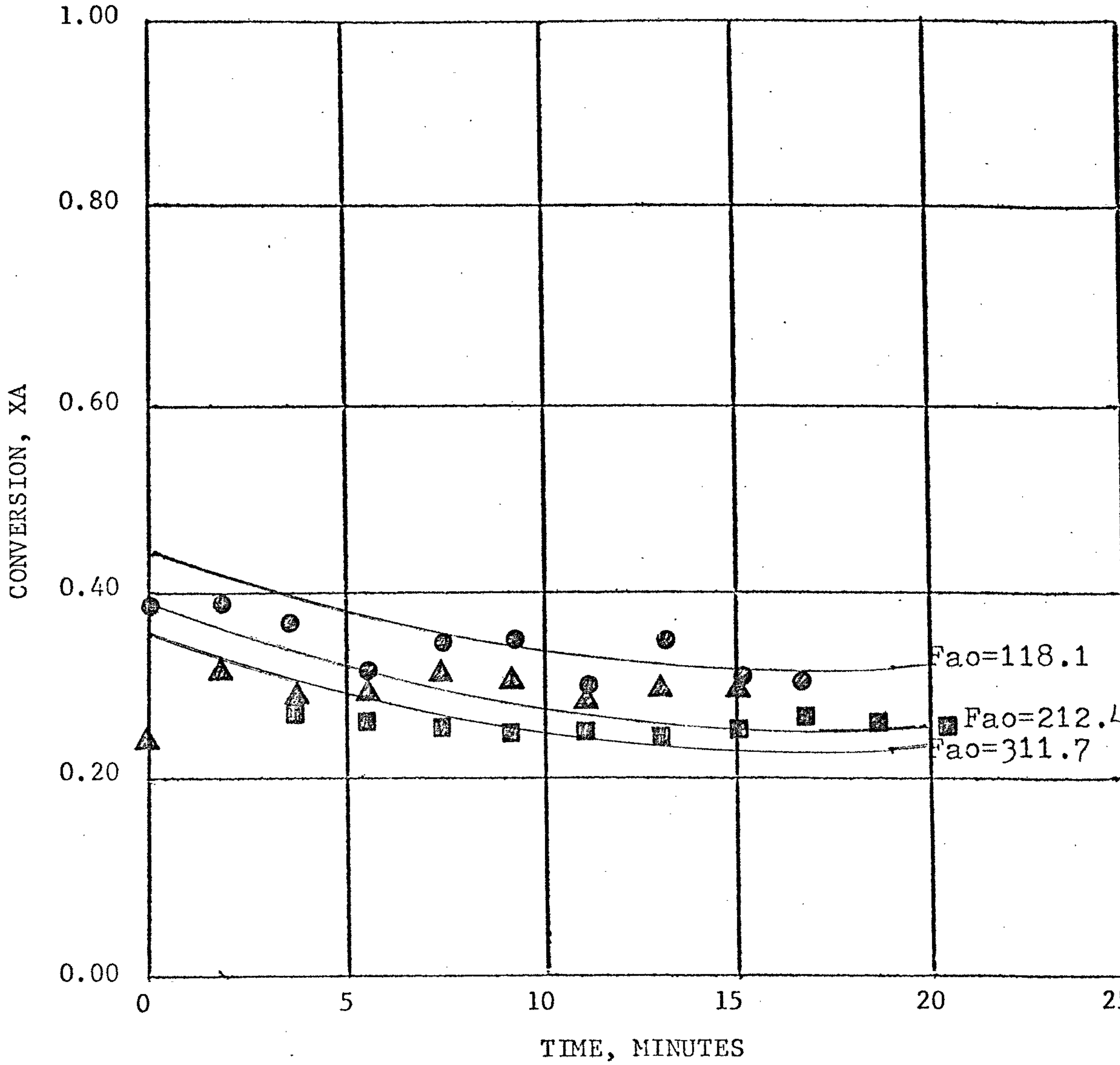
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	900	deg. F.
	ULTRASOUND	=	26,000	cycles/sec.
● Represents	W/FAO	=	14000	g.cat-sec/gmole
	FAO	=	113.4	gm./hr.
▲ Represents	W/Fao	=	7343	g.cat-sec/gmole
	Fao	=	216.3	gm./hr.
■ Represents	W/Fao	=	5464	g.cat-sec/gmole
	Fao	=	290.6	gm./hr.

FIGURE NO. 52

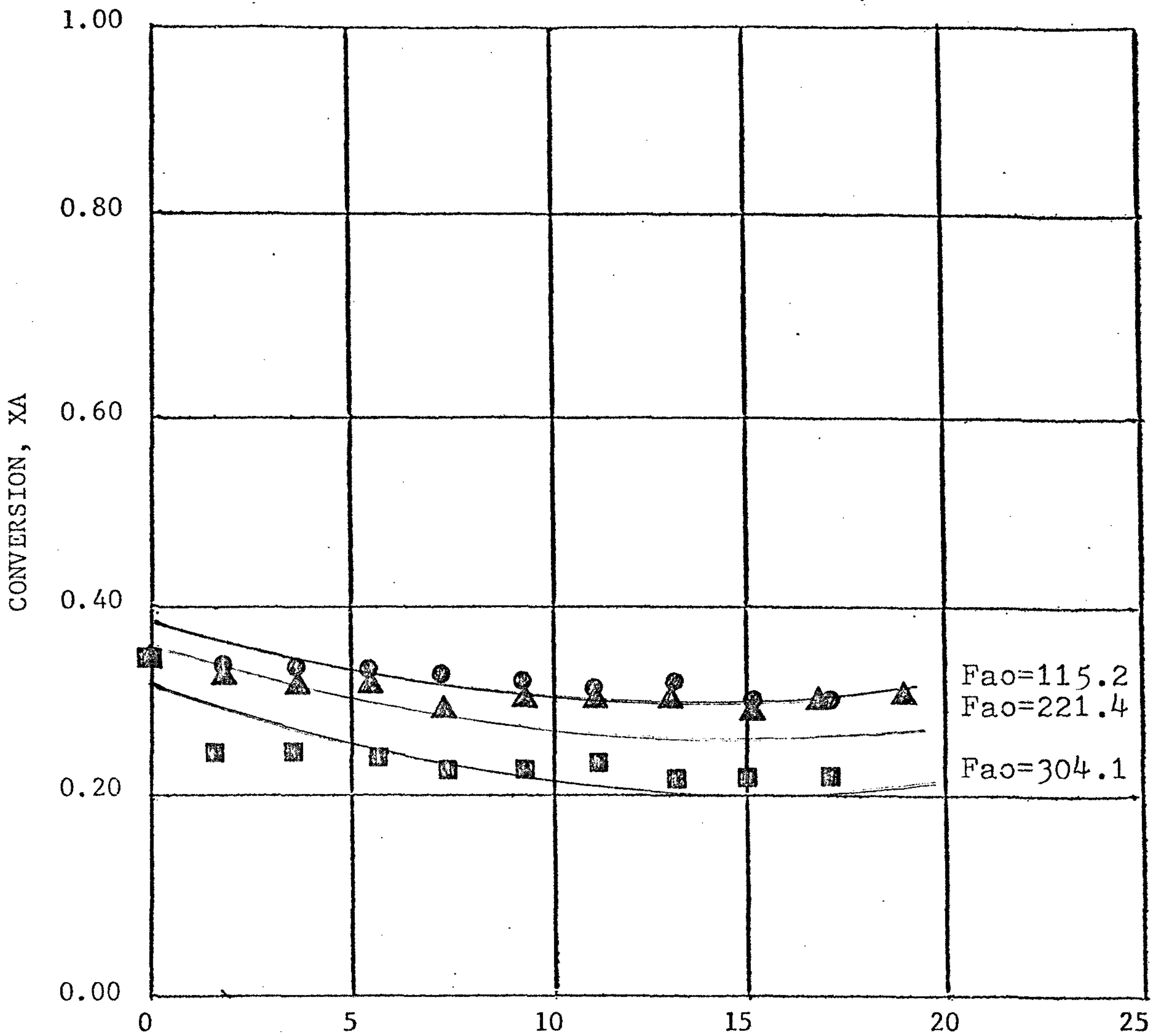
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	900	deg. F.
	ULTRASOUND	=	39,000	cycles/sec.
⊗ Represents	W/FAO	=	13449	g.cat-sec/gmole
	FAO	=	118.1	gm./hr.
▲ Represents	W/Fao	=	7476	g.cat-sec/gmole
	Fao	=	212.4	gm./hr.
■ Represents	W/Fao	=	5096	g.cat-sec/gmole
	Fao	=	311.7	gm./hr.

FIGURE NO. 53

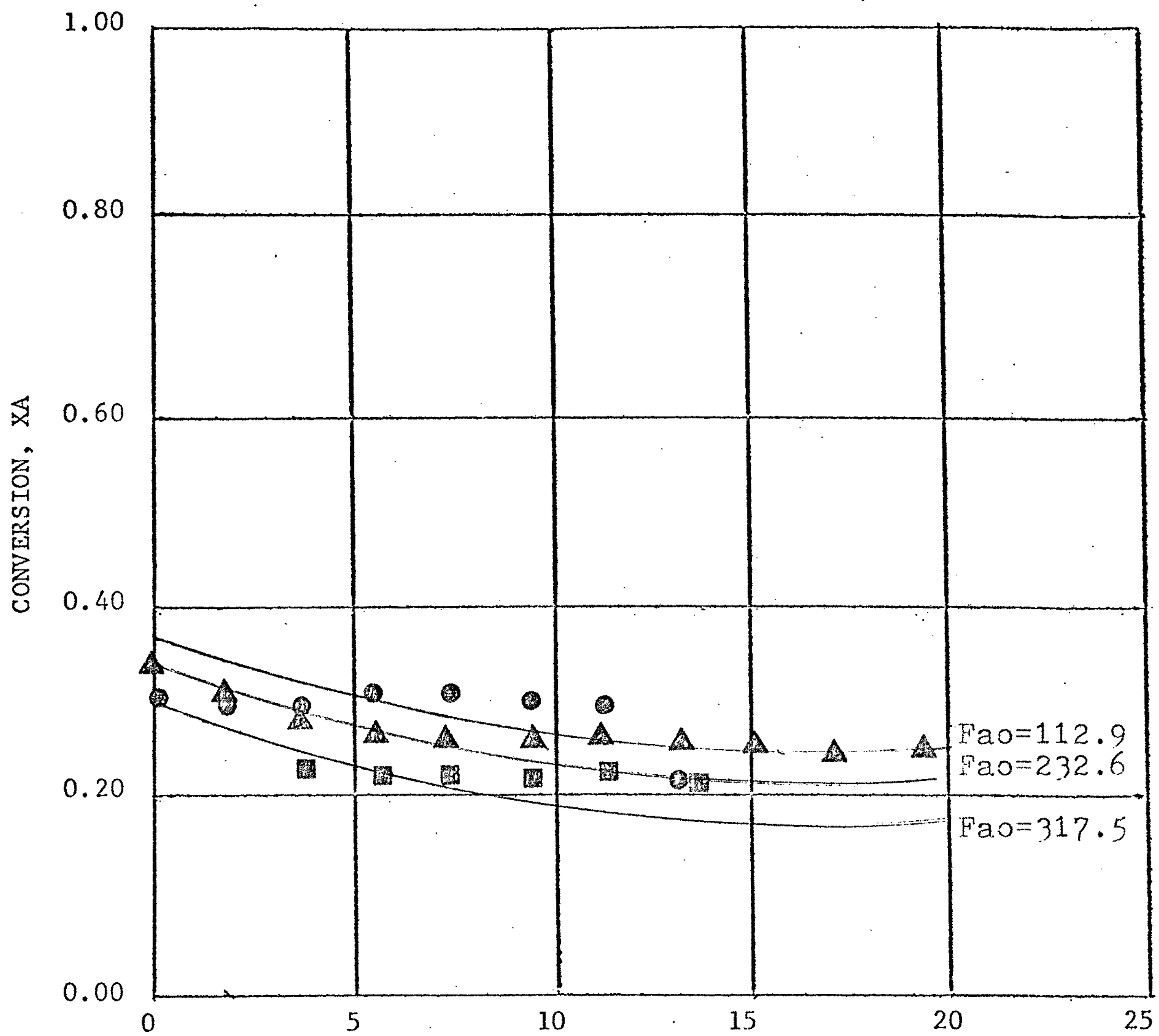
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	925	deg. F.
	ULTRASOUND	=	0	cycles/sec.
● Represents	W/FAO	=	13789	g.cat-sec/gmole
	FAO	=	115.2	gm./hr.
▲ Represents	W/Fao	=	7174	g.cat-sec/gmole
	Fao	=	221.4	gm./hr.
■ Represents	W/Fao	=	5222	g.cat-sec/gmole
	Fao	=	304.1	gm./hr.

FIGURE NO. 54

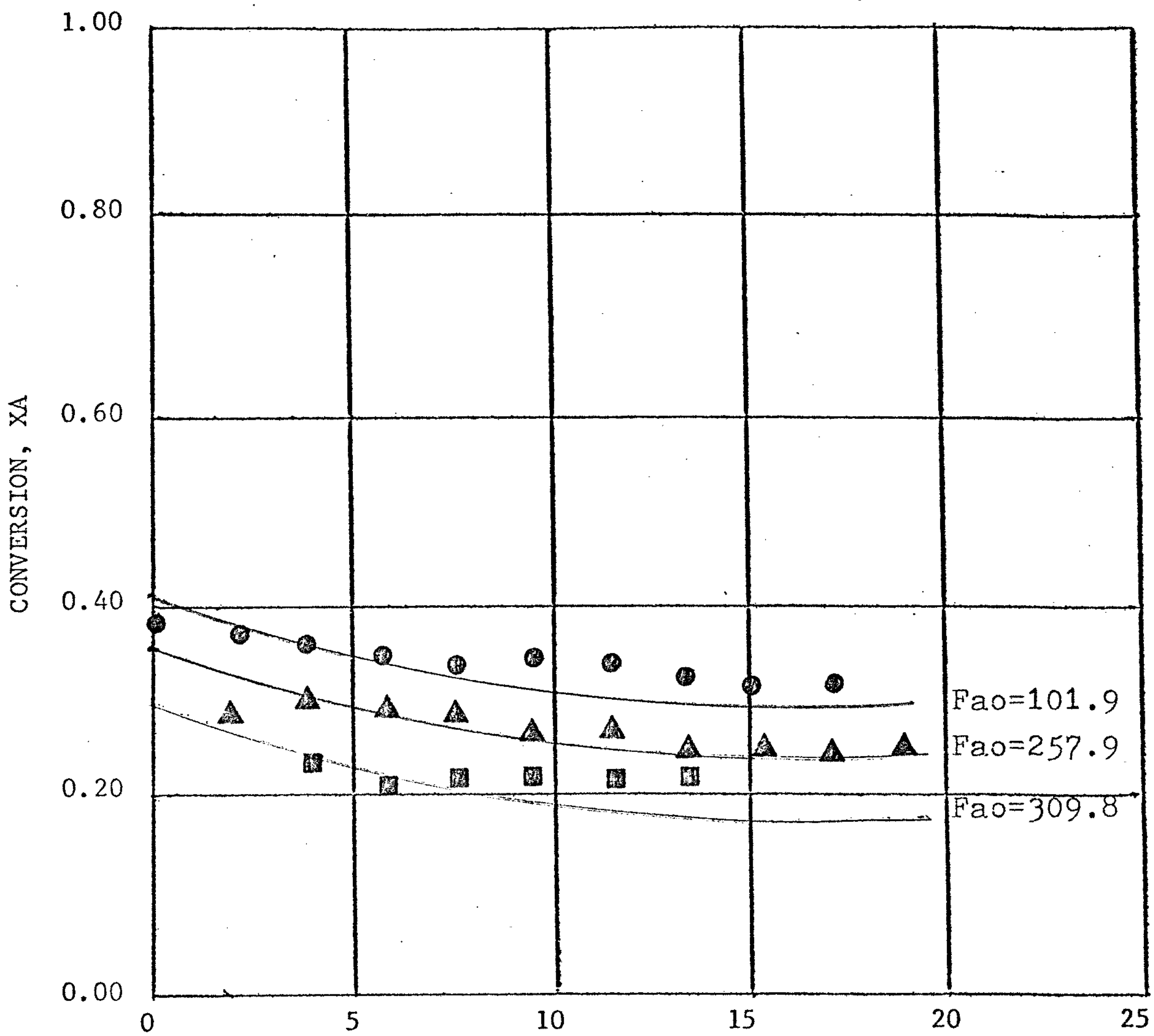
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	925	deg. F.
	ULTRASOUND	=	26,000	cycles/sec.
● Represents	W/FAO	=	14072	g.cat-sec/gmole
	FAO	=	112.9	gm./hr.
▲ Represents	W/Fao	=	6829	g.cat-sec/gmole
	Fao	=	232.6	gm./hr.
■ Represents	W/Fao	=	5001	g.cat-sec/gmole
	Fao	=	317.5	gm./hr.

FIGURE NO. 55

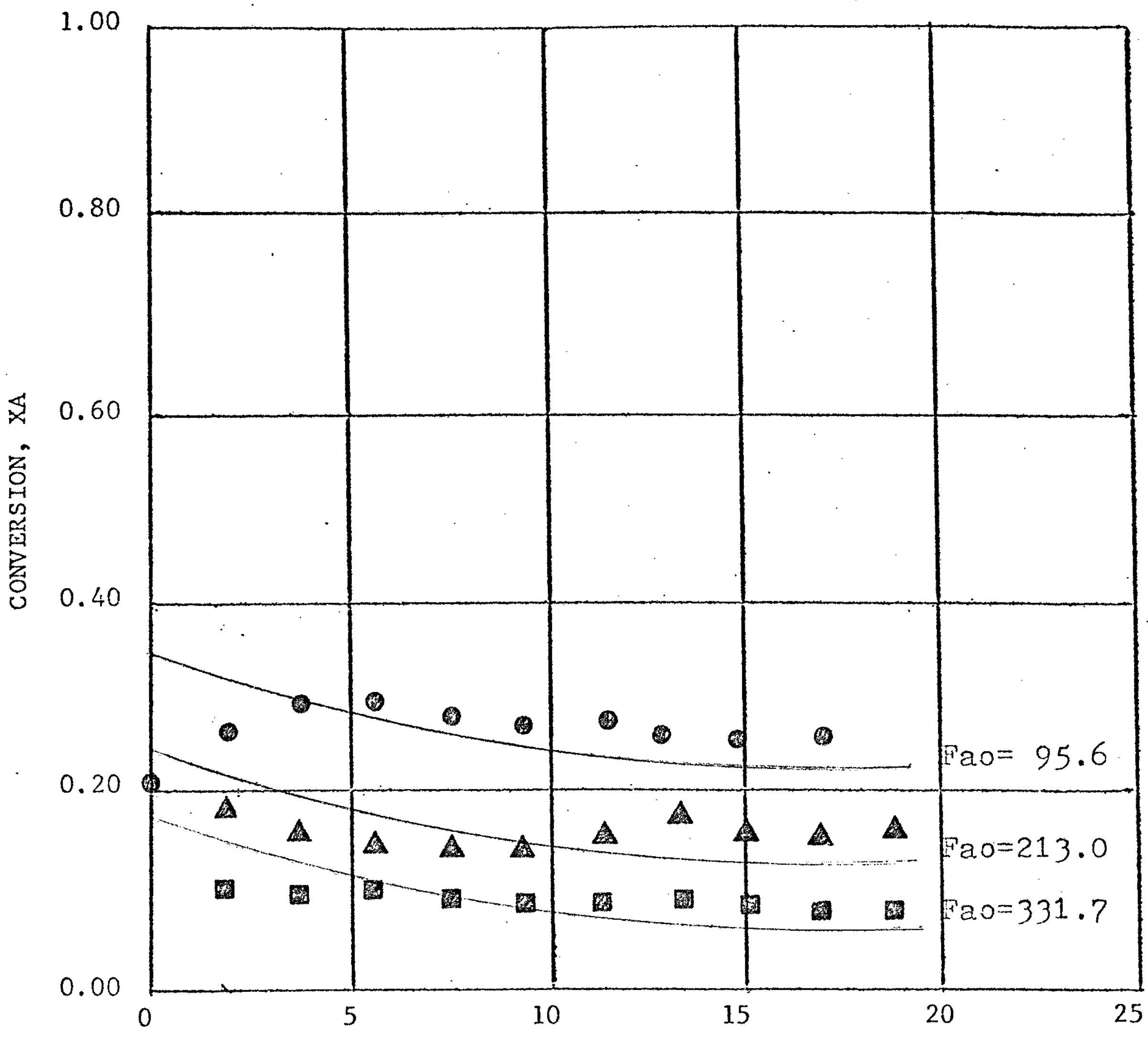
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0841	cm.
	TEMPERATURE	=	925	deg. F.
	ULTRASOUND	=	39,000	cycles/sec.
● Represents	W/FAO	=	15587	g.cat-sec/gmole
	FAO	=	101.9	gm./hr.
▲ Represents	W/Fao	=	6157	g.cat-sec/gmole
	Fao	=	257.9	gm./hr.
■ Represents	W/Fao	=	5127	g.cat-sec/gmole
	Fao	=	309.8	gm./hr.

FIGURE NO. 56

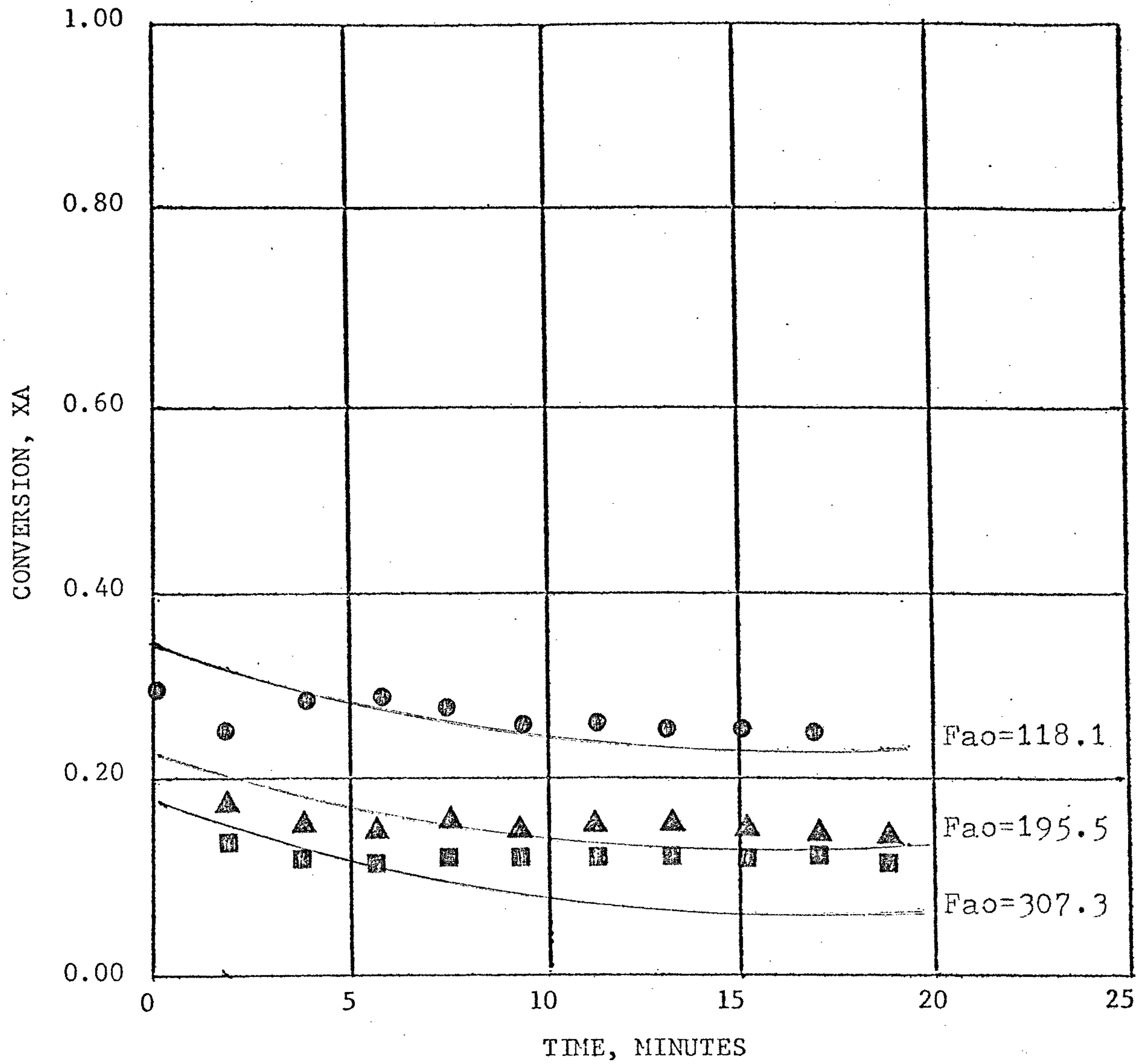
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	875	deg. F.
	ULTRASOUND	=	0	cycles/sec.
● Represents	W/FAO	=	16608	g.cat-sec/gmole
	FAO	=	95.6	gm./hr.
▲ Represents	W/Fao	=	7156	g.cat-sec/gmole
	Fao	=	213.0	gm./hr.
■ Represents	W/Fao	=	4826	g.cat-sec/gmole
	Fao	=	331.7	gm./hr.

FIGURE NO. 57

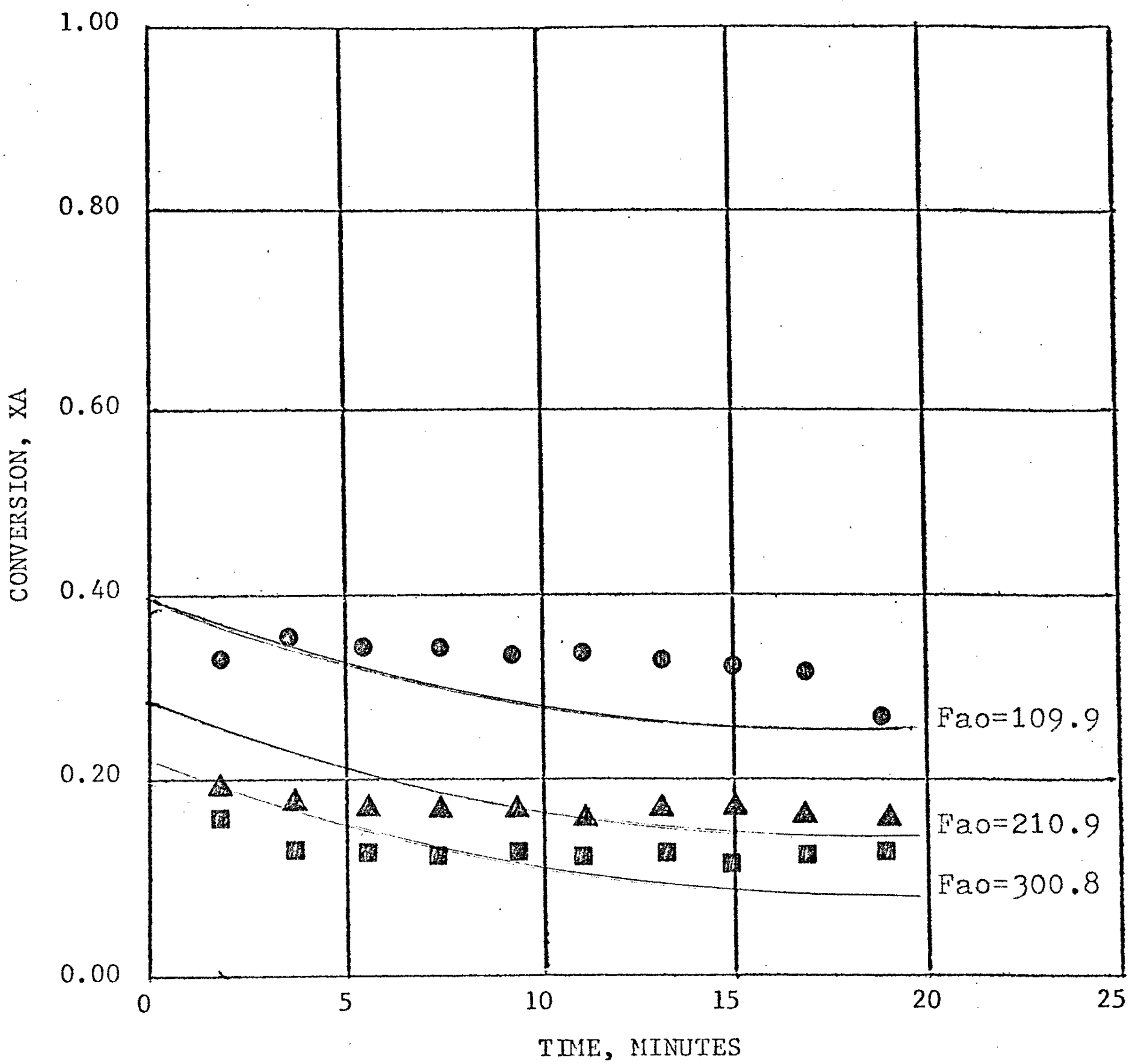
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	875	deg. F.
	ULTRASOUND	=	26,000	cycles/sec.
● Represents	W/FAO	=	13561	g.cat-sec/gmole
	FAO	=	118.1	gm./hr.
▲ Represents	W/Fao	=	8191	g.cat-sec/gmole
	Fao	=	195.5	gm./hr.
■ Represents	W/Fao	=	5209	g.cat-sec/gmole
	Fao	=	307.3	gm./hr.

FIGURE NO. 58

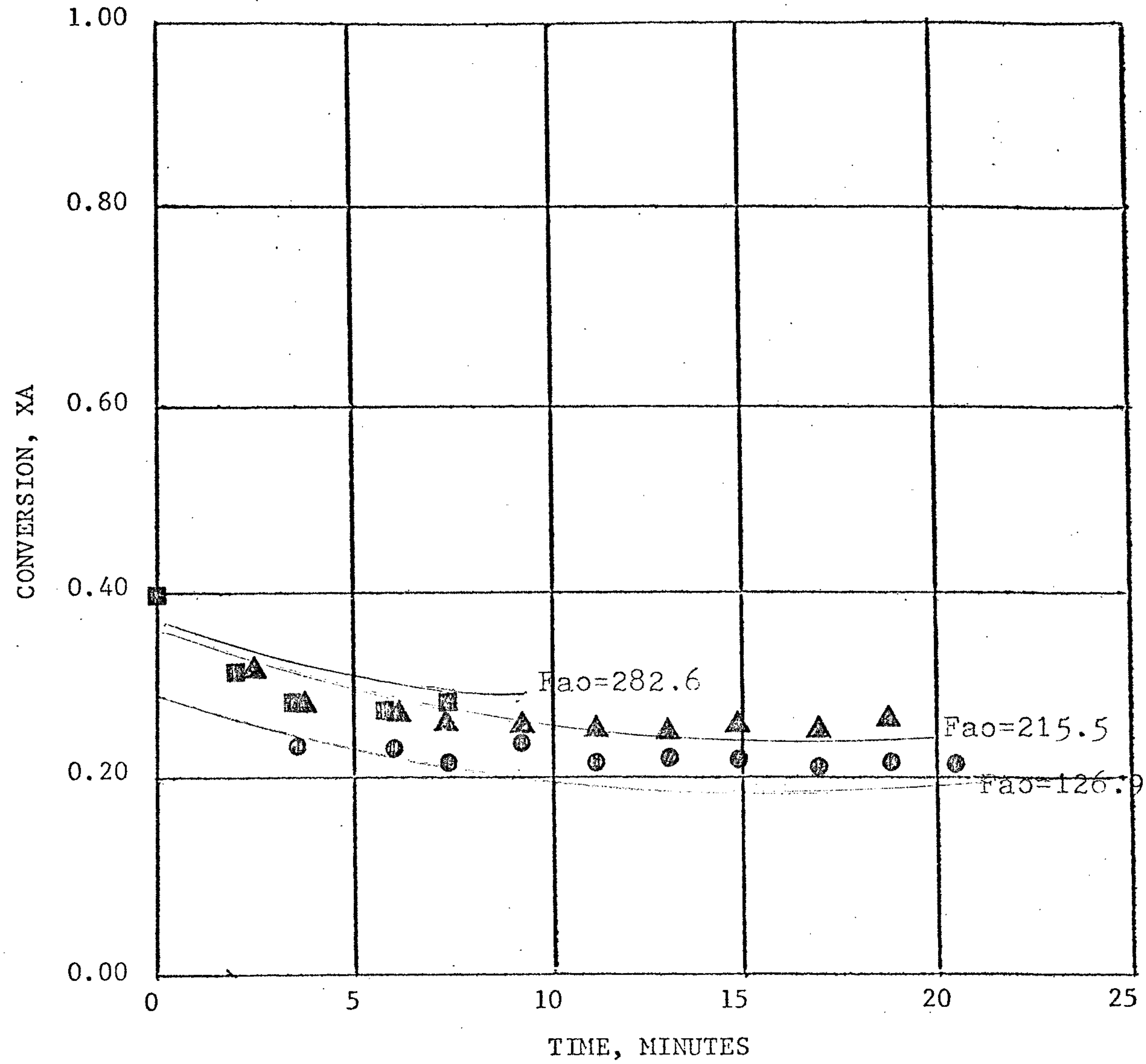
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	875	deg. F.
	ULTRASOUND	=	39,000	cycles/sec.
● Represents	W/FAO	=	14570	g.cat-sec/gmole
	FAO	=	109.9	gm./hr.
▲ Represents	W/Fao	=	7590	g.cat-sec/gmole
	Fao	=	210.9	gm./hr.
■ Represents	W/Fao	=	5322	g.cat-sec/gmole
	Fao	=	300.8	gm./hr.

FIGURE NO. 59

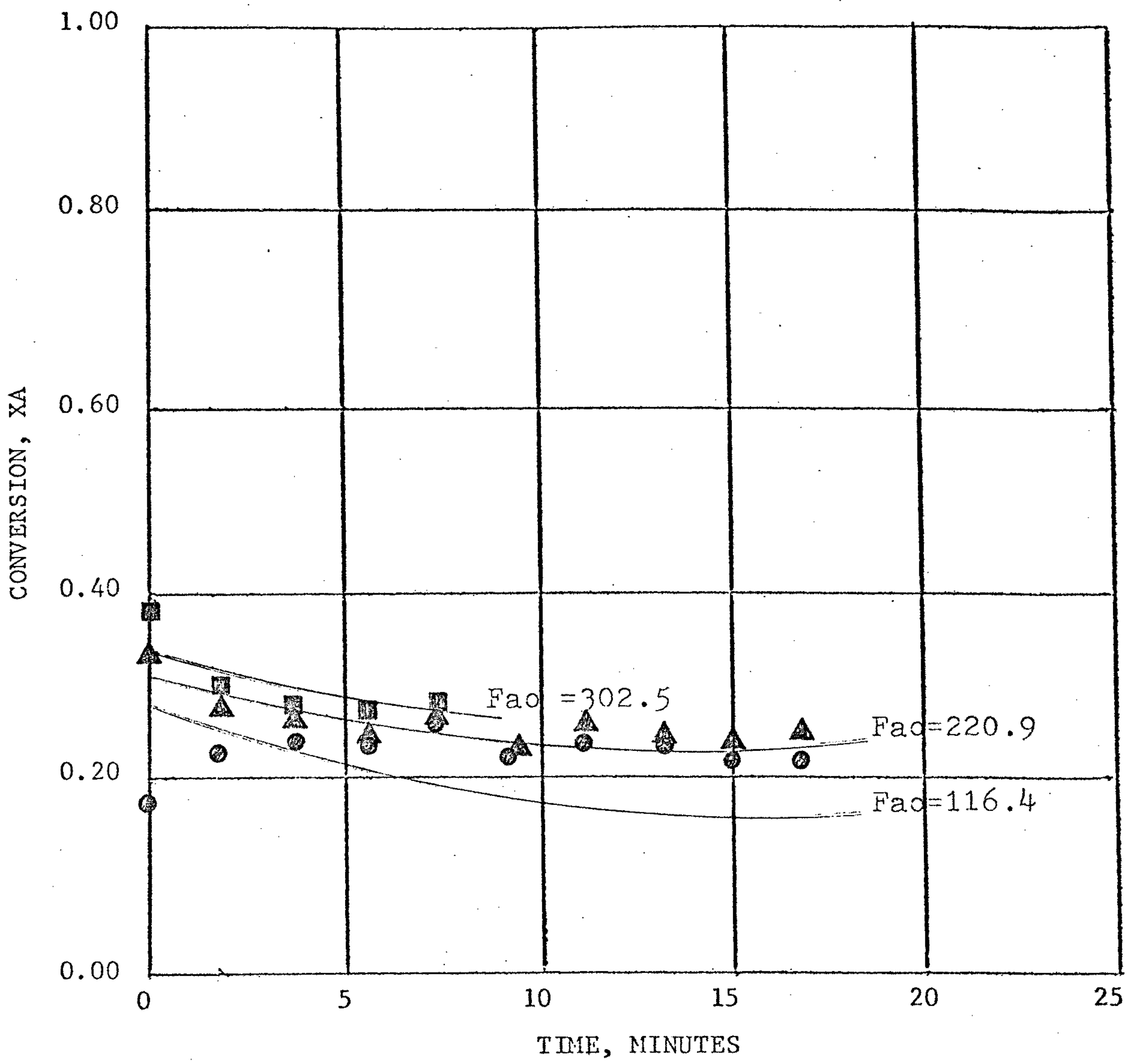
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	900	deg. F.
	ULTRASOUND	=	0	cycles/sec.
● Represents	W/FAO	=	12616	g.cat-sec/gmole
	FAO	=	126.9	gm./hr.
▲ Represents	W/Fao	=	7429	g.cat-sec/gmole
	Fao	=	215.5	gm./hr.
■ Represents	W/Fao	=	5666	g.cat-sec/gmole
	Fao	=	282.6	gm./hr.

FIGURE NO. 60

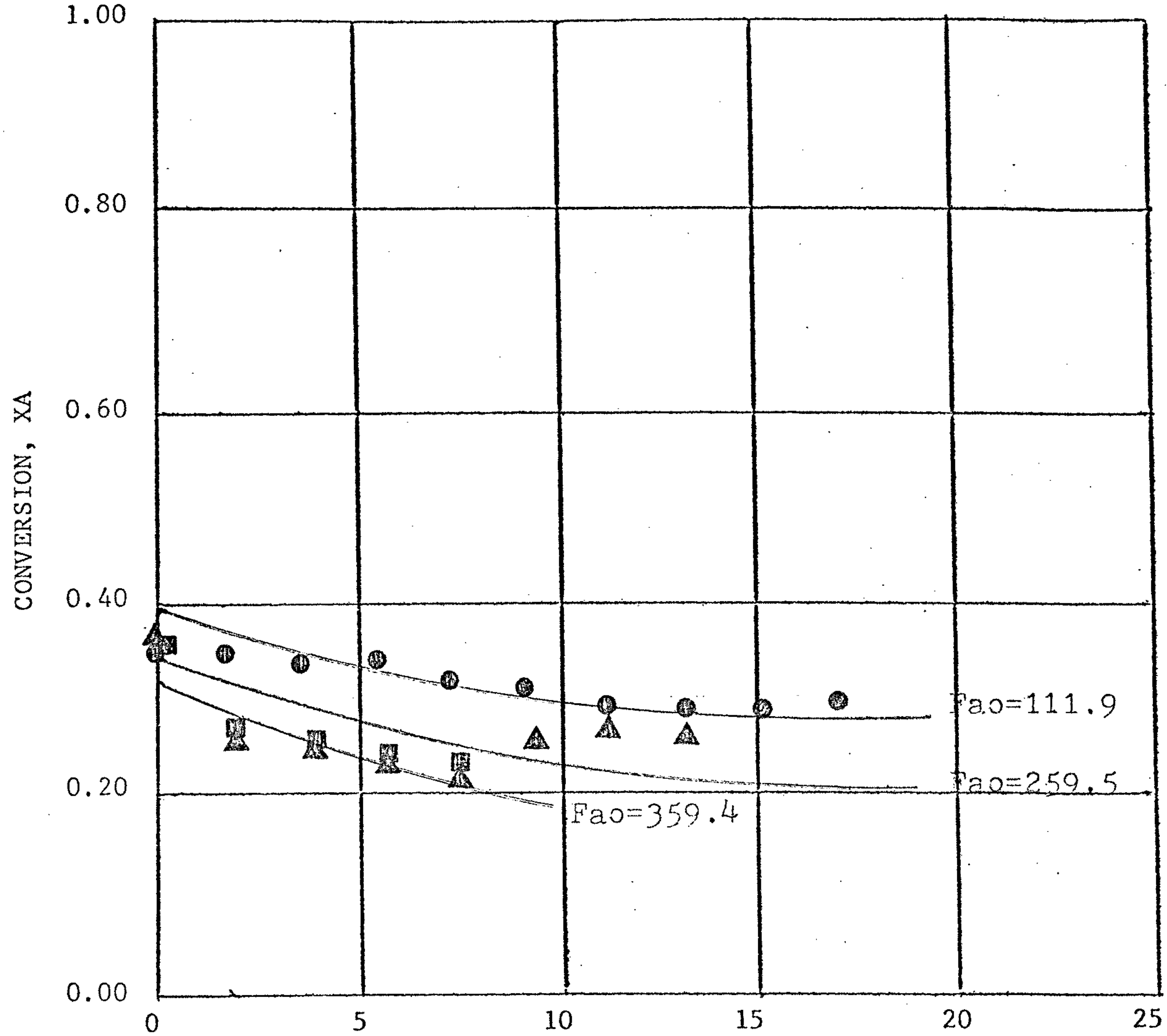
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	900	deg. F.
	ULTRASOUND	=	26,000	cycles/sec.
● Represents	W/FAO	=	13761	g.cat-sec/gmole
	FAO	=	116.4	gm./hr.
▲ Represents	W/Fao	=	7148	g.cat-sec/gmole
	Fao	=	220.9	gm./hr.
■ Represents	W/Fao	=	5293	g.cat-sec/gmole
	Fao	=	302.5	gm./hr.

FIGURE NO. 61

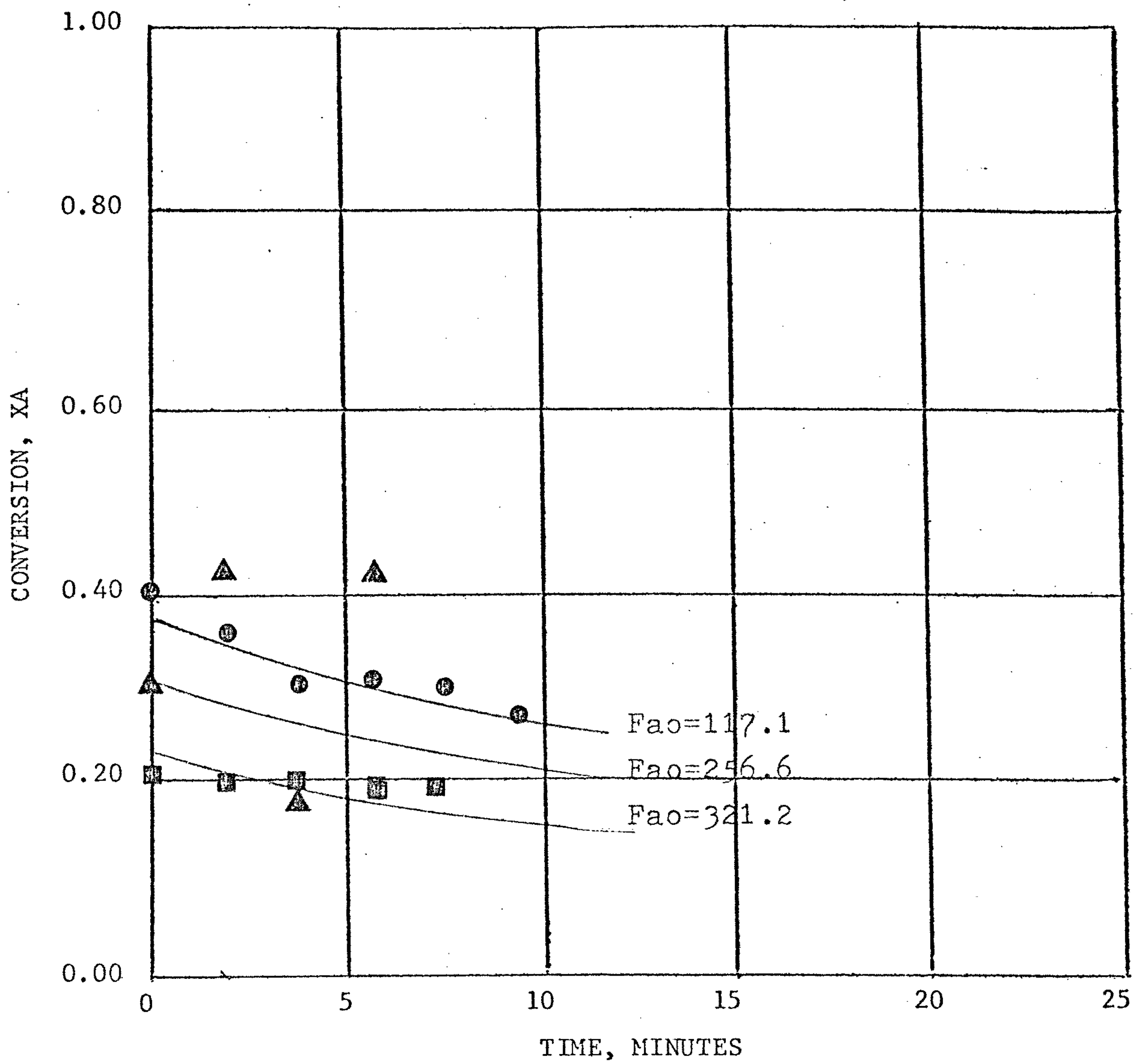
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	39,000	cycles.sec. -
	ULTRASOUND	=	900	deg. F.
● Represents	W/FAO	=	14309	g.cat-sec/gmole
	FAO	=	111.9	gm./hr.
▲ Represents	W/Fao	=	6169	g.cat-sec/gmole
	Fao	=	259.5	gm./hr.
■ Represents	W/Fao	=	4455	g.cat-sec/gmole
	Fao	=	359.4	gm./hr.

FIGURE NO. 62

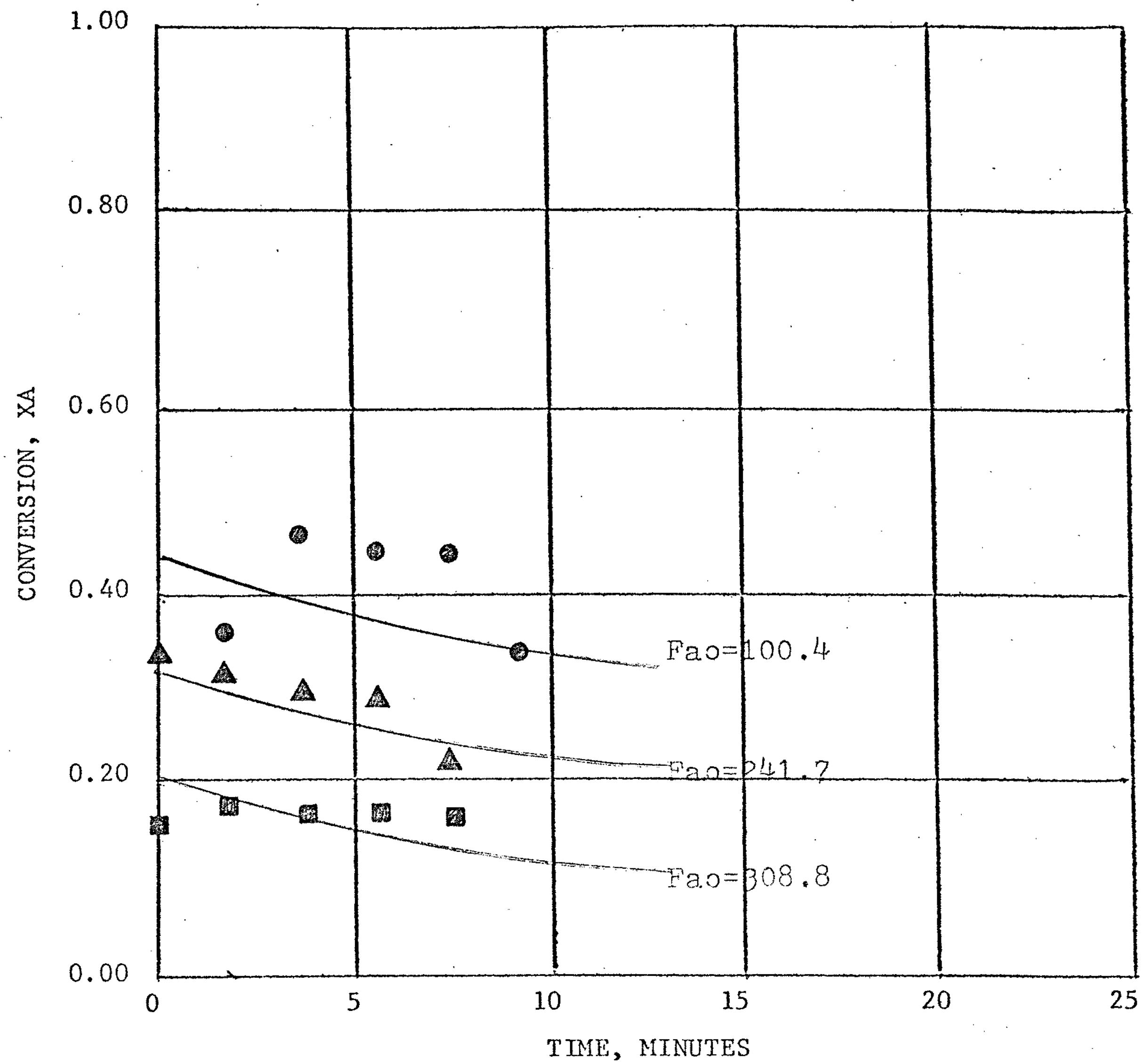
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	925	deg. F.
	ULTRASOUND	=	0	cycles/sec.
● Represents	W/FAO	=	13673	g.cat-sec/gmole
	FAO	=	117.1	gm./hr.
▲ Represents	W/Fao	=	5936	g.cat-sec/gmole
	Fao	=	256.6	gm./hr.
■ Represents	W/Fao	=	4742	g.cat-sec/gmole
	Fao	=	321.2	gm./hr.

FIGURE NO. 63

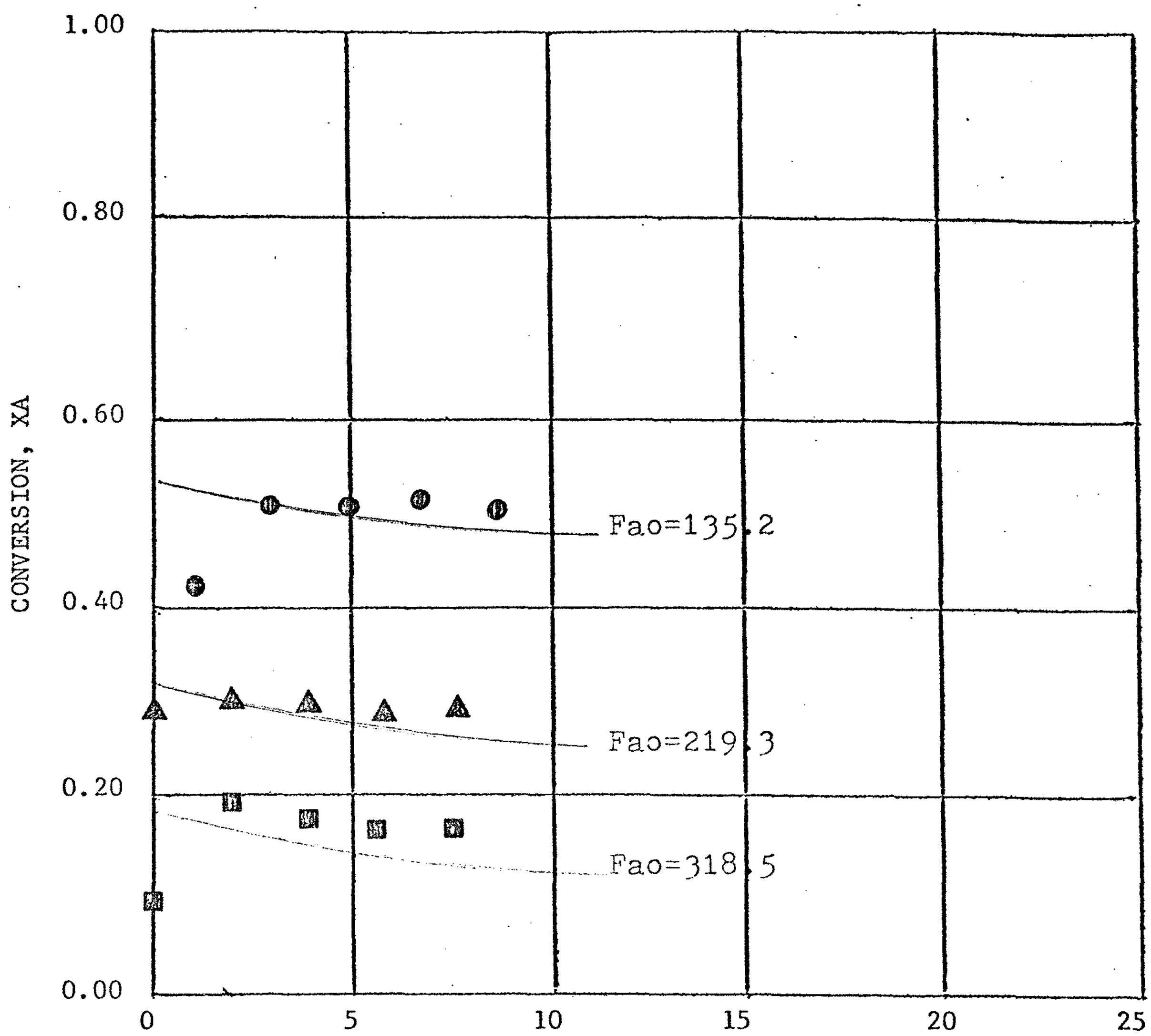
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	925	deg. F.
	ULTRASOUND	=	26,000	cycles/sec.
● Represents	W/FAO	=	15177	g.cat-sec/gmole
	FAO	=	100.4	gm./hr.
▲ Represents	W/Fao	=	6303	g.cat-sec/gmole
	Fao	=	241.7	gm./hr.
■ Represents	W/Fao	=	4932	g.cat-sec/gmole
	Fao	=	308.8	gm./hr.

FIGURE NO. 64

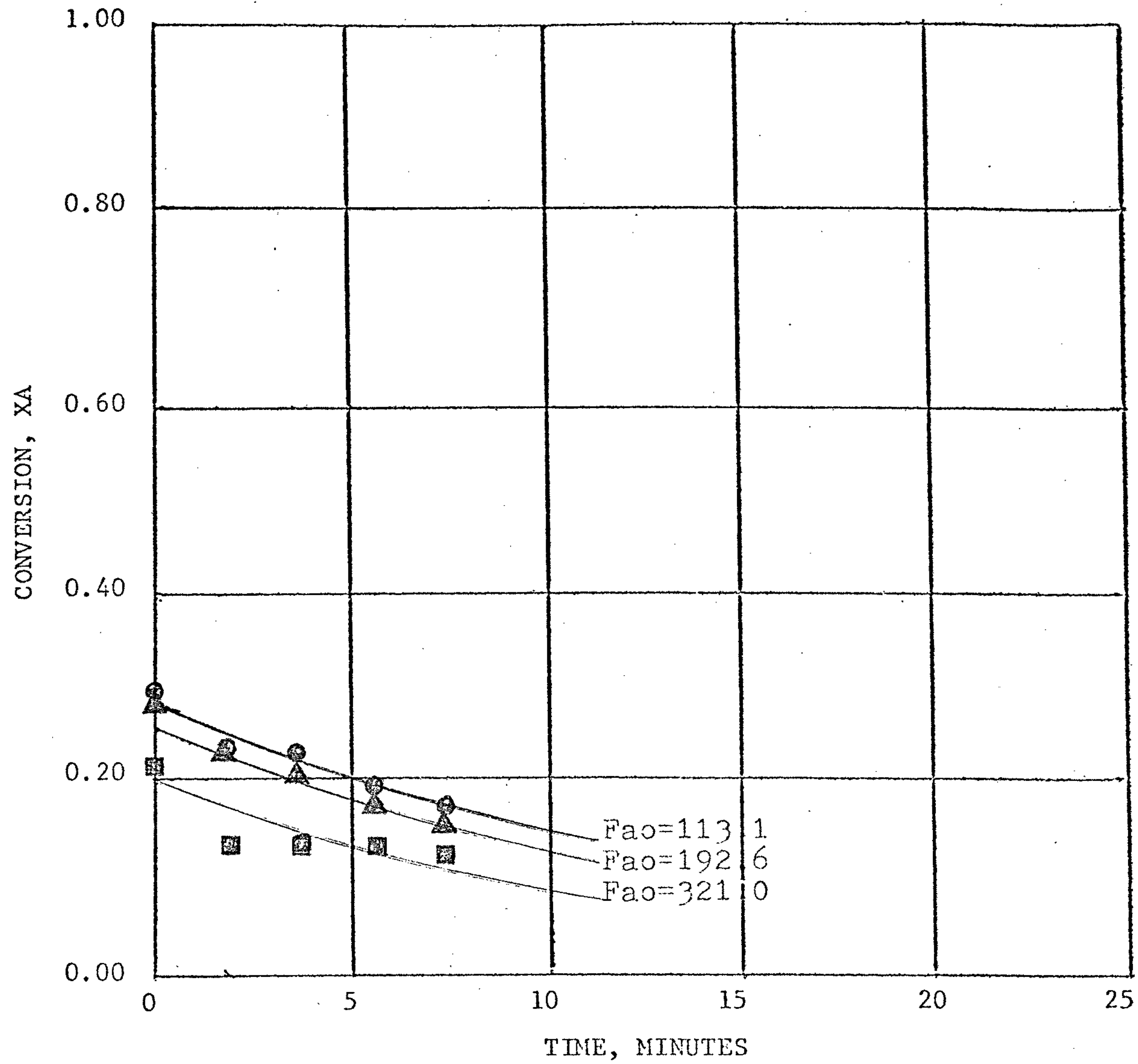
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0419	cm.
	TEMPERATURE	=	925	deg. F.
	ULTRASOUND	=	39,000	cycles/sec.
● Represents	W/FAO	=	11263	g.cat-sec/gmole
	FAO	=	135.2	gm./hr.
▲ Represents	W/Fao	=	6947	g.cat-sec/gmole
	Fao	=	219.3	gm./hr.
■ Represents	W/Fao	=	4782	g.cat-sec/gmole
	Fao	=	318.5	gm./hr.

FIGURE NO. 65

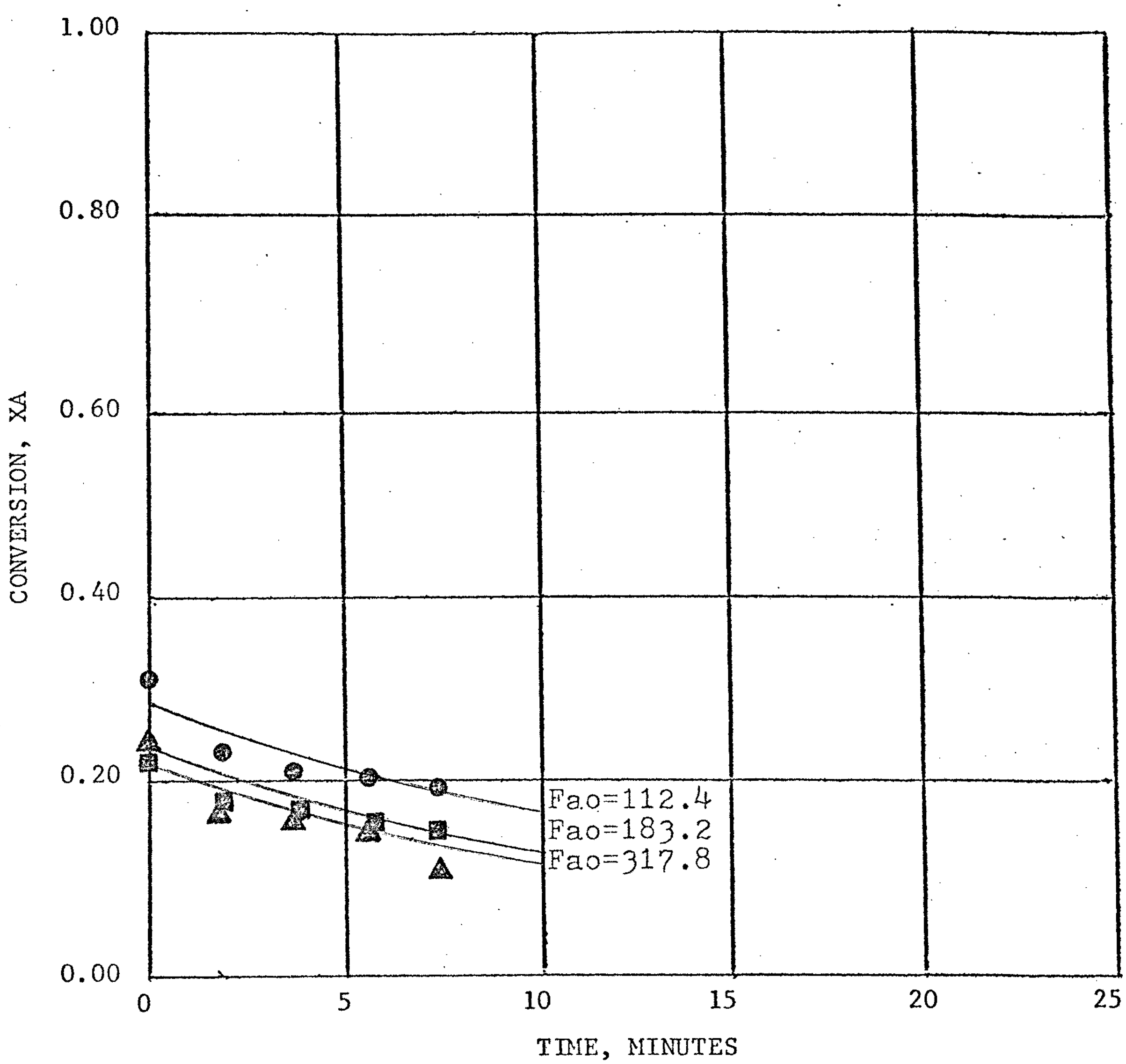
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0209	cm.
	TEMPERATURE	=	850	deg. F.
	ULTRASOUND	=	0	cycles/sec.
⊘ Represents	W/FAO	=	8034	g.cat-sec/gmole
	FAO	=	113.1	gm./hr.
▲ Represents	W/Fao	=	4719	g.cat-sec/gmole
	Fao	=	192.6	gm./hr.
▩ Represents	W/Fao	=	2831	g.cat-sec/gmole
	Fao	=	321.0	gm./hr.

FIGURE NO. 66

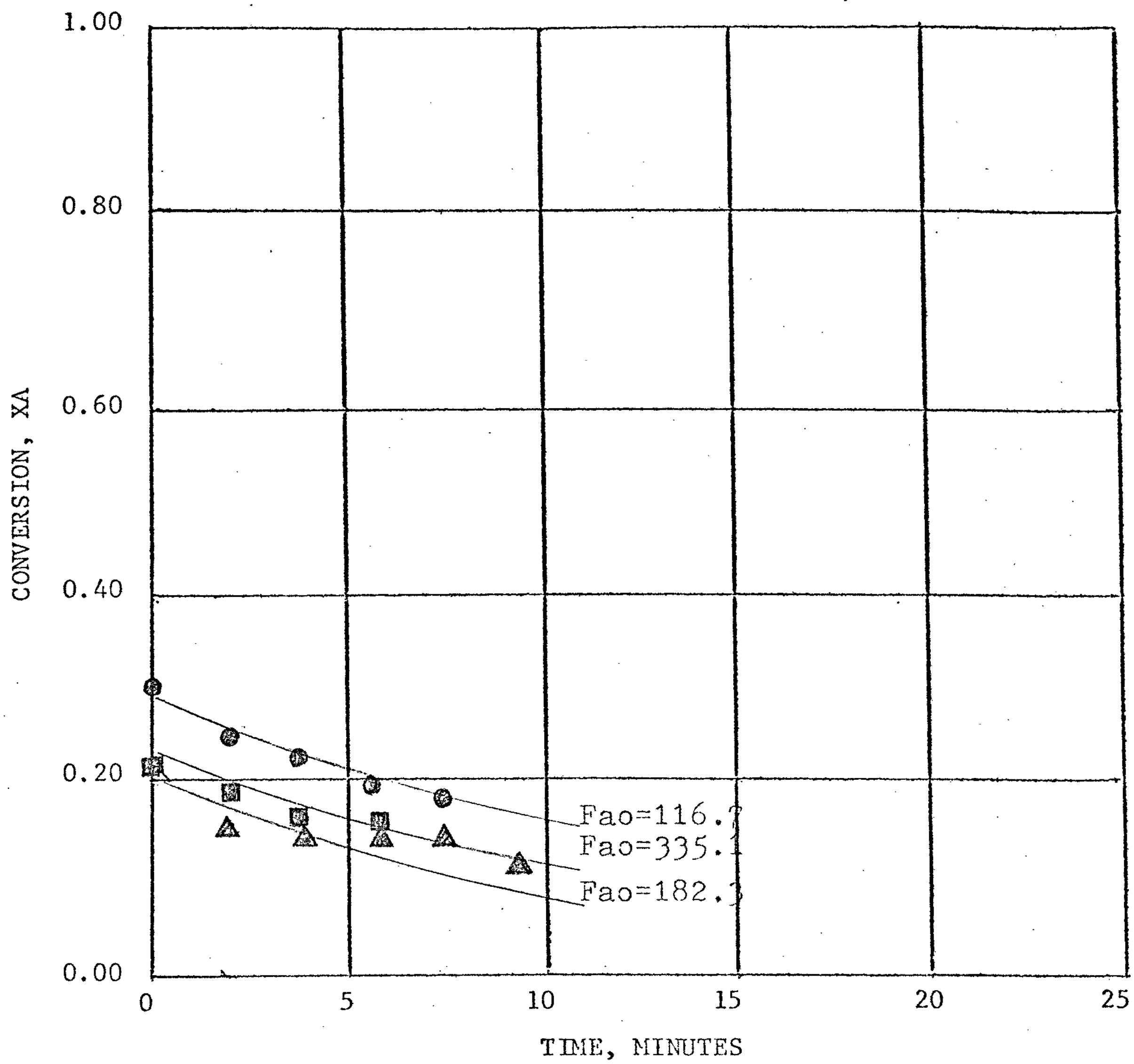
CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0209	cm.
	TEMPERATURE	=	850	deg. F.
	ULTRASOUND	=	26,000	cycles/sec.
● Represents	W/FAO	=	8087	g.cat-sec/gmole
	FAO	=	112.4	gm./hr.
▲ Represents	W/Fao	=	4961	g.cat-sec/gmole
	Fao	=	183.2	gm./hr.
■ Represents	W/Fao	=	2860	g.cat-sec/gmole
	Fao	=	317.8	gm./hr.

FIGURE NO. 67

CONVERSION, XA VERSUS TIME



	PARTICLE DIAMETER	=	0.0209	cm.
	TEMPERATURE	=	850	deg. F.
	ULTRASOUND	=	39,000	cycles/sec.
● Represents	W/FAO	=	7788	g.cat-sec/gmole
	FAO	=	116.7	gm./hr.
▲ Represents	W/Fao	=	4984	g.cat-sec/gmole
	Fao	=	182.3	gm./hr.
■ Represents	W/Fao	=	2712	g.cat-sec/gmole
	Fao	=	335.1	gm./hr.

TABLE NO. 31

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	850	deg. F.
Ultrasound	=	0	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	-----	0	-----	0	-----
2	.2774	2	-----	2	-----
4	.2532	4	.1470	4	.1075
6	.2371	6	.1384	6	.0886
8	.2305	8	.1210	8	.0858
10	.2211	10	.1097	10	.0680
		12	.1042	12	.0635
				14	.0464
				16	.0420
				18	.0493
				20	.0337

Fao	= 115.6	= 175.6	= 351.0
W/Fao	= 13730	= 9039	= 4518

A	= 0.28648	= 0.17777	= 0.13828
B	= -0.02738	= -0.04603	= -0.06841

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 32

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	850	deg. F.
Ultrasound	=	26,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	-----	0	-----	0	-----
.5	.3964	.5	-----	.5	-----
2	.3085	2	-----	2	.1375
4	.2519	4	.1772	4	.1253
6	.2389	6	.1444	6	.1234
8	.2320	8	.1144	8	.1070
10	.1993	10	.1125	10	.0901
12	.1863	12	.0964	12	.0657
14	.1716	14	-----	14	.0657
16	.1703			16	.0604
18	.1523			18	.0466
				20	.0540

Fao	= 130.5	= 156.0	= 268.0
W/Fao	= 12165	= 10166	= 5922
A	= 0.34055	= 0.22657	= 0.16306
B	= -0.04761	= -0.07336	= -0.06269

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 33

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	850	deg. F.
Ultrasound	=	39,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	-----	0	-----	0	-----
2	.2243	2	-----	2	.1264
4	.1653	4	.1710	4	.0874
6	.1589	6	.1297	6	.0506
8	.1745	8	.1224	8	.0483
10	.1566	10	.1190	10	.0473
12	.1442	12	.1129	12	.0511
14	.1365			14	.0349
				16	.0287
				18	.0319

Fao	= 120.9	= 198.8	= 281.7
W/Fao	= 13130	= 7982	= 5633

A	= 0.21121	= 0.18689	= 0.11171
B	= -0.03174	= -0.04582	= -0.07954

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 34

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	875	deg. F.
Ultrasound	=	0	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3548	0	.3470	0	-----
2	.3346	2	.3249	1	.2731
4	.3194	4	.3000	3	.2272
6	.2964	6	.2705	5	.1839
8	.2850	8	.2710	7	.1789
10	.2690	10	.2626	10	.1573
12	.2668	12	.2421	12	.1500
14	.2417	14	.2337	14	.1475
16	.2374	16	.2410	16	.1280
18	.2552	18	.2021	18	.1183
				20	.1204
Fao	= 98.2		= 171.0		= 350.5
W/Fao	= 16158		= 9242		= 4528
A	= 0.34453		= 0.33642		= 0.25014
B	= -0.02162		= -0.02597		= -0.04061

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 35

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	875	deg. F.
Ultrasound	=	26,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.2644	0	-----	0	-----
2	.3449	2	.4218	2	.2661
4	.2974	4	.3966	4	.2590
6	.2696	6	.3647	6	.2499
8	.2564	8	.3456	8	.2401
10	.2295	10	.3163	10	.2453
12	.2228	12	.3197	12	.2323
14	.2113	14	.2869	14	.2234
16	.2096	16	.2988	16	.2306
18	.1983	18	.2710	18	.2222
20	-----	20	.2925	20	.2313
Fao	= 217.2		= 127.2		= 357.8
W/Fao	= 7303		= 12465		= 4436
A	= 0.31104		= 0.42144		= 0.26487
B	= -0.02566		= -0.02274		= -0.00911

Above Coefficients Fit
Exponential Equation $X_a = Ae^{Bt}$

TABLE NO. 36

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	875	deg. F.
Ultrasound	=	39,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.5209	0	.4022	0	.3537
2	.4124	2	.3103	2	.3680
4	.3658	4	.2772	4	.3433
6	.3505	6	.2521	6	.3331
8	.3324	8	.2370	8	.3173
10	.3315	10	.2352	10	.3229
12	.3296	12	.2294	12	.3102
14	.3114	14	.2184	14	.3078
16	.3024	16	.2110	16	.2998
18	.2974	18	.2145	18	.3084
Fao =	131.0	=	224.8	=	369.1
W/Fao =	12129	=	7077	=	4302
A =	0.43849	=	0.33173	=	0.35752
B =	-0.02487	=	-0.02982	=	-0.01033

Above Coefficients Fit
Exponential Equation $X_a = Ae^{Bt}$

TABLE NO. 37

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	900	deg. F.
Ultrasound	=	0	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.4955	0	.2931	0	-----
2	.4689	2	.2891	2	.4055
4	.4467	4	.2686	4	.3260
6	.4443	6	.2681	6	.2992
8	.4282	8	.2716	8	.2839
10	.4359	10	.2765	10	.2905
12	.4241	12	.2660	12	.2833
14	.4257	14	.2720	14	.2860
16	.4903	16	.2744	16	.2914
18	.4050	18	.2551	18	.2858
20	-----	20	-----	20	.2888
Fao =	136.6	=	313.4	=	145.6
W/Fao =	11625	=	5068	=	10907
A =	0.47660	=	0.28511	=	0.34660
B =	-0.00948	=	-0.00472	=	-0.01246

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 38

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	900	deg. F.
Ultrasound	=	26,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3799	0	.3914	0	-----
2	.4119	2	.3304	2	-----
4	.3762	4	.3091	4	.2917
6	.4086	6	.2988	6	.2697
8	.3865	8	.3014	8	.2915
10	.3958	10	.3089	10	.2822
12	.3829	12	.2927	12	.2933
14	.3918	14	.2998	14	.2926
16	.3564	16	.3063	16	.2943
18	.3474	18	.3082	18	.2996
				20	.2964
				22	.3105
Fao	= 113.4	=	216.3	=	290.6
W/Fao	= 14000	=	7343	=	5464
A	= 0.40237	=	0.33919	=	0.27773
B	= -0.00541	=	-0.00870	=	-0.00360

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 39

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	900	deg. F.
Ultrasound	=	39,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3962	0	.2605	0	-----
2	.3847	2	.3268	2	-----
4	.3742	4	.3029	4	.2870
6	.3256	6	.2946	6	.2718
8	.3526	8	.3124	8	.2739
10	.3551	10	.3164	10	.2800
12	.3035	12	.3083	12	.2725
14	.3603	14	.3069	14	.2670
16	.3162	16	.3122	16	.2577
18	.3118	18	.3104	18	.2732
				20	.2532
				22	.2555
Fao	= 118.1		= 212.4		= 311.7
W/Fao	= 13449		= 7476		= 5096
A	= 0.3858		= 0.29181		= 0.28903
B	= -0.01188		= +0.00452		= -0.00553

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 40

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	925.	deg. F.
Ultrasound	=	0	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3370	0	-----	0	.3373
2	.3282	2	.3354	2	.2561
4	.3388	4	.3171	4	.2532
6	.3328	6	.3207	6	.2419
8	.3434	8	.2850	8	.2294
10	.3212	10	.3029	10	.2342
12	.3154	12	.2971	12	.2245
14	.3177	14	.2986	14	.2099
16	.2975	16	.2942	16	.2177
18	.3039	18	.3018	18	.2129
20	-----	20	.3071	20	-----

Fao	= 115.2	= 221.4	304.1
W/Fao	= 13789	= 7174	= 5222

A	= 0.34295	= 0.32082	= 0.28532
B	= -0.00657	= -0.00439	= -0.01945

Above Coefficients Fit
Exponential Equation $X_a = Ae^{Bt}$

TABLE NO. 41

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	925.	deg. F.
Ultrasound	=	26,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3128	0	.3494	0	-----
2	.3036	2	.3163	2	-----
4	.3025	4	.2915	4	.2343
6	.3195	6	.2797	6	.2276
8	.3184	8	.2827	8	.2260
10	.3022	10	.2794	10	.2201
12	.3017	12	.2688	12	.2275
14	.2228	14	.2710	14	.2216
		16	.2760		
		18	.2732		
Fao =	112.9	=	232.6	=	317.5
W/Fao =	14072	=	6829	=	5001
A =	0.32761	=	0.31813	=	0.23522
B =	-0.01436	=	-0.01110	=	-0.00438

Above Coefficients Fit
Exponential Equation $X_a = Ae^{Bt}$

TABLE NO. 42

CONVERSION VERSUS TIME

Particle Diameter	=	0.0841	cm.
Temperature	=	925.	deg. F.
Ultrasound	=	39,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversin	time	Conversion	time	Conversion
0	.3805	0	-----	0	-----
2	.3651	2	.2887	2	-----
4	.3552	4	.3072	4	.2344
6	.3447	6	.2945	6	.2156
8	.3397	8	.2887	8	.2200
10	.3392	10	.2697	10	.2219
12	.3337	12	.2681	12	.2219
14	.3227	14	.2373	14	.2140
16	.3168	16	.2471		
18	.3173	18	.2466		
		20	.2455		
Fao	= 101.9		257.9		309.8
W/Fao	= 15587		6157		5127
A	= 0.37209		= 0.31144		= 0.23169
B	= -0.00972		= -0.01354		= -0.00515

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 43

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	875.	deg. F.
Ultrasound	=	0	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	-----	0	-----	0	-----
2	.3303	2	.1992	2	.1482
4	.3572	4	.1817	4	.1308
6	.3367	6	.1724	6	.1324
8	.3427	8	.1713	8	.1242
10	.3320	10	.1729	10	.1297
12	.3364	12	.1762	12	.1234
14	.3310	14	.1810	14	.1318
16	.3191	16	.1716	16	.1181
18	.3975	18	.1757	18	.1303
20	.2664	20	.1645	20	.1292
Fao	= 95.6	=	213.0	=	331.7
W/Fao	= 16608	=	7156	=	4826
A	= 0.36334	=	0.18733	=	0.13718
B	= -0.01013	=	-0.00544	=	-0.00517

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 44

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	875.	deg. F.
Ultrasound	=	26,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.2937	0	-----	0	-----
2	.2468	2	.1724	2	.1291
4	.2870	4	.1486	4	.1196
6	.2886	6	.1432	6	.1157
8	.2805	8	.1621	8	.1144
10	.2630	10	.1402	10	.1164
12	.2682	12	.1608	12	.1230
14	.2606	14	.1582	14	.1161
16	.2536	16	.1621	16	.1190
18	.2591	18	.1487	18	.1168
20	------	20	.1428	20	.1097
Fao =	118.1	=	195.5	=	30[illegible].[illegible]
W/Fao =	13561	=	8191	=	5209
A =	0.28251	=	0.15882	=	0.12313
B =	-0.05166	=	-0.00305	=	-0.00405

Above Coefficients Fit
Exponential Equation $X_a = Ae^{Bt}$

TABLE NO. 45

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	875.	deg. F.
Ultrasound	=	39,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.2149	0	-----	0	-----
2	.2640	2	.1860	3	.1433
4	.2967	4	.1527	5	.1196
6	.1958	6	.1472	7	.1232
8	.2840	8	.1406	9	.1184
10	.2693	10	.1358	11	.1265
12	.2673	12	.1582	13	.1256
14	.2584	14	.1783	15	.1242
16	.2606	16	.1642	17	.1245
18	.2545	18	.1588	19	.1234
20	-----	20	.1749	21	.1265
Fao	= 109.9		= 210.9		= 300.8
W/Fao	= 14570		= 7590		= 5322
A	= 0.22888		= 0.15303		= 0.12866
B	= -0.01126		= -0.00343		= -0.00217

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 46

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	900.	deg. F.
Ultrasound	=	0	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	-----	0	-----	0	.4105
2	-----	2	.3130	2	.3183
4	.2266	4	.2816	4	.2799
6	.2306	6	.2734	6	.2767
8	.2190	8	.2722	8	.2803
10	.2429	10	.2651		
12	.2169	12	.2663		
14	.2197	14	.2576		
16	.2143	16	.2644		
18	.2126	18	.2581		
20	.2220	20	.2728		
2[illegible]	.2226				
Fao =	126.9	=	215.5	=	282.6
W/Fao =	12616	=	7429	=	5666
A =	0.23094	=	0.29251	=	0.37068
B =	-0.00284	=	-0.00659	=	-0.04515

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 47

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	900.	deg. F.
Ultrasound	=	26,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.1685	0	.3369	0	.3926
2	.2215	2	.2859	2	.3043
4	.2375	4	.2709	4	.2793
6	.2332	6	.2552	6	.2791
8	.2516	8	.2599	8	.2742
10	.2303	10	.2350		
12	.2397	12	.2712		
14	.2403	14	.2630		
16	.2222	16	.2669		
18	.2213	18	.2574		
Fao	= 116.4		= 220.9		= 302.5
W/Fao	= 13761		= 7148		= 5293
A	= 0.21043		= 0.29183		= 0.35587
B	= -0.00756		= -0.00900		= -0.04022

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 48

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	900.	deg. F.
Ultrasound	=	39,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
Time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3587	0	.3818	0	.3634
2	.3507	2	.2624	2	.2745
4	.3408	4	.2516	4	.2616
6	.3379	6	.2716	6	.2460
8	.3227	8	.2256	8	.2348
10	.3191	10	.2649		
12	.2925	12	.2729		
14	.2941	14	.2712		
16	.2995				
18	.2927				

Fao	= 111.9	= 259.5	= 359.4
W/Fao	= 14309	= 6169	= 4455
A	= 0.35798	= 0.29887	= 0.33192
B	= -0.01247	= -0.01327	= -0.04916

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 49

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	925.	deg. F.
Ultrasound	=	0	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3956	0	.3088	0	.1940
2	.3602	2	.4393	2	.1979
4	.3004	4	.1783	4	.2012
6	.3114	6	.4335	6	.1957
8	.2966	8	-----	8	.1836
10	.2705	10	-----	10	-----

Fao	= 117.1	= 256.6	= 321.2
W/Fao	= 13675	= 5936	= 4742
A	= 0.38961	= 0.31463	= 0.19916
B	= -0.03632	= -0.00574	= -0.00607

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 50

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	925	deg. F.
Ultrasound	=	26,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	-----	0	.3630	0	------
2	.3695	2	.3401	2	.1558
4	.4747	4	.3039	4	.1673
6	.4671	6	.3006	6	.1706
8	.4604	8	.2388	8	.1799
10	.3755	10	-----	10	.1637

Fao	= 100.8	= 241.7	= 308.8
W/Fao	= 15177	= 6303	= 4932

A	= 0.42660	= 0.37113	= 0.15888
B	= -0.00008	= -0.04805	= -0.00858

Above Coefficients Fit
Exponential Equation $X_a = Ae^{Bt}$

TABLE NO. 51

CONVERSION VERSUS TIME

Particle Diameter	=	0.0419	cm.
Temperature	=	925.	deg. F.
Ultrasound	=	39,000	cycles/sec.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
1	.4312	0	.2457	0	.0970
3	.5170	2	.2526	2	.1945
5	.5180	4	.2573	4	.1776
7	.5206	6	.2458	6	.1783
9	.5137	8	.2432	8	.1670

Fao	= 135.[illegible]	= 219.3	= 318.5
W/Fao	= 11863	= 6947	= 4782

A	0.456220	= 0.25125	= 0.12971
B	+0.017853	= -0.00239	= +0.04980

Above Coefficients Fit
Exponential Equation $X_a = Ae^{Bt}$

TABLE NO. 52

CONVERSION VERSUS TIME

Particle Diameter	=	0.0209	cm.
Temperature	=	850.	deg. F.
Ultrasound	=	0	cycles/sec.
Feed Rate	=	Fao	gms/hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3001	0	.2839	0	.2169
2	.2341	2	.2327	2	.1356
4	.2231	4	.1952	4	.1324
6	.1948	6	.1733	6	.1308
8	.1617	8	.1613	8	.1185

Fao	= 113.1	= 192.6	= 321.0
W/Fao	= 803[illegible]	= 4719	= 2831

A	= 0.28979	= 0.18378	= 0.27239
B	= -0.07103	= -0.06225	= -0.071275

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 53

CONVERSION VERSUS TIME

Particle Diameter	=	0.0209	cm.
Temperature	=	850.	deg. F.
Ultrasound	=	26000.	cycles/sec.
Feed Rate	=	Fao	gms/hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3172	0	.2314	0	.2231
2	.2323	2	.1674	2	.1620
4	.2186	4	.1563	4	.1526
6	.2010	6	.1384	6	.1592
8	.1895	8	.0968	8	.1472

Fao	= 112.4	= 183.2	= 317.8
W/Fao	= 8057	= 4961	= 2860
A	= 0.28316	= 0.22374	= 0.19771
B	= -0.058751	= -0.09666	= -0.04245

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

TABLE NO. 54

CONVERSION VERSUS TIME

Particle Diameter	=	0.0209	cm.
Temperature	=	850.	deg. F.
Ultrasound	=	39,000	cycles/se.
Feed Rate	=	Fao	gms./hr.
Space Velocity	=	W/Fao	gm.cat.-sec./gmole
time	=	t	minutes

time	Conversion	time	Conversion	time	Conversion
0	.3034	0	-----	0	.2080
2	.2557	2	.1437	2	.1890
4	.2297	4	.1475	4	.1667
6	.1893	6	.1439	6	.1558
8	.1774	8	.1383	8	-----
10	-----	10	.1114	10	-----

Fao	= 116.7	= 182.3	= 335.1
W/Fao	= 7788	= 498[illegible]	= 2712
A	0.29872	= 0.16136	= 0.20745
B	= -0.06890	= -0.02858	= -0.04962

Above Coefficients Fit
Exponential Equation $Xa = Ae^{Bt}$

APPENDIX VII

CARBON OXYGEN REACTION

THE CARBON-OXYGEN REACTION

During several of the initial runs in this study, a problem was encountered with carbonization of the cumene at reaction temperatures of 1000°F. and subsequent plugging of the reactor and fouling of the catalyst. Carbonization was sometime so severe that it was often very difficult to remove the preheater from the reactor to clean it.

This problem was solved by purging the reactor with air at reaction temperature for 12 hours after each run to burn off the carbon.

The Carbon-Oxygen Reaction Rate Equation

For the reaction

$$C + O_2 \qquad CO_2$$
$$B(S) + A(g) \qquad \text{gaseous product,}$$

Parker and Hottell have shown that the rate equation for surface reaction controlling is as follows:

$$-r_B = \frac{4.32 \times 10^{14} C_{Ag}}{T^{\frac{1}{2}}} e^{\frac{-44.000}{RT}}$$

$$r_B = \frac{\text{gm.moles carbon reacted}}{\text{sec-cm}^2}$$

$T = {}^{\circ}K.$

C_{Ag} = concentration of oxygen, $\frac{\text{gm-moles}}{\text{cm}^3}$

$R = 1.98 \frac{\text{cal}}{\text{gm mole-}^{\circ}K}$

Calculation of Rate Constant, k_s

$$k_s = \frac{4.32 \times 10^{14}}{T^{\frac{1}{2}}} e^{-\frac{44,000}{RT}}$$

k_s = rate constant, $\frac{cm}{sec}$

$T^{\frac{1}{2}} = (850^oF.)^{\frac{1}{2}} = (727^oK)^{\frac{1}{2}} = 27^oK^{\frac{1}{2}}$

$$k_s = \frac{4.32 \times 10^{14}}{27} e^{-\frac{44,000 \frac{cal}{gm\ mole}}{(1.98 \frac{cal}{gm\ mole\text{-}^oK})(727^oK)}}$$

$$= 0.1598 \times 10^{14}\ e^{-30.6}$$

$$= (0.1598 \times 10^{14})(5.137 \times 10^{-14}) = 0.821 \frac{cm}{sec}$$

Calculation of Oxygen Concentration, C_{A_g}

$$C_{A_g} = \frac{(1.0\ amt.)\ (0.21)}{(0.0821 \frac{liter\text{-}atm.}{gm\ mole\text{-}^oK})(727^oK)(1000 \frac{cm^3}{liter})}$$

$$= 3.52 \times 10^{-6} \frac{gm\text{-}moles}{cm^3}$$

Calculation of Reaction Rate

$$-r_B = k_s C_{A_g} = (0.821 \frac{cm}{sec})(3.52 \times 10^{-6} \frac{gm\text{-}moles}{cm^3})$$

$$= 2.89 \times 10^{-6} \frac{gm\text{-}moles}{cm^2\text{-}sec}$$

Calculation of Maximum Weight of Carbon

Assume 5% carbonization at a feed rate of 600 gms/hr. cumene for 30 minutes.

$$\text{gms. carbon} = \frac{(600\ \frac{\text{gms}}{\text{hr}})(0.05)(0.5\ \text{hrs.})(12.011\ \frac{\text{gms}}{\text{gm mole}})}{(120.12\ \frac{\text{gms}}{\text{gm mole}})}$$

$$= 1.5\ \text{gms. carbon}$$

Calculation of Available Surface Area

Reactor

$$S_R = \frac{(0.767\ \text{in})(20.5\ \text{in})}{(2.54\ \frac{\text{cm}}{\text{in}})^2} = 3.26\ \text{cm}^2$$

Preheater

$$S_P = \frac{(0.767\ \text{in})(20.5\ \text{in})}{(2.54\ \frac{\text{cm}}{\text{in}})^2} = 7.66\ \text{cm}^2$$

Catalyst

$$S_C = (13.1\ \frac{\text{cm}^2}{\text{gm}}\ \_(5.748\ \text{gms}) = 75.30\ \text{cm}^2$$

Total area = 86.22 cm^2

Required Reaction Time

$$t = \frac{(1.5\ \text{gms})}{(12.011\ \frac{\text{gms}}{\text{gm-mole}})\ (2.89\text{x}10^{-6}\frac{\text{gmmoles}}{\text{cm}^2\text{-sec}})(60\frac{\text{sec}}{\text{min}})(86.22\ \text{cm}^2)}$$

$$= 8.4\ \text{min}$$

APPENDIX VIII

EFFECTIVENESS FACTOR CALCULATIONS

Method 1 for determining the effectiveness factor uses equation 15.

$$\epsilon = \frac{3}{h_s}\left[\frac{1}{\tanh h_s} - \frac{1}{h_s}\right] \qquad (15)$$

where h_s is the thiele modulus and is defined as:

$$h_s = r_p\left[\frac{S_V k'_s}{D_e}\right]^{\frac{1}{2}} \qquad (14)$$

the surface reaction rate constant k'_s is determined by equation 13.

$$k'_s = \frac{\epsilon L k_2 K_A \pi}{(1 + K_A \pi) C_{A_o} S_g} \qquad (13)$$

Tables 55 through 58 contain the results from performing the above calculations for three temperatures and three ultrasounds. Figures 68 through 70 are the results plotted as Log ϵ versus Log h_s.

TABLE NO. 56

EFFECTIVENESS FACTORS AT VARIOUS PARTICLE DIAMETERS

Ultrasound = 0 cps

Temperature = 925 deg. F.

Diameter cm.	$Lk_2 \times 10^4$	$k_s \times 10^6$	h_s	tanh h_s	
.0032	4.6044	7.9783	.352	.3377	.992
.0209	3.0511	5.2174	1.857	.9524	.826
.0419	2.4551	4.1983	3.338	.9975	.632
.0841	1.8554	3.1727	5.825	1.0000	.427
.2000	1.1152	1.9070	10.740	1.0000	.253
.3580	.6352	1.0861	14.509	1.0000	.192

Temperature = 875 deg. F.

.0032	1.4973	2.5050	.199	.1964	.997
.0209	1.2018	2.1007	1.165	.8226	.920
.0419	1.0772	1.8022	2.2105	.9762	.776
.0841	.9376	1.5686	4.1394	.9995	.550
.2000	.7331	1.2265	8.7050	1.0000	.305
.358	.5727	.9409	13.647	1.0000	.204

Temperature = 850 deg. F.

.0032	.7635	1.2502	.141	.1402	.999
.0209	.7151	1.1748	.894	.7132	.950
.0419	.6919	1.1368	1.762	.9428	.840
.0841	.6640	1.0909	3.465	.9980	.618
.2000	.6178	1.0159	7.949	1.0000	.330
.358	.5727	.9740	13.936	1.0000	.200

TABLE NO. 56

EFFECTIVENESS FACTORS VERSUS PARTICLE DIAMETERS

Ultrasound = 39,000 cps

Temperature = 925 deg. F.

Diameter cm.	$Lk_2 \times 10^4$	$k_s \times 10^6$	h_s	tanh h_s	
.0032	3.9364	6.7313	.322	.3121	.993
,0209	2.6680	4.5623	1.736	.9400	.843
.0419	2.1863	3.7386	3.150	.9963	.653
.0841	1.6928	2.8947	5.564	.9999	.442
.2000	1.0655	1.8220	10.498	1.0000	.259
.358	.6405	1.0952	14.570	1.0000	.192

Temperature = 875 deg. F.

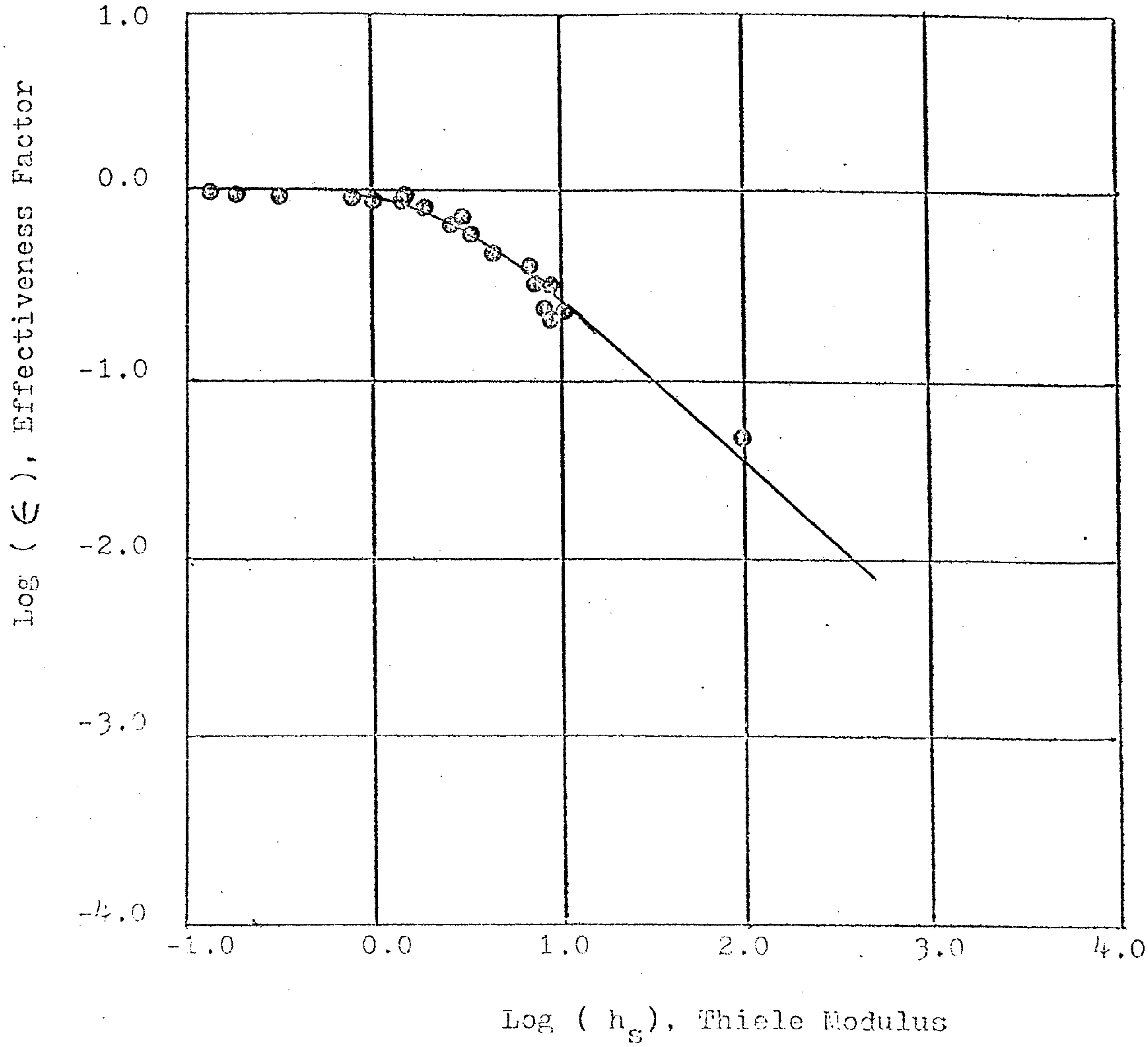
.0032	1.1698	1.9571	.176	.1742	.998
.0209	1.0255	1.7157	1.076	.7916	.930
.0419	.9608	1.6075	2.088	.9697	.793
.0841	.8851	1.4808	4.022	.9994	.561
.2000	.7661	1.2817	8.898	1.0000	.299
.358	.6214	1.0396	12.345	1.0000	.195

Temperature = 850 deg. F.

.0032	.6691	1.0993	.132	.1316	.999
.0209	.6149	1.0088	.828	.6795	.957
.0419	.6112	1.0207	1.670	.9316	.853
.0841	.6304	1.0357	3.377	.9977	.627
.2000	.6221	1.0222	7.977	1.0000	.329
.358	.6637	1.0905	14.749	1.0000	.190

FIGURE NO. 68

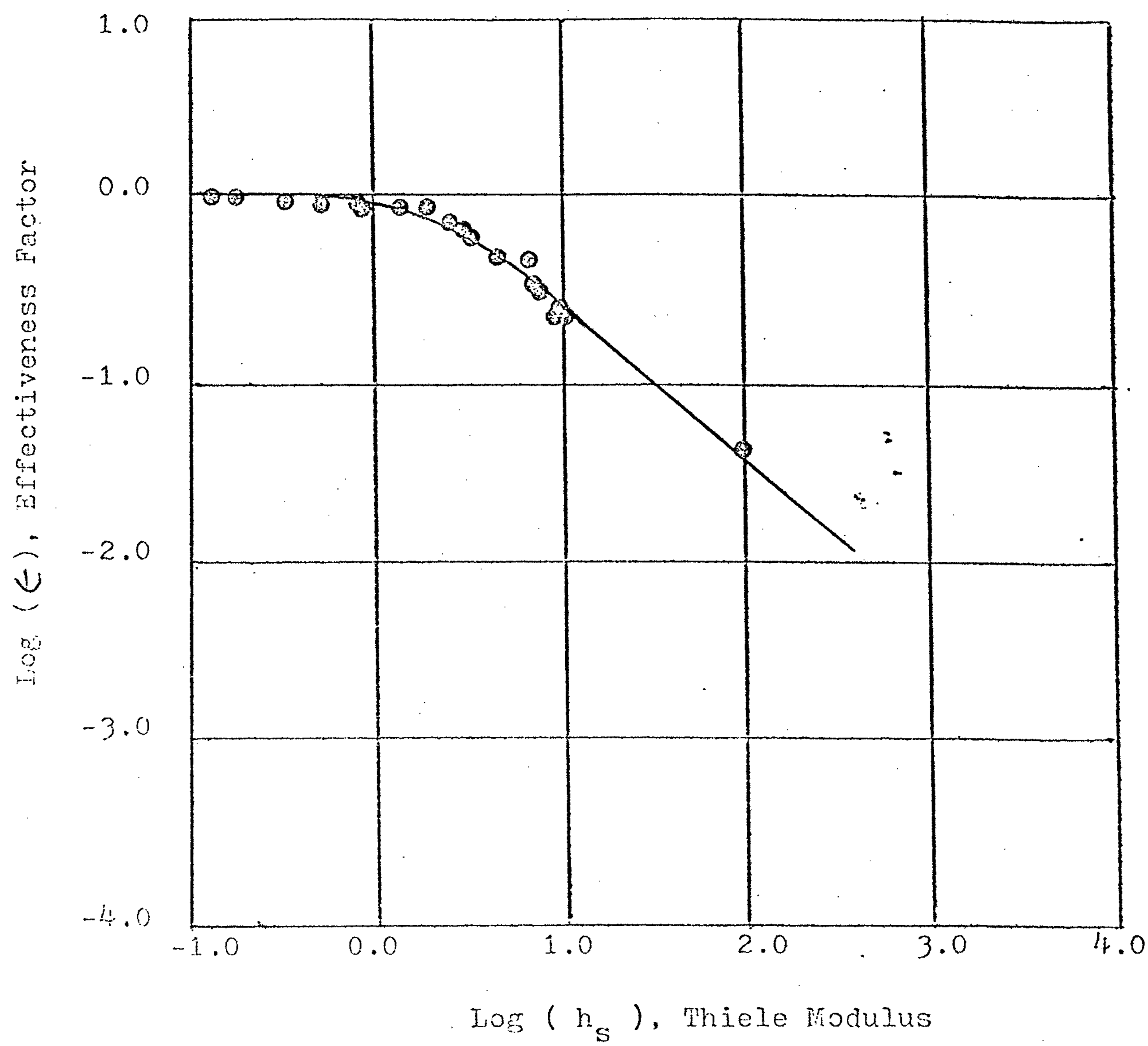
EFFECTIVENESS FACTOR VERSUS THIELE MODULUS



Ultrasound = 0 cps

FIGURE NO. 69

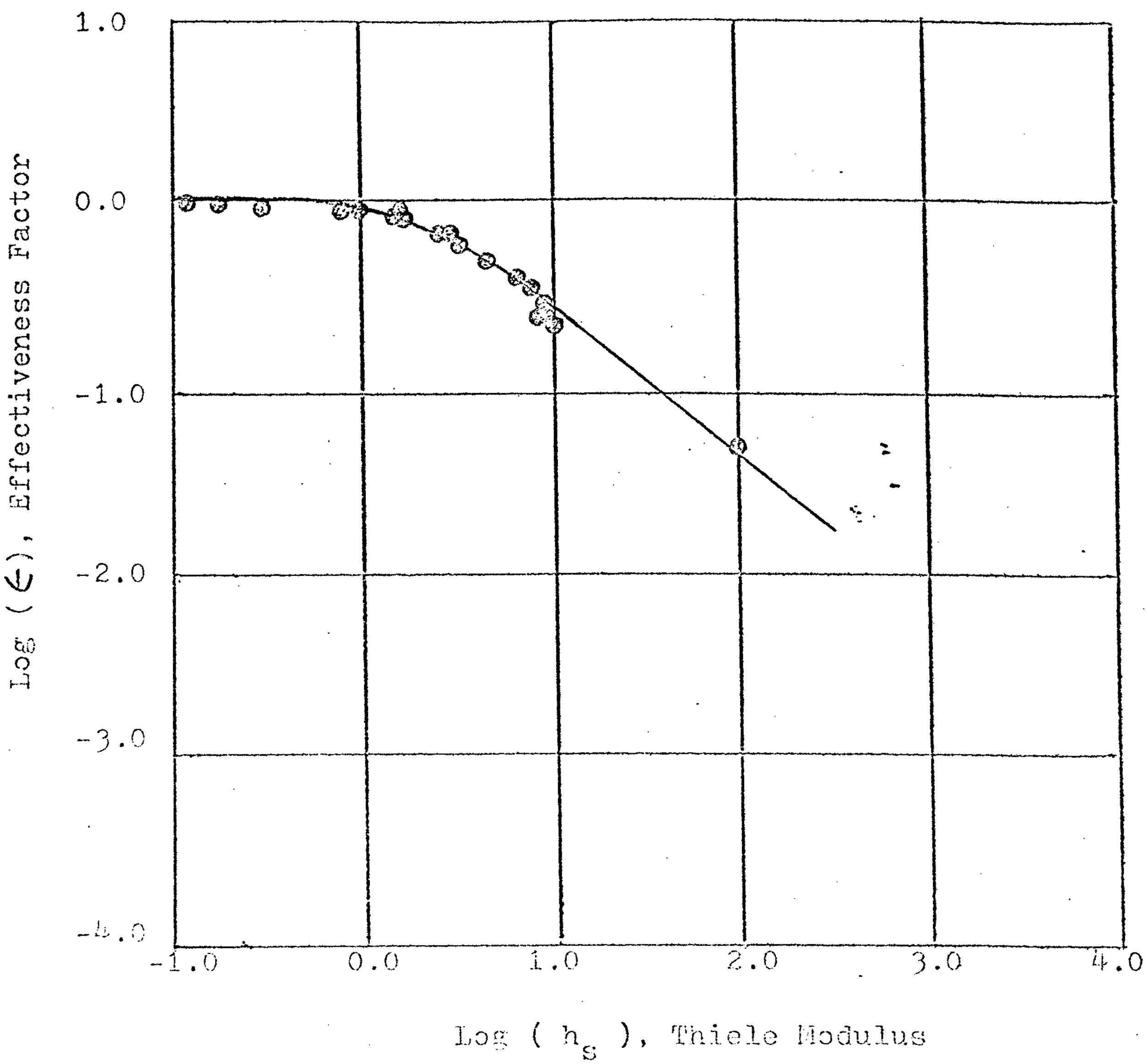
EFFECTIVENESS FACTOR VERSUS THIELE MODULUS



Ultrasound = 26,000 cps

FIGURE NO. 70

EFFECTIVENESS FACTOR VERSUS THIELE MODULUS



Ultrasound = 39,000 cps

TABLE NO. 57

EFFECTIVENESS FACTORS VERSUS PARTICLE DIAMETERS

Ultrasound = 26,000 cps

Temperature = 925 deg. F.

Diameter cm.	$Lk_2 \times 10^4$	$k_s \times 10^6$	h_s	$\tanh h_s$	
.0032	4.0039	6.8466	.326	.3146	.993
.0209	2.7154	4.6433	1.751	.9415	.841
.0419	2.2190	3.7946	3.174	.9960	.651
.0841	1.7118	2.9273	5.596	.9999	.440
.2000	1.0701	1.8298	10.521	1.0000	.258
.358	.6381	1.0911	14.542	1.0000	.192

Temperature = 875 deg. F.

.0032	1.2659	2.1179	.183	.1810	.998
.0209	1.0748	1.7982	1.101	.8010	.927
.0419	.8798	1.4720	1.998	.9639	.806
.0841	.7463	1.2486	4.042	.9994	.559
.2000	.6157	1.0300	8.782	1.0000	.303
.358	.6157	1.0300	14.279	1.0000	.195

Temperature = 850 deg. F.

.0032	.6691	1.0994	.132	.1316	.999
.0209	.6613	1.0865	.859	.6960	.954
.0419	.6520	1.0713	1.711	.9368	.847
.0841	.6406	1.0525	3.403	.9978	.624
.2000	.6212	1.0206	7.971	1.0000	.329
.358	.6015	.9883	14.041	1.0000	.198

Method 2 (Corrigan, 1953) for determining the effectiveness factor is based on the assumption that at constant conversion, pressure, and temperature the reactor design equation reduces to equation

$$W/Fao = (1/\epsilon)\, C$$

For the same conditions listed above but for different catalyst sizes the equation reduces to:

$$\frac{(W/Fao)_1}{(W/Fao)_2} = \frac{C/\epsilon_1}{C/\epsilon_2}$$

Obtain enough data from the the above steps to plot as W/Fao versus particle diameter, d_p, at constant conversion amd extrapolate to $d_p = 0$. Divide all W/Fao values by this extrapolated value to determine the values of ϵ as shown in equation .

If we assume that only the outside surface of the catalyst is effective them:

$$\epsilon = C_2 \alpha$$

from which it can be shown that

$$d_p = C_3 (1/\epsilon)$$

A plot of d_p versus 1/ should yield a straight line if this assumption is true. Table 55 contains the calculated results from Method 2.

TABLE NO. 55

EFFECTIVENESS FACTORS VERSUS PARTICLE DIAMETERS

Temperature = 925 deg. F.

Diameter cm.	0	26,000	39,000
.0032	.960	.972	.984
.0209	.785	.842	.902
.0419	.645	.727	.821
.0841	.475	.571	.696
.2000	.276	.358	.490
.3580	.175	.238	.349

Temperature = 875 deg. F.

.0032	.991	.989	.907
.0209	.942	.931	.600
.0419	.890	.871	.428
.0841	.800	.770	.272
.2000	.628	.585	.135
.358	.486	.440	.081

Temperature = 850 deg. F.

.0032	.995	.993	.998
.0209	.974	.977	.986
.0419	.951	.958	.973
.0841	.907	.932	.947
.2000	.806	.835	.883
.358	.700	.741	.803

APPENDIX IX

COMPUTER PROGRAMS

```
C       PROGRAM PLOT
C
        DIMENSION T(30),Y(30)
        DIMENSION A(3)
        NP=9
        N=21
        DO 1000 I=1,N
        READ 5000,TEMP,SIZE,US,FAO
C       TEMP = TEMPERATURE IN DEG. F.
C       SIZE = PARTICLE SIZE OF CATALYST IN TYLER NO.
C       US = ULTRASOUND IN CPS.
C       FAO = FLOW RATE IN GRAMS/HOUR.
  5000  FORMAT(4F10.2)
        READ 2000,(A(JJ),JJ=1,3)
  2000  FORMAT(2F10.5)
        A(1)=A(1)*1.E-02
        A(2)=A(2)*1.E-04
        A(3)=A(3)*1.E-08
C       A(I) = COEFFICIENTS OF XA VS. W/FAO POLYNOMIAL.
        TT=0.
        PRINT 2040
  2040  FORMAT('1')
        DO 4000 K=1,NP
        T(K)=TT
        Y(K)=A(1)+A(2)*TT+A(3)*TT**2.
  8000  FORMAT(I5,F10.0,E17.7)
        TT=TT+3000.
  4000  CONTINUE
        DO 3000J=1,NP
        PRINT 8000, J,T(J),Y(J)
  3000  CONTINUE
        CALL XYPLOT(NP,T,Y)
        PRINT 5100,TEMP,SIZE,US,FAO
  5100  FORMAT(//,15X,'PLOT OF CONVERSION VERSUS W/FAO',
       Z/,15X,'FOR TEMPERATURE =',F10.0,/,15X,'FOR PARTICLE',
       Z'SIZE =',F9.0,/,15X,'FOR ULTRASOUND =',F11.0,
       Z/,15X,'FOR FLOW RATE OF',F12.1)
  1000  CONTINUE
        STOP
        END
```

```
C      PROGRAM CUMENE
C
       REAL*4 KA,K,KR,KG(100),KS(100)
       REAL*4 XA(100),ELK2(100),AA(3),WFAO(100)
       MM=25
       A=13.1
       PIE=1.
       DO 1000 KK=1,MM
       WW=0.
       READ 1,TEMPE,(AA(I),I=1,3)
C      TEMPE = TEMPERATURE IN DEG. F.
1      FORMAT(4F10.5)
       READ,M
C       M = NO. OF ITTERATIONS FOR CALCULATING W/FAO.
       PRINT 400
       AA(1)=AA(1)*1.E-02
       AA(2)=AA(2)*1.E-04
       AA(3)=AA(3)*1.E-08
C      AA(I) = COEFFICIENTS OF XA VERSUS W/FAO POLY.
       AUG=0.
       DO 101 I=1,M
       WW=WW+1000.
       WFAO(I)=WW
       XA(I)=WFAO(I)**2.*AA(3)+WFAO(I)*AA(2)+AA(1)
       T=TEMPE+460.
       K =10.**(7.126-8927./T)
       KA=10.**(700./T-.179)
       KR=10.**(2195/T-1.286)
       GAMMA2=( 1./(KA*PIE) +1. )/WFAO(I)
       BETA2= ( 2./(KA*PIE) + KR/KA ) /WFAO(I)
       DELTA = SQRT( 1. + PIE/K )
       D2= DELTA*DELTA
       D3 = D2*DELTA
       RATIO = ALOG( (1.+XA(I)*DELTA) / (1.-XA(I)*DELTA) )
       ELK2(I)=GAMMA2*((1./(2.*DELTA) -1./(D3*2.)) *
      ZRATIO + XA(I)/D2) + BETA2*(1./(2.*D3)*RATIO -
      Z1./(2.*D2)*ALOG(1. -D2*XA(I)*XA(I)-XA(I)/D2))
       KS(I)=(ELK2(I)*T*82.03)/(1.8*A)
       KS(I)=1./KS(I)
       XAO=(1.-XA(I))/(1.+XA(I))
       YALM=(1.-XAO)/ALOG(1./XAO)
       KG(I)=(6.26*T*XA(I))/(WFAO(I)*1.8*ALOG(1.+YALM))
       KG(I)=1./KG(I)
400    FORMAT(5X,'W/FAO             CONVERSION      KINETIC RATE CO
NSTANT')
       PRINT 4,I,WFAO(I),XA(I),ELK2(I)
101    CONTINUE
300    FORMAT(5X,'INTRINSIC RATE CONSTANT    MASS TRANSFER COEF
FICIENT')
       DO 102 I=1,M
3      FORMAT(I5,2F15.5)
4      FORMAT(I5,F15.0,F10.5,E20.7)
       AUG=AUG+ELK2(I)
102    CONTINUE
       AUG=AUG/M
       PRINT 4001,AUG
4001   FORMAT(/,' THE AVERAGE VALUE FOR ELK2 =',E20.7)
1000   CONTINUE
```

NOMENCLATURE

A = reference to cumene

A = area, cm^2

a = superficial surface area of catalyst, $\frac{cm^2}{gm}$

a = transverse acceleration, $\frac{cm}{sec^2}$

C = total concentration of A + R + S, $\frac{gm\text{-}moles}{cm^3}$

C_A = concentration of cumene, $\frac{gm\text{-}moles}{cm^3}$

C_{Ae} = equilibrium concentration of benzene, $\frac{gm\text{-}moles}{cm^3}$

C_{Al} = concentration of active sites occupied by A, $\frac{cm^2}{gm\text{-}cat}$

C_{A_s} = concentration of cumene on catalyst surface, $\frac{gm\text{-}moles}{cm^3}$

C_L = total concentration of available active sites, $\frac{cm^2}{gm\ cat}$

C_l = concentration of unoccupied active sites, $\frac{cm^2}{gm\ cat}$

C_p = heat capacity of gas at constant pressure, $\frac{cal}{gm\text{-}^\circ C.}$

C_R = concentration of benzene, $\frac{gm\text{-}moles}{cm^3}$

CR_e = equilibrium concentration of benzene, $\frac{gm\ moles}{cm^3}$

C_{Rl} = concentration of active sites occupied by R, $\frac{cm^2}{gm\ cat}$

C_S = concentration of propylene, $\frac{gm\text{-}moles}{cm^3}$

C_{Sl} = concentration of active sites occupied by S, $\frac{cm^2}{gm\ cat}$

C_V = heat capacity of gas at constant volume, $\frac{cal}{gm\text{-}^\circ C.}$

D_{AB} = diffusivity of A in A + R + S, $\frac{cm^2}{sec}$

D_{AR} = diffusivity of cumene in benzene, $\frac{cm^2}{sec}$

D_{AS} = diffusivity of cumene in propylene, $\frac{cm^2}{sec}$

D_e = effective pore diffusivity, $\frac{cm^2}{sec}$

D_K = Knudsen diffusivity, $\frac{cm^2}{sec}$

D_s = combined diffusivity, $\frac{cm^2}{sec}$

d = average diameter of catalyst pore, cm

d_p = diameter of catalyst particle, cm.

E = activation energy, $\frac{gm\ cal}{gm\text{-}mole}$

F = feed rate, $\frac{gms}{hr}$

F = force, dynes

F_{AO} = initial cumene feed rate, $\frac{gm\text{-}moles}{hr.}$ or $\frac{gm\text{-}moles}{sec.}$

f = frequency, $\frac{cycles}{sec.}$

G = superficial mass velocity of gas normal to catalyst bed, $\frac{gms}{cm^2\text{-}sec}$

g_C = conversion factor, 980 $\frac{dynes}{gm.}$

h_S = Thiele modulus = $mr_p = r_p \left(\frac{k_s S_V}{D_e}\right)^{\frac{1}{2}}$, dimensionless

I = intensity, $\frac{erg}{cm^2\text{-}sec}$, $\frac{dyne\text{-}cm.}{cm^2\text{-}sec}$ $\left(10^{-7}\ \frac{watt\text{-}sec}{erg}\right)$

I_o = $10^{-16}\ \frac{watts}{cm^2}$

K = equilibrium constant for overall reaction, atm.

K_2 = equilibrium constant for surface reaction, atm.

K_3 = equilibrium desorption constant for R, atm.

K_A = equilibrium adsorption constant for A, $\frac{1}{atm.}$

K_R = equilibrium adsorption constant for R, $\frac{1}{atm.}$

k = forward reaction rate constant for overall reaction,

$\frac{\text{gm moles}}{\text{gm cat-atm-sec}}$

k = compressibility, $\frac{cm^2}{dyne}$, $\frac{cm\text{-}sec^2}{gm}$ (dyne = $\frac{gm\text{-}cm}{sec^2}$)

k' = reverse reaction rate constant for overall reaction,

$\frac{\text{gm moles}}{\text{gm cat-atm}^2\text{-sec}}$

k_0 = constant, $\frac{cm}{sec}$

k_1 = rate constant for adsorption of A, $\frac{\text{gm moles}}{cm^2\text{- atm-sec}}$

k'_1 = rate constant for desorption of A, $\frac{\text{gm moles}}{cm^2\text{-sec}}$

k_2 = forward reaction rate constant for surface reaction, $\frac{\text{gm moles}}{cm^2\text{-sec}}$

k'_2 = reverse reaction rate constant for surface reaction, $\frac{\text{gm moles}}{cm^2\text{-atm-sec}}$

k_3 = equilibrium desorption constant for R, atm.

k'_3 = rate constant for adsorption of R, $\frac{\text{gm moles}}{cm^2\text{-atm-sec}}$

k_g = $\frac{DAB}{\delta}$, mass transfer coefficient, $\frac{cm}{sec}$

k_p = pseudo first order forward reaction rate constant, $\frac{cm^3}{\text{gm cat-sec}}$

k'_p = pseudo first order reverse reaction rate ~~xx~~ constant, $\frac{cm^3}{\text{gm cat-sec}}$

k_s = forward intrinsic rate constant for surface reaction, $\frac{cm}{sec}$

k'_s = reverse intrinsic rate constant for surface reaction, $\frac{cm^4}{gm\ mole-sec}$

L = reactor length, cm/

L = total concentration of active sites, $\frac{cm^2}{gm\ cat}$

l = unoccupied active catalyst site, dimensionless

M = molecular weight, $\frac{gms}{gm\ mole}$

m = mass, gms.

N_A = number ofmoles of A, gm moles

N_{A_O} = initial number of moles of A, gm moles

N_{Af} = final number of moles of A, gm moles

N_{A_z} = rate of mass transfer of A in z direction, $\frac{gm-moles}{cm^2-sec}$

N_{B_z} = rate of mass transfer of R + S in z direction, $\frac{gm-moles}{cm^2-sec}$

N_T = total number of moles, gm-moles

n = 1,3,5,7,9, etc.

P = vapor pressure, mm. Hg

p = partial pressure, atm

p = pressure, $\frac{dynes}{cm^2}$

PC = critical pressure, atm.

p_{max} = maximum pressure caused by sound wave, $\frac{dynes}{cm^2}$

p_T = total pressure, atm.

R = ideal gas constant, 82.06 $\frac{cm^3-atm}{gm\ mole-{}^oK}$.

R = referene to benzene

R = ideal gas constant, 1.987 $\frac{\text{gm-cal}}{\text{gm mole-}^\circ\text{K}}$

R = 8.31×10^7 $\frac{\text{ergs}}{\text{gm mole-K}}$, $\frac{\text{dyne-cm.}}{\text{gm mole-K}}$

(erg = dyne-cm = $\frac{\text{gm-cm}^2}{\text{sec}^2}$)

R_e = Reynold's number, dimensionless

R_g = ideal gas constant, 8.3×10^7 $\frac{\text{gm-cm}^2}{\text{gm mole-}^\circ\text{K-sec}^2}$

R_{max} = maximum reaction rate, $\frac{\text{gm moles}}{\text{sec.}}$

R_P = rate of diffusion into catalyst pellet, $\frac{\text{gm-moles}}{\text{sec.}}$

r_o = initial rate of reaction, $\frac{\text{gm-moles}}{\text{gm cat-sec}}$

r_A = gm moles A diffusing toward catalyst surface per second per gm catalyst, $\frac{\text{gm-moles}}{\text{gm. sec}}$

$(-r_{A1})$ = reaction rate, $\frac{\text{gm moles A}}{\text{gm cat-sec}}$

r_e = equivalent radius of pore, cm.

r_P = radius of catalyst particle, cm.

S = reference to propylene

S_{EX} = external surface area of catalyst, cm^2

S_g = total surface area of porous catalyst, $\frac{\text{cm}^2}{\text{gm}}$

S_V = total surface of porous catalyst = $\rho_P S_g$, $\frac{\text{cm}^2}{\text{cm}^3}$

T = Temperture, °K

T = Period, $\frac{\text{sec}}{\text{cycle}}$

t = time, sec.

t = temperature, °C .

T_C = critical temperature, °C.

V = velocity of propagation of wave form, $\frac{cm}{sec}$

V_b = molar volume at the normal boiling point, $\frac{cm^3}{gm\ mole}$

V_C = critical molar volume, $\frac{cm^3}{gm\text{-}mole}$

V_g = pore volume, $\frac{cm^3}{gm}$

v = transverse velocity, $\frac{cm}{sec}$

v = volume, cm^3

W = weight catalyst, gms.

W = work done on A system dyne-cm, ergs.

W_C = weight of catalyst, gms

X = distance traversed by wave form, cm.

X_A = conversion of A, dimensionless

X_{A_e} = equilibrium conversion of cumene, dimensionless

X_{A_f} = final conversion of A

X_{A_o} = initial conversion of A

Y = mole fraction in gas phase

Y = amplitude, cm

Y_A = mole fraction of A, dimensionless

Y_{A_b} = mole fraction of A in bulk stream, dimensionless

$Y_{A_{LM}}$ = log mean mole fraction of cumene in the bulk stream dinemsionless

Y_{As} = mole fraction of A at catalyst surface, dimensionless

y = displacement, cm.

z = distance in z direction, cm.

β = sound intensity level, decibels

γ = $\frac{C_p}{C_v}$

δ = thickness of stagnant gas film between main gas stream and external surface of catalyst, cm.

ε = void fraction in packed catalyst bed, dimensionless

ϵ = catalyst effectiveness factor, dimensionless

ϵ/K = Lennard-Jones parameter, °K

Θ = catalyst internal void fraction, dimensionless

λ = wave length, $\frac{cm.}{cycle}$

π = total pressure, atm.

ρ = fluid density, $\frac{gms}{cm^3}$

ρ_B = bulk density of catalyst bed, $\frac{gms}{cm^3}$

ρ_o = initial gas density, $\frac{gms}{cm^3}$

ρ_P = catalyst particle density, $\frac{gms}{cm^3}$ of particle volume

ρ_t = true density of solid material in porous catalyst, $\frac{gms}{cm^3}$

σ = Lennard-Jones parameter, Å

τ = tortuosity factor, dimensionless

μ_C = critical viscosity, $\frac{gm.}{cm\text{-}sec}$

Ω_D = collision integral

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