CHAPTER 5

EXPERIMENTAL RESULT

5.1 Testing of apparatus for styrene synthesis

Using the blank test method to check the apparatus for styrene synthesis. The steps are as follows.

1. Checking each apparatus for styrene synthesis system.
2. Set up the apparatus for styrene synthesis system.
3. Checking the leakage of the system at each joint.
4. Feeding ethylbenzene to the reactor without loading catalyst in the reactor.
5. Varying the flow rate of ethylbenzene at fix reactor temperature.
6. Varying the reactor temperature from 300 °C to 560 °C.
7. Analysis of the ethylbenzene and the products at each temperature by using the gas chromatography.

From the blank test, it is found that at the temperature above 500 °C, ethylbenzene is cracking to yield styrene monomer (this is the thermal cracking). Thus, in the experiment, we will avoid the reaction due to thermal cracking by running the experiment in the range of reaction temperature, 360-440 °C.

5.2 Differential reactor test

Once the apparatus for styrene synthesis is set, it is necessary to ensure that the reactor is a differential type.

Theorectically, if it is the differential reactor, we will obtain the rate of equation as (13).

$$r = \frac{XF}{W} \qquad (1)$$

or

$$X = \frac{rW}{F} \qquad (2)$$

where r = rate of reaction per weight of catalyst

F = flow rate of reactant

W = weight of catalyst

X = conversion of reactant

From the equation, X = rW/F, the correlation between X and W/F is linear and slope is equal to the rate of reaction per weight of catalyst. Thus, if X VS W/F is plotted, for the differential reactor, the correlation must be linear.

Operating condition

Partial pressure of ethylbenzene	11.75	mm Hg
Reactor temperature	360	°C
Weight of catalyst	0.26	gm

Table 5.1

Test differential reactor data

W/F (gm.s/mole)	%X
1,942,327	2.886
1,230,827.5	1.812
920,842.9	1.363
710,304.9	1.047
590,560.1	0.922

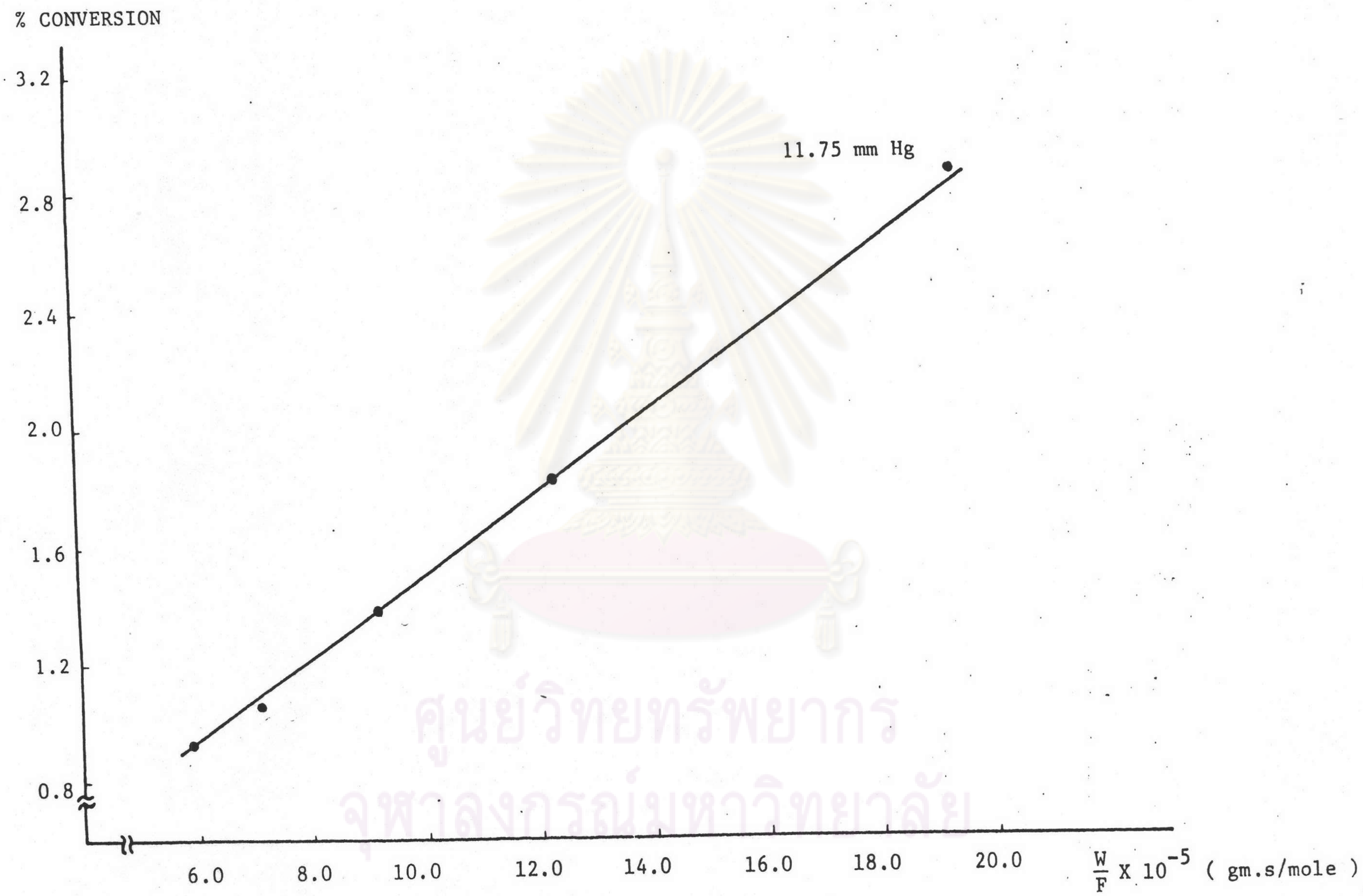

FIG 5.1 DIFFERENTIAL REACTOR TEST

5.3 Data

Before collecting the data, the catalyst must be stabilized by passing the ethylbenzene to the catalyst at the reactor temperature of 360 °C for 60 hours. The product is taken to gas chromatography for each two hours to analyze the styrene. This is to ensure that the catalyst is stable by lokking at the amount of styrene as shown in figure 5.2

After stabilizing the catalyst, the differential reactor is verified and then the data are collected.

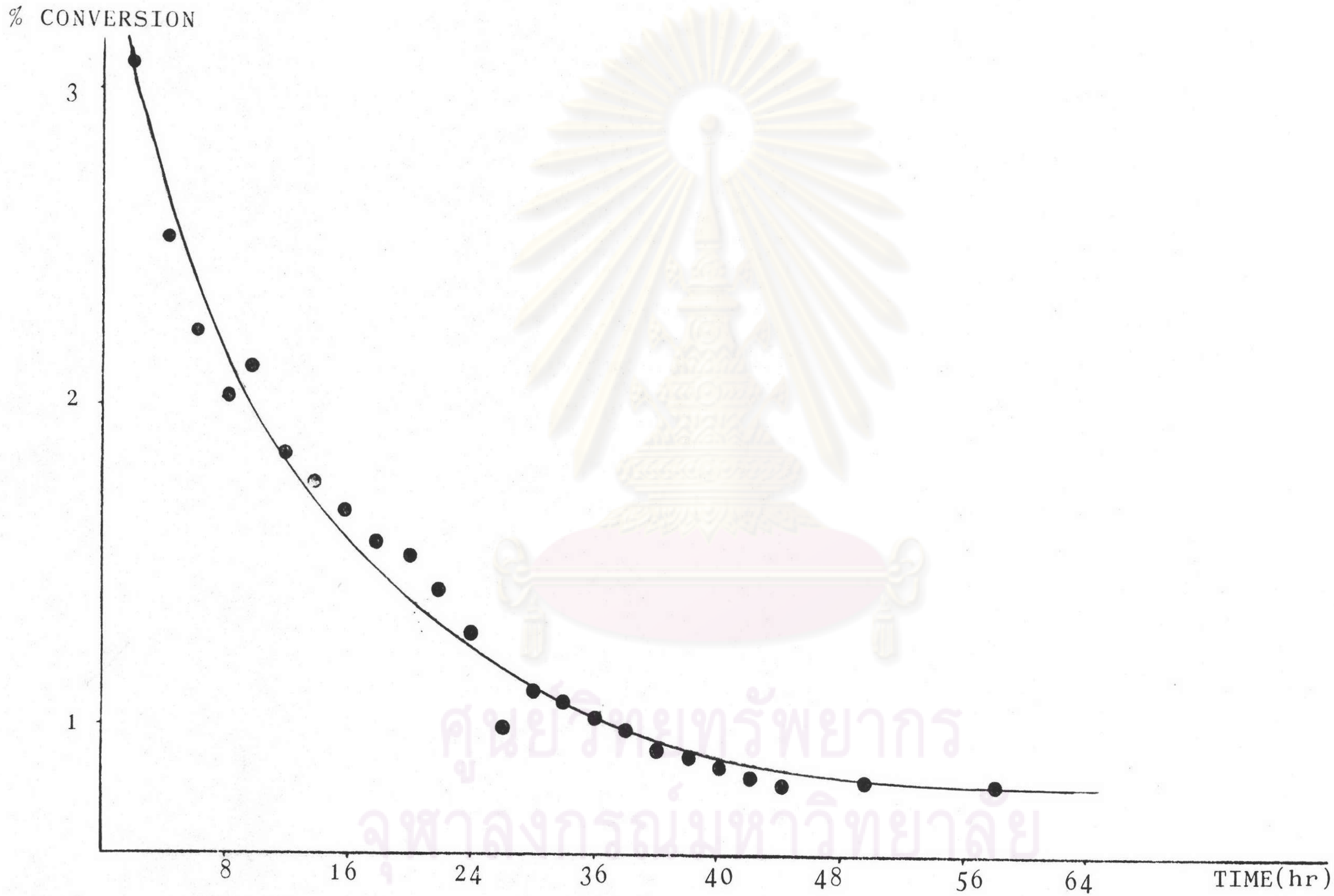

FIG 5.2 STABILIZE THE CATALYST

5.3.1 Determine the rate of reaction

From the equation (2) in appendix D

$$r = \frac{kb_E P_E}{1+b_E P_E}$$

or

$$\frac{1}{r} = \frac{1}{k} + \frac{1}{kb_E P_E}$$

For the above rate equation, the correlation between 1/r and $1/P_E$ is linear which

intercept = 1/k

slope = $1/kb_E$

The correlation between 1/r and $1/P_E$ is plotted in graph as shown in figure 5.3

Operating condition

Partial pressure of ethylbenzene	11.15-38.6	mm Hg
Flow rate of ethylbenzene	2.15×10^{-7}-7.1×10^{-7}	mole/sec
Flow rate of CO_2	1.465×10^{-5}	mole/sec
Weight of catalyst	0.26	gm

Table 5.2

Determine the rate equation data

Reactor temperature (°C)	1/r (gm.s/mole)	$1/P_E$ (mm Hg^{-1})
360	84,295,867	0.0897
	64,379,477	0.06192
	51,993,052	0.04141
	42,414,964	0.03284
	36,853,713	0.02591

Reactor temperature (°C)	1/r (gm.s/mole)	$1/P_E$ (mm Hg^{-1})
380	74,965,393	0.0897
	56,506,991	0.6192
	44,216,303	0.04141
	36,373,977	0.03284
	35,215,214	0.02714
400	65,636,000	0.0897
	49,451,308	0.06192
	39,385,680	0.04141
	32,708,599	0.03284
	28,620,138	0.02714
420	48,358,883	0.0897
	36,900,963	0.06192
	28,368,765	0.04141
	25,851,884	0.03284
	22,604,476	0.02714
440	26,540,854	0.0897
	22,201,916	0.06192
	18,247,525	0.04141
	15,668,501	0.03284
	14,493,486	0.02714

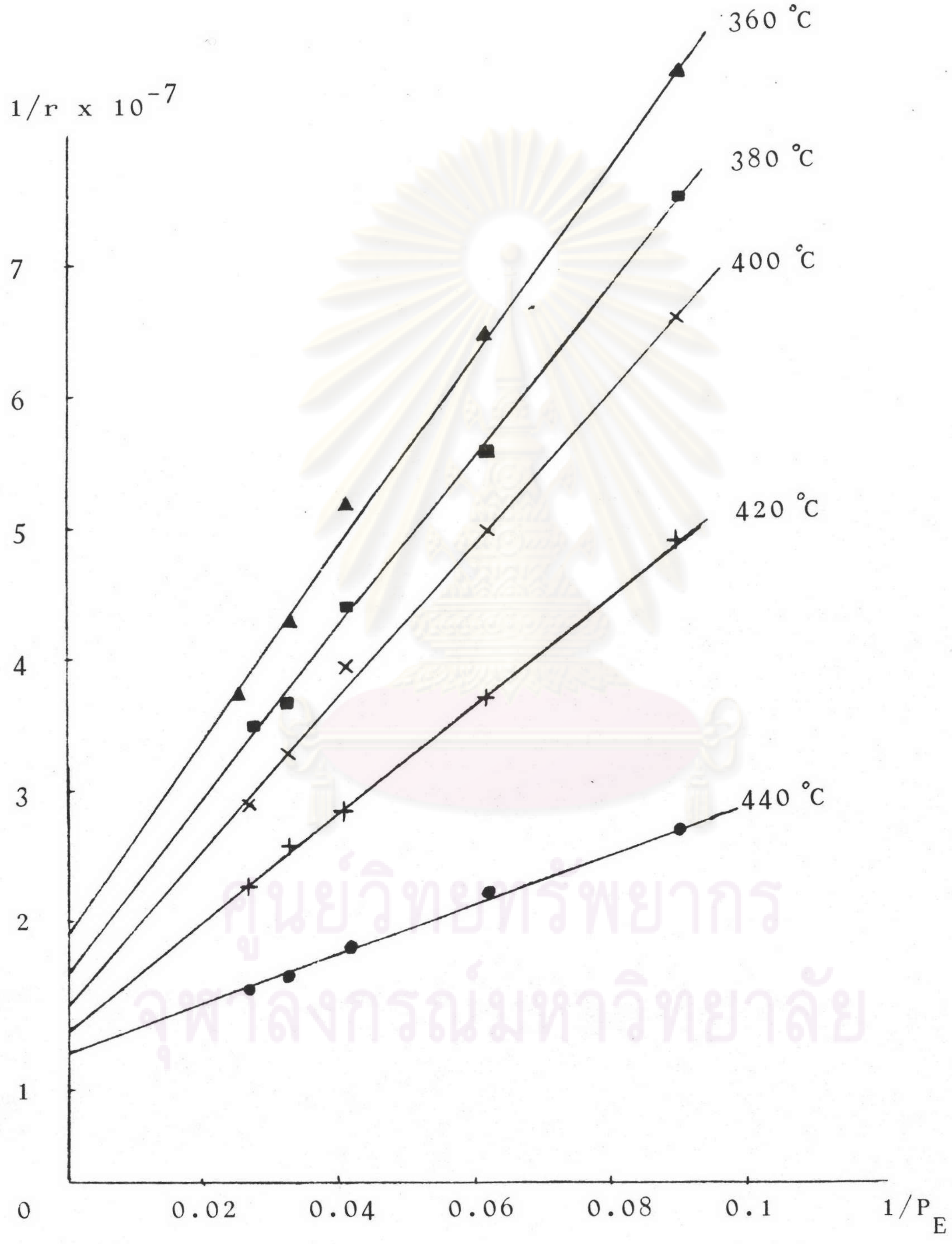

FIG 5.3 THE CORRELATION BETWEEN $1/r$ AND $1/P_E$

The above data show that the correlation between $1/r$ and $1/P_E$ is linear. Thus, the rate equation for dehydrogenation of ethylbenzene to styrene is

$$r = \frac{kb_E P_E}{1+b_E P_E}$$

From the above data, the value of k are obtained

Table 5.3

The value of the rate constant (k)

k	ln k	T (K)	1/T (K^{-1})
5.388×10^{-8}	-16.736	633	1.5797×10^{-3}
6.017×10^{-8}	-16.626	653	1.5314×10^{-3}
7.233×10^{-8}	-16.442	673	1.4859×10^{-3}
8.417×10^{-8}	-16.290	693	1.443×10^{-3}
1.000×10^{-7}	-16.118	713	1.4025×10^{-3}

From Arrhenius' law

$$k = Ae^{-E_a/RT}$$

or $$\ln k = \ln A - E_a/RT$$

where k = rate constant of the reaction

A = constant or frequency factor

E_a = activation energy

R = gas constant

T = absolute temperature

From the above equation, the correlation between ln k and 1/T is linear where

$$\text{intercept} = \ln A$$

$$\text{slope} = -E_a/R$$

The correlation between ln k and 1/T is shown in figure 5.4

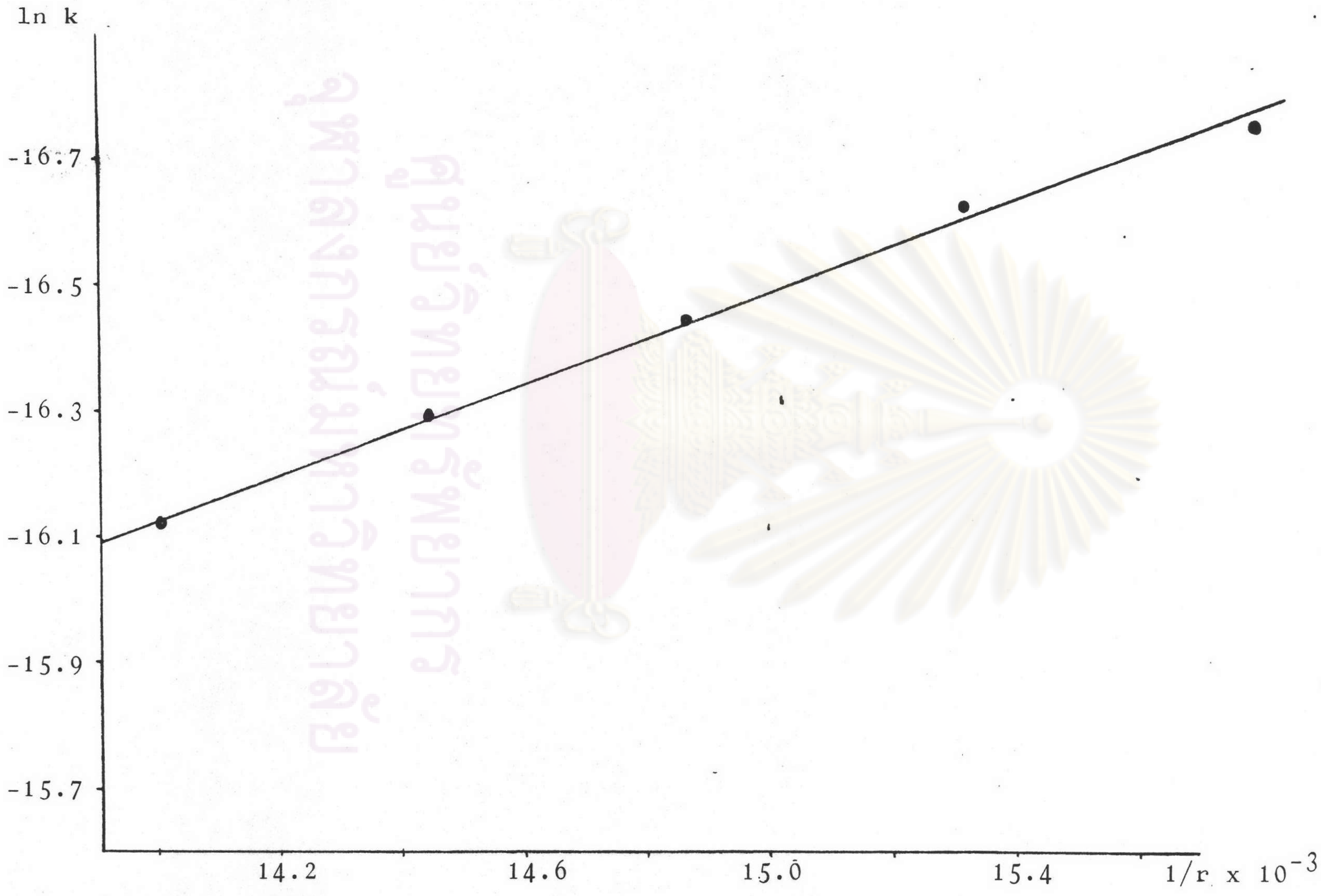

FIG 5.4 THE CORRELATION BETWEEN Ln k AND 1/T

5.3.2 Study the effect of partial pressure on rate of reaction

Operation condition

Partial pressure of ethylbenzene	11.15-38.6	mm Hg
Flow rate of ethylbenzene	2.15×10^{-7}-7.1×10^{-7}	mole/sec
Flow rate of CO_2	1.465×10^{-5}	mole/sec
Weight of catalyst	0.26	gm

Table 5.4

Effect of partial pressure on rate of reaction

Reaction temperature (°C)	P_E (mm Hg)	%X
360	11.15	1.41383
	16.15	1.2697
	24.15	1.04
	30.45	1.0025
	38.6	0.937
380	11.15	1.59
	16.15	1.447
	24.15	1.223
	30.45	1.169
	36.85	0.989
400	11.15	1.816
	16.15	1.653
	24.15	1.373
	30.45	1.3
	36.85	1.2169

Reaction temperature (°C)	P_E (mm Hg)	%X
420	11.15	2.4648
	16.15	2.215
	24.15	1.906
	30.45	1.645
	36.85	1.541
440	11.15	4.491
	16.15	3.682
	24.15	2.9635
	30.45	2.7138
	36.85	2.606

The correlation between P_E and %X is shown in figure 5.5

From the above data, its found that as the increasing of partial pressure of ethylbenzene, the conversion of ethylbenzene is increased.

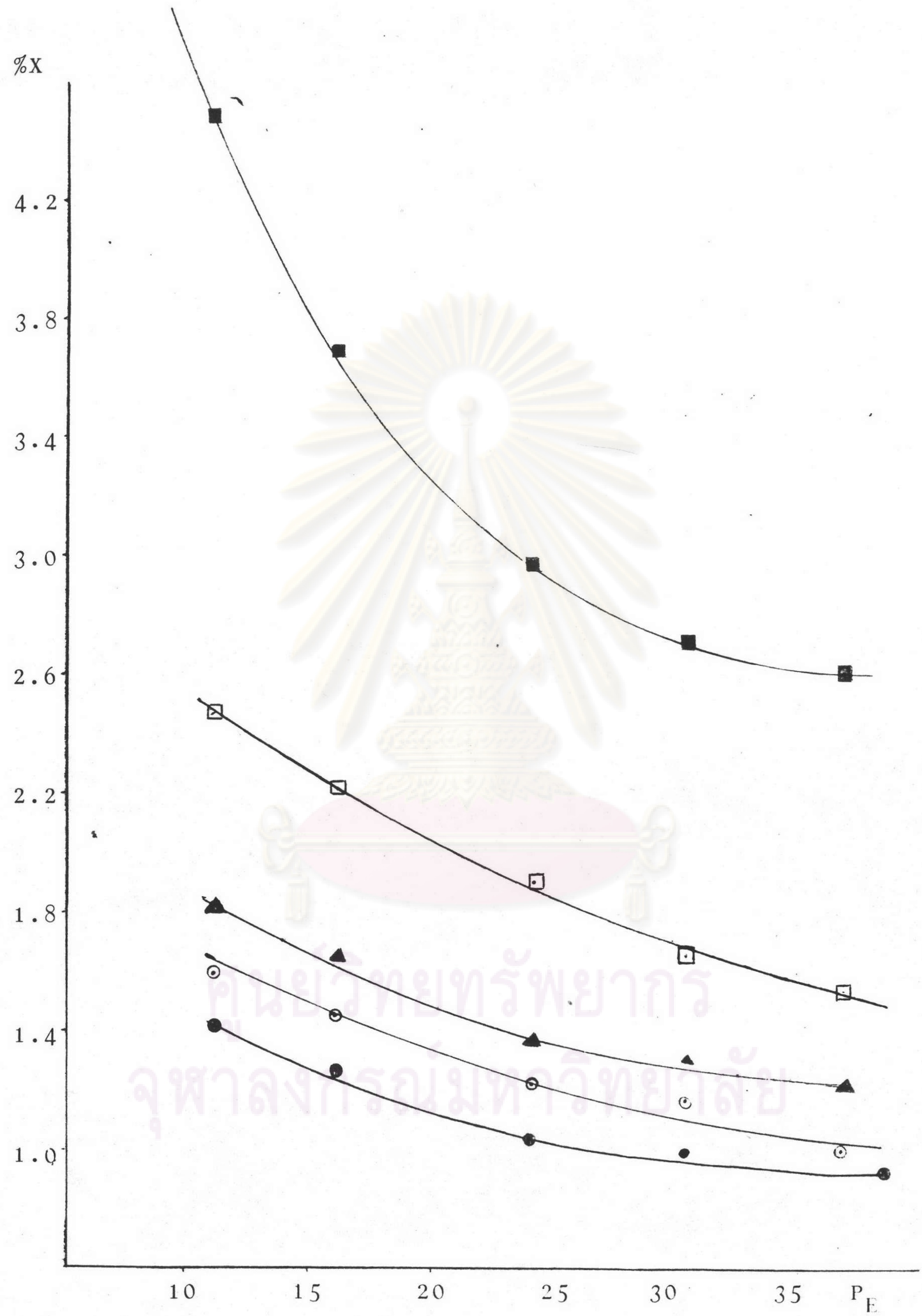

FIG 5.5 THE CORRELATION BETWEEN %X AND P_E

5.3.3 Study the effect of temperature on rate of reaction

Operating condition

Partial pressure of ethylbenzene	11.15-38.6	mm Hg
Flow rate of ethylbenzene	2.15×10^{-7}-7.1×10^{-7}	mole/sec
Flow rate of CO_2	1.465×10^{-5}	mole/sec
Reaction temperature	360-440	^{o}C
Weight of catalyst	0.26	gm

Table 5.5

Effect of temperature on rate of reaction

P_E (mm Hg)	Reaction temperature (^{o}C)	%X
11.15	360	1.41383
	380	1.59
	400	1.816
	420	2.4648
	440	4.491
16.15	360	1.2697
	380	1.447
	400	1.651
	420	2.215
	440	3.682
24.15	360	1.04
	380	1.223
	400	1.373
	420	1.906
	440	2.9635

P_E (mm Hg)	Reaction temperature (°C)	%X
30.45	360	1.0025
	380	1.169
	400	1.3
	420	1.645
	440	3.7138
36.85	380	0.989
	400	1.2169
	420	1.541
	440	2.606

The correlation between %X and T is plotted as shown in figure 5.6

From the above data, its found that as the increasing of the reaction temperature, the conversion of the ethylbenzene is increased.

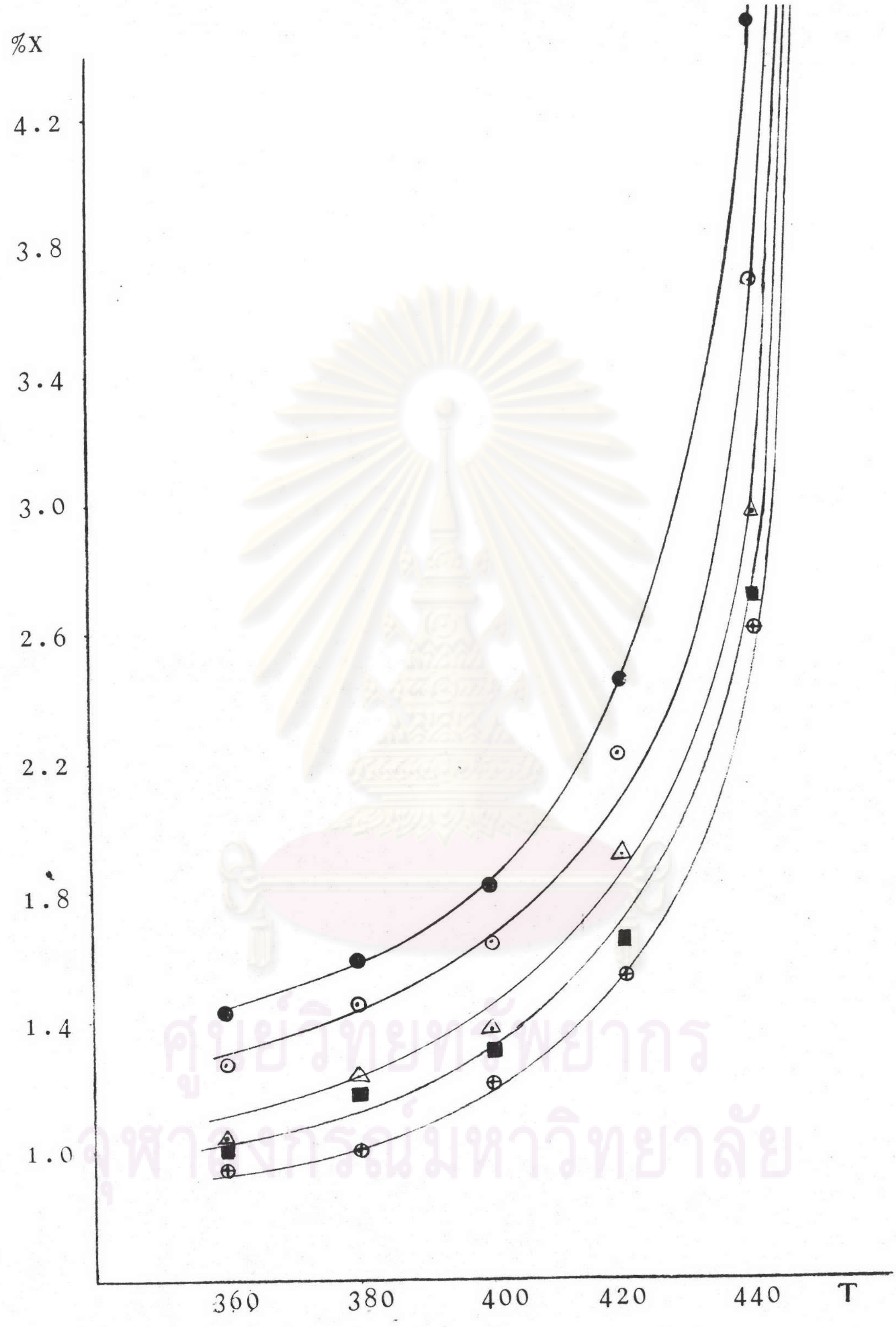

FIG 5.6 THE CORRELATION BETWEEN %X AND T

5.3.4 Study the effect of diluent on rate of reaction

Table 5.6

Effect of diluent on rate of reaction at 380 °C

Diluent	1/r (gm.s/mole)	$1/P_E$ (mm Hg^{-1})
N_2+steam	29,630,148	0.084
	30,204,464	0.08683
	34,052,679	0.09093
	35,928,985	0.10688
	42,933,903	0.12299
	42,038,472	0.1256
CO_2+steam	31.047,416	0.0723
	34,008,097	0.07998
	35,517,124	0.08577
	38,527,643	0.08926
	39,962,920	0.09555

Table 5.7

Effect of diluent on rate of reaction at 440 °C

Diluent	1/r (gm.s/mole)	$1/P_E$ (mm Hg^{-1})
N_2+steam	10,402,159	0.08681
	10,104,739	0.0843
	12,471,634	0.10122
	13,094,081	0.1161
	13,719,596	0.12394
	15,498,650	0.1276
	15,802,957	0.14173

Diluent	1/r (gm.s/mole)	$1/P_E$ (mm Hg^{-1})
CO_2+steam	12,267,002	0.08056
	13,824,318	0.0813
	16,618,287	0.10618
	17,062,446	0.10937
	16,607,060	0.11765

The correlation between 1/r and $1/P_E$ is plotted as shown in figure 5.7, 5.8

From the data, the effect of the diluent on the rate constant of the reaction is $CO_2 < CO_2$+steam $< N_2$+steam

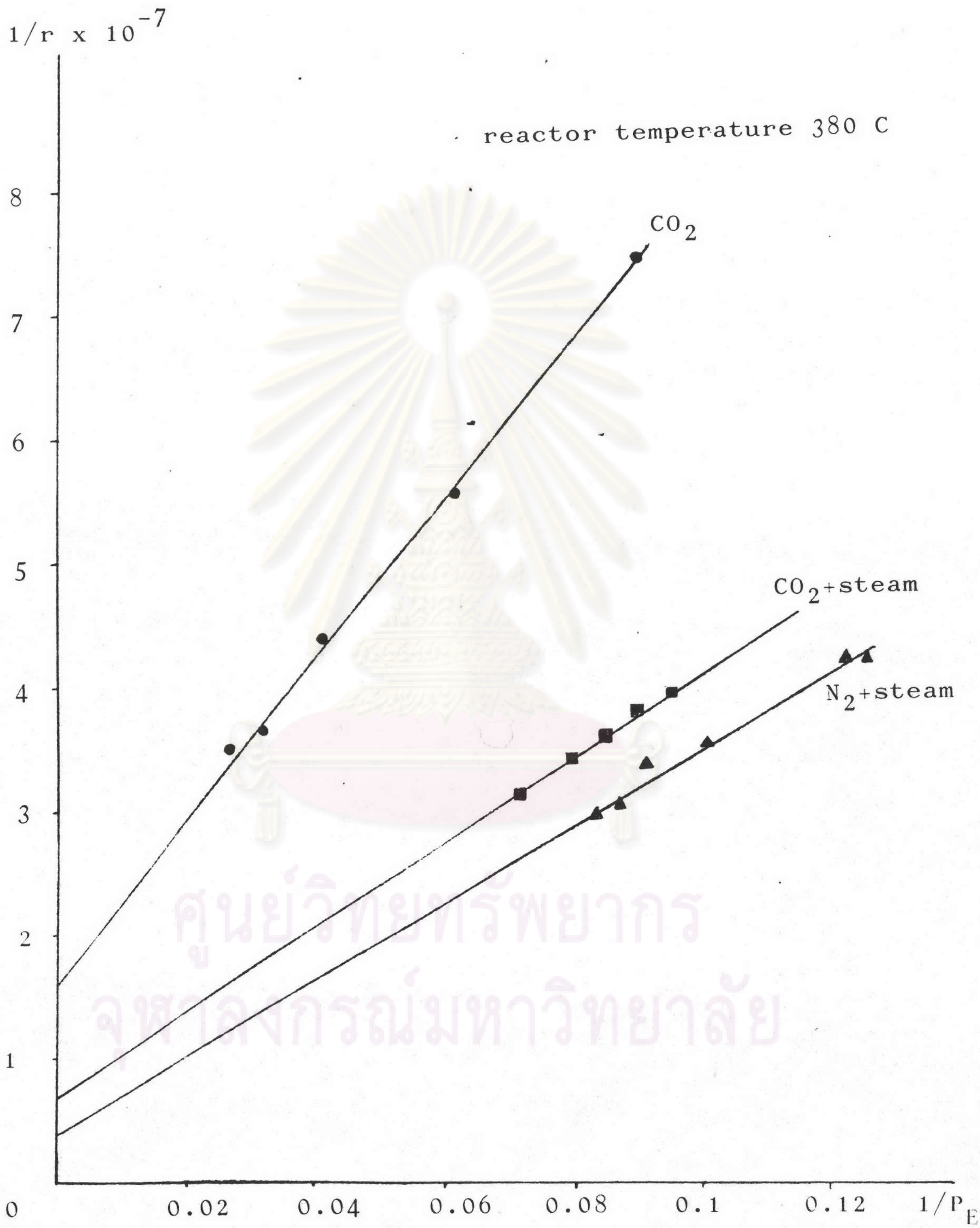

FIG 5.7 THE CORRELATION BETWEEN 1/R AND $1/P_E$

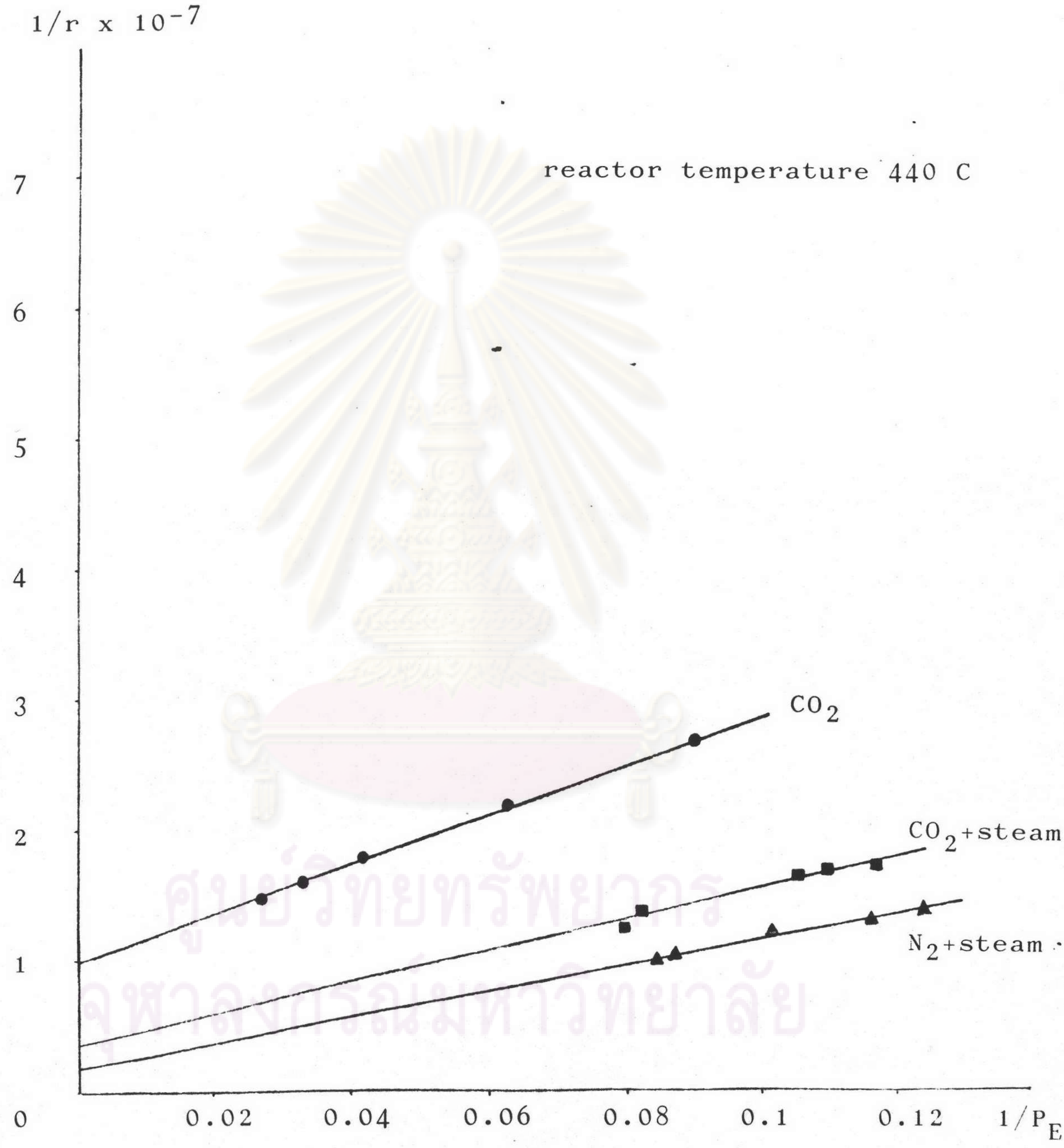

FIG 5.8 THE CORRELATION BETWEEN 1/R AND $1/P_E$