APPENDICES

Appendix A. Calculation of activation energy

From Arrhenius Equation

$$k(T) = Ae^{-(E/RT)}$$

$$\ln(k) = \ln(A) - E/RT$$

whereas;

rate	=	gPP/mmoleZr.hr
k	=	rate constant
E	=	Activation Energy (cal/mole)
R	=	Rate of reaction (1.987 cal/mole/^{o}K)
T	=	Temperature (^{o}K)
A	=	Constant

$$\text{rate} \propto k(T)$$

Due to the corresponding between rate of reaction and rate constant (k) which both are function of temperature and were got from concentration constant for each polymerization, the activity or rate of reaction (gPP/mmoleZr.hr) was used to plot versus 1/T to determine the slope for activation energy calculation.

But the constant (A) were not obtained from the intercept of this plot.

From Arrhenius plot (Figure 5.1) between natural logarithm of activity or rate of reaction versus 1/T, the slope -6666.6 was obtained.

$$\text{Slope} = -(E/RT)$$

$$E = \text{Slope} \times R = 13.25 \text{ kcal/mole}$$

<u>Appendix B</u>. Conversion calculation

Conversion (%) = grams of propylene used per grams of propylene feed x 100

Yield (as mole of PP) = Weight of PP obtained per molecular weight of PP (1)

Mole of propylene per mole of PP = Ratio of PP molecolar weight to propylene molecular weight (2)

Mole of propylene used = (1) x (2) mole

Grams of propylene used = (1) x (2) x 42 grams

Temp. (oC)	Yield (grams PP)	Yield (moles PP)	mole propylene /mole PP	Grams of propylene used	Conversion (%)
50	110.98	0.008712	303.30952	110.98	55.5
40	71.06	0.004227	400.23810	71.06	35.5
30	53.69	0.003125	409.04762	53.69	26.8
20	34.855	0.001941	427.52381	34.855	17.4
10	9.16	0.000463	471.42857	9.16	4.6
-10	1.3	0.000041	761.90476	1.3	0.7
-20	0.92	0.000053	410.92857	0.92	0.5

** Molecular weight of propylene = 42 g/mole

**Propylene feed = 200 grams

Appendix C. Grams polypropylene produced per gram zirconium calculation

M_w of Zr = 91.22

Temp. (°C)	Activity*	gPP.	Mn	mmole of Zr	mgrams of Zr	gPP./gZr
50	22196	110.98	12739	5	0.4561	243323.83
40	14212	71.06	16810	5	0.4561	155799.17
30	10738	53.69	17180	5	0.4561	117715.41
20	6971	34.855	17956	5	0.4561	76419.64
10	1832	9.16	19800	5	0.4561	20083.32
-10	260	1.3	32000	5	0.4561	2850.25
-20	92	0.92	17259	10	0.9122	1008.55

*gPP/mmoleZr.hr

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