

Memo 3

DIVERSIFIED CHEMICAL PRODUCTS**Specialty Products Division****Cambridge MA 02139**

TO: U. R. Engineer
FROM: Hyung Ko Op
DATE: 2007 Sep 10
SUBJECT: Analysis of Kinetic Experiments for Reaction 1

Per your request, I applied the techniques of Fogler (p. 209) to analyze the kinetic data we obtained from Blacksburg. I assumed reaction rate expressions of the form: $\text{rate} = k * R1^\alpha R2^\beta$. I used the data from the eleven experiments to regress values for α , β , and k for each reaction (formation of A and C). The numerical results for the fitted parameters are given below. The values for the parameters showed large variations from experiment to experiment. No attempt was made to correlate the kinetic rate constant, k , to the temperature because the values obtained seemed clearly unrelated to the temperature.

REACTION 1A (FORMATION OF A):

R1/R2	Temp., °C	CAT, mL	k	α	β	<i>err2/N</i>
1:1	80.0	0.22	1.64e+00	2.689	-4.690	0.027
	85.0	0.22	1.36e+00	2.374	-3.697	0.021
	90.0	0.22	1.29e+00	2.211	-3.041	0.018
2:1	80.0	0.22	2.12e-11	25.780	-18.454	0.011
	85.0	0.22	2.01e+02	-5.557	5.397	0.139
	90.0	0.22	7.10e+02	-6.475	5.174	0.051
3:1	80.0	0.22	1.13e+05	-7.992	3.767	0.047
	85.0	0.22	1.01e+03	-4.516	2.256	0.033
	90.0	0.22	1.65e+02	-3.066	1.619	0.025
2:1	85.0	0.11	1.99e-14	33.978	-24.781	0.045
	85.0	0.33	1.20e+04	-9.528	7.382	0.087

REACTION 1B (FORMATION OF C):

R1/R2	Temp., °C	CAT, mL	k	α	β	<i>err2/N</i>
1:1	80.0	0.22	1.06e-01	0.614	-1.440	0.048
	85.0	0.22	1.71e-01	0.484	-1.141	0.031
	90.0	0.22	3.22e-01	0.573	-1.336	0.019
2:1	80.0	0.22	1.43e-06	11.392	-8.357	0.019
	85.0	0.22	4.50e-02	1.024	-0.162	0.044
	90.0	0.22	2.14e+01	-4.697	3.275	0.026
3:1	80.0	0.22	4.16e+00	-2.895	1.499	0.041
	85.0	0.22	7.92e+00	-2.901	1.299	0.028
	90.0	0.22	2.46e+01	-3.277	1.221	0.031
2:1	85.0	0.11	1.04e-09	19.983	-14.995	0.015
	85.0	0.33	2.12e+00	-2.848	2.243	0.035