Kinetics and Reactor Design HW5

Daniel Naumov

Assigned: March 1, 2023
Due: March 8, 2023

1 Problem Statement

1.1 P6-11$_B$ (a, b, d, f)

P6-11$_B$ Pure butanol is to be fed into a *semibatch reactor* containing pure ethyl acetate to produce butyl acetate and ethanol. The reaction

$$CH_3COOC_2H_5 + C_4H_9OH \rightleftharpoons CH_3COOC_4H_9 + C_2H_5OH$$

is elementary and reversible. The reaction is carried out isothermally at 300 K. At this temperature, the equilibrium constant is 1.08 and the specific reaction rate is 9×10^{-5} dm^3/mol·**s.** Initially, there is 200 dm^3 of ethyl acetate in the vat, and butanol is fed at a volumetric rate of 0.05 dm^3/s. The feed and initial concentrations of butanol and ethyl acetate are 10.93 mol/dm^3 and 7.72 mol/dm^3, respectively.

(a) Plot and analyze the equilibrium conversion of ethyl acetate as a function of time.
(b) Plot and analyze the conversion of ethyl acetate, the rate of reaction, and the concentration of butanol as a function of time.
(c) Rework part **(b)**, assuming that ethanol evaporates (reactive distillation) as soon as it forms. (This is a graduate level question.)
(d) Use Polymath or some other ODE solver to learn the sensitivity of conversion to various combinations of parameters (e.g., vary F_{B0}, N_{A0}, v_0).
(e) Apply one or more of the six ideas in Preface Table P-4, page xxvii, to this problem.
(f) Write a question that requires critical thinking and then explain why your question requires critical thinking. (*Hint*: See Preface Section G.)

Figure 1

1.2 P7-10_C

P7-10_C The reactions of ozone were studied in the presence of alkenes [from R. Atkinson et al., *Int. J. Chem. Kinet.*, *15(8)*, 721]. The data in Table P7-9_C are for one of the alkenes studied, *cis*-2-butene. The reaction was carried out isothermally at 297 K. Determine the rate law and the values of the rate-law parameters.

TABLE P7-9_C RATE AS A FUNCTION OF OZONE AND BUTENE CONCENTRATIONS

Run	*Ozone Rate* ($mol/s \cdot dm^3 \times 10^7$)	*Ozone Concentration* (mol/dm^3)	*Butene Concentration* (mol/dm^3)
1	1.5	0.01	10^{-12}
2	3.2	0.02	10^{-11}
3	3.5	0.015	10^{-10}
4	5.0	0.005	10^{-9}
5	8.8	0.001	10^{-8}
6	4.7*	0.018	10^{-9}

**Hint*: Ozone also decomposes by collision with the wall.

Figure 2

1.3 P7-12_A

P7-12_A The thermal decomposition of isopropyl isocyanate was studied in a *differential packed-bed reactor*. From the data in Table P7-11_A, determine the reaction-rate-law parameters.

TABLE P7-11_A RAW DATA†

Run	*Rate* ($mol/s \cdot dm^3$)	*Concentration* (mol/dm^3)	*Temperature* *(K)*
1	4.9×10^{-4}	0.2	700
2	1.1×10^{-4}	0.02	750
3	2.4×10^{-3}	0.05	800
4	2.2×10^{-2}	0.08	850
5	1.18×10^{-1}	0.1	900
6	1.82×10^{-2}	0.06	950

† *Jofostan Journal of Chemical Engineering*, Vol. 15, page 743 (1995).

Figure 3

2 Problem Solution

2.1 P6-11$_B$ (a, b, d, f)

a) At equilibrium, r is equal to 0, and since we know the reaction is elementary and semibatch, we can do the following:

$$C_A C_B = \frac{C_C C_D}{K_c} \tag{1}$$

$$V = V_0 + v_0 t \tag{2}$$

$$C_A = \frac{N_{A0}(1-X)}{V} = \frac{C_{A0}(1-X)}{V/V_0} = \frac{C_{A0}(1-X)}{1+v_0 t/V_0} \tag{3}$$

$$C_B = \frac{C_{B0}\frac{v_0 t}{V_0} - C_{A0}X}{1+v_0 t/V_0} \tag{4}$$

$$C_C = C_D = \frac{C_{A0}X}{1+v_0 t/V_0} \tag{5}$$

$$\left(\frac{C_{A0}(1-X)}{1+v_0 t/V_0}\right) \times \left(\frac{C_{B0}\frac{v_0 t}{V_0} - C_{A0}X}{1+v_0 t/V_0}\right) = \frac{\left(\frac{C_{A0}X}{1+v_0 t/V_0}\right)^2}{K_C} \tag{6}$$

$$t = \frac{V_0 C_{A0}}{v_0 C_{B0}}\left(\frac{X^2}{K_C(1-X)} + X\right) \tag{7}$$

We are given all the necessary values to solve for t as a function of X now.

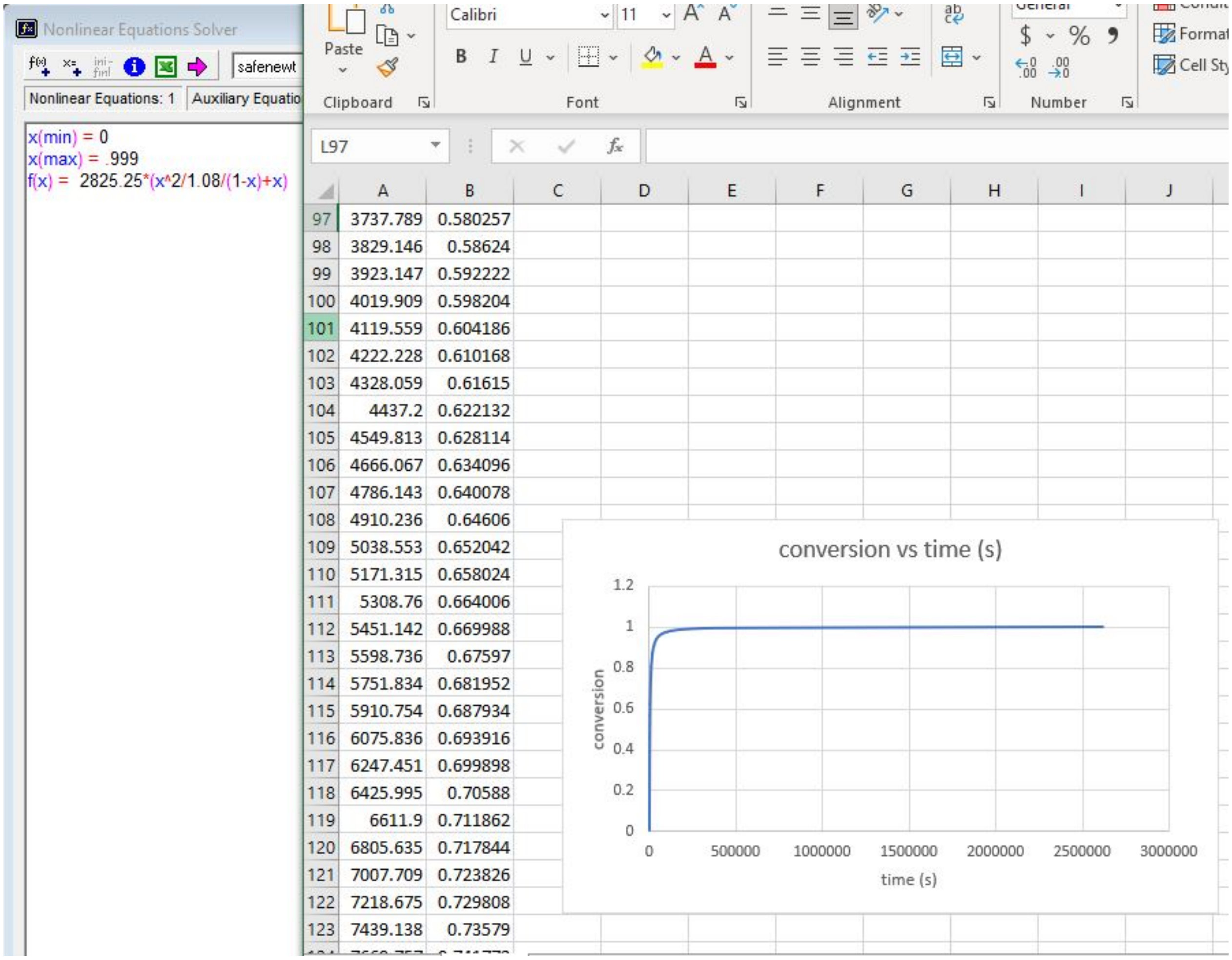

Figure 4: My graph for conversion as a function of time for this problem

b)

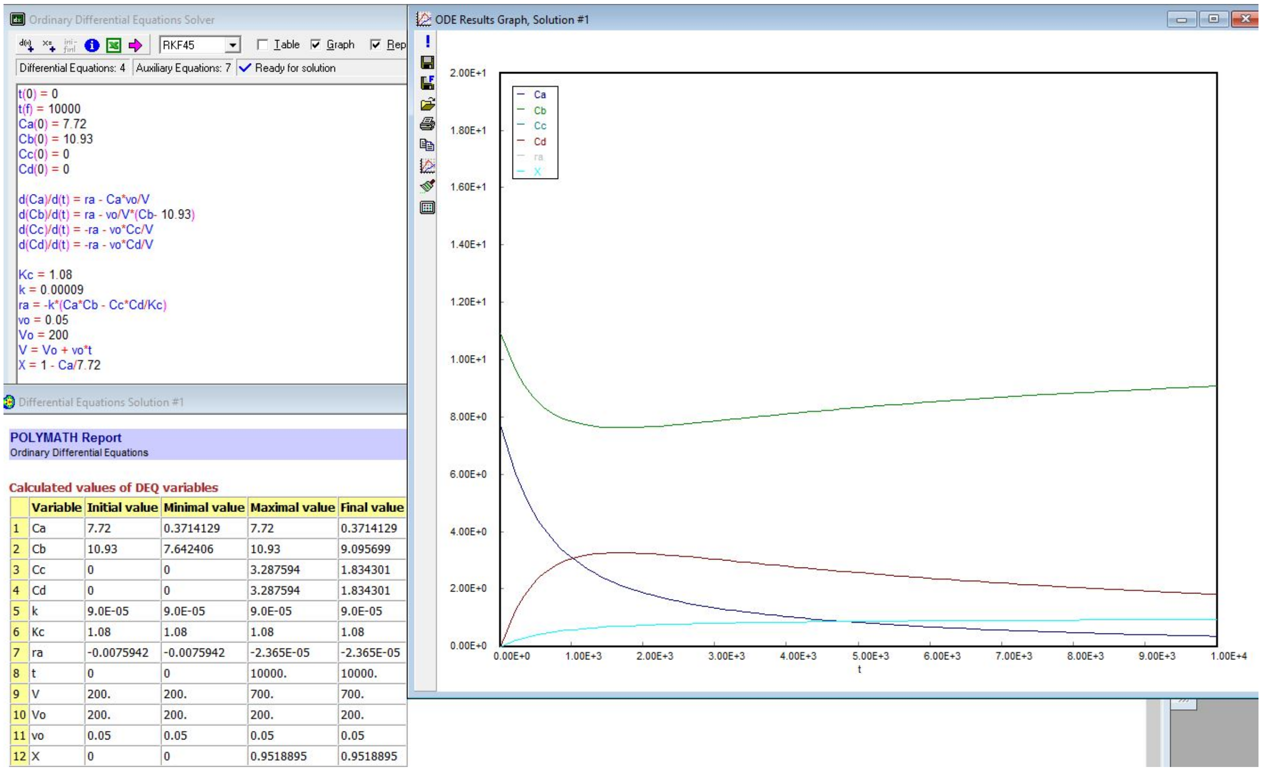

Figure 5: My graph for concentrations and conversions as functions of time

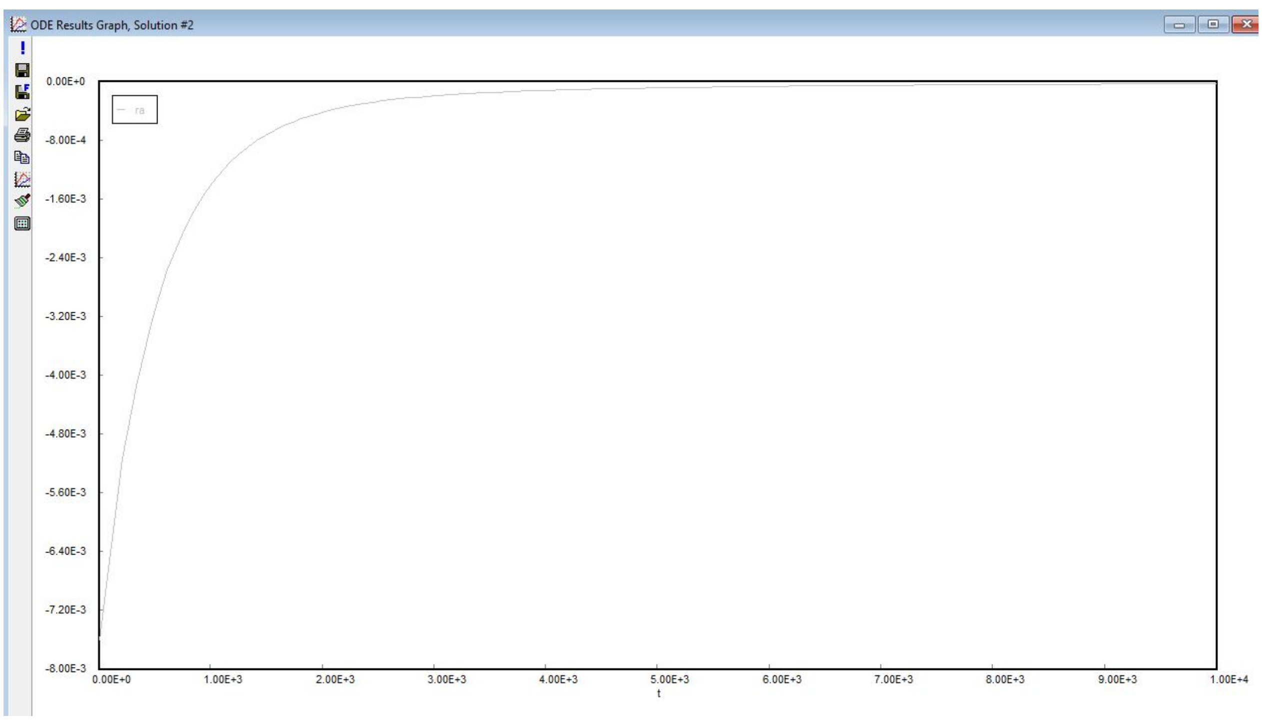

Figure 6: My graph for ra as a function of time

d)

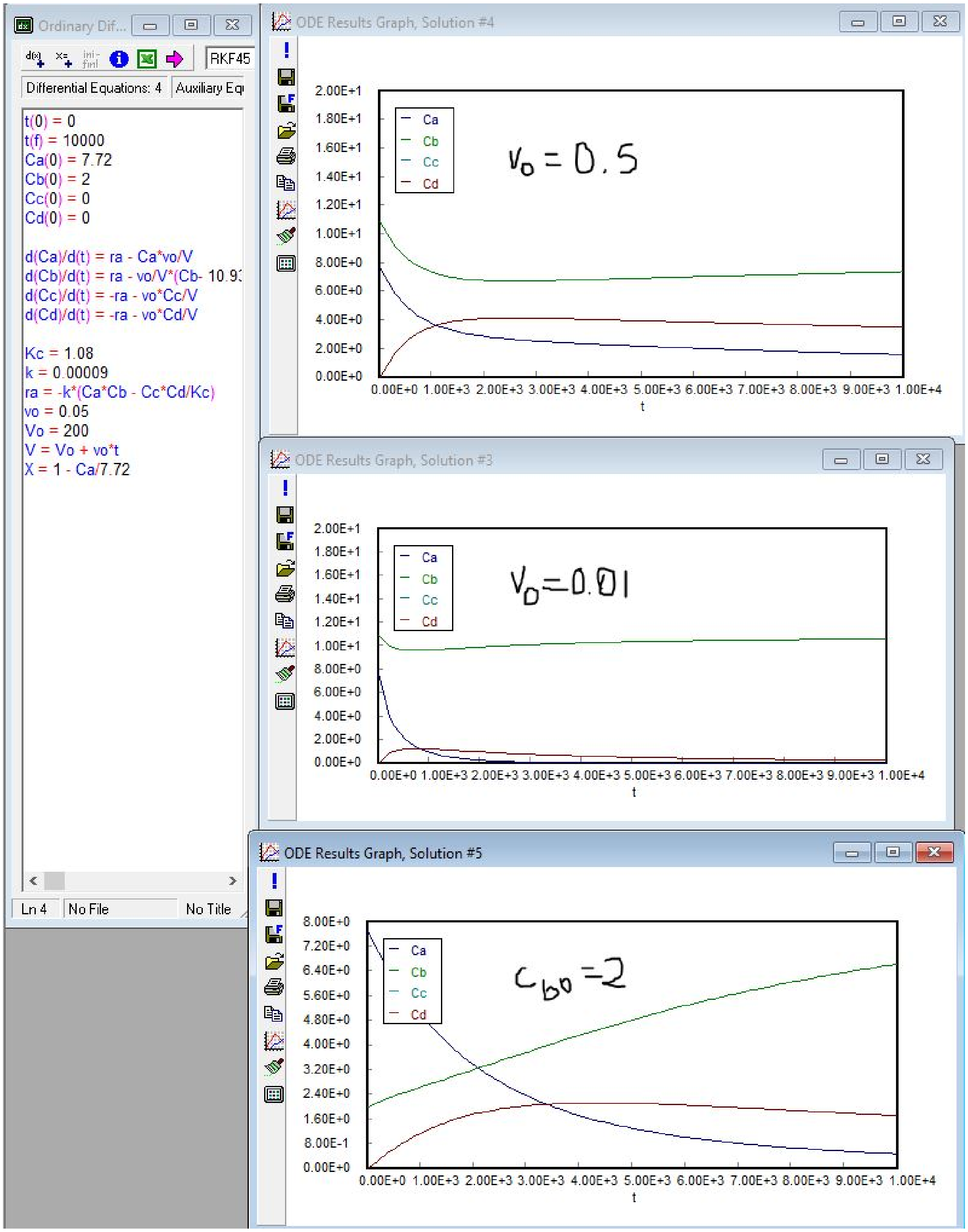

Figure 7: My graphs that showcase the changes that come with changing some parameters

f) How would we determine an adequate size for the reactor such that an accident is very unlikely to occur? This question requires critical thinking as we need to apply information such as conversion rate and time to know when to extract the product, and then adjust the size of the reactor while keeping that in mind.

2.2 P7-10$_C$

Two reactions going on here - ozone can either decompose by hitting the wall, or react by hitting butene. So we can express the rate law as such:

$$-r = \frac{dC_A}{dt} = k_1 C_A + k_2 C_A^{\alpha} C_B^{\beta} \tag{8}$$

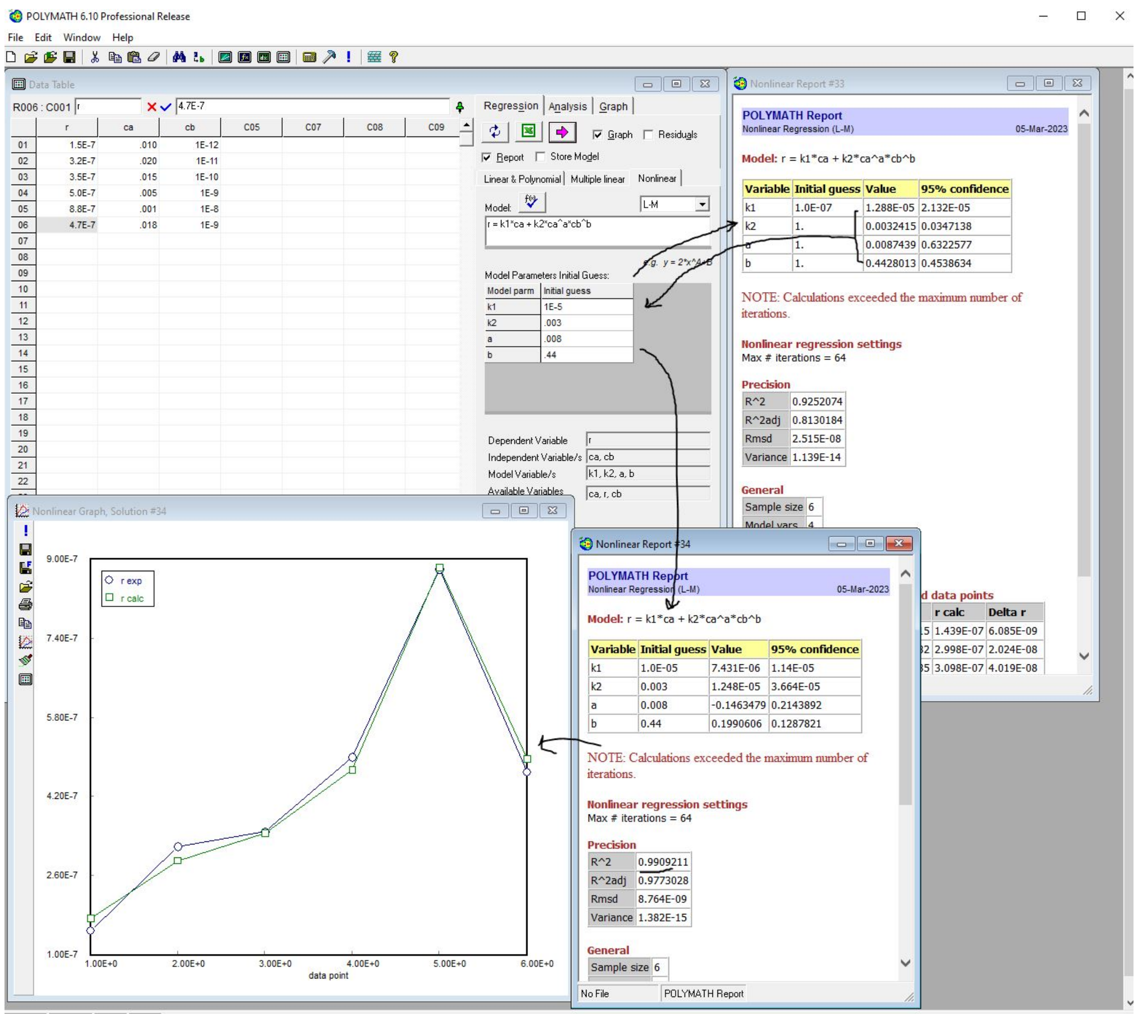

Figure 8: Nonlinear regression using given data. 2 iterations.

$$-r = \frac{dC_A}{dt} = 7.43 \times 10^{-6} C_A + 1.25 \times 10^{-5} C_A^{-0.15} C_B^{0.20} \tag{9}$$

2.3 P7-12$_A$

We're given temperatures, so k will have an Arrhenius equation type of dependence. So, the rate law is:

$$-r_A = Ae^{-E/RT}C_A^{\alpha} \tag{10}$$

We know R is 8.314 J/molK. Nonlinear regression to find A, E, and α.

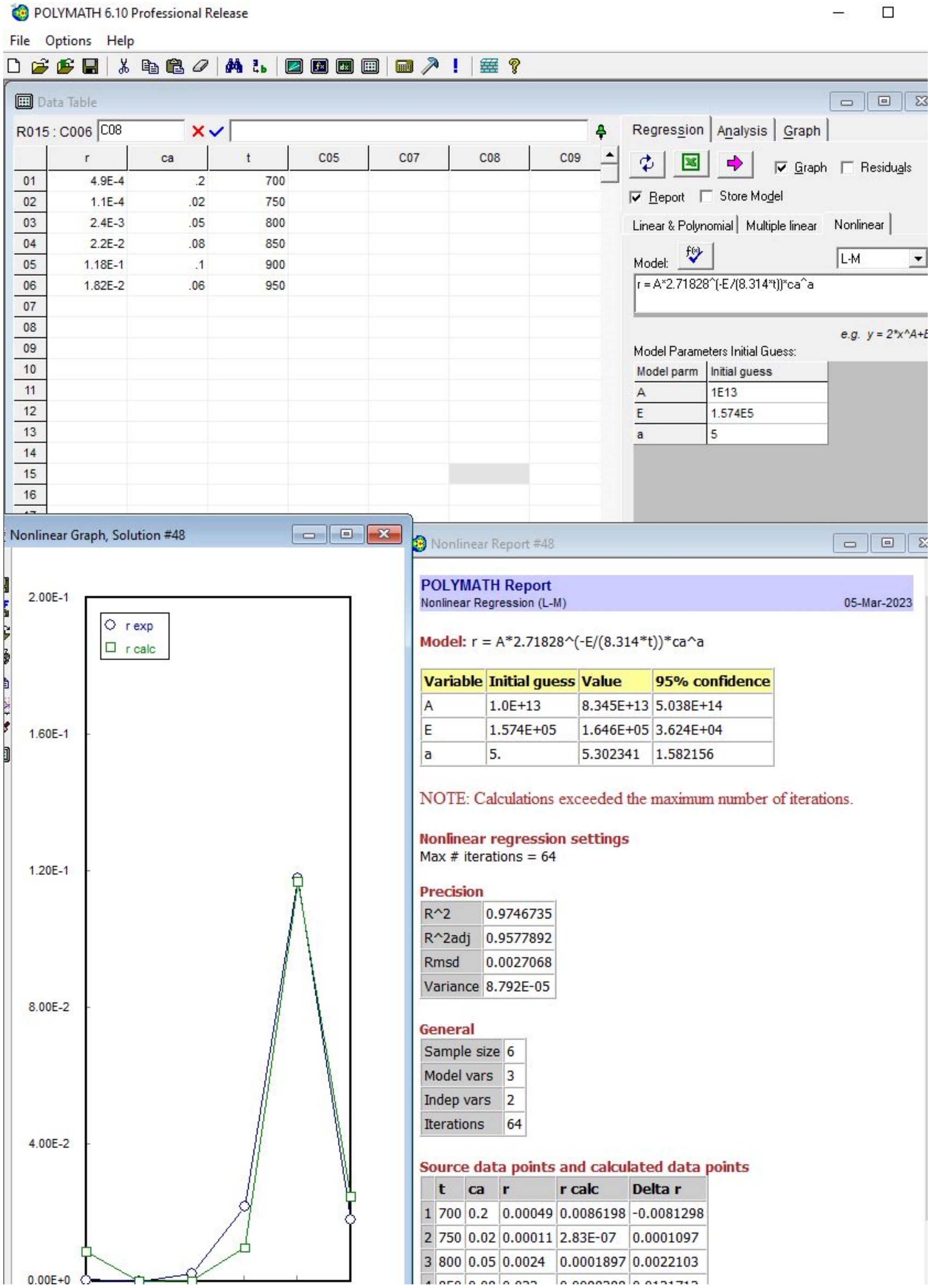

Figure 9: Nonlinear regression using given data. Around 10 iterations were needed to get to a good R^2 value.

$$-r_A = 1.0 \times 10^{13} e^{-(1.5\times 10^5)/RT} C_A^5 \tag{11}$$