ChE 344
Chemical Reaction Engineering
Winter 1999
Final Exam

Solution

(25 pts) 1) The gas phase irreversible reaction

$$A + B \quad C$$

is elementary. The entering flow rate of A is 10 mol/min and is equal molar in A and B. The entering concentration of A is 0.4 mol/dm³.

a) What is the CSTR reactor volume necessary to achieve 90% conversion?
b) What PFR volume is necessary to achieve 90% conversion?

Additional Information

$$k = 2 \text{ dm}^3/\text{mol} \cdot \text{min}$$
$$T_0 = 500 \text{ K}$$

Note: You do **not** need to use POLYMATH, but if you do write your program below in case you do not obtain the correct answer.

a) $$F_{A0} X = (-r_A)V$$

$$F_{A0} = 10$$
$$x = 0.9$$
$$V = ?$$

$$-r_A = kC_A C_B = 2C_{A0}^2 (1-X)^2 / \quad 1 - \frac{X}{2}^{\;2}$$

$$= 2 \quad (0.4)^2 \quad \frac{(0.1)^2}{(0.55)^2} = 0.01057$$

$$V = \frac{10 \times 0.9}{0.01057} = 851 \text{ dm}^3$$

b) $$F_{A0} \; dX = (-r_A)dV$$

$$\int_0^{0.9} \frac{dX \; 1 - \frac{X}{2}^{\;2}}{(1-X)^2} = \frac{kC_{A0}^2}{F_{A0}} \quad V$$

$$2 \quad -\frac{1}{2} \quad 1-\frac{1}{2} \quad \ln(1-0.9) + \quad -\frac{1}{2}^{\;2} 0.9 + \frac{\left(1-\tfrac{1}{2}\right)^2 0.9}{1-0.9} = \frac{2 \quad 0.4^2 V}{10}$$

$$V = \frac{3.63 \quad 10}{2 \quad 0.4^4} = 113.3 \text{ dm}^3$$

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Equations: <u>Initial value</u>
d(X)/d(V)=-ra/Fao   0
Fao=10
k=2
Cao=0.4
eps=(1-1-1)*0.5
Ca=Cao*(1-X)/(1+eps*X)
ra=-k*Ca^2
V1=Fao*X/(-ra)
$V_0 = 0,$ $V_f = 125$

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X	V	V1
0.88385918	100	637.73656
0.88598907	101.5625	660.85219
0.88804985	103.125	684.46088
0.89004458	104.6875	708.56481
0.89197617	106.25	733.16608
0.89384737	107.8125	758.26674
0.89566078	109.375	783.86879
0.89741884	110.9375	809.97417
0.89912391	112.5	836.58475
0.90077817	114.0625	863.70237
0.90238373	115.625	891.32882
0.90394257	117.1875	919.46584
0.90545658	118.75	948.11511
0.90692755	120.3125	977.27829
0.90835718	121.875	1006.957
0.90974708	123.4375	1037.1527
0.9110988	125	1067.8671

W'99FinalExam

(15 pts) 2) The irreversible zero order gas phase dimerization

$$2A \longrightarrow A_2$$

is carried out in a packed bed reactor with 5 kg of catalyst. The entering pressure is 10 atm and the exit pressure is 1 atm. Pure A enters at a flow rate of 10 mol/min. The reaction is zero order in A.
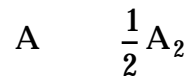
$P_0 = 10$ atm $\qquad\qquad\qquad\qquad\qquad$ P = 1 atm

$F_{A0} = 10$ mol/min $\qquad\qquad\qquad\qquad$ X = ?
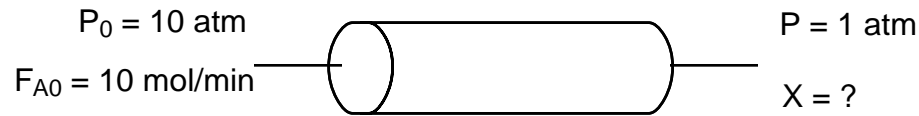
a) What is the pressure drop parameter α?
b) What is the exit conversion?

Additional Information

$k = 1.5$ mol/kg•min
$T_0 = 500$ K

Note: You do not need to use POLYMATH, but if you do write your program below in case you do not obtain the correct answer.

$$A \longrightarrow \frac{1}{2}A_2$$

$$F_{A0}\frac{dX}{dW} = (-r_A)$$

$$\int_0^x dX = \frac{k}{F_{A0}}W$$

$$X = \frac{1.5}{10}W = 0.15W$$

$$\frac{dy}{dw} = -\frac{\alpha}{2}\frac{(1+\varepsilon X)}{y}$$

$$\int_0^x 2y\,dy = -\int_0^5 \left(1-\frac{1}{2}\right)0.15W\,\alpha\,dW$$

$$y^2\Big|_1^{0.1} = -\alpha\left[W-\frac{0.15}{4}w^2\right]_0^5$$

$$-0.99 = -\alpha\left[5-\frac{0.15\cdot25}{4}\right]$$

$$= -\alpha\,4.0625$$

$$\alpha = 0.2437\ \text{kg}^{-1}$$

$$X = 0.15\cdot5 = 0.75$$

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(10 pts) 3) The species A and B react to form species C, D, and E in a packed bed reactor. The catalyst does not decay. The reaction is elementary. The following profiles were obtained
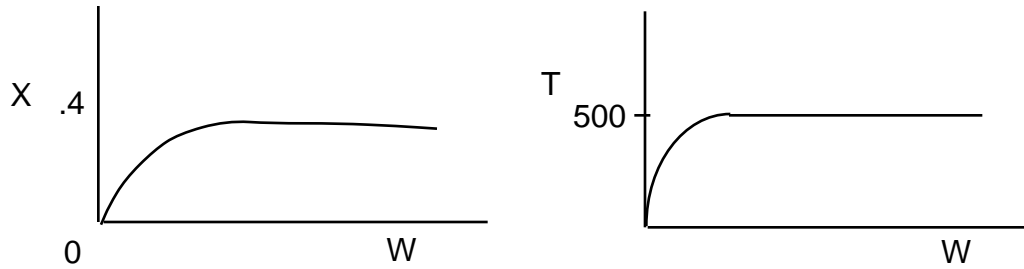
Circle the correct true (T) or False (F) answer for this system

(T) F   a) The above profiles could represent an adiabatic system where the addition of inerts will increase the conversion.

T (F)   b) The above profiles could represent a system where decreasing the flow rate will increase the conversion.

T (F)   c) The above profiles could represent a system where if the feed temperature is increased, one cannot tell from the above profiles whether or not the conversion will increase or decrease.

(T) F   d) There could be a heat exchanger on the reactor for which the heat flow is

$$\frac{d\dot{Q}}{dW} = \frac{1000 \text{ kJ}}{\text{kg s K}} (T - 500)$$

(T) F   e) The above reaction may be an excellent candidate for reactor staging.

a) The reaction is exothermic and adiabatic. Addition of inerts will lower the exit temperature and hence will increase the conversion.

b) Decreasing the flow rate will not change the exit condition because it is an equilibrium condition.

c) Equilibrium is reached early in the reaction, so increase temperature, decrease equilibrium conversion.

d) Because the ambient temperature is 500, same as final equilibrium temperature.

e) Yes, because it may be an exothermic reversible reaction.

W'99FinalExam

(3 pts)   4) The gas phase reaction

$$2A + B \quad \longrightarrow \quad C$$

is carried out in a PFR. The feed is equal molar in A and B and the entering temperature is 500K and the entering pressure is 16.4 atm. If the exit conversion is X, then the exit concentration of B (in mol/dm^3) is
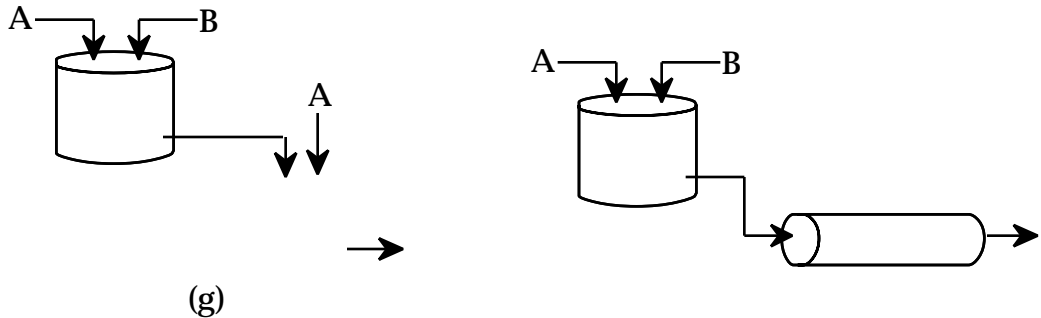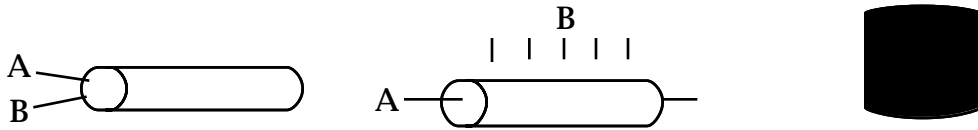
a) $C_B = 0.4\,(1-X)/(1-.5X)$
b) $C_B = 0.4\,(1-X)(1-1.5X)$
c) $C_B = 0.4$
d) $C_B = 0.4\,(1-0.5X)/(1-X)$
e) None of the above
f) Cannot be calculated without knowing the exit conversion.

$$A + \frac{1}{2}B \quad \longrightarrow \quad \frac{1}{2}C$$

$$\varepsilon = y_{A0}\,\delta = \frac{1}{2}\left[\frac{1}{2} - \frac{1}{2} + 1\right]$$

$$= -\frac{1}{2}$$

$$C_B = \frac{C_{A0}\left[\Theta_B - \dfrac{X}{2}\right]}{(1 + \varepsilon X)} = \frac{C_{A0}\left[1 - \dfrac{X}{2}\right]}{1 - \dfrac{X}{2}}$$

$$= C_{A0} = 0.2$$

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(6 pts)   5)   a)   The following elementary liquid phase reactions are to be carried out

$$A + B \quad\longrightarrow\quad R$$

$$R + B \quad\longrightarrow\quad S$$
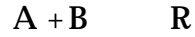
Species R is the desired product. Which of the following schemes should be used?

(g)

b)   In the reactors

$$A \quad\longrightarrow\quad B \qquad r_B = k_B C_A^2$$

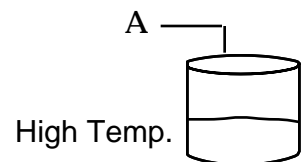$$A + B \quad\longrightarrow\quad 2C \qquad r_C = k_C C_A C_B$$
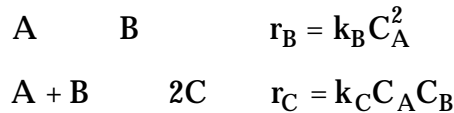
What is the instantaneous selectivity of C to B? Which reactor or combination of reactors and at what temperatures would you use for the following reaction system?
C is the desired product.

Data for Part (b)

$C_{A0} = 4 \ mol/dm^3$ $k_B = 1 \ dm^3/mol$ min at 300K with $E = 4000cal/mol$

$k_C = 1 \ dm^3/mol$ min at 300K with $E = 12000cal/mol$

High Temp.

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(a)

$$r_{1R} = k_{1R}C_A C_B$$

$$r_{2R} = k_{2R}C_R C_B$$

$$S_{RS} = \frac{r_R}{k_{2S}} = \frac{r_{1R} + r_{2R}}{r_{2S}} = \frac{k_{1R}C_A C_B - k_{2S}C_R C_B}{k_{2S}C_R C_B}$$

$$\frac{k_{1R}}{k_{2R}} = \frac{C_A}{C_R} - 1$$

We can maximize S_{RS} by keeping C_A high and C_R low. For keeping C_R low, keep C_B low because

$$r_R = r_{1R} + r_{2R}$$

$$= \left(k_{1R}C_A - k_{2S}C_R\right)C_B$$

$$\boxed{r_R \quad C_B}$$

Hence, use either (b) or (d).

(b)

$$S_{CB} = \frac{r_C}{r_B} = \frac{k_C C_A C_B}{k_B C_A^2 - \frac{1}{2}K_C C_A C_B}$$
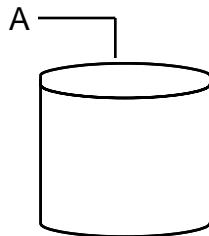
$$= \frac{1}{\dfrac{k_B}{k_C}\dfrac{C_A}{C_B} - \dfrac{1}{2}}$$

$$= \frac{1}{\exp\dfrac{8000}{RT}\dfrac{C_A}{C_B} - \dfrac{1}{2}}$$
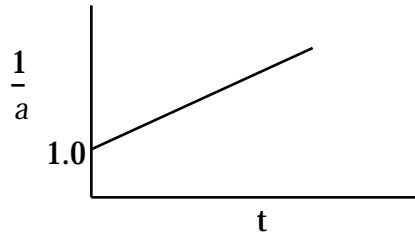
We can maximize S_{CB} by keeping

T high
C_A low
C_B high

Use semibatch
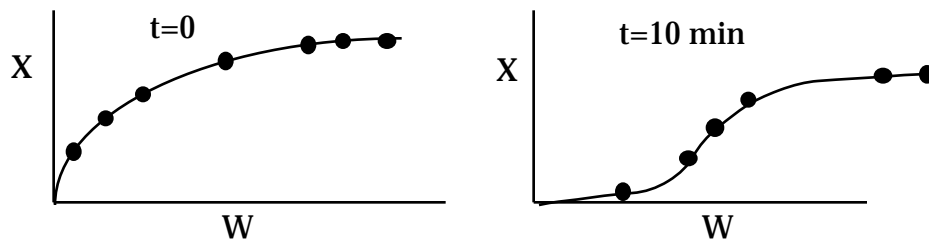

and high reactor temperature.

7

(8 pts) 6) a) The following plot of activity as a function of time was obtained.

What type of decay would best describe to data? (circle the correct answer)
1) Poisoning
2) Sintering
3) Coking
4) None of the above

b) The following profiles were measured in a PBR

The type of catalyst decay can best be described by (circle the correct answer)
1) Poisoning
2) Sintering
3) Coking
4) None of the above

c) The following catalyst activity profile was measured in a PBR for the isomerization of A to B.

The decay law that best describes this data is (circle the correct answer)

1) $\dfrac{da}{dt} = -ka$

2) $\dfrac{da}{dt} = -ka^2$

3) $\dfrac{da}{dt} = -ka\ C_A$

4) $\dfrac{da}{dt} = -ka^2\ C_B$
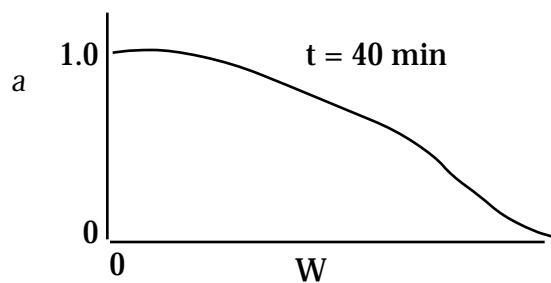
5) None of the above

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(8 pts) 7) (P10-4) The rate law for the hydrogenation (H) of ethylene (E) to form ethane (A) over a cobalt-molybdenum catalyst [*Collection Czech. Chem. Commun.*, **51, 2760** (1988)] is

$$-r_E = \frac{kP_E P_H}{1 + K_E P_E}$$

Suggest a mechanism and rate-limiting step consistent with the rate law. (Can be done by inspection.)

$$E + S \qquad E \cdot S$$

$$E \cdot S + H_2 \qquad A + S \text{ (rate limiting step)}$$
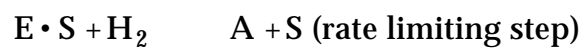
Suppose the heat exchanger in Example E8-12 became fouled so that the overall heat transfer coefficient was reduced by 50%?
What would be the new steady state temperatures inside the reactor?
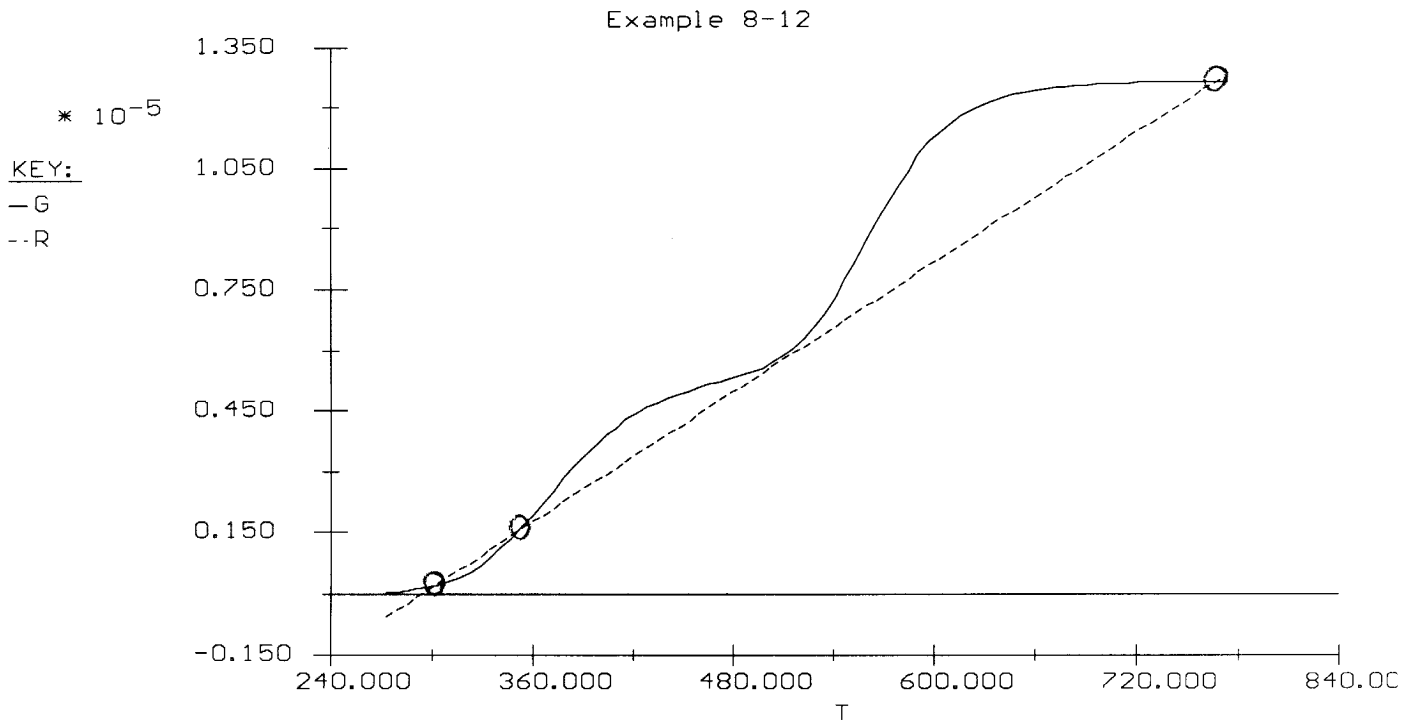
Example 8-12

Example 8-12

T	G	R
273	348.95093	-5800
279.25	523.32713	-4133.3333
285.5	769.89762	-2466.6667
291.75	1111.8544	-800
298	1577.0101	866.66667
304.25	2197.4646	2533.3333
310.5	3008.5355	4200
316.75	4046.7083	5866.6667
323	5346.445	7533.3333
329.25	6935.8923	9200
335.5	8831.8671	10866.667
341.75	11034.913	12533.333
348	13525.569	14200
354.25	16263.058	15866.667
360.5	19187.252	17533.333
366.75	22223.951	19200

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Example 8-12 -- Page 5

T	G	R
673	124704.86	100866.67
679.25	124965.12	102533.33
685.5	125181.44	104200
691.75	125361.86	105866.67
698	125512.9	107533.33
704.25	125639.8	109200
710.5	125746.83	110866.67
716.75	125837.45	112533.33
723	125914.49	114200
729.25	125980.24	115866.67
735.5	126036.57	117533.33
741.75	126085.03	119200
748	126126.89	120866.67
754.25	126163.17	122533.33
760.5	126194.76	124200
766.75	126222.36	125866.67

(20 pts) 9) The elementary liquid phase reactions

$$(1) \quad A \quad B$$

$$(2) \quad 2A \quad C$$

are carried out in a 100 dm^3 PFR where species B is the desired product. Pure A enters at a molar flow rate of 40.0 mol/min and at a concentration of 4.0 mol/dm^3.

Additional Information

$$C_{P_A} = C_{P_B} = 20 \text{ cal/mol/K}$$

$$C_{P_C} = 40 \text{ cal/mol/K}$$

$$H_{Rx1A} = +10,000 \text{ cal/mol}$$

$$H_{Rx2A} = -20,000 \text{ cal/mol}$$

$$Ua = 100 \frac{cal}{dm^3 \ min \ K} \text{ with } T_a = 400K$$

$$k_{1A} = 0.05 \text{ min}^{-1} \text{ at } 400K \text{ with } E = 10,000 \text{ cal/mol}$$

$$k_{2C} = 0.0005 \text{ dm}^3/\text{mol}/\text{min at } 400K \text{ with } E = 19,000 \text{ cal/mol}$$

a) For a feed temperature of 450K, what are the exit concentrations and temperature

$$C_A = \underline{\ 2.55\ }, \ C_B = \underline{\ 1.35\ }, \ C_C = \underline{\ 0.05\ }, \ T = \underline{\ 391\ } K$$

b) The feed temperature can be varied between 400 and 700. What feed temperature do you recommend to maximize the exit molar flow rate of B?

T(K)	F_B (mol/min
400	12.03
500	18.06
600	2.29
550	3.78
525	5.73
505	15.49
495	16.81

75% Marks for setting up the problem correctly with all correct equations and numbers in <u>POLYMATH Notation</u>

25% Final Answer

(9)

Equations: Initial values

d(T)/d(V)=(r1a*dh1a+r2a*dh2a+Ua*(Ta-T))/((Fa+Fb+2*Fc)*Cp   450
    a)

d(Fa)/d(V)=r1a+r2a   40

d(Fb)/d(V)=-r1a   0

d(Fc)/d(V)=-0.5*r2a   0

vo=10

dh1a=10000

dh2a=-20000

Ua=100

Ta=400

Cpa=20

k1a=0.05*exp(-10000/1.987*(1/T-1/400))

k2a=0.001*exp(-19000/1.987*(1/T-1/400))

Ca=Fa/vo

Cb=Fb/vo

Cc=Fc/vo

$$r1a=-k1a*Ca$$

$$r2a=-k2a*Ca^2$$

$$V_0 = 0, \quad V_f = 100$$

Variable	Initial value	Maximum value	Minimum value	Final value
V	0	100	0	100
T	450	450	389.499	391.014
Fa	40	40	25.466	25.466
Fb	0	13.53	0	13.53
Fc	0	0.502042	0	0.502042
vo	10	10	10	10
dh1a	10000	10000	10000	10000
dh2a	-20000	-20000	-20000	-20000
Ua	100	100	100	100
Ta	400	400	400	400
Cpa	20	20	20	20
k1a	0.20235	0.20235	0.0356163	0.0374452
k2a	0.0142414	0.0142414	0.000524915	0.000577311
Ca	4	4	2.5466	2.5466
Cb	0	1.353	0	1.353
Cc	0	0.0502042	0	0.0502042

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a) True because initially the reactor temperature decreases.

b) False because in this case, the temperature should not come back to the initial value.

c) True. The reaction is endothermic and it shows a decrease in temperature first and then the heat exchanger take sit back to the initial temperature.

    (a) (2) second order (sintering?)
    (b) (3) coking
    (c) activity profile missing
    (d)

Variable	Initial value	Maximum value	Minimum value	Final value
V	0	100	0	100
T	450	450	389.499	391.014
Fa	40	40	25.466	25.466
Fb	0	13.53	0	13.53
Fc	0	0.502042	0	0.502042
vo	10	10	10	10
dh1a	10000	10000	10000	10000
dh2a	−20000	−20000	−20000'	−20000
Ua	100	100	100	100
Ta	400	400	400	400
Cpa	20	20	20	20
k1a	0.20235	0.20235	0.0356163	0.0374452
k2a	0.0142414	0.0142414	0.000524915	0.000577311
Ca	4	4	2.5466	2.5466
Cb	0	1.353	0	1.353
Cc	0	0.0502042	0	0.0502042