HW 24.-2

POLYMATH Report
Ordinary Differential Equations

RTD-for 2 CSTR
06-Dec-2011

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	C1	0.1	9.357E-15	0.1	9.357E-15
2	C2	0	0	0.0249176	3.059E-08
3	E	0	0	0.249176	3.059E-07
4	ELT	0	0	0.249176	3.059E-07
5	Et	0	0	0.5198615	9.177E-06
6	Et2	0	0	1.909397	0.0002753
7	t	0	0	30.	30.
8	tau1	1.	1.	1.	1.
9	tau2	2.	2.	2.	2.
10	v	10.	10.	10.	10.
11	V1	10.	10.	10.	10.
12	V2	20.	20.	20.	20.

Differential equations

1 d(C2)/d(t) = 1/tau2*(C1-C2)
2 d(C1)/d(t) = -1/tau1*C1

Explicit equations

1 V1 = 10
2 V2 = 20
3 v = 10
4 tau1 = V1/v
5 tau2 = V2/v
6 E = v*C2
7 Et = v*C2*t
8 Et2 = v*C2*t^2
9 ELT = 1/(tau1-tau2)*(exp(-t/tau1)-exp(-t/tau2))

14-13 (c), (f), & (g)

(g) X by RTD & by mole Balance

$\sigma^2 = 75.4$, $\tau = 9.93$

$\sigma_\theta^2 = 0.765$

(c) 1st order,

$$\frac{C_A}{C_0} = 1 - X = \frac{1}{(1+k\tau_i)^n} = \frac{1}{(1+(0.1)(7.59)]^{1.31}} = 0.477$$

$X = 1 - 0.477 = 0.52$

$$\sigma_\theta^2 = \frac{\sigma^2}{\tau^2} = \frac{75.4}{(9.93)^2} = 0.765$$

TIS model, $\sigma_\theta^2 = \frac{1}{n}$, $n = \frac{1}{\sigma_\theta^2} = 1.31$

$$\tau_i = \frac{\tau}{n} = \frac{9.93}{1.31} = 7.59$$

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by interpolation

1-CSTR:

$$\frac{C_A}{C_{A0}} = \frac{1}{1+k\tau} = \frac{1}{1+(0.1)(9.93)} = 0.517 \quad , \quad X_1 = 0.482$$

2-CSTR

$$\frac{C_A}{C_{A0}} = \frac{1}{(1+k_i\tau_i)^2} = \frac{1}{[1+(0.1)(9.93)/2]^2} = 0.446$$

$X_2 = 553$.

$$X = 0.482 + \left(\frac{0.553 - 0.482}{2}\right)(0.31)$$

$= 0.493$

POLYMATH Report
Ordinary Differential Equations

14-13-f
24-Nov-2010

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	a	1.13	1.13	1.13	1.13
2	C1	0.02014	7.607E-13	0.02014	7.607E-13
3	C2	0	0	0.007847	1.044E-12
4	E	0	0	0.0784698	1.044E-11
5	Et2	0	0	2.553558	3.773E-07
6	k1	0.1	0.1	0.1	0.1
7	k2CA0	0.1	0.1	0.1	0.1
8	t	0	0	200.	200.
9	Tau	0	0	9.929513	9.929513
10	tau	9.93	9.93	9.93	9.93
11	v	10.	10.	10.	10.
12	var	0	0	75.45451	75.45451
13	vartheta	0	0	0.7652207	0.7652207
14	X1	0	0	1.	1.
15	X1bar	0	0	0.5257559	0.5257559
16	X2	0	0	0.952381	0.952381
17	X2bar	0	0	0.4240153	0.4240153

Trial & Error

Assume a
Do Polymath calc
See if $\sigma_\theta^2 = 0.765$
If not, repeat

$= \sigma_\theta^2$

← 1st order

← 2nd order

Differential equations

1 d(C2)/d(t) = 2*(a+1)/tau*(C1-C2)
2 d(C1)/d(t) = 2*a*C2/tau-2*(a+1)/tau*C1
3 d(Tau)/d(t) = E*t
4 d(X1bar)/d(t) = X1*E
5 d(X2bar)/d(t) = X2*E
6 d(var)/d(t) = Et2

$v = a v_0 = 1.13 \times 10 = 11.3$

Explicit equations

1 a = 1.13
2 tau = 9.93
3 v = 10
4 E = v*C2
5 Et2 = E*(t-tau)^2
6 vartheta = var/tau^2
7 k2CA0 = 0.1
8 k1 = 0.1
9 X1 = 1-exp(-k1*t)
10 X2 = k2CA0*t/(1+k2CA0*t)

2nd order

RTD method

→ X_2 (2nd order) = ~~0.424~~ 0.422

Mole Balance Method

X_2 = ~~0.424~~ 0.424

T_{1S} =

POLYMATH Report
Nonlinear Equations

No Title
24-Nov-2010

Calculated values of NLE variables

	Variable	Value	f(x)	Initial Guess
1	CA1	0.6780498	-7.332E-09	0.5
2	CA2	0.5953475	-1.171E-08	0.5

	Variable	Value
1	a	1.13
2	CA0	1.
3	rA1	-0.0459752
4	rA2	-0.0354439
5	v	10.
6	V1	49.7
7	V2	49.7
8	X1	0.3219502
9	X2	0.4046525

Nonlinear equations

1 f(CA1) = v*CA0+a*v*CA2+V1*rA1-(a+1)*v*CA1 = 0

2 f(CA2) = (a+1)*v*CA1+V2*rA2-(a+1)*v*CA2 = 0

Explicit equations

1 V1 = 49.7

2 V2 = 49.7

3 v = 10

4 CA0 = 1

5 a = 1.13

6 rA1 = -0.1*CA1^2

7 rA2 = -0.1*CA2^2

8 X1 = 1-CA1

9 X2 = 1-CA2

General Settings

Total number of equations	11
Number of implicit equations	2
Number of explicit equations	9
Elapsed time	0.0000 sec
Solution method	SAFENEWT
Max iterations	150
Tolerance F	0.0000001
Tolerance X	0.0000001
Tolerance min	0.0000001

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