

Solution of a System of ODEs with POLYMATH and Excel, Parametric Studies with Excel

The canonical form of a system of n simultaneous first-order ordinary differential equations ODE with specified initial values (initial value problem) is:

$$\frac{dy_1}{dx} = f_1(y_1, y_2, \dots, y_n, x)$$

$$y_1(x_0) = y_{1,0}$$

$$\frac{dy_2}{dx} = f_2(y_1, y_2, \dots, y_n, x)$$

$$y_2(x_0) = y_{2,0}$$

⋮

⋮

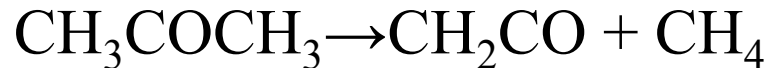
$$\frac{dy_n}{dx} = f_n(y_1, y_2, \dots, y_n, x)$$

$$y_n(x_0) = y_{n,0}$$

where x is the independent variable and y_1, y_2, \dots, y_n are dependent variables

Adiabatic Operation of a Tubular Reactor for Cracking of Acetone

The irreversible, vapor-phase cracking of acetone (A) to ketene (B) and methane (C) that is given by the reaction:



is carried out adiabatically in a tubular reactor. The reaction is first order with respect to acetone and the specific reaction rate can be expressed by

$$\ln k = 34.34 - \frac{34222}{T}$$

The acetone feed flow rate to the reactor is F_A mol/s, the inlet temperature is $T = 1150$ K and the reactor operates at the constant pressure of $P = 162$ kPa (1.6 atm). The volume of the reactor is $V = 4$ m³. Inert gas (nitrogen) is fed at the rate of F_N mol/s.

Adiabatic Operation of a Tubular Reactor for Cracking of Acetone - Assignments

- (a) Calculate the flow-rates (in mol/s) and the mole fractions of acetone, ketene and methane along the reactor for the case where **pure toluene** is being fed at the rate of $F_A = 38.3$ g-mol/s. Use Polymath to calculate and plot the conversion and reactor temperature (in K) versus volume.
- (b) The conversion in the reactor in part (a) is very low in adiabatic operation because the reactor content cools down very quickly. It is suggested that feeding nitrogen along with the acetone might be beneficial in maintaining a higher temperature. Compare the final conversions and temperatures for the cases where **28.3, 18.3, 8.3, 3.3 and 0.0 mol/s nitrogen** is fed into the reactor (the total molar feed rate is 38.3 mol/s in all the cases).

Adiabatic Operation of a Tubular Reactor for Cracking of Acetone – Model Equations

POLYMATH 6.10 Educational Release - [Ordinary Differential Equations Solver]

File Program Edit Format Problem Examples Window Help

dx= x= init/init RKF45 Table Graph Report

Differential Equations: 4 Auxiliary Equations: 15 Ready for solution

```
d(FA)/d(V) = rA # Differential mass balance on acetone
d(FB)/d(V) = -rA # Differential mass balance on ketene
d(FC)/d(V) = -rA # Differential mass balance on methane
d(T)/d(V) = (-deltaH) * (-rA) / (FA * CpA + FB * CpB + FC * CpC + FN * CpN) # Differential enthalpy balance
XA = (FA0-FA)/FA0 # Conversion of acetone
rA = -k * CA # Reaction rate in g-mol/m3-s
FA0 = 38.3 # Feed rate of acetone in g-mol/s
FN = 38.3 - FA0 # Feed rate of nitrogen in g-mol/s
P = 162 # Pressure kPa
CA = yA * P * 1000 / (8.31 * T) # Concentration of acetone in k-mol/m3
yA = FA / (FA + FB + FC + FN) # Mole fraction of acetone
yB = FB / (FA + FB + FC + FN) # Mole fraction of ketene
yC = FC / (FA + FB + FC + FN) # Mole fraction of methane
k = 8.2E14 * exp(-34222 / T) # Reaction rate constant in s-1
deltaH = 80770 + 6.8 * (T - 298) - .00575 * (T ^ 2 - 298 ^ 2) - 1.27e-6 * (T ^ 3 - 298 ^ 3) # Heat of reaction in J/mol-K
CpA = 26.6 + .183 * T - 45.86e-6 * T ^ 2 # Heat capacity of acetone in J/mol-K
CpB = 20.04 + 0.0945 * T - 30.95e-6 * T ^ 2 # Heat capacity of ketene in J/mol-K
CpC = 13.39 + 0.077 * T - 18.71e-6 * T ^ 2 # Heat capacity of methane in J/mol-K
CpN = 6.25 + 8.78e-3 * T - 2.1e-8 * T ^ 2 # Heat capacity of nitrogen in J/mol-K
FB(0) = 0 # Feed rate of ketene in g-mol/s
FA(0) = 38.3 # Feed rate of acetone in g-mol/s
FC(0) = 0 # Feed rate of methane in g-mol/s
T(0) = 1035 # Inlet reactor temperature in K
V(0) = 0 # Reactor volume in m3
V(f) = 4
```

Ln 6 P4-3B.POL ADIABATIC OPERATION OF A TUBULAR REACTOR FOR CRACKING OF ACETONE

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Export to Excel

The POLYMATH code provides complete and clear documentation

Adiabatic Operation of a Tubular Reactor for Cracking of Acetone – Solution for $F_A = 38.3$ mol/s

POLYMATH 6.10 Educational Release - [Differential Equations Solution #1]

POLYMATH Report ADIABATIC OPERATION OF A TUBULAR REACTOR FOR
Ordinary Differential Equations

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	CA	18.83535	12.68959	18.83535	12.68959
2	CpA	166.8786	154.9084	166.8786	154.9084
3	CpB	84.69309	80.3113	84.69309	80.3113
4	CpC	73.04238	67.86058	73.04238	67.86058
5	CpN	15.3148	14.20092	15.3148	14.20092
6	deltaH	7.876E+04	7.876E+04	7.977E+04	7.977E+04
7	FA	38.3	28.44647	38.3	28.44647
8	FA0	38.3	38.3	38.3	38.3
9	FB	0	0	9.853527	9.853527
10	FC	0	0	9.853527	9.853527
11	FN	0	0	0	0
12	k	3.580818	0.0344545	3.580818	0.0344545
13	P	162.	162.	162.	162.
14	rA	-67.44594	-67.44594	-0.4372133	-0.4372133
15	T	1035.	907.5422	1035.	907.5422
16	V	4.	0	4.	4.
17	XA	0	0	0.2572723	0.2572723
18	yA	1.	0.5907454	1.	0.5907454
19	yB	0	0	0.2046273	0.2046273
20	yC	0	0	0.2046273	0.2046273

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Drop of ~120 K in the temperature reduces the reaction rate by two orders of magnitude

Low conversion of the reactant

Adiabatic Operation of a Tubular Reactor – Exporting to Excel and Adding the ODE Solver

Polymath DEQ Migration Document

	Variable	Value	Polymath Equation
Explicit Eqs	XA	0	$XA = (FA_0 - FA) / FA_0$
	rA	-17.60990721	$rA = -k * CA$
	FA0	10	$FA_0 = 10$
	FN	28.3	$FN = 38.3 - FA_0$
	P	162	$P = 162$
	CA	4.917845344	$CA = yA * P * 1000 / (8.31 * T)$
	yA	0.261096606	$yA = FA / (FA + FB + FC + FN)$
	yB	0	$yB = FB / (FA + FB + FC + FN)$
	yC	0	$yC = FC / (FA + FB + FC + FN)$
	k	3.580817609	$k = 8.2E14 * \exp(-34222 / T)$
	deltaH	78758.21631	$\text{delta}H = 80770 + 6.8 * (T - 298) - 0.0001 * T^2$
	CpA	166.8786215	$CpA = 26.6 + .183 * T - 45.86e-6 * T^2$
	CpB	84.69308625	$CpB = 20.04 + 0.0945 * T - 30.95e-6 * T^2$
	CpC	73.04238025	$CpC = 13.39 + 0.077 * T - 18.71e-6 * T^2$
	CpN	15.31480428	$CpN = 6.25 + 8.78e-3 * T - 2.1e-8 * T^2$
Integration Vars	FA	10	$FA(0) = 10$
	FB	0	$FB(0) = 0$
	FC	0	$FC(0) = 0$
	T	1035	$T(0) = 1035$
ODE Eqs	d(FA)/d(V)	-17.60990721	$d(FA)/d(V) = rA$
	d(FB)/d(V)	17.60990721	$d(FB)/d(V) = -rA$
	d(FC)/d(V)	17.60990721	$d(FC)/d(V) = -rA$
	d(T)/d(V)	-659.7507676	$d(T)/d(V) = (-\text{delta}H) * (-rA) / (FA * CpA + FB * CpB + FC * CpC + FN * CpN)$
Indep Var	V	0	$V(0) = 0; V(f) = 4$

Add-Ins

Add-Ins available:

- Analysis ToolPak
- Analysis ToolPak - VBA
- Conditional Sum Wizard
- Euro Currency Tools
- Internet Assistant VBA
- Lookup Wizard
- Ode Solver
- Solver Add-in

Solver Add-In should be removed

Separate Worksheets are Prepared for the Various Cases

Ready

Adiabatic Operation of a Tubular Reactor – ODE Solver Add In Communication Box

Microsoft Excel - Example-4

File Edit View Insert Format Tools Data Window Help

Type a question for help

100%

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	A	B	C	D	E	F
1	POLYMATH DEQ Migration Document					
2		Variable	Value		Polymath Equation	Comments
3	Explicit Eqs	XA	0		$XA=(FA0-FA)/FA0$	Conversion of acetone
4		rA	-17.60990721		$rA=-k * CA$	Reaction rate in g-mol/m ³ -s
5		FA0	10		$FA0=10$	Feed rate of acetone in g-mol/s
6		FN	28.3		$FN=3$	in g-mol/s
7		P	162		$P=162$	one in k-mol/m ³
8		CA	4.917845344		$CA=yA$	ne
9		yA	0.261096606		$yA=FA$	e
10		yB	0		$yB=FB$	ne
11		yC	0		$yC=FC$	ne
12		k	3.580817609		$k=8.2$	t in s-1
13		deltaH	78758.21631		$deltaH$	mol-K
14		CpA	166.8786215		$CpA=$	one in J/mol-K
15		CpB	84.69308625		$CpB=$	ne in J/mol-K
16		CpC	73.04238025		$CpC=$	ane in J/mol-K
17		CpN	15.31480428		$CpN=$	gen in J/mol-K
18	Integration Vars	FA	10		$FA(0)=$	ance on acetone
19		FB	0		$FB(0)=$	ance on ketene
20		FC	0		$FC(0)=$	ance on methane
21		T	1035		$T(0)=$	Differential enthalpy balance
22	ODE Eqs	d(FA)/d(V)	-17.60990721		$d(FA)/d(V) = rA$	
23		d(FB)/d(V)	17.60990721		$d(FB)/d(V) = -rA$	
24		d(FC)/d(V)	17.60990721		$d(FC)/d(V) = -rA$	
25		d(T)/d(V)	-659.7507676		$d(T)/d(V) = (-deltaH) * (-rA) / (FA * CpA + FB * CpB + FC * CpC + FN * CpN)$	
26	Indep Var	V	0		$V(0)=0; V(f)=4$	
27						

Polymath ODE

ODE initial values vector (Y)

ODE equations vector (Y')

Differential variable cell

Diff. variable final value

Show Report

Intermediate Cells to Store

Data Points

Exit Clear Adv. Help Solve

Sheet1 Sheet2 Sheet3

Adiabatic Operation of a Tubular Reactor – Comparison of results for $F_N = 0$ and $F_N = 28.3$

Microsoft Excel - Example-4

File Edit View Insert Format Tools Data Window Help

Type a question for help

E27

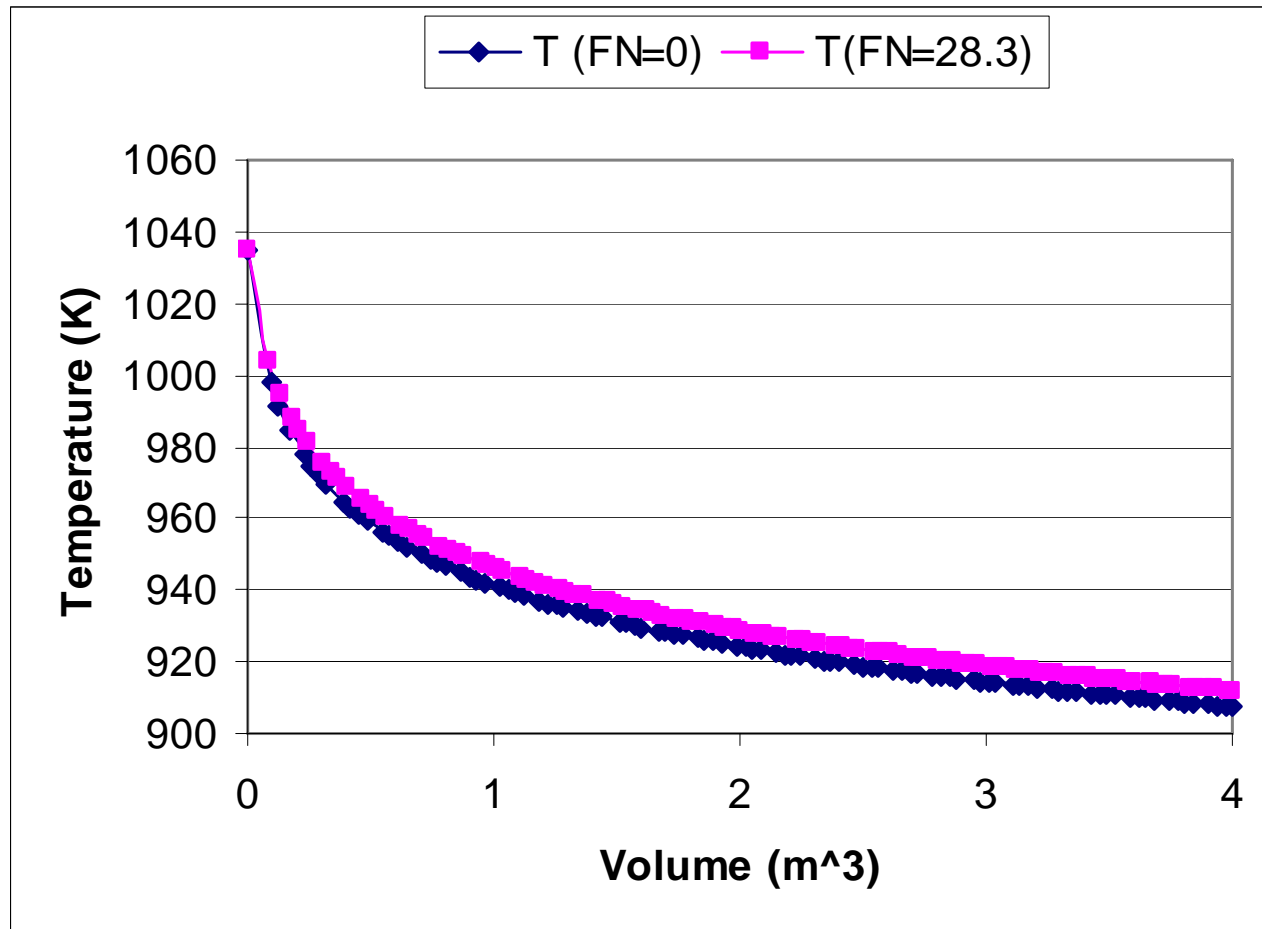
POLYMATH DEQ Migration Document						
	Variable	value	value	Equation	Comments	
3	Explicit Eqs	XA	0.313552401	0.257272258	FA0	Conversion of acetone
4		rA	-0.145866418	-0.437213285		Reaction rate in g-mol/m ³ -s
5		FA0	10	38.3		Feed rate of acetone in g-mol/s
6		FN	28.3	0		
7		P	162	162		
8		CA	3.541783023	12.68958732	$000 / (8.3 \times 10^{-3})$	
9		yA	0.165666446	0.590745352	$FB + FC + FA$	
10		yB	0.075672363	0.204627324	$FB + FC + FA$	
11		yC	0.075672363	0.204627324	$FB + FC + FA$	
12		k	0.041184459	0.034454492	$k(-34222)$	
13		deltaH	79744.527	79773.92861	$0 + 6.8 \times 10^4$	
14		CpA	155.3379823	154.9084155	$183 \times T - 445.0$	
15		CpB	80.47607044	80.3112995	$0.094 \times T -$	
16		CpC	68.04592572	67.86057679	$0.07 \times T -$	
17		CpN	14.2386407	14.2009238	$0.78 \times 10^{-3} \times T -$	
18	Integration Vars	FA	6.864475993	28.44647253		Differential mass balance on acetone
19		FB	3.135524007	9.853527468		Differential mass balance on ketene
20		FC	3.135524007	9.853527468		Differential mass balance on methane
21		T	911.8567009	907.5421516		Differential enthalpy balance
22	ODE Eqs	d(FA)/d(V)	-0.145866418	-0.437213285		
23		d(FB)/d(V)	-0.145866418	-0.437213285	rA	
24		d(FC)/d(V)	0.145866418	0.437213285	rA	
25		d(T)/d(V)	-6.011513678	-5.945205114	$\text{deltaH} \times (-rA) / (FA \times CpA + FB \times CpB + FC \times CpC + FN \times CpN)$	
26	Indep Var	V	4	4		

Ready

FN=0 FN=3.3 FN=8.3 FN=18.3 FN=28.3 DEQ Solution (1) Sheet1

No significant change in the temperature profile and the conversion occurs because of the addition of the inert gas.

Adiabatic Operation of a Tubular Reactor – Comparison of results for $F_N = 0$ and $F_N = 28.3$



Adiabatic Operation of a Tubular Reactor – Comparison of results for $F_N = 0$ and $F_N = 28.3$

