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:

$$\frac{dy_1}{dx} = f_1(y_1, y_2, \ldots y_n, x) \qquad y_1(x_0) = y_{1,0}$$

$$\frac{dy_2}{dx} = f_2(y_1, y_2, \ldots y_n, x) \qquad y_2(x_0) = y_{2,0}$$

$$\vdots \qquad\qquad \vdots$$

$$\frac{dy_n}{dx} = f_n(y_1, y_2, \ldots y_n, x) \qquad y_n(x_0) = y_{n,0}$$

where x is the independent variable and $y_1, y_2, \ldots y_n$ 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:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4$$

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

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

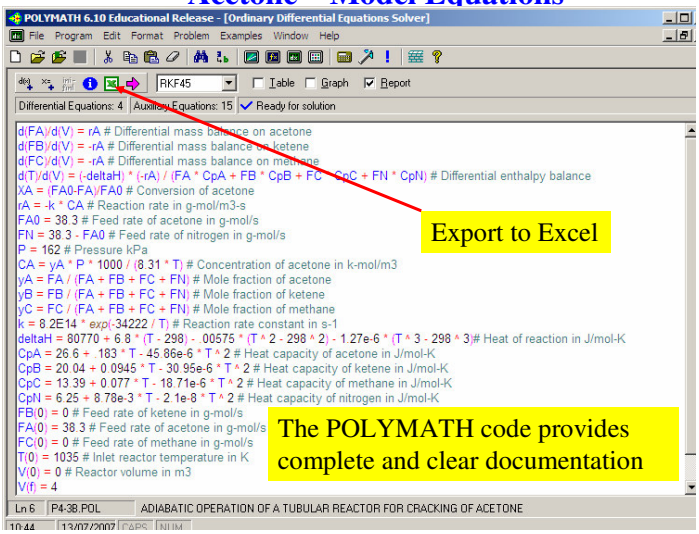
The acetone feed flow rate to the reactor is F_A mol/s, the inlet temperature is $T = 1150$ K and the reactor operates at the constant pressure of $P = 162$ kPa (1.6 atm). The volume of the reactor is $V = 4$ m^3. Inert gas (nitrogen) is fed at the rate of F_N mol/s.

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



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]

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POLYMATH Report ADIABATIC OPERATION OF A TUBULAR REACTOR F

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	1.	0	4.	1.
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

Microsoft Excel - Book1

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E27

POLYMATH DEQ Migration Document

		Variable	Value	Polymath Equation
2				
3	Explicit Eqs	XA	0	XA=(FA0-FA)/FA0
4		rA	-17.60990721	rA=-k * CA
5		FA0	10	FA0=10
6		FN	28.3	FN=38.3 - FA0
7		P	162	P=162
8		CA	4.917845344	CA=yA * P * 1000 / (8.31 * T)
9		yA	0.261096606	yA=FA / (FA + FB + FC + FN)
10		yB	0	yB=FB / (FA + FB + FC + FN)
11		yC	0	yC=FC / (FA + FB + FC + FN)
12		k	3.580817609	k=8.2E+4 * exp(-34222 / T)
13		deltaH	78758.21631	deltaH=80770 + 6.8 * (T - 298) - .0
14		CpA	166.8786215	CpA=26.6 + .183 * T - 45.86e-6 * T
15		CpB	84.69308625	CpB=20.04 + 0.0945 * T - 30.95e-
16		CpC	73.04238025	CpC=13.39 + 0.077 * T - 18.71e-6
17		CpN	15.31480428	CpN=6.25 + 8.78e-3 * T - 2.1e-8 *
18	Integration Vars	FA	10	FA(0)=10
19		FB	0	FB(0)=0
20		FC	0	FC(0)=0
21		T	1035	T(0)=1035
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
26	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
Ode_Solver
Solver Add-in

OK Cancel Browse... Automation...

Ode_Solver

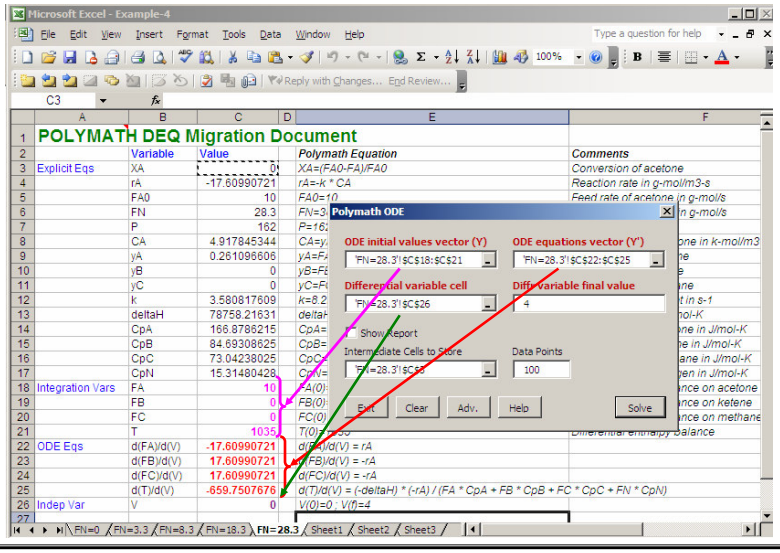
FN=0 FN=3.3 FN=8.3 FN=18.3 FN=28.3 Sheet1 Sheet2 Sheet3

Ready

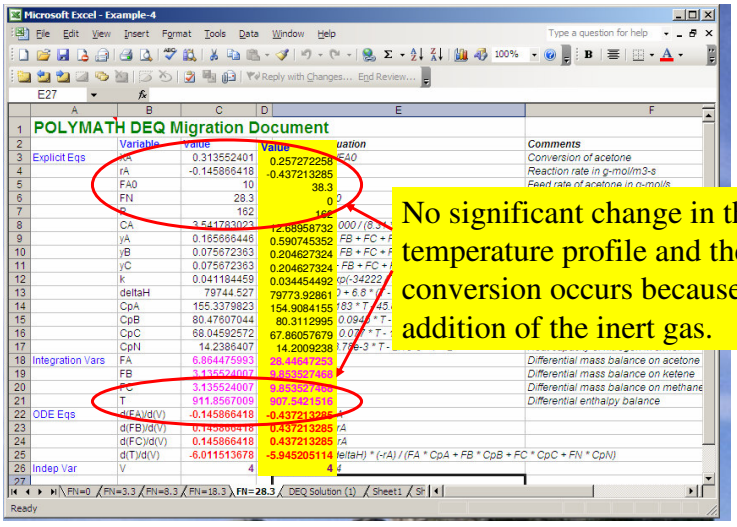
Solver Add-In should be removed

Separate Worksheets are Prepared for the Various Cases

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

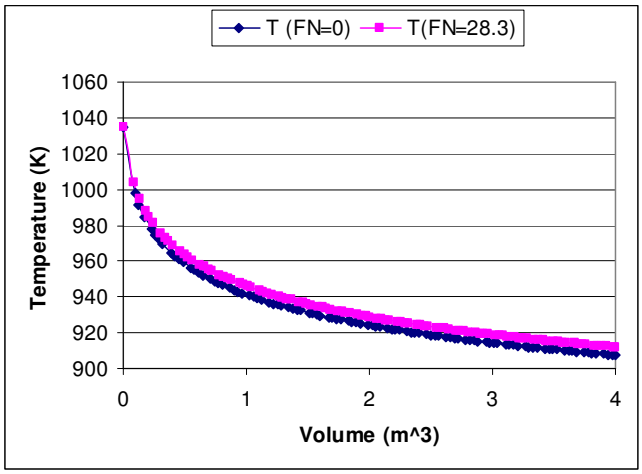


Adiabatic Operation of a Tubular Reactor – Comparison of results for $F_N = 0$ and $F_N = 28.3$



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 $F_N = 28.3$