

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

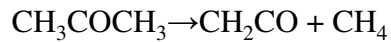
The canonical form of a system of n simultaneous first-order ordinary differential equations ODE with specified initial values (initial value problem) is:

$$\begin{array}{ll} \frac{dy_1}{dx} = f_1(y_1, y_2, \dots, y_n, x) & y_1(x_0) = y_{1,0} \\ \frac{dy_2}{dx} = f_2(y_1, y_2, \dots, y_n, x) & y_2(x_0) = y_{2,0} \\ \vdots & \vdots \\ \frac{dy_n}{dx} = f_n(y_1, y_2, \dots, y_n, x) & y_n(x_0) = y_{n,0} \end{array}$$

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

Run Stop Breakpoint Insert Breakpoint Help

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) - 0.0675 * (T^2 - 298^2) - 1.27E-6 * (T^3 - 298^3) # Heat of reaction in J/mol-K
CpA = 26.6 + 0.183 * 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(tf) = 4
  
```

Export to Excel

The POLYMATH code provides complete and clear documentation

Ln 6 P4:38.POL ADIABATIC OPERATION OF A TUBULAR REACTOR FOR CRACKING OF ACETONE

10.44 13/07/2007 10:40:11

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

POLYMATH Report
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 | 0 | 0 | 4. | 0.2572723 |
| 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 |

No File POLYMATH Report
1/15/13 13:02/2007 /CARS/ NJIM

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

File Edit View Insert Format Tools Data Window Help

Type a question for help

100%

Reply with Changes... Egd Review...

E27

POLYMATH DEQ Migration Document

| Variable | Value | Polymath Equation |
|------------------|--------------|--|
| Explicit Eqs | | |
| XA | 0 | XA=(FA0-FA)/FA0 |
| rA | -17.60990721 | RA=k * CA |
| FA0 | 10 | FA0=10 |
| FN | 28.3 | FN=38.3 - FA0 |
| P | 162 | P=162 |
| CA | 4.917845344 | CA=A * P * 1000 / (8.31 * T) |
| yA | 0.261095806 | 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=8.25E4 * exp(-34222 / T) |
| deltaH | 78758.21631 | deltaH=80770 + 6.8 * (T - 298) - 0. |
| CpA | 166.8786215 | CpA=26.6 + 183 * T - 45.86e-6 * T |
| CpB | 84.69308625 | CpB=20.04 + 0.0945 * T - 30.95e-6 |
| CpC | 73.04238025 | CpC=13.39 + 0.077 * T - 18.71e-6 |
| CpN | 15.31480428 | CpN=6.25 + 8.79e-3 * T - 2.1e-8 |
| 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) | -659.7507678 | d(T)/d(V) = (-deltaH) * (rA) / (FA * CpA + FB * CpB + FC * CpC + FN * CpN) |
| Indep Var | 0 | V(0)=0, V(f)=4 |

Ready

W:\Nrc0\Nrc=3\FN=28.3\FN=18.3\FN=28.3\Sheet1 Sheet2 Sheet3

Add-Ins available:

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

OK Cancel Browse... Automation...

Ode Solver

Solver Add-In should be removed

Separate Worksheets are Prepared for the Various Cases

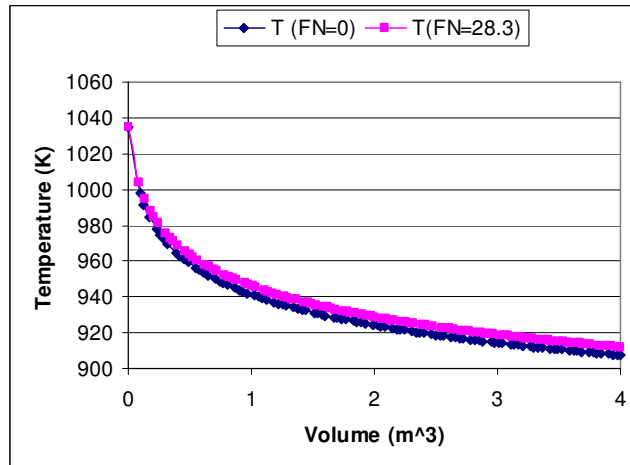
Adiabatic Operation of a Tubular Reactor – ODE Solver Add In Communication Box

The screenshot shows the POLYMATH DEQ Migration Document in Microsoft Excel. The document is a table with columns for Variable, Value, Polymath Equation, and Comments. It includes sections for Explicit Eqs, Integration Vars, ODE Eqs, and Indep Var. A Polymath ODE dialog box is open, showing initial values and equations for variables Y1, Y2, Y3, and Y4. The dialog box has fields for 'ODE initial values vector (Y)' and 'ODE equations vector (Y)', and a 'Solve' button.

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

The screenshot shows the POLYMATH DEQ Migration Document in Microsoft Excel. The document is a table with columns for Variable, Value, Polymath Equation, and Comments. It includes sections for Explicit Eqs, Integration Vars, ODE Eqs, and Indep Var. A yellow callout box highlights the text: "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 $F_N = 28.3$

