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Review Paper

Modeling and Simulation Study of the CSTR for Complex Reaction by Using Polymath

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Abstract

This paper deals with basic simulation studies on of the common used devices in chemical industry Continuous Stirred Tank Reactor (CSTR). Simulations on mathematical models has several advantages over the experiment on a real model or system. The mathematical model is developed from material balances. Simulation is very important and popular tool now a days, when computation speed of computers increases exponentially every day numerical mathematics is used for steady-state analysis and dynamic analysis. Simulation results are used for choosing of an optimal working point and an external linear model of this nonlinear plant. This paper deals with simulation experiments on one type of nonlinear systems, CSTR reactor. This simulations results in optimal working point, external linear model and they will be later used for choosing of an optimal working point and mainly for control purpose.

Keywords: Polymath, CSTR, steady-state, dynamics, Runge-Kutta's method.

Introduction

There are several types of stirred reactors used in chemical or biochemical industry. Continuous Stirred Tank Reactors (CSTR) are common used because of their technological paramers. Reaction inside flows continuously and we can control this reaction by for example volumetric flow rate of the reactant (Ingham et al. 2000). The first step is introducing of the mathematical model which describes relations between state variables in the mathematical way. This mathematical model comes from material or heat balances inside the reactor. In our case of isothermal reactor with complex reaction (Russell and Denn 1972) is mathematical model the set of ordinary differential equations (ODE). Simulation usually consists of steady-state analysis which observes behaviour of the system in steady-state and dynamic analysis which shows dynamic behavior after the step change of the input quantity (Ingham et al. 2000, Luyben 1989).

Model of the Reactor

Reactor under the consideration is isothermal reactor with complex reaction. Reactions inside the reactor can be described by following reactions:

$$A + B \xrightarrow{k_1} X \quad (1)$$

$$B + X \xrightarrow{k_2} Y \quad (2)$$

$$B + Y \xrightarrow{k_3} Z \quad (3)$$

This reaction has sequential $A \rightarrow X \rightarrow Y \rightarrow Z$,
As well as parallel characteristics $B \rightarrow X,\ B \rightarrow Y,\ B \rightarrow Z$

Mathematical description of all variables is of course very complicated. Therefore there must be introduced some simplifications before we start to build the mathematical model of the plant. We expect, that reactant inside the tank is perfectly mixed and volume of the reactant is constant during the reaction. The mathematical model of the system is then derived from the material balances inside the reactor. All three reactions are assumed to follow second order kinetics.

Tacking component balance on A, We get.

$$\frac{d(V*C_A)}{d(t)} = (F_0 * C_{A0} - F * C_A) - k_1 * C_A * C_B * V \quad (4)$$

Dividing by V on both side

$$\frac{d(C_A)}{d(t)} = \frac{F_0*C_{A0}-F*C_A}{V} - k_1 * C_A * C_B \quad (5)$$

Tacking component balance on B, We get.

$$\frac{d(V*C_B)}{d(t)} = (F_0 * C_{B0} - F * C_B) - k_1 * C_A * C_B * V - k_2 * C_B * C_X * V - k_3 * C_B * C_Y * V \quad (6)$$

Dividing by V on both side

$$\frac{d(C_B)}{d(t)} = (F_0 * C_{B0} - F * C_B)/V - k_1 * C_A * C_B - k_2 * C_B * C_X - k_3 * C_B * C_Y \quad (7)$$

Similarly, We can write for component X, Y, Z

$$\frac{d(C_X)}{d(t)} = \frac{(F_0*C_{X0}-F*C_X)}{V} + k1 * C_A * C_B - k_2 * C_B * C_X \quad (8)$$

$$\frac{d(C_Y)}{d(t)} = \frac{(F_0*C_{Y0}-F*C_Y)}{V} + k_2 * C_B * C_X - k_3 * C_B * C_Y \quad (9)$$

$$\frac{d(C_Z)}{d(t)} = \frac{(F_0*C_{Z0}-F*C_Z)}{V} + k_3 * C_B * C_Y \quad (10)$$

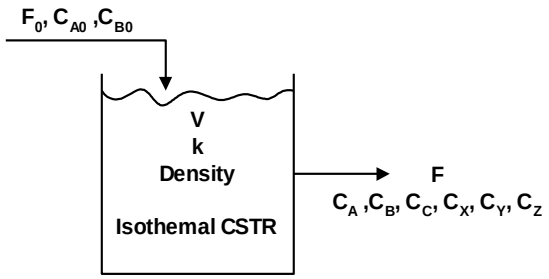

Figure- 1
Isothermal CSTR

This set of nonlinear ODE describes behavior of the state variables which are in this case concentrations of components *A, B, X, Y* and *Z* are C_A, C_B, C_C, C_X, C_Y and C_Z in time t respectively. We can say, that this CSTR belongs to the class of nonlinear lumped-parameters systems. In above equation no.(4) to equation no. (10), F denotes volumetric flow rate, V is volume of the tank, k means rate constants and C are concentrations. Numerical subscripts 1, 2 and 3 represent reaction steps. Assuming inlet flow rate is equal to outlet flow rate i.e. $F_0 = F$. Some technological parameters and constants are shown in table 1.

Table- 1
Parameters of the Reactor

Sr.no.	Parameter	Value of parameter with unit
1.	k_1	5×10^{-4} (m^3/kmol.s)
2.	k_2	5×10^{-2} (m^3/kmol.s)
3.	k_3	2×10^{-2} (m^3/kmol.s)
4.	C_{A0}	0.4 (kmol/m^3)
5.	C_{B0}	0.6 (kmol/m^3)
6.	C_{X0} , C_{Y0}, C_{Z0}	0 (kmol/m^3)
7.	V	1 (m^3)
8.	F	0.01 (m^3/s)

Simulation Results

There were done two basic simulation studies steady state analysis and dynamic analysis. Both analyses use numerical methods for computation.

Steady-state analysis: Steady-state analysis means computation of the state variables in time $t \to \infty$, where we expect that the value of this quantity is stable. From the computation point of view it means, that all derivatives with respect to time are equal to zero, i.e. $d(\cdot)/dt = 0$.

$$\frac{d(C_A)}{d(t)} = 0 = \frac{F*C_{A0}-F*C_A}{V} - k_2 * C_A * C_B$$

$$C_A = F * C_{A0}/(F + V * k_1 * C_B) \quad (11)$$

Similarly, equation (7) to (10) we get, steady state equations of C_A, C_B, C_X, C_Y, and C_Z

$$C_B = F * C_{B0}/(F + k_1 C_A * V + k_2 * C_X * V + k_3 * C_Y * V \quad (12)$$

$$C_X = (F * C_{X0} + V * k_1 * C_A * C_B)/(F + k_2 C_B * V \quad (13)$$

$$C_Y = (F * C_{Y0} + V * k_2 * C_B * C_X)/(F + k_3 * C_B * V \quad (14)$$

$$C_Z = (F * C_{Z0} + k_3 * C_B * C_Y)/F \quad (15)$$

Figures 2 represent course of the computed steady-state values of the state variables. As it can been seen, value is computed value is stable nearly around t=1000 sec, after that the concentration values are not changed.

Table-2
Calculated values of steady state concentrations

	Variable	Initial value	Minimal value	Maximal value	Final value
1	t	0	0	1500.	1500.
2	CA	0.4	0.3888017	0.4	0.3888017
3	CB	0.6	0.5760397	0.6	0.5760397
4	CX	0	0	0.0029114	0.002886
5	CY	0	0	0.0038744	0.0038624
6	CZ	0	0	0.0044498	0.0044498
7	F	0.01	0.01	0.01	0.01
8	V	1.	1.	1.	1.
9	CA0	0.4	0.4	0.4	0.4
10	CB0	0.6	0.6	0.6	0.6
11	CX0	0	0	0	0
12	CY0	0	0	0	0
13	CZ0	0	0	0	0
14	k1	0.0005	0.0005	0.0005	0.0005
15	k2	0.05	0.05	0.05	0.05
16	k3	0.02	0.02	0.02	0.02

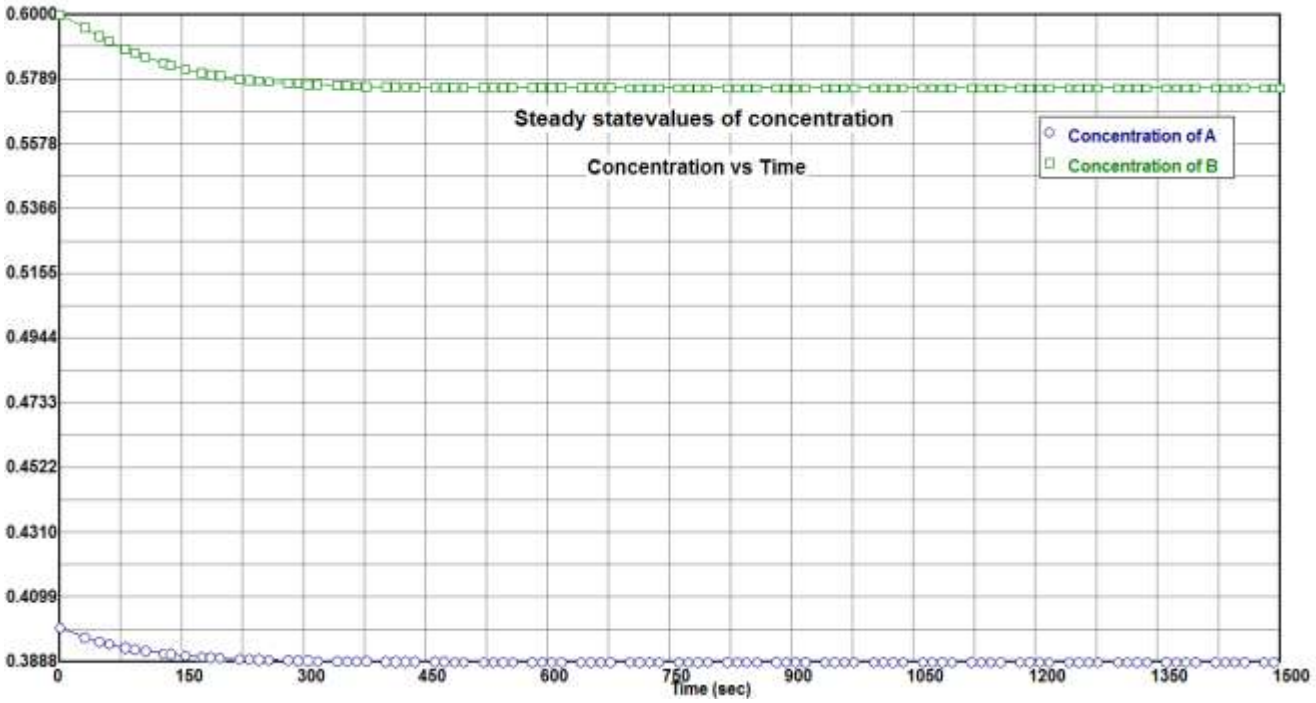

Figure-2
Steady state concentration profile vs time

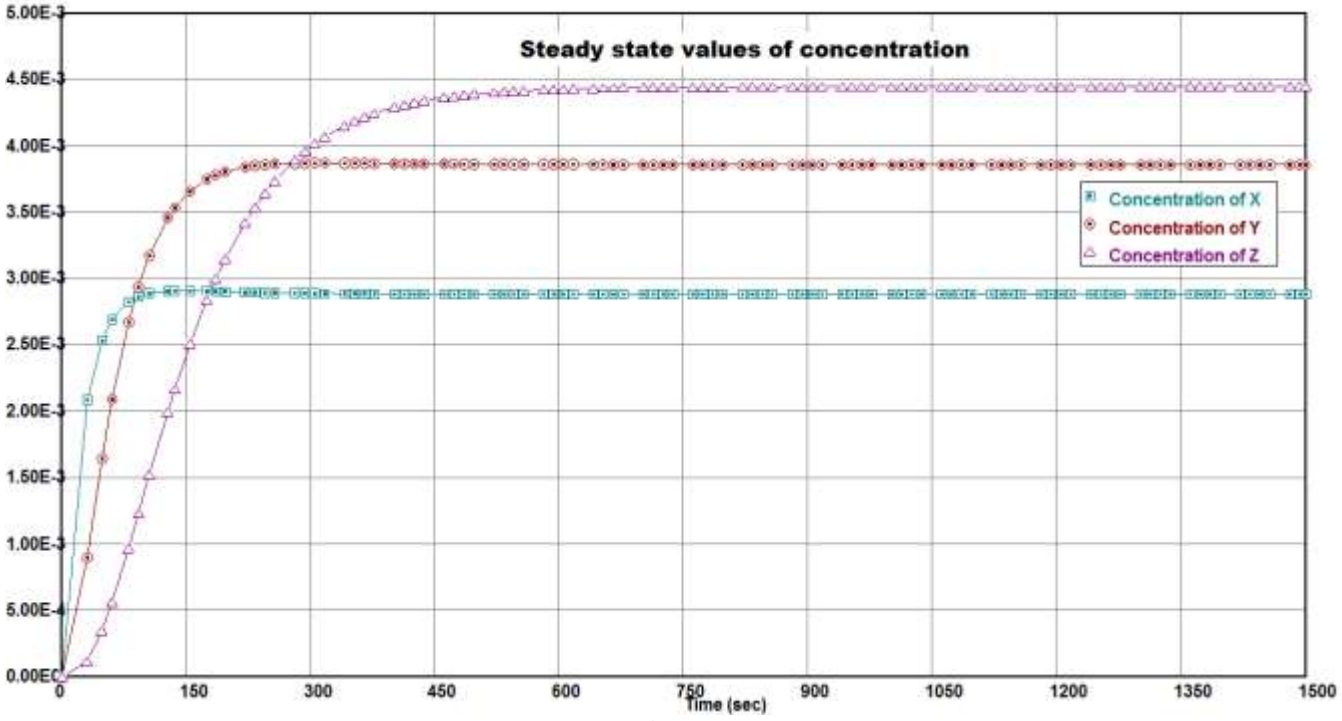

Figure-3
Steady state concentration of C_X, C_Y, and C_Z vs time

The second analysis were done for various flow rates in the range F=<0, 0.01> m^3/s. the main goal of the static analysis is to find optimal volumetric flow rate. Optimal in this case means point where product concentration is maximal.

Only concentrations C_X and C_Y has maximum in this case, concentration C_Z s has decreasing progress which is not very relevant for us. Maximum values of all concentrations and appropriate volumetric flow rate q are given below. This flow rate is used lately for the dynamic analysis. Steady state values of the state variables in the working point are, F=0.0025 (m^3/s), C_A= 0.3369774 (kmol/m^3), C_B= 0.4246187 (kmol/m^3), C_X= 0.0032226 (kmol/m^3), C_Y= 0.0072414 (kmol/m^3).

Table-3
Steady state values of concentrations for different flow rates

F(m^3/s)	C_A	C_B	C_X	C_Y	C_Z
0	0.2913335	0.2874315	0.0029428	0.0075455	0.0981782
0.001	0.3369774	0.4246187	0.0032226	0.0072414	0.0525587
0.002	0.3574784	0.4858989	0.0033037	0.0068562	0.0323617
0.003	0.3683311	0.5179965	0.0033011	0.006401	0.0219668
0.004	0.3748571	0.5370401	0.0032626	0.0059435	0.0159368
0.005	0.3791706	0.5494394	0.0032079	0.0055118	0.0121097
0.006	0.3822247	0.5580807	0.0031458	0.005115	0.0095145
0.007	0.384499	0.5644126	0.0030808	0.004754	0.0076662
0.008	0.3862581	0.5692315	0.0030151	0.0044269	0.0062998
0.009	0.3876593	0.5730086	0.0029499	0.0041308	0.0052599
0.01	0.3888017	0.5760397	0.002886	0.0038624	0.0044498

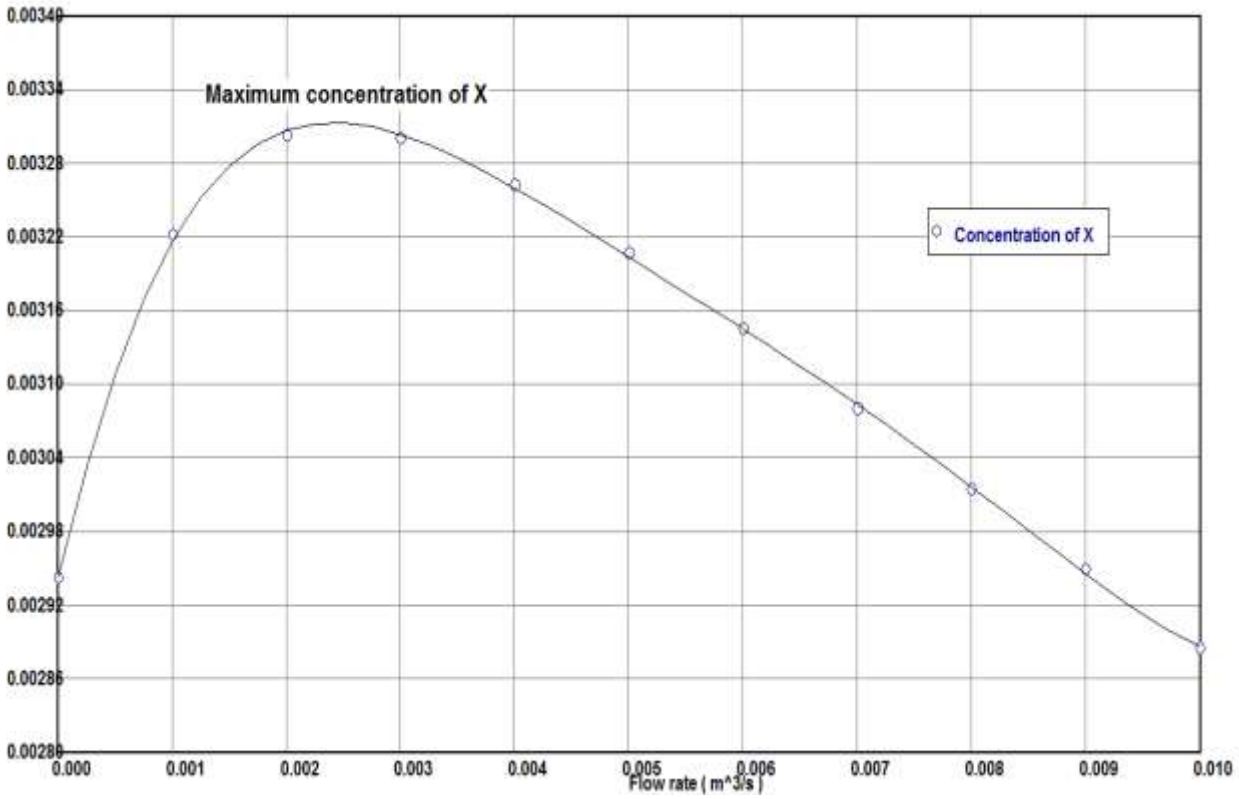

Figure-4

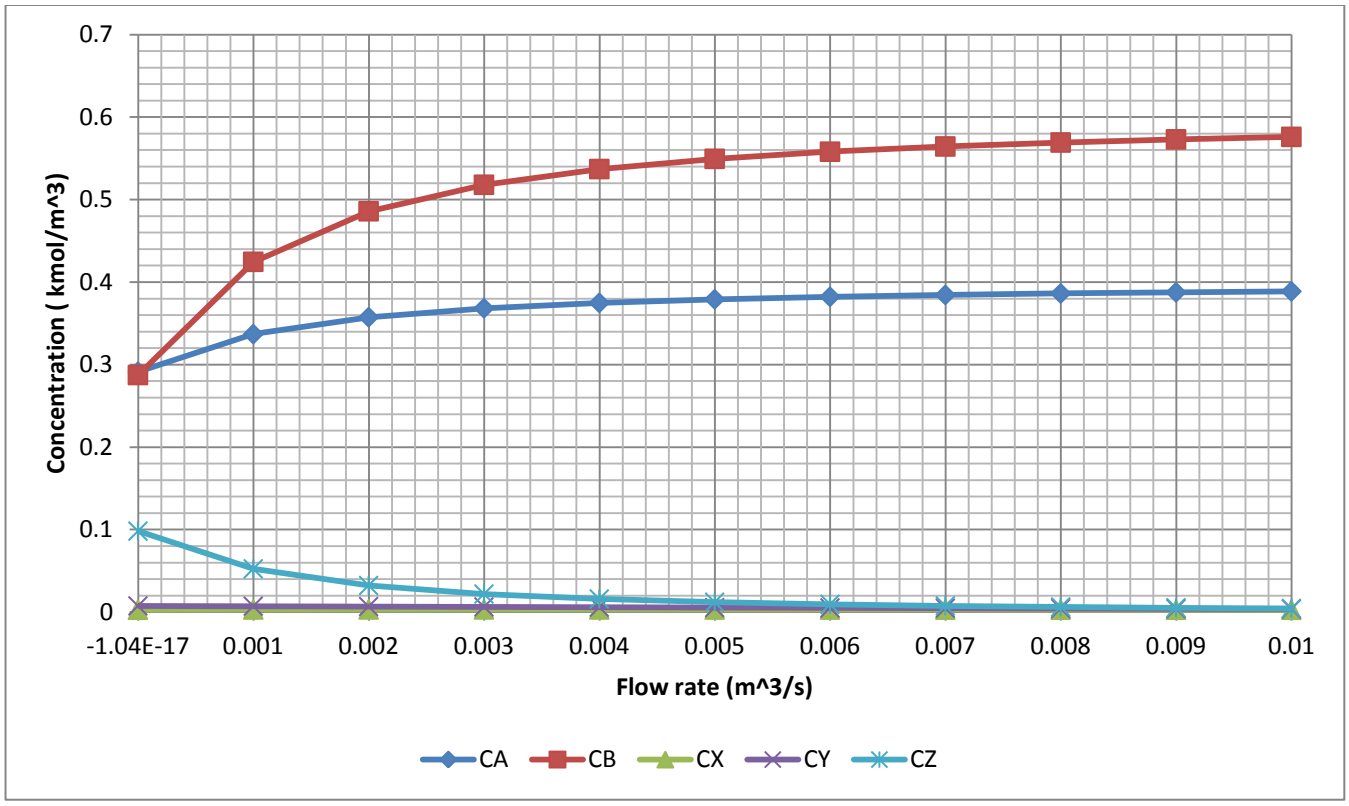

Figure- 5
Steady-state values of the concentrations C_A , C_B , C_X , C_Y and C_Z for different volumetric flow rate F

Dynamic Analysis: The next step after the steady-state analysis is usually dynamic analysis which observes behavior of the system after the step change of the input variable. In this case is input variable step change of the volumetric flow rate ΔF. Mathematically dynamic analysis means numerical solving of the set of ODE with some convenient method. Runge Kutta's standard method was used for solving of this problem (Shampire 1994). This Method belongs to the class of the high-order, it is self-started and should be used both for computing of initial assessments and final solutions too. Despite the fact, that in Polymath, in which Runge- Kutta's method build-in function RKF56, RKF45 etc. Computation was done with the general description of Runge-Kutta's standard method. This method uses first four parts of Taylor series

The polymath programs used the following equation and RKF45 is used for the simulation purpose.

The fourth order runge-kutta algorithm is widely used in chemical engineering. The Runge-kutta algorithm is given below

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) + O(h^5) \quad (16)$$

$$k_1 = h\, f(x_i,\ y_i)$$

$$k_2 = h\, f(x_i + \frac{h}{2},\ y_i + \frac{k_1}{2})$$

$$k_3 = h\, f(x_i + \frac{h}{2},\ y_i + \frac{k_2}{2})$$

$$k_4 = h\, f(x_i + h,\ y_i + k_3$$

k_1, k_2, k_3, k_4 are approximate derivative values computed on the interval $x_i \le x \le x_{i+1}$ and h is the step size

$$x_{i+1} = x_i + h$$

Where local error term for the fourth order Runge-kutta is $O(h^5)$

Simulation took time t = <0; 20 000> s and integration step was h = 10 s. Steady-state values of the state variables C_A, C_B, C_X, C_Y and C_Z computed from the previous steady-state analysis for this concreat working point were used as initial conditions. There were done four step changes of the input variable volumetric flow rate of the reactant, F, -50% of its steady-state value (i.e. -0.0005 m^3/s); -25% (-0.00025 m^3/s); 25% (0.00025 m^3/s) and 50% (0.0005 m^3/s). Outputs y_{1-3} in table below difference between actual value of the output and its initial value

$$y_1 = C_X(t) - C_x^{(s)}$$

$$y_2 = C_Y(t) - C_Y^{(s)}$$

$$y_3 = C_Z(t) - C_Z^{(s)}$$

This difference is made only because of better display of outputs they started in zero point.

Table-4
Main program used for finding out concentration

```
# Main Program
d(CA)/d(t) = (F * (CA0 - CA) / V) - (k1 * CA * CB) # Concentration of A
CA(0) = .4
d(CB)/d(t) = (F * (CB0 - CB) / V) - (k1 * CA * CB) - (k2 * CB * CX) - (k3 * CB * CY) # Concentration of B
CB(0) = 0.6
d(CX)/d(t) = (F * (CX0 - CX) / V) + (k1 * CA * CB) - (k2 * CB * CX) # Concentration of X
CX(0) = 0
d(CY)/d(t) = (F * (CY0 - CY) / V) + (k2 * CB * CX) - (k3 * CB * CY) # Concentration of Y
CY(0) = 0
d(CZ)/d(t) = (F * (CZ0 - CZ) / V) + (k3 * CB * CY) # Concentration of Z
CZ(0) = 0

# The explicit equations
F = 0.01 # Mass flow rate (m^3/sec)
V = 1 # Volume of reactor(m^3)
CA0 = 0.4 # Initial concentration of A
CB0 = 0.6 # Initial concentration of B
CX0 = 0 # Initial concentration of X
CY0 = 0 # Initial concentration of Y
CZ0 = 0 # Initial concentration of Z
k1 = 5 * 10 ^ -4 # Rate constant for reaction 1
k2 = 5 * 10 ^ -2 # Rate constant for reaction 2
k3 = 2 * 10 ^ -2 # Rate constant for reaction 3
# Initial/final values of the independent differentiation variable
t(0) = 0
t(f) = 1500
```

Differential equations

1 d(CA)/d(t) = (F * (CA0 - CA) / V) - (k1 * CA * CB)
Concentration of A

2 d(CB)/d(t) = (F * (CB0 - CB) / V) - (k1 * CA * CB) - (k2 * CB * CX) - (k3 * CB * CY)
Concentration of B

3 d(CX)/d(t) = (F * (CX0 - CX) / V) + (k1 * CA * CB) - (k2 * CB * CX)
Concentration of X

4 d(CY)/d(t) = (F * (CY0 - CY) / V) + (k2 * CB * CX) - (k3 * CB * CY)
Concentration of Y

5 d(CZ)/d(t) = (F * (CZ0 - CZ) / V) + (k3 * CB * CY)
Concentration of Z

Parameters used for Programming

Total number of equations	15	Solution method	RKF_45
Number of differential equations	5	Step size guess. h	0.000001
Number of explicit equations	10	Truncation error tolerance. eps	0.000001
Elapsed time	0.000 sec		

Conclusion

Paper deals with simulation of the CSTR which is typical nonlinear system with lumped parameters. Mathematical model of the plant comes from material balances inside the reactor which results in the set of nonlinear ODE. Simple Polymath programming is used for solving of a steady-state. All results are shown in result are done by polymath software The steady-state analysis for different value of input volumetric flow rate shows nonlinear properties of the system and the optimal working point is for volumetric flow rate F is 0.001 m^3/s where the concentration of the product Y has its maximum.

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