PROGRAM FOR SIMULATION OF A CONTINUOUS STIRRED TANK REACTOR IN MATLAB'S GUI

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Abstract

This contribution presents program in MATLAB's Graphical User Interface (GUI) which can be used for investigating of the static and dynamic behaviour and adaptive control of the nonlinear system represented by Continuous Stirred Tank Reactor (CSTR). Program provides computation for various values of the input variables which made this program universal for the wide range of the users without theoretical knowledge about the modeling, simulation and control.

1   Introduction

Simulation is the technical discipline which shows the behavior and reactions of any system on its model [1]. There are many types of models; the main categories are real models and computer models.

Based on this division, also simulation can be done for a real model is investigation of its behavior as a result of input stimulation. These simulations are done on the real model of the system. Computer simulation has a great importance today and MATLAB is big tool which can help you with computer simulation. It starts with creation of a mathematical model and the obtained equations are solved by using an appropriate calculation method. The importance of computer simulation will grow in the future when computers are faster.

The most of the chemical processes has nonlinear properties. Computer simulation is one way how to examine this behaviour which is obtained by steady-state and dynamic analysis. Model of the system is usually represented by the set of the partial or ordinary the differential equations.

2   Description of the system

The examined system is represented by Continuous Stirred Tank Reactor (CSTR) which is widely used in the praxis. A graphical diagram of the CSTR reactor is shown in Figure 1.
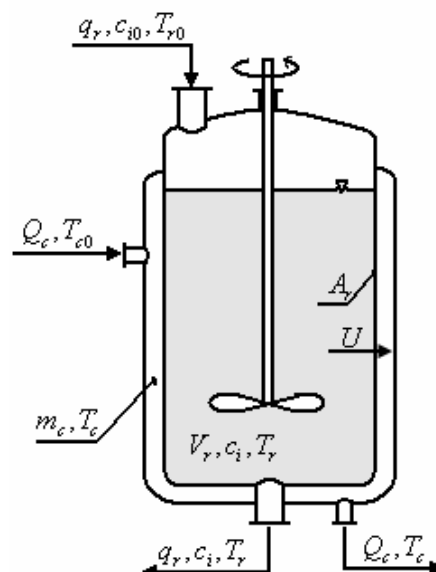

Figure 1: Continuous Stirred Tank reactor

The reaction inside the reactor is called *van der Vusse reaction.* This reaction can be described by the following scheme:

$$A \xrightarrow{\;k_1\;} B \xrightarrow{\;k_2\;} C$$
$$2A \xrightarrow{\;k_3\;} D \tag{1}$$

The mathematical model of this reactor is described by the set of four Ordinary Differential Equations (ODE) which come from material and heat balances inside the reactor:

$$\frac{dc_A}{dt} = \frac{q_r}{V_r}\left(c_{A0} - c_A\right) - k_1 c_A - k_3 c_A^{\;2}$$

$$\frac{dc_B}{dt} = -\frac{q_r}{V_r} c_B + k_1 c_A - k_2 c_B$$

$$\frac{dT_r}{dt} = \frac{q_r}{V_r}\left(T_{r0} - T_r\right) - \frac{h_r}{\rho_r c_{pr}} + \frac{A_r U}{V_r \rho_r c_{pr}}\left(T_c - T_r\right) \tag{2}$$

$$\frac{dT_c}{dt} = \frac{1}{m_c c_{pc}}\left(Q_c + A_r U \left(T_r - T_c\right)\right)$$

where $c_A \geq 0$, $c_B \geq 0$.

In the set of equations (2) t is the time, c are concentrations, T represents temperatures, c_p is used for specific heat capacities, q represents volumetric flow rate, Q_c is heat removal, V are volumes, ρ represents densities, A_r is the heat exchange surface and U is the heat transfer coefficient. Indexes $(\cdot)_A$ and $(\cdot)_B$ belong to compounds A and B, $(\cdot)_r$ denotes the reactant mixture, $(\cdot)_c$ cooling liquid and $(\cdot)_0$ are feed (inlet) values.

The model of the reactor belongs to the class of *lumped-parameter nonlinear systems.* Nonlinearity can be found in reaction rates (k_j) which are described via Arrhenius law:

$$k_j\left(T_r\right) = k_{0j} \cdot \exp\left(\frac{-E_j}{R T_r}\right), \text{ for } j = 1, 2, 3 \tag{3}$$

where k_0 represent pre-exponential factors and E are activation energies.

The reaction heat (h_r) in the equation (2) is expressed as:

$$h_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B + h_3 \cdot k_3 \cdot c_A^2 \tag{4}$$

where h_i means reaction enthalpies.

Parameters of the reactor are given in Table 1 [1].

Table 1: PARAMETERS OF THE REACTOR

$k_{01} = 2.145 \cdot 10^{10}$ min^{-1}	$k_{02} = 2.145 \cdot 10^{10}$ min^{-1}	$k_{03} = 1.5072 \cdot 10^{8}$ min^{-1}mol^{-1}
$E_1/R = 9758.3$ K	$E_2/R = 9758.3$ K	$E_3/R = 8560$ K
$h_1 = -4200$ kJ.kmol^{-1}	$h_2 = 11000$ kJ.kmol^{-1}	$h_3 = 41850$ kJ.kmol^{-1}
$V_r = 0.01$ m^3	$\rho_r = 934.2$ kg.m^{-3}	$c_{pr} = 3.01$ kJ.kg^{-1}.K^{-1}
$U = 67.2$ kJ.min^{-1}m^{-2}K^{-1}	$c_{pc} = 2.0$ kJ.kg^{-1}.K^{-1}	$A_r = 0.215$ m^2
$c_{A0} = 5.1$ kmol.m^{-3}	$T_{r0} = 387.05$ K	$U = 67.2$ kJ.min^{-1}m^{-2}K^{-1}
$m_c = 5$ kg	$c_{B0} = 0$ kmol.m^{-3}	

3   Simulation program

Simulation program was made in the MATLAB version 6.5 with the usage of the Graphic User Interface (GUI). The main program's window is shown in Figure 2.
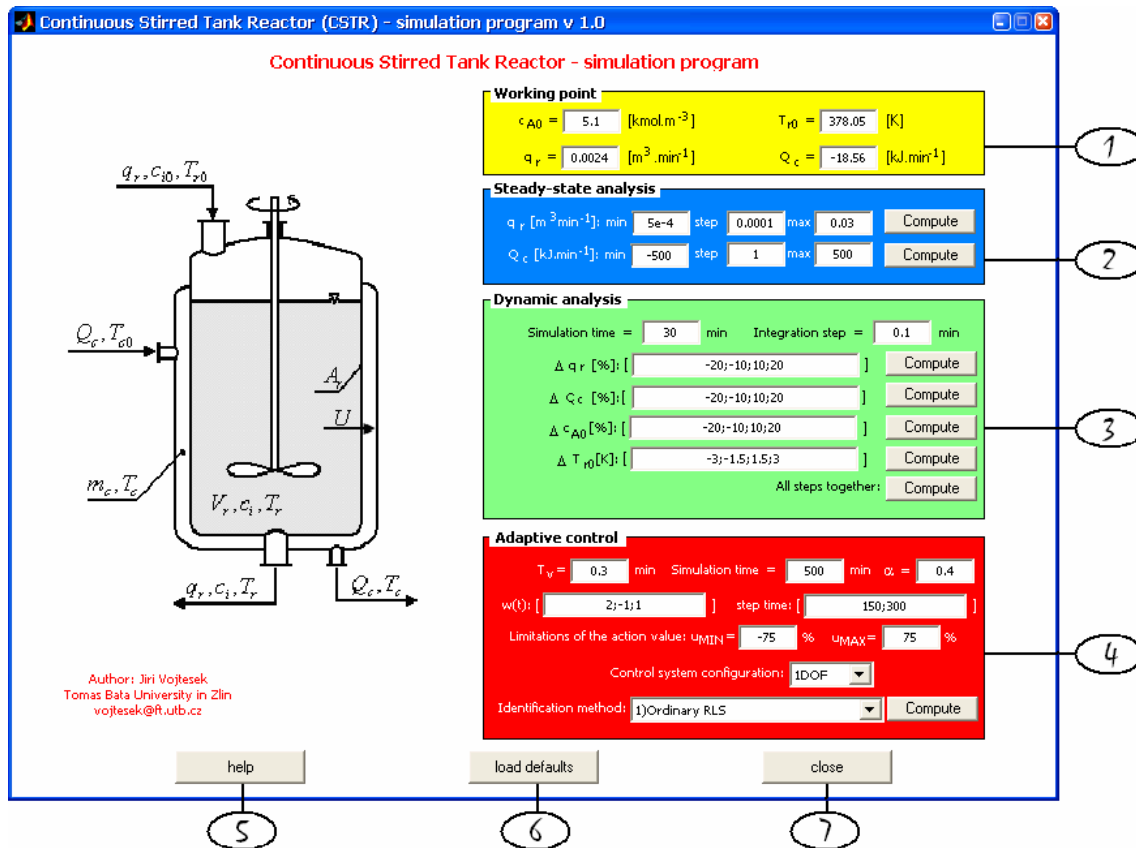
Figure 2: Main window of the program

Main window has 7 main parts:

1. Working point: Here you can define working point of the system represented by:

   - input concentration of the compound A c_{A0}

   - input concentration of the reactive temperature T_{r0}

   - volumetric flow rate of the reactive compound q_r

   - heat removal of the cooling liquid Q_c

These parameters can be changed in the edit windows and all constants like densities, volumes, heat capacities are stored in the separate M-file **const_allg.m**.

2. Steady-state analysis:

In this part you can compute steady-state analysis of the system. Steady-state analysis for stable systems involves computing values of state variables in time $t \rightarrow \infty$, when changes of these variables are equal to zero. That means, that the set of ODEs (2) is solved with the condition $\partial(\cdot)/\partial t = 0$. A simple iteration method was used to solve this problem. You can examine steady values of quantities for various rates of the volumetric flow of the reactant, q_r, and heat removal of the cooling liquid, Q_c, by pressing the button "Compute" in appropriate row.

3. Dynamic analysis:

For this nonlinear lumped-parameter system dynamic analysis involves solving the set of nonlinear ODE. Runge-Kutta's standard method with a fixed step was used for solving equations (2). At first you can specify simulation parameters – simulation time and integration step. The behaviour of the system is then solved for various step changes of the input quantities Δq_r, ΔQ_c, Δc_{A0} and ΔT_{r0}.

You can specify arbitrary number of steps separated by the semicolon or brake and computation is executed again by the pressing the button "Compute" in each row. If you want to observe dynamic analysis for all steps together, press button "Compute" in the last row of the Dynamic analysis sub-window.

Plotted outputs represent the difference of state variables c_A, c_B, T_r and T_c from their steady state values c_A^s, c_B^s, T_r^s and T_c^s, i.e.

$$y_1 = c_A - c_A^s; \quad y_2 = c_B - c_B^s; \quad y_3 = T_r - T_r^s; \quad y_2 = T_c - T_c^s \tag{5}$$

4. Adaptive control:

The adaptive control [3] with usage of polynomial synthesis [4] and pole-placement method was used for control of this reactor. This method could be used for systems with negative control properties such as non-minimum phase behaviour or transport delay.

Adaptive approach in this work is based on choosing of the External Linear Model (ELM) of the nonlinear process, parameters of which are estimated recursively [5]. The resulted regulator works in continuous-time and its parameters are tuned according to estimated parameters of the ELM.

There was used δ-model as an ELM in this work. This model belongs to the class of discrete models but its properties are different according to classical discrete model in Z-plain.

You can choose two control system configurations one degree-of-freedom (1DOF) and two degrees-of-freedoms. Both configurations are displayed in Figure 3.
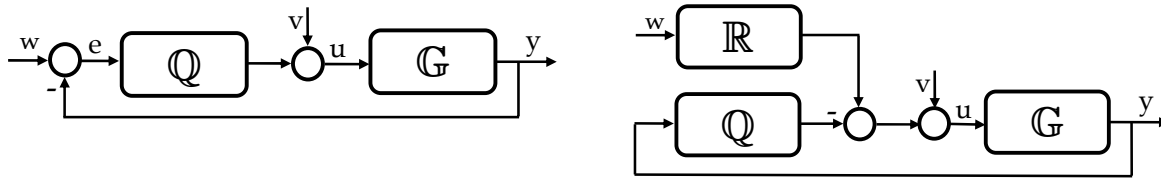

Figure 3: 1DOF and 2DOF configurations

Transfer functions of the feedback and feedforward parts of the controllers have following forms:

$$Q(s) = \frac{q(s)}{s \cdot p(s)}, R(s) = \frac{r(s)}{s \cdot p(s)} \tag{6}$$

Where parameters of the polynomials $p(s)$, $q(s)$ and $r(s)$ are computed from the diophantine equations [6]

$$a(s) \cdot s \cdot p(s) + b(s) \cdot q(s) = d(s)$$
$$t(s) \cdot s + b(s) \cdot r(s) = d(s) \tag{7}$$

These equations ensures stability, asymptotic tracking of the reference signal and disturbance attenuation. Polynomial $d(s)$ on the right side of the (7) is stable polynomial. Roots of this polynomial are poles of the closed-loop and the control quality is determined by the placement of these poles. A method, where poles were connected to parameters of the controlled system was used to set poles of the characteristic polynomial. Then, the polynomial $d(s)$ could be rewritten for aperiodical processes to the form

$$d(s) = n(s) \cdot (s + \alpha)^{\deg d - \deg n} \tag{8}$$

for $\alpha > 0$ be an optional coefficient reflecting closed-loop poles and stable polynomial $n(s)$ is obtained from the spectral factorization of the polynomial $a(s)$

$$n^*(s) \cdot n(s) = a^*(s) \cdot a(s) \tag{9}$$

Changes of the heat removal were used as manipulated variable and the controlled output was the temperature of the reactant:

$$y(t) = T_r(t) - T_r^s(t)[K]; u(t) = 100 \cdot \frac{Q_c(t) - Q_c^s(t)}{Q_c^s(t)} [\%] \tag{10}$$

Dynamic analysis of the output temperature shows that ELM could be expressed by a second order system with the relative order one described by the transfer function

$$G(s) = \frac{b_1 s + b_0}{s^2 + a_1 s + a_0} \tag{11}$$

You can choose sampling period T_v, simulation time, the placement of the root α, values of the wanted value (reference signal $w(t)$) and time where step change of the $w(t)$ arise and limitation of the input variable $u(t)$. First step change arise at the start time and it means that if the number of steps is n, the number of the time steps is $(n-1)$. You can make again as much steps as you like.

As it is written above, adaptivity of the control process is fulfilled by continuous parameter estimation during the control. Recursive Least Squares (RLS) methods [7], [8] with modifications (exponential and directional forgetting) were used for this parameter estimation. You can choose method from the popup window shown in Figure 4.
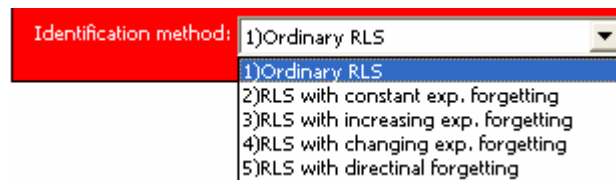

Identification method: 1)Ordinary RLS

1)Ordinary RLS
2)RLS with constant exp. forgetting
3)RLS with increasing exp. forgetting
4)RLS with changing exp. forgetting
5)RLS with directinal forgetting

Figure 4: Popup window for identification method

5. **Button "help":** displays HTML of this program

6. **Button "load defaults":** rewrites values in the edit windows with the default values.

7. **Button "close":** closes all windows and quit the program

4 Conclusion

This paper presents simulation program for simulation of the steady-state, dynamics and adaptive control of the CSTR reactor which is typical member of the nonlinear lumped-parameters system. Program provides computing without the deepest theoretical knowledge about the system which is the main advantage of this system. User can change control configuration, identification methods and the most of the important parameters of the control. Program is available by writing to the author's e-mail vojtesek@ft.utb.cz.

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