MATLAB Simulation for Continuous Stirred Tank Reactor.

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ABSTRACT

This paper presents control of the nonlinear system represented by a Continuous Stirred Tank Reactor (CSTR) using MATLAB's® Graphical User Interface (GUI). This simulation 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 modeling, simulation, and control.

(Keywords: adaptive control, simulation, modeling, CSTR, continuous stirred tank reactor, MATLAB®)

INTRODUCTION

Simulation is the technical discipline which shows the behavior and reactions of any system on its model [1]. While there are many types of models the main categories are real models and computer models. Based on this division, simulation can be done for a real model as 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 useful tool which can help with computer simulation. The process 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 as computers continue to get faster. Most of the chemical processes have nonlinear properties. Computer simulation is one way how to examine this behavior which is obtained by steady-state and dynamic analysis.

Models of the system are usually represented by the set of the partial or ordinary differential equations.

CONTINUOUS STIRRED TANK REACTOR

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

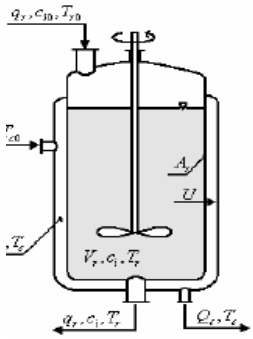

Figure 1: Continuous Stirred Tank Reactor.

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

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$
$$2A \xrightarrow{k_3} D \qquad (1)$$

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:

$$\frac{dc_A}{dt} = \frac{q_r}{V_r}(c_{A0} - c_A) - k_1 c_A - k_3 c_A^2$$
$$\frac{dc_B}{dt} = -\frac{q_r}{V_r} c_B + k_1 c_A - k_2 c_B$$
$$\frac{dT_r}{dt} = \frac{q_r}{V_r}(T_{r0} - T_r) - \frac{h_r}{\rho_r c_{pr}} + \frac{A_r U}{V_r \rho_r c_{pr}}(T_c - T_r)$$
$$\frac{dT_c}{dt} = \frac{1}{m_c c_{pc}}(Q_c + A_r U(T_r - T_c)) \quad \textbf{(2)}$$

where $cA \geq 0$, $cB \geq 0$.

In the set of Equations (2) *t* is the time, *c* are concentrations, *T* represents temperatures, *cp* is used for specific heat capacities, *q* represents volumetric flow rate, *Qc* is heat removal, *V* are volumes which represent densities, *Ar* is the heat exchange surface, and *U* is the heat transfer coefficient. Indexes *(·)A* and *(·)B* belong to compounds A and B, *(·)r* denotes the reactant mixture, *(·)c* cooling liquid, and *(·)*0 are feed (inlet) values.

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

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

Where k_0 represents pre-exponential factors and *E* represents activation energies. The reaction heat (*hr*) in Equation (2) is expressed as:

$$h_r = h_1 \cdot k_1 \cdot c_A + h_2 \cdot k_2 \cdot c_B + h_3 \cdot k_3 \cdot c_A^2 \quad \textbf{(4)}$$

where *hi* means reaction enthalpies. Parameters of the reactor are given in Table 1 [1].

Table 1: Parameters of the Reactor.

*k*01=2.145·1010 min-1 *E1/R* = 9758.3 K *h*1 =-4200 kJ.kmol-1 *Vr* = 0.01 m3 *U*=67.2 kJ.min-1m-2K-1 *cA*0 = 5.1 kmol.m-3 *mc* = 5 kg	*k*02=2.145·1010 min-1 *E2/R* = 9758.3 K *h*2=11000 kJ.kmol-1 ρ*r* =934.2 kg.m-3 *cpc*=2.0 kJ.kg-1.K-1 *Tr*0 = 387.05 K *cB*0 = 0 kmol.m	*k*03=1.5072·108 min-1 mol-1 *E3/R* = 8560 K *h*3 = 41850 kJ.kmol-1 *cpr* = 3.01 kJ.kg-1.K-1 *Ar* = 0.215 m2 *U*= 67.2 kJ.min-1m-2K-1

SIMULATION PROGRAM

The 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

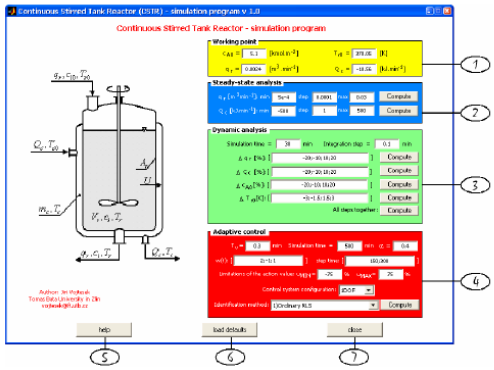

Figure 2: Main Window of the Program.

The main window has 7 main parts:

1. Working point:

Here you can define the working point of the system represented by: input concentration of the compound A *cA0*- input concentration of the reactive temperature *Tr0*- volumetric flow rate of the reactive compound *qr* - heat removal of the cooling liquid *Qc.* These parameters can be changed in the editor window**.**

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 $t \to \infty$, 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, *qr*, and heat removal of the cooling liquid, *Qc*, by pressing the button "Compute" in the 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 behavior of the system is then solved for various step changes of the input quantities *Δqr*, *ΔQc*, *ΔcA0,* and *ΔTr0*. The user can specify an arbitrary number of steps separated by the semicolon or brake and the computation is executed again by the pressing the button "Compute" in each row. If one wants to observe dynamic analysis for all steps together, press "Compute" button in the last row of the Dynamic Analysis sub window. Plotted outputs represent the difference of state variables *cA, cB*, *Tr* and *Tc* from their steady state values .

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 behavior or transport delay. An 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.

The δ-model was used 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. One can choose two control system configurations, one degree-of-freedom (1DOF) and two degrees-of-freedoms. Both configurations are displayed in Figure 3.

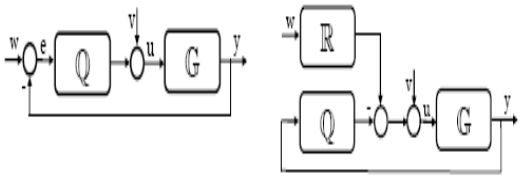

Figure 3: 1DOF and 2DOF Configurations.

Transfer functions of the feedback and feed forward parts of the controllers have following:

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

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

$$\begin{aligned} a(s)\cdot s\cdot p(s)+b(s)\cdot q(s)&=d(s)\\ t(s)\cdot s+b(s)\cdot r(s)&=d(s)\end{aligned} \qquad \textbf{(7)}$$

These equations ensure stability, asymptotic tracking of the reference signal, and disturbance attenuation. Polynomial *d*(*s*) on the right side of Equation (7) is a 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 a periodical process to the form:

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

for *á* > 0 be an optional coefficient reflecting closed-loop poles and stable polynomial *n*(*s*) is:

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

obtained from the spectral factorization of the polynomial *a*(*s*). Changes of the heat removal were used as manipulated variable and the controlled output was the temperature of the reactant:

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

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:

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

One can choose sampling period Tv, simulation time, the placement of the root á, 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). The first step change

arises at the start time and it means that if the number of steps is n, the number of the time steps is (n – 1). One can employ as many steps as required.

As it is written above, adaptability 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. One can choose the method from the popup window shown in Figure 4.

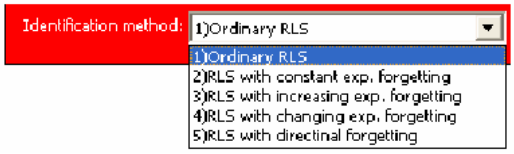

Figure 4: Popup Window for Identification Method.

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

CONCLUSION

This paper presents a 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. The program provides computing without the deepest theoretical knowledge about the system, which is the main advantage of this system. The user can change control configuration, identification methods, and most of the important parameters of the control.

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