Use of Differential Equations In Modeling and Simulation of CSTR

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Abstract: - The paper presents the use of differential equations in the computer modeling and simulation which technical filed with big future nowadays. The first part gives an overview to the process of the mathematical modeling and especially the construction of the mathematical model. This model usually consists of linear or nonlinear algebraic or differential equations which are then solved numerically to obtain information about the system's behaviour. The simple iteration method was used for the steady-state analysis and the Runge-Kutta's methods are employed in the dynamic analysis for solving of the set of Ordinary Differential Equations. Proposed methods were tested on the mathematical model of Continuous Stirred-Tank Reactor.

Key-Words: - Differential equation, Mathematial model, Steady-state analysis, Dynamic analysis, Simple iteration method, Runge-Kutta's method.

1 Introduction

The mathematical equations generally, not only differential equations, can be found everywhere. The high importance of the mathematical equations is in the field of modeling and simulation of the real systems [1], [2]. Not every property of the controlled system is known before we start and that is why we perform simulation experiments on the system.

The model of the process is a simplified version of the real system and includes all variables and relations of the system which are important for the investigation [3]. The mathematical and physical models are two main types of models used nowadays. The mathematical model is abstract representation of the real process which uses input, state or output variables and reactions between them for collecting of the set of mathematical equations [4].

Differential equations are very often used because of their accuracy of the description. Unfortunately, the major group of DE are nonlinear [5]. There can be found a lot of methods for solving of the nonlinear DE such as Euler's method, Taylor's method or Runge-Kutta's methods [6] which are very popular because of their simplicity and easy programmability.

The chemical reactors are equipments very often used in the chemical or biochemical industry for production of several products [1]. The most common used ones are Continuous Stirred-Tank Reactors (CSTR) of tubular reactors. The first type belongs to the class of lumped-parameters systems mathematical model of which is described by the set of Ordinary Differential Equations (ODE) while the tubular reactor is typical member of the distributed-parameters systems where the mathematical model consists of Partial Differential Equations.

All simulations performed in this paper are done in the mathematical software Matlab, version 7.0.1.

2 Modeling and Simulation

There exist two basic types of models – (I.) real models and (II.) abstract models. The first group is represented by the small or similar copy of the original one which is then subjected to the experiments while it is supposed that the results are similar to results on the real one [2].

The other, safer and cheaper way is to create mathematical model as an abstract representation of the real system. Simulation of the behaviour of the mathematical model is then nothing more than numerical solving of the set of equations.

The full mathematical description of the process is usually very complex as there are numerous variables which can vary during time of in the space. Very important part of the modeling procedure is selecting of state variables and relations between them and on the contrary introduce constants and simplifications other variables which reduces complexity of the system. The best mathematical model describe real system

in the most proper way and moreover it is the simplest one from the range of available models. The compromise between this properness and simplicity is one of the most important parts of the modeling.

2.1 Mathematical Balances

Mathematical balances are used as a common tool for constructing of the mathematical model. They usually include kinetic equations for reaction rates of the reactions in the chemical reactor, heat rates, heat transfers and equations which represents property changes [4].

The equation of the material balance as a first type has general word formulation:

[Mass flow of the component into the system] = [Mass flow of the component out of the system] + [Rate of accumulation of mass in the system] (1)

Some processes, especially in the chemical equipment include chemical reaction and the material balance is in this case

[Mass flow of the component into the system] = [Mass flow of the component out of the system] + [Rate of accumulation of mass in the system] − [Rate of production of the component by the reaction] (2)

Both previous equations are reduced in the steady-state state to the form

[Mass flow of the component into the system] = [Mass flow of the component out of the system] (3)

The second type of the balances, heat balances, describes temperature changes caused by the reaction inside systems with chemical reactions. This balance can be then described as

[Heat in the input flow] + [Heat arrised during the reaction] = [Heat in the output flow] + [Heat accumulated inside] − [Heat transfered from or into the surrounds] (4)

2.2 Mathematical Description

The equations above are in the word form. If we want to transform them into the mathematical meaning, we can use the simple algebraic equations or more complex differential equations. Both types are linear or nonlinear. Unfortunately, major group of the systems in the nature has nonlinear behaviour which could cause problems in the solving. Differential equations are divided into two main groups – ordinary, where state variables depend only on one variable (usually time dependence) while partial equations depend two or more variables (time and space variable for example). There are two types of systems from the differential equation point of view. The first, systems with lumped parameters, are described by one or more, usually set of ordinary differential equations. The second type of systems is described by one or more partial differential equations and these types of systems are called systems with distributed parameters.

As the area of mathematical models is very wide, let us focus on the nonlinear time-invariant systems with lumped parameters. Such systems could be described generally by the set

$$\begin{aligned} \dot{\boldsymbol{x}}(t) &= \boldsymbol{f}[\boldsymbol{x}(t), \boldsymbol{u}(t)] \\ \boldsymbol{y}(t) &= \boldsymbol{g}[\boldsymbol{x}(t), \boldsymbol{u}(t)] \end{aligned} \tag{5}$$

where $\boldsymbol{x}(t) = [x_1(t), x_2(t), \ldots x_n(t)]^T$ represents state vector, $\boldsymbol{u}(t) = [u_1(t), u_2(t), \ldots u_m(t)]^T$ is input vector, t is time, $\boldsymbol{f} = [f_1, f_2, \ldots f_n]^T$ and $\boldsymbol{g} = [g_1, g_2, \ldots g_n]^T$ are nonlinear vector functions while $\boldsymbol{y}(t)$ represents output vector.

The mathematical model in (5) is then for defined initial conditions. Each state variable needs as many initial conditions as is the highest order of the derivative in the differential equation (5). This concrete system has initial condition:

$$\boldsymbol{x}(0) = \boldsymbol{x}^s \tag{6}$$

where $\boldsymbol{x}^s$ is obtained from the steady-state analysis.

2.3 Steady-state Analysis

Steady-state analysis for the stable systems involves computing values of state variables in the time close to infinity, when changes of these variables are equal to zero. Mathematically talking, differences with respect to time in the differential equations are equal to zero, i.e.

$$\frac{d(\cdot)}{dt} = 0 \tag{7}$$

The set of nonlinear differential equations (5) is then transformed to the set of nonlinear algebraic equations. Despite the fact, that there is a possibility to solve nonlinear algebraic equations analytically, some cases are not solvable this way. The iterative methods [5] lead to the exact solution for appropriate choice of the initial iteration and fullfiled convergence condition.

The simple iteration method for the differential equation

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{f}[\boldsymbol{x}(t), \boldsymbol{u}(t)] \tag{8}$$

with initial condition (6) leads the solving of the steady-state model

$$\boldsymbol{f} = (\boldsymbol{x}^s, \boldsymbol{u}^s) = 0 \tag{9}$$

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where $\boldsymbol{u}^s$ is vector of known input variables and unknown parameters are component of the vector $\boldsymbol{x}^s$ which is called working point of the system.

Nonlinear function in the equation (9) could be rewritten to

$$\boldsymbol{f}(\boldsymbol{x})=0 \tag{10}$$

and we can obtain with the separation of the unknown parameter $\boldsymbol{x}$ to the left side new nonlinear equation

$$\boldsymbol{x}=\boldsymbol{\phi}(\boldsymbol{x}) \tag{11}$$

Where $\boldsymbol{\phi}=\left[\phi_1,\phi_2,\ldots\phi_n\right]^T$ is new nonlinear function and (11) leads to the iterative equation in the form of

$$\boldsymbol{x}^{k+1}=\boldsymbol{\phi}(\boldsymbol{x}^k) \quad \text{for k = 0,1,...} \tag{12}$$

which leads to the exact solution only if the convergence condition is satisfied. Let the vector function $\boldsymbol{\phi}$ be defined in the closed convex region $D\subset\Re^n$ and if $\boldsymbol{x}\in D$ so $\boldsymbol{\phi}\in D$ too. Moreover, let functions $\boldsymbol{\phi}$ have continuous partial differential derivations of all variables $x_1\div x_n$ in the region D, then there exists matrix

$$\varphi'(\boldsymbol{x})=\frac{d\varphi}{d\boldsymbol{x}}=\begin{vmatrix} \frac{d\varphi_1}{dx_1} & \frac{d\varphi_1}{dx_2} & \cdots & \frac{d\varphi_1}{dx_n} \\ \frac{d\varphi_2}{dx_1} & \frac{d\varphi_2}{dx_2} & \cdots & \frac{d\varphi_2}{dx_n} \\ \vdots & & \ddots & \\ \frac{d\varphi_n}{dx_1} & \frac{d\varphi_n}{dx_2} & \cdots & \frac{d\varphi_n}{dx_n} \end{vmatrix} \tag{13}$$

If matrix (13) fulfils the condition $\left\|\varphi'(x)\right\|<1$ for any $\boldsymbol{x}\in D$, there is only one solution $\boldsymbol{x}^*\in D$ of the equation (12).

There could be of course thousands of iterations during the computation but from the practical point of view it is convenient to stop the computation in case where the difference between values of actual and previous iteration is sufficiently small, i.e. condition

$$\left\|\boldsymbol{x}^{(k)}-\boldsymbol{x}^{(k-1)}\right\|<\varepsilon \tag{14}$$

is fulfilled for accuracy $\varepsilon>0$.

2.4 Dynamic Analysis

Once we have solved steady-state of the system, we can move to the solution of the differential equations described as (5).

Let us introduce first ordinary differential equation in the form of

$$\frac{dy}{dx}=f(x,y) \tag{15}$$

with initial condition $y(0) = y_0$ which is called Cauchy Problem.

Although there are a lot of single-step and multi-step methods for solving of the differential equations, the Runge-Kutta's methods [6] are very often used because of their simplicity and easy programmability.

Runge-Kutta's methods comes from the Taylor series of the (15):

$$\begin{aligned} y_{i+1}=y_i+\left.\frac{dy}{dx}\right|_{x_i,y_i}(x_{i+1}-x_i)+\ldots \\ +\frac{1}{2!}\left.\frac{d^2y}{dx^2}\right|_{x_i,y_i}(x_{i+1}-x_i)^2+\ldots \end{aligned} \tag{16}$$

and the order of the Runge-Kutta's method depends on the number of parts taken from the Taylor's series. For example, the most commonly used, the fourth order Runge-Kutta's method, employs first four parts of the Taylor's series and the value of output variable is computed from:

$$y_{i+1}=y_i+\frac{1}{6}\cdot(g_1+2g_2+2g_3+g_4) \tag{17}$$

where variables $g_{1\text{-}4}$ are computed from

$$\begin{aligned} g_1&=h\cdot f(x_i,y(x_i)) \\ g_2&=h\cdot f\left(x_i+\frac{1}{2}h,y(x_i)+\frac{1}{2}g_1\right) \\ g_3&=h\cdot f\left(x_i+\frac{1}{2}h,y(x_i)+\frac{1}{2}g_2\right) \\ g_4&=h\cdot f(x_i+h,y(x_i)+g_3) \end{aligned} \tag{18}$$

and h is optional integration step and $y(x_i)$ is value of the output variable for state variable x_i.

Although the Runge-Kutta's methods are build-in functions in the major mathematical software such as MATLAB (functions ode23, ode45 etc.) [7] or MATHEMATICA (DSolve, NDSolve etc.), the computation procedure described by equations (17) and (18) is easily programmable with the use of common computation tools as it will be presented in the practical part.

3 Simulation Example

Proposed simulation methods were tested on the mathematical model of the Continuous Stirred-Tank Reactor (CSTR) as a typical member of the group of nonlinear systems with lumped parameters.

Graphical representation is this reactor shown in Fig. 1.

The reaction inside is simple exothermic reaction with the scheme $A \rightarrow B \rightarrow C$ and the cooling jacket is used. Consequently, we supposed that the volume V, densities ρ, the heat transfer coefficient α and heat capacities of the reactant c_{pr} and the cooling c_{pc}

are constant during the reaction because of the simplification.

Input variables are input concentrations of compounds A and B, c_{A0} and c_{B0}, input temperatures of the reactant and the coolant, T_{r0} and T_{c0}, and the volumetric flow rates of the reactant and the coolant, q_r and q_c.

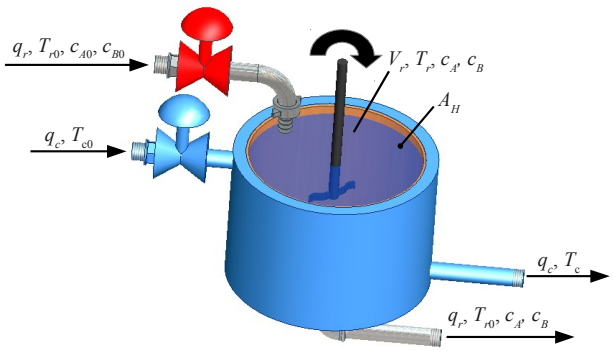

Fig. 1: Scheme of the Continuous Stirred-Tank Reactor

State variables are concentrations of compounds A and B, c_A and c_B, the temperature of the reactant T_r and the temperature of the coolant T_c.

3.1 Mathematical Model

Now we have introduced the most important variables which is base for the mathematical modelling.

Material balances of compounds A and B rewritten from the word form (2) are:

$$q\,c_{A0} = q\,c_A + V\,k_1\,c_A + V\,\frac{dc_A}{dt} \tag{19}$$

for the compound A and

$$q\,c_{B0} = q\,c_B - V\,k_1\,c_A + V\,k_2\,c_B + V\,\frac{dc_A}{dt} \tag{20}$$

for the second compound B.

The third differential equation comes from the heat balance (3) with the mathematical description

$$q_r\rho_r c_{pr} T_{r0} + V\,h_r = q_r\rho_r c_{pr} T_r + \ldots$$
$$\ldots + A_h\,\alpha\left(T_r - T_c\right) + V_r\,\rho_r\,c_{pr}\,\frac{dT_r}{dt} \tag{21}$$

where A_h represents heat exchange surface and hr is reaction heat, $h_r = h_1 k_1 c_A + h_2 k_2 c_B$ for h_1 and h_2 as a reaction enthalpies.

Finally, the last equation represents heat balance of the coolant (4):

$$q_c\rho_c c_{pc} T_{c0} + A_h\,\alpha\left(T_r - T_c\right) = q_c\rho_c c_{pc} T_c + \ldots$$
$$\ldots + V_c\,\rho_c\,c_{pc}\,\frac{dT_c}{dt} \tag{22}$$

If we separate derivatives of the state variables with respect to time on the left side and the rest parts on the right side we obtain mathematical model as a set of ODE:

$$\begin{aligned}
\frac{dc_A}{dt} &= -\left(\frac{q_r}{V_r} + k_1\right)c_A + \frac{q_r}{V_r}c_{A0} \\
\frac{dc_B}{dt} &= -\left(\frac{q_r}{V_r} + k_2\right)c_B + \frac{q_r}{V_r}c_{B0} + k_1 c_A \\
\frac{dT_r}{dt} &= \frac{q_r}{V_r}\left(T_{r0} - T_r\right) + \frac{h_r}{\rho_r c_{pr}} + \frac{A_h\,\alpha}{V_r\rho_r c_{pr}}\left(T_r - T_c\right) \\
\frac{dT_c}{dt} &= \frac{q_c}{V_c}\left(T_{c0} - T_c\right) + \frac{A_h\alpha}{V_c\rho_c c_{pc}}\left(T_r - T_c\right)
\end{aligned} \tag{23}$$

Very important variables which were not mentioned until now are reaction rates, k_1 and k_2 computed from the Arrhenius law

$$k_j = k_{j0}\cdot\exp\left(\frac{-E_j}{R\,T_r}\right) \quad \text{for } j = 1, 2 \tag{24}$$

Where k_{j0} represents pre-exponential factors, E_j are activation energies and R is universal gas constant.

Mainly presence of these reaction rates form nonlinearity of this system – see reaction temperature T_r as a state variable in denominator of the exponential function in (24).

The fixed parameters of the reactor are shown in Table 1 [8].

$V_r = 1.2\ m^3$	$h_1 = 4.8\cdot10^4\ kJ.kmol^{-1}$
$V_c = 0.64\ m^3$	$h_2 = 2.2\cdot10^4\ kJ.kmol^{-1}$
$\rho_r = 985\ kg.m^{-3}$	$U = 43.5\ kJ.min^{-1}m^{-2}K^{-1}$
$\rho_c = 998\ kg.m^{-3}$	$c_{A0} = 2.85\ kmol.m^{-3}$
$c_{pr} = 4.05\ kJ.kg^{-1}.K^{-1}$	$c_{B0} = 0\ kmol.m^{-3}$
$c_{pc} = 4.18\ kJ.kg^{-1}.K^{-1}$	$T_{r0} = 323\ K$
$A_h = 5.5\ m^2$	$T_{c0} = 293\ K$
$E_1/R = 13477\ K$	$q_r = 0.08\ m^3.min^{-1}$
$E_2/R = 15290\ K$	$q_c = 0.08\ m^3.min^{-1}$

Table 1: Fixed parameters of the reactor

3.2 Steady-state Analysis

As it is written in the theoretical part 2.3, the mathematical meaning of the steady-state analysis is to solve the set of ODE (23) in the condition $d(\cdot)/dt = 0$. Some of the variables are constant and we can group them into the constants $b_{0\text{-}4}$:

$$\begin{aligned}
b_0 &= \frac{q_r}{V_r} \quad b_1 = \frac{A_h\,\alpha}{V_r\rho_r c_{pr}} \\
b_2 &= \rho_r c_{pr} \quad b_1 = \frac{A_h\,\alpha}{V_c\rho_c c_{pc}} \quad b_4 = \frac{q_c}{V_c}
\end{aligned} \tag{25}$$

The resulted nonlinear steady-state model is then:

$$c_A^s = \frac{b_0 c_{A0}}{b_0 + k_1} \qquad c_B^s = \frac{k_1 c_A^s + b_0 c_{B0}}{b_0 + k_2}$$
$$T_r^s = \frac{\frac{h_r}{b_2} + b_0 T_{r0} + b_1 T_c^s}{b_0 + b_1} \qquad T_c^s = \frac{b_3 T_r^s + b_4 T_{c0}}{b_3 + b_4} \tag{26}$$

Where index $(\cdot)^s$ represents steady-state value.

This set is also in the form of (11) which means that we can use Simple iteration method (12) for solving of this set of nonlinear algebraic equations. The convergence condition (13) is fulfilled and we can compute steady-state values for initial values $T_r(0) = T_{r0}$ and $T_c(0) = T_{c0}$ from iteration cycle

$$k_1(k) = k_{10} \cdot \exp\left(\frac{-E_j}{R T_r(k)}\right)$$
$$k_2(k) = k_{20} \cdot \exp\left(\frac{-E_j}{R T_r(k)}\right)$$
$$c_A(k) = \frac{b_0 c_{A0}}{b_0 + k_1(k)}$$
$$c_B(k) = \frac{k_1(k) c_A(k) + b_0 c_{B0}}{b_0 + k_2(k)} \tag{27}$$
$$h_r(k) = h_1 k_1(k) c_A(k) + h_2 k_2(k) c_B(k)$$
$$T_r(k) = \frac{\frac{h_r(k)}{b_2} + b_0 T_{r0} + b_1 T_c(k)}{b_0 + b_1}$$
$$T_c(k) = \frac{b_3 T_r(k) + b_4 T_{c0}}{b_3 + b_4}$$

For $k = 0,1,2,...,N$ where N is optional maximal number of iterations, e.g. $N = 100$. Values of the variables c_A^s, c_B^s, T_r^s and T_c^s are shown in following Fig. 2 and 3.

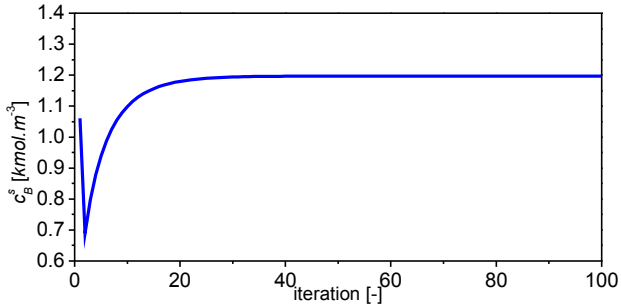

Fig. 2: The course computed steady-state value of c_B^s during iterations

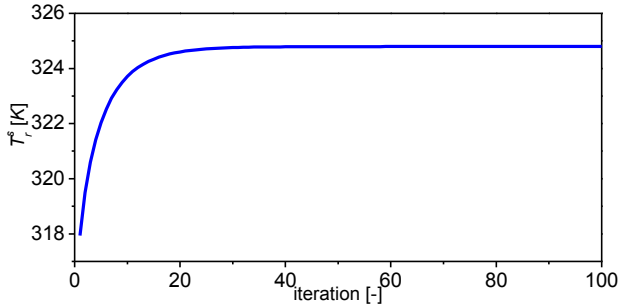

Fig. 3: The course computed steady-state value of T_r^s during iterations

As it can be seen from graphs, the iteration process converge quite quickly. If we introduce condition (14), the computation could end after approximately 30-40 iterations.

The steady-state values of the state variables for the defined working-point in Table 1 are

$$c_A^s = 1.5801\ kmol.m^{-3} \qquad T_r^s = 324.8\ K$$
$$c_B^s = 1.1971\ kmol.m^{-3} \qquad T_c^s = 306.28\ K \tag{28}$$

3.3 Dynamic Analysis

The dynamic analysis discovers the behaviour of the system after the step change of the input variable. As it is written above, there are six possible input variables – concentrations c_{A0} and c_{B0}, temperatures T_{r0} and T_{c0} and volumetric flow rates q_r and q_c.

The changes of concentrations and temperatures has mainly theoretical meaning. The step change could be performed but it is inapplicable from the control point of view, where we need numerous changes of the input variable. On the other hand, changes of the volumetric flow rate are ideal and easily realizable by the valves on the pipes. That is why we perform step changes of the input volumetric flow rate of the reactant or cooling, Δq_r or Δq_c, in this part. The practical solution of the set of ODE is:

1. Defining of the simulation time t_h and integration step h, in our case $t_h = 200\ min$ and $h = 0.5\ min$.
2. Computation of the initial values which are steady-state values of the state variables in the defined working point.
3. Change input according to change Δq_r or Δq_c
4. Iteration cycle which computes values of variables $g_{1\text{-}4}$ according to (18).
5. Compute values of output variables at the end of the integration step from (17).
6. Set computed output variables from the previous point as an input variables for the next integration step and jump to the point 4.

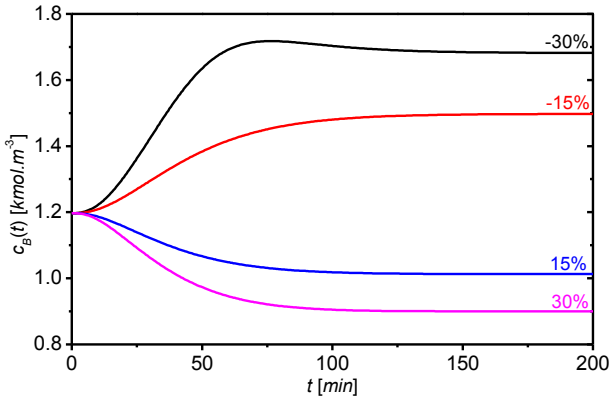

Fig. 4:The course of the concentration c_B after the step changes of input volumetric flow rate q_r

7. Compute values of output variables until final time t_h.

The first dynamic analysis was done for four step changes Δq_r = -30%, -15%, 15% and 30% from the working point value q_r = 0.08 $m^3.min^{-1}$. The results are shown in Fig. 4 and Fig. 5.

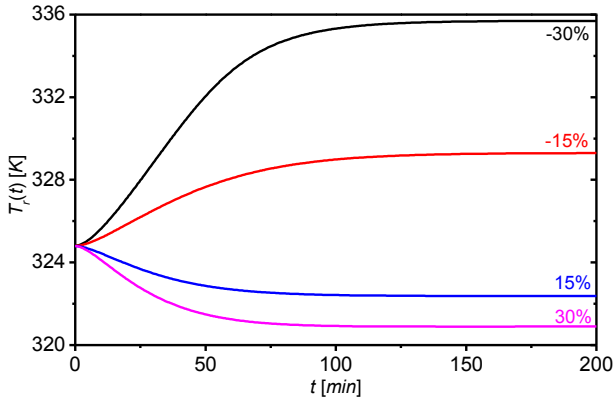

Fig. 5: The course of the temperature T_r after the step changes of input volumetric flow rate q_r

The second analysis was done for the same step changes but for the volumetric flow rate of the coolant Δq_c from its working-point value q_c = 0.08 $m^3.min^{-1}$ – see results in Fig. 6 and Fig. 7.

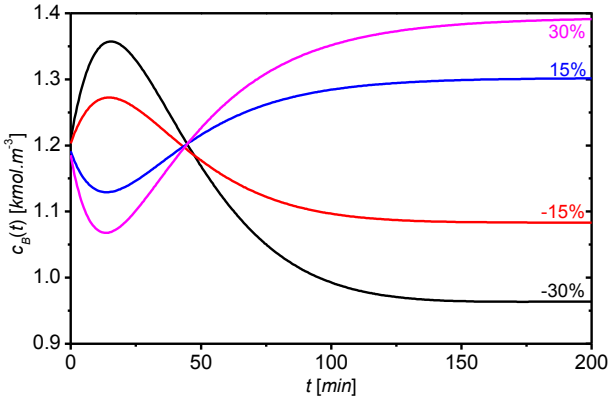

Fig. 6:The course of the concentration c_B after the step changes of input volumetric flow rate q_c

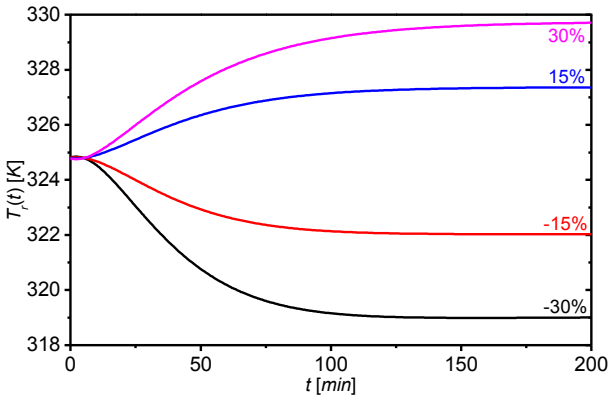

Fig. 7: The course of the temperature T_r after the step changes of input volumetric flow rate q_c

Dynamic analyses for both step changes presented in Fig. 4 - 7 have shown behaviour of the system which can be mathematically described by the first or the second order transfer functions. This could be important for the designing of the adaptive controller – see [8].

5 Conclusion

The goal of this paper was to show one field, where we can find differential equations – in the modelling and computer simulation. The process of modelling with the use of material and heat balances inside the system results in the mathematical model which is then subjected to the steady-state state and dynamic analyses. Presented experiments have shown usability of the Simple iteration method for static analysis. Fulfilled convergence condition guarantee solution within few iterations. The Runge-Kutta's method used for numerical solution of the set of ODE have good results although the mathematical model is highly nonlinear. All proposed methods have one big advantage – they are easily programmable. The practical experiment consists of steady-state and dynamic analysis performed on the Continuous Stirred-Tank Reactor as a typical nonlinear system from the praxis.

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