Control Structure of Chemical Reactor

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This paper presents a control structure which can be used effectively for control of chemical reactors. This structure is a multilayer control structure. It is characterized by the dividing of process control into several algorithms on the various layers. The algorithms are interfering with the different time intervals.

Multilayer control structures are characterized by the different way of the control activity [1]. The individual layers are hierarchically arranged. This organization is given by results of the vertical decomposition. The ability to reduce information from the lower to the higher layers is guaranteed by the hierarchical structure. The activities of subsystems on the lower layer are coordinated by subsystems on the higher layer. The information from the lower layer, which is needed for the higher layer organization, is sent to the higher layer. This is realized by the information channel (Fig. 1). After vertical decomposition, various forms of the connecting of subsystems can be acquired [2]. The relatively independent subsystems are controlled so that their own goals are fulfilled. The acquirement of the global optimum is ensured by the hierarchical form of the multilayer structure. The respective contradictions of the individual subsystems goals and the changes of the external condition are removed by the multilayer structure.

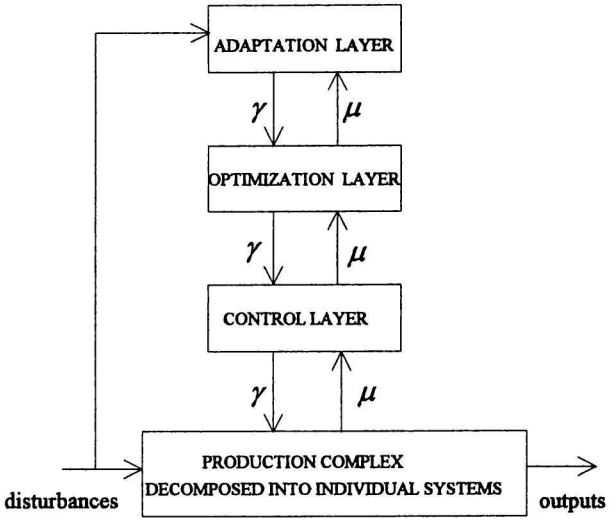

Fig. 1. Block scheme of multilayer structure, γ – coordination variables, μ – information variables.

THEORETICAL

Individual Layer Analysis

The arranging of system layers is connected with the decomposition of the controlled system. The specifying of goals for individual parts of the system is included in this arranging. So, several subproblems of the whole problem are obtained. The individual subproblems are solved by different methods. The type of problem, physical structure or frequency, and the greatness of disturbances entering into the system are the base for dividing the problem. Every layer works with different sampling period.

The adaptation layer works with sampling period τ_3. This layer is connected with disturbances and process variable boundaries. The disturbances influence process parameters. The introduction of β-parameters and α-parameters is the task of adaptation layer. The β-parameters are installed to simplify the optimization problem. Unknown control process parameters are represented by α-parameters. α- and β-parameters are included in modified description of the system.

The basic layer of multilayer structure is the optimization layer. The static optimization is done on this layer so that the disturbances are taken into account. These disturbances can influence the choice of a process performance function. The sampling period of optimization layer is τ_2. The trajectories of reference variables y_α and u_α are determined on the optimization layer.

The third layer is the layer of the direct control. Here, the trajectories of control variable u_α are found so that the output y of the controlled process reaches reference values y_α from the optimization layer [3].

The type of control algorithm is determined on the adaptation layer. The sampling period of the direct control layer is τ_1. The connection between sampling periods τ_1, τ_2, τ_3 can be expressed [2] by inequality $\tau_1 < \tau_2 < \tau_3$.

Problem Formulation

Consider a controlled system in the form

$$\begin{aligned} \frac{\mathrm{d}\boldsymbol{x}(t)}{\mathrm{d}t} &= \mathbf{A}\boldsymbol{x}(t) + \mathbf{B}\boldsymbol{u}(t) + \boldsymbol{z}(t) \\ \boldsymbol{y}(t) &= \mathbf{C}\boldsymbol{x}(t) \end{aligned} \tag{1}$$

where $\boldsymbol{x}(t)$ is n-dimensional state vector, $\boldsymbol{u}(t)$ is m-dimensional control input vector, $\boldsymbol{z}(t)$ is p-dimensional disturbance vector, $\boldsymbol{y}(t)$ is r-dimensional output response vector, $\mathbf{A}$ is system matrix $(n \times n)$, $\mathbf{B}$ is control matrix $(n \times m)$, $\mathbf{C}$ is output matrix $(r \times n)$.

The process boundaries are

$$\boldsymbol{h}[\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{z}(t)] \geqq \boldsymbol{h}_0 \tag{2}$$

where $\boldsymbol{h}, \boldsymbol{h}_0$ are vector functions of parameters of the controlled technological process. The problem of our interest is to find $\boldsymbol{u}(t)$ which minimizes a performance function when disturbances slowly change. The performance function is chosen as the quadratic criterion in the form [10]

$$J(\boldsymbol{u}) = \frac{1}{2}\int_{t_0}^{\infty} [\boldsymbol{x}(t)^T \mathbf{Q}\boldsymbol{x}(t) + \boldsymbol{u}(t)^T \mathbf{R}\boldsymbol{u}(t)]\mathrm{d}t \tag{3}$$

where $\mathbf{Q}$ is diagonal constant positive semidefinite matrix $(n \times n)$, $\mathbf{R}$ is diagonal constant positive definite matrix $(m \times m)$.

The performance function (3) is for mathematical reasons [10] one of the most used performance criteria in the process control design.

Layer Activities

Optimization Layer

The slowly changing disturbances are approximated by their predicted value $\boldsymbol{z}_N(t) = \boldsymbol{z}_N = \text{const}$, which is determined on the adaptation layer. For the optimization layer, we can use the modified description of the system dynamics [4] in the form

$$\frac{\mathrm{d}\boldsymbol{x}_m(t)}{\mathrm{d}t} = \mathbf{A}\boldsymbol{x}_m(t) + \mathbf{B}\boldsymbol{u}_m(t) + \boldsymbol{z}_N \tag{4}$$

The optimal processing of control $\boldsymbol{u}_m(t)$ is influenced by the prediction of disturbances $\boldsymbol{z}_N$ and by the initial state of system $\boldsymbol{x}_0$. For the predicted constant value $\boldsymbol{z}_N$ we have to minimize on the optimization layer the function

$$J_s = \frac{1}{2}[\boldsymbol{x}_s^T \mathbf{Q}\boldsymbol{x}_s + \boldsymbol{u}_s^T \mathbf{R}\boldsymbol{u}_s] \tag{5}$$

with respect to the following boundaries

$$\begin{aligned} \boldsymbol{h}_s[\boldsymbol{x}_s, \boldsymbol{u}_s, \boldsymbol{z}_N] &= \boldsymbol{h}_0 \\ \mathbf{A}\boldsymbol{x}_s + \mathbf{B}\boldsymbol{u}_s + \boldsymbol{z}_N &= \mathbf{0} \end{aligned} \tag{6}$$

The optimal values of the state vector $\boldsymbol{x}_N$ and control vector $\boldsymbol{u}_N$ are obtained on this layer [4, 5].

Direct Control Layer

The reaching of the optimal values $\boldsymbol{u}_N, \boldsymbol{x}_N$ is the goal of the direct control layer. We can use various methods for the direct control. They can be *e.g.* the optimal control or decentralized control with the control variables compounded of local and global components [4]. For this layer we can choose again the quadratic criterion and the controlled system description as it is in (7)

$$\begin{aligned} J(\boldsymbol{u}) &= \frac{1}{2}\int_{t_0}^{\infty} [\Delta\boldsymbol{x}(t)^T \mathbf{Q}\Delta\boldsymbol{x}(t) + \Delta\boldsymbol{u}(t)^T \mathbf{R}\Delta\boldsymbol{u}(t)]\mathrm{d}t \\ \frac{\mathrm{d}\Delta\boldsymbol{x}(t)}{\mathrm{d}t} &= \mathbf{A}\Delta\boldsymbol{x}(t) + \mathbf{B}\Delta\boldsymbol{u}(t) \\ \Delta\boldsymbol{x}(t) &= \boldsymbol{x}(t) - \boldsymbol{x}_N \\ \Delta\boldsymbol{u}(t) &= \boldsymbol{u}(t) - \boldsymbol{u}_N \end{aligned} \tag{7}$$

The control law is, see *e.g.* [1, 2]

$$\Delta\boldsymbol{u}(t) = -\mathbf{R}^{-1}\mathbf{B}^T\mathbf{K}\Delta\boldsymbol{x}(t) \tag{8}$$

and the symmetric matrix $\mathbf{K}$ is the solution of Riccati equation [1]

$$\mathbf{K}\mathbf{A} - \mathbf{A}^T\mathbf{K} + \mathbf{K}\mathbf{B}\mathbf{R}^{-1}\mathbf{B}^T\mathbf{K} - \mathbf{Q} = \mathbf{0} \tag{9}$$

Adaptation Layer

The prediction of disturbances is changed on the adaptation layer if the boundaries of these disturbances are overstepped. The new optimization process will be evoked and new optimal (nominal) values of state and control variables will be determined. These values take into account the changed situation.

RESULTS AND DISCUSSION

The above described control structure was implemented on the continuous stirred tank reactor with reactions A → B → C [6]. We consider that it is the nonlinear system with the dynamical model in the form

$$\begin{aligned} \frac{\mathrm{d}c_\mathrm{A}(t)}{\mathrm{d}t} &= \frac{q}{V}c_\mathrm{Av} - \frac{q}{V}c_\mathrm{A}(t) + r_\mathrm{A}(t) \\ \frac{\mathrm{d}c_\mathrm{B}(t)}{\mathrm{d}t} &= \frac{q}{V}c_\mathrm{Bv} - \frac{q}{V}c_\mathrm{B}(t) + r_\mathrm{B}(t) \\ \frac{\mathrm{d}T(t)}{\mathrm{d}t} &= \frac{q}{V}T_\mathrm{v}(t) + \frac{Q_\mathrm{r}}{V\rho c_p} - \frac{q}{V}T(t) - \frac{Q_\mathrm{c}}{Vc_p\rho} \\ \frac{\mathrm{d}T_\mathrm{c}(t)}{\mathrm{d}t} &= \frac{q_\mathrm{c}}{V_\mathrm{c}}T_\mathrm{cv}(t) + \frac{Q_\mathrm{c}}{V_\mathrm{c}\rho_\mathrm{c}c_\mathrm{pc}} - \frac{q_\mathrm{c}}{V_\mathrm{c}}T_\mathrm{c}(t) \end{aligned} \tag{10}$$

where

$$Q_c = f\alpha_t(T - T_c),\ Q_r = V(H_1 r_1 + H_2 r_2)$$
$$k_i = k_{0i} \exp\left(-\frac{g_i}{T}\right)$$
$$r_1 = k_1 c_A,\ r_2 = k_2 c_B,\ r_B = r_1 - r_2,\ r_A = -r_1 \quad (11)$$

Constants of the nonlinear model are listed in Symbols.

The individual variables are:
control variables: q_c
state variables: c_A, c_B, T, T_c
output variables: T, c_B
input variables: c_{Av}, c_{Bv}, T_v, T_{cv}

The multilayer control structure uses for control design of nonlinear reactor the linearized model. The linearized model is in the form

$$\frac{d\Delta \boldsymbol{x}(t)}{dt} = \mathbf{A}\Delta \boldsymbol{x}(t) + \mathbf{B}\Delta \boldsymbol{u}(t) + z_N$$
$$\Delta \boldsymbol{x}^T(t) = [\Delta c_A, \Delta c_B, \Delta T, \Delta T_c] \quad (12)$$
$$\Delta \boldsymbol{u}(t) = \Delta q_c$$

In the surrounding of the steady state defined by

$q_c = 0.11$ [m^3 min^{-1}]; $c_A = 1.285$ [kmol m^{-3}];
$c_B = 4.125$ [kmol m^{-3}]; $T = 345.68$ [K];
$T_c = 310.62$ [K]

the system matrix and the control matrix are

$$\mathbf{A} = \begin{bmatrix} -0.753 & 0 & -0.044 & 0 \\ 1.173 & -0.174 & 0.037 & 0 \\ 2.899 & 0.029 & 0.011 & 0.061 \\ 0 & 0 & 0.086 & -0.258 \end{bmatrix} \quad (13)$$

$$\mathbf{B} = [-27.531]$$

The changes of the input concentration of the components A, B and the changes of the input temperature and the temperature of the cooling medium were considered to be disturbances and their changes evoke the new optimization process. These changes are registered by adaptation layer. The adaptation layer checks the technological boundaries, too. On the optimization layer, the optimal values of control and state variables are calculated by gradient method, which is one of the often used static optimization methods [7]. The goal function

$$J_s = \frac{1}{2}(q_1 x_{1s}^2 + q_2 x_{2s}^2 + q_3 x_{3s}^2 + q_4 x_{4s}^2 + r u_s^2) \quad (14)$$

is minimized with respect to the boundaries resulting from the linearized static model

$$a_{11}x_{1s} + a_{13}x_{3s} + z_{1N} = 0 \quad (15)$$
$$a_{21}x_{1s} + a_{22}x_{2s} + a_{23}x_{3s} + z_{2N} = 0 \quad (16)$$
$$a_{31}x_{1s} + a_{32}x_{2s} + a_{33}x_{3s} + a_{34}x_{4s} + z_{3N} = 0 \quad (17)$$
$$Bu + a_{43}x_{3s} + a_{44}x_{4s} + z_{4N} = 0 \quad (18)$$

The following relations for the state variables were obtained

$$x_1 = f_{11}(\boldsymbol{u}) + f_{12}(\boldsymbol{z})$$
$$x_2 = f_{21}(\boldsymbol{u}) + f_{22}(\boldsymbol{z})$$
$$x_3 = f_{31}(\boldsymbol{u}) + f_{32}(\boldsymbol{z}) \quad (19)$$
$$x_4 = f_{41}(\boldsymbol{u}) + f_{42}(\boldsymbol{z})$$

From these relations the optimal values u_N and $x_{1N}, x_{2N}, x_{3N}, x_{4N}$ were calculated for different changes of input variables. We considered the elements of weighting matrix $\mathbf{Q}$ and matrix $\mathbf{R}$ to be $q_1 = 0.01$, $q_2 = 0.01$, $q_3 = 0.0001$, $q_4 = 0.0001$, $r = 1$. The selection of weighting matrices elements follows from properties of the controlled process and is connected with its technological parameters.

The direct control layer ensures that the desired values of state and control variables, calculated on the optimization layer, are achieved [8, 9].

The decentralized control law was used in the form

$$\Delta \boldsymbol{u}(t) = \boldsymbol{u}^1(t) + \boldsymbol{u}^g(t)$$
$$\boldsymbol{u}^1(t) = -\mathbf{R}^{-1}\mathbf{B}^T\mathbf{K}\Delta \boldsymbol{x} \quad (20)$$
$$\boldsymbol{u}^g(t) = -\mathbf{B}^{-1}\mathbf{H}\Delta \boldsymbol{x}$$
$$\boldsymbol{u}(t) = \Delta \boldsymbol{u}(t) + \boldsymbol{u}_n$$

where $\mathbf{H}$ is the interaction matrix. Control responses of the continuous stirred tank reactor achieved by the described control structure are in Figs. 2—5. The control variable is shown in Fig. 6. The controlled outputs reach their set points in spite of existing disturbances in the controlled system.

CONCLUSION

It is very important from the viewpoint of its industrial utilization to have a good control structure for chemical processing plants. The multilayer control structure was applied to control a chemical reactor. This structure effectively accepts various disturbances which enter into the controlled process. In the chemical reactor these disturbances can be represented by

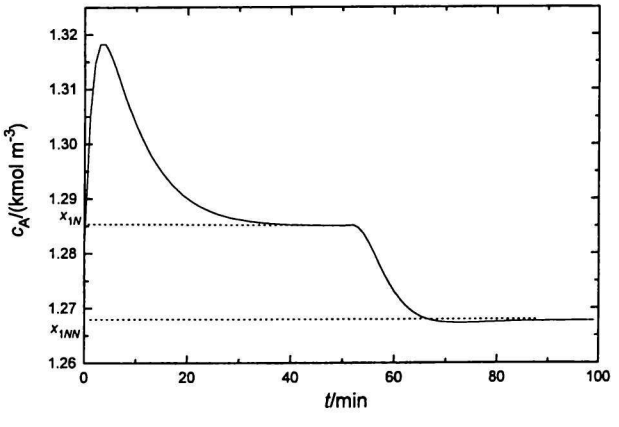

Fig. 2. Control responses of concentration of component A.

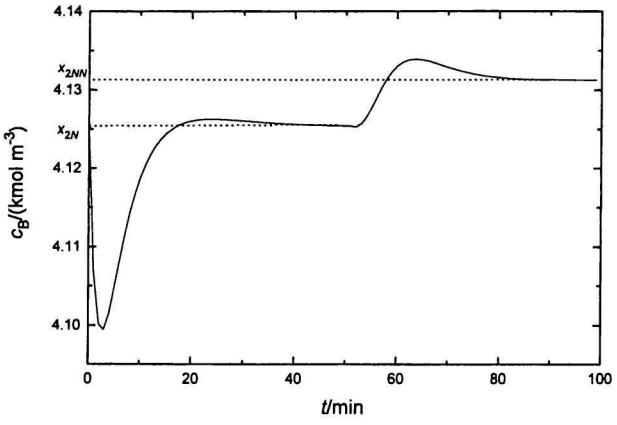

Fig. 3. Control responses of concentration of component B.

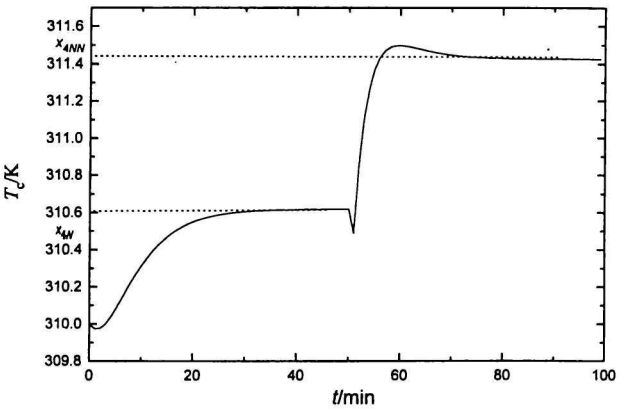

Fig. 5. Control responses of temperature of cooling medium.

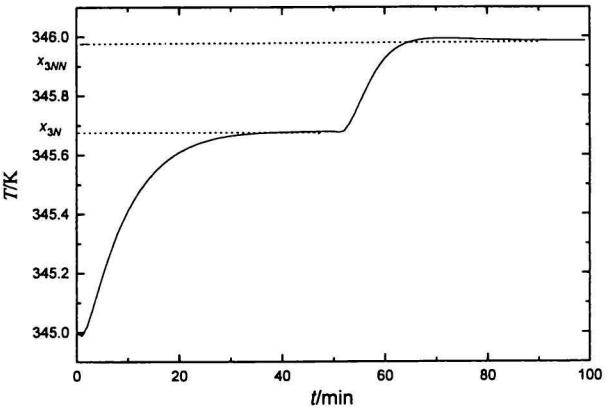

Fig. 4. Control responses of temperature of reaction mixture.

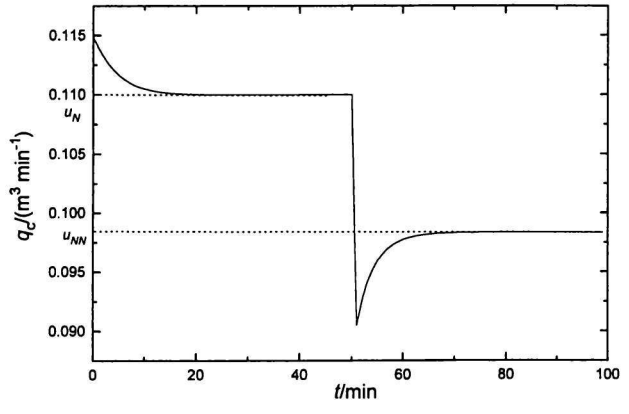

Fig. 6. Control variable.

changes of the input variables during the process control. The obtained simulation results demonstrate the convenience of the described multilayer control structure for control of such systems as chemical reactors. The convergence properties of the proposed algorithms for all layers of the multilayer control structure are very good.

SYMBOLS
of numerical values of physical quantities [unit]

α, β		adaptation layer parameters
τ_i		sampling period
γ, μ		coordination, information quantities
$q = 0.21$	[m^3 min^{-1}]	volume flow rate of reaction mixture
$q_c = 0.11$	[m^3 min^{-1}]	volume flow rate of cooling medium
$V = 1.2$	[m^3]	volume of reaction mixtures
$V_c = 0.64$	[m^3]	volume of cooling medium
$r = 796$	[kg m^{-3}]	density of reaction mixture
$r_c = 998$	[kg m^{-3}]	density of cooling medium
$c_p = 3.94$	[kJ kg^{-1} K^{-1}]	measuring heat of reaction mixture
$c_{pc} = 4.182$	[kJ kg^{-1} K^{-1}]	measuring heat of cooling medium
$f = 5.6$	[m^2]	transfer area
$\alpha_t = 41.2$	[kJ m^{-2} K^{-1} min^{-1}]	coefficient of heat transfer
$k_{01} = 2.703 \times 10^8$		frequency factor
$k_{02} = 2.223 \times 10^{27}$		frequency factor

$g_1 = 6896$	[K]	constant
$g_2 = 23453$	[K]	constant
$H_1 = 15500$	[kJ kmol^{-1}]	reaction enthalpy
$H_2 = 12000$	[kJ kmol^{-1}]	reaction enthalpy
r_A, r_B	[kmol m^{-3} min^{-1}]	reaction rates
c_A, c_B, c_{Av}, c_{Bv}	[kmol m^{-3}]	concentration and input concentration of components A, B
T_c, T, T_v	[K]	temperature of cooling medium, reaction mixture, input temperature

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