

## CONTROL SYSTEMS USING MATHEMATICAL MODELS OF TECHNOLOGICAL OBJECTS IN THE CONTROL LOOP

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### ABSTRACT

The control problems for technological objects with distributed state variables and large dead times are discussed in the present article. The creation of control systems using the object model in the control loop is considered. It is shown that the most effective approach for the development of models of chemical-processing facilities is a method of heat flow calorimetry for the creation of kinetic models of processes in multiphase systems and the use of simplified hydrodynamics models to describe mass transport processes. The demonstration of the successful application of this approach for creating mathematical models and their use in control systems has been shown for two important industrial processes, namely, the sintering process in the preparation of cement clinker in tubular rotating kilns and the modification process for epoxy resins with 1,4-butanediol to obtain epoxy polymers with improved physical and mechanical properties. Such mathematical models make it possible to specify the optimal operating modes of the considered processes.

**Key words:** the objects with delay, models for control, kinetics, heat flux calorimetry, cement clinker, epoxy resins.

### INTRODUCTION

Closed control systems on deviation that work with a feedback loop are widely used in many industries [1-5].

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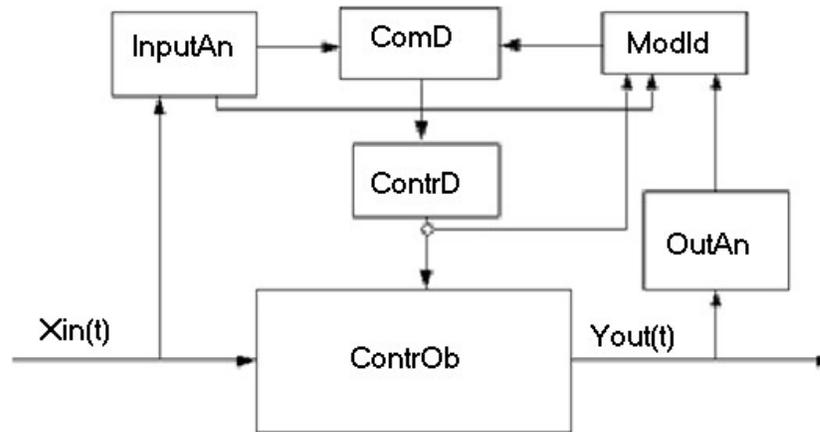


However, they cannot be successfully used for controlling objects with distributed state variables and large dead times, such as tubular and tower reactors, shell tubular heat exchangers, and distillation columns, if it is necessary to support controlled variables at the apparatus output [6]. Additionally, deviation control systems may not always may be used to control for potentially dangerous objects because deviation-regulated parameters from given values are not permitted with consideration for the safety processes [8, 9].

## **METHODS**

The control of objects with distributed parameters requires the use of predictive control systems that can generate control actions with compensatory actions for input disturbances while regulating channels. The generation of such control signals is based on analysis of the input variables of the object and exact knowledge of the order transformation of input variables into output variables. With the availability of such information, it is possible to use calculation methods that consider transfer functions of conduction disturbances through the regulation channel [5-7]. In these cases, the control system may generate control actions that support regulated values for a given level. When a computer is present in the control loop, it is possible to use a mathematical model of the object to predict the object behaviour with input disturbances. In this case, such a control system is called a control system with a “fast model” in the control loop. Because the solution of the mathematical model for the object provides a response of the object that is faster than the real object response, it is possible to analyse the response and generate an optimal control action, allowing for compensation of possible deviation-regulated variables from set points.

In Fig. 1, the total structure of the scheme control system with a “fast model” in the control loop is shown.



**Fig.1.** Structural scheme of disturbance control using the “fast model” in the control loop.

ContrOb – control object; ContrD – control device; InputAn – input analyser; OutAn – output analyser; ModId – model identifier; ComD – computing device;  $X_{in}(t)$  – vector-function of input variables; and  $X_{out}(t)$  – vector-function of output variables.

Input variables pass through the InputAn (input analyser). After the input variables vector and the input disturbance vector are entered into this device, the process proceeds to the computing device (ComD) and into ModId (model identifier). In this device (model identifier), information about the current values of the control vector come is generated. In ModId, the inverse task is solved, and current parameters of the mathematical model are specified. The delay time must be considered for every signal, which is a very important feature of the identification procedure. The real delay time may be specified or may be determined using the results of a passive experiment on objects or the results of active experiments. In this case, special planned disturbances act on the object. By observing these disturbances with various actions, it is possible to specify the exact values for the delay time for every control channel.

After the identification model is transferred to the computer, optimal values for the control actions are calculated. These optimal control actions correspond to the current state of the controlled object. At present, such control schemes are applied to control complicated and responsible processes characterized by variegated disturbances of input variables. Based on experience with operating such systems, it is possible to specify the critical deviation state variables that demand an identification procedure for the mathematical model. This process allows for decreased use of complete identification, which increases the processing speed of the control system.

**Creation models for control systems.**

With creation models for control systems, such feature models are very important for providing performance predictions in a wide interval change of variables. For these aims, it is very helpful to create model equations of chemicals kinetics and hydrodynamics. Simplified hydrodynamics models are commonly used, such as the ideal mixing model, the plug flow model and combinations of these models. For creation kinetics models, heat flux calorimetry can be helpful. The use of calorimetry for an investigation kinetics chemical reaction is based on the observation that the rate of heat generation is related to the rates of chemical reactions as follows:

$$\frac{dQ_{gen}}{dt} = \sum w_{ij} \cdot H_j \quad (1)$$

$$\frac{dc_i}{dt} = \sum_{j=1}^R \sum_{i=1}^N w_{ij} \quad (2)$$

$$w_{ij} = -k_j \cdot \prod_{i=1}^{N_r} c_i^{n_i} + k_{-j} \cdot \prod_{i=N_r+1}^{N_p} c_i^{n_i} \quad (3)$$

where  $Q_{gen}$  / kJ is the total heat absorbed (or generated) in the chemical process;

$w_{ij}$  /  $kmol \cdot m^{-3} \cdot min^{-1}$  is the rate of transformation of  $i$ -th component of reaction mixture in  $j$ -th chemical reaction;

$k_j = \exp(\ln(k_{0,j}) - (E_j / RT)) / (kmol \cdot m^{-3})^{n-1} min^{-1}$  is the rate constant of the forward reaction;

$k_{-j} = \exp(\ln(k_{0,-j}) - (E_{-j} / RT)) / (kmol \cdot m^{-3})^{n-1} min^{-1}$  is the rate constant of the reverse reaction;  $n$  is the reaction order;  $H_j$  /  $kJ \cdot kmol^{-1}$  is the heat effect of the chemical reaction; and  $t$  / min is the current time of the process.

The procedure that is usually used to specify kinetics parameters from experimental data is included in the selection of kinetics parameters from condition minimal mismatch between experimental data and process modelling results. For such mismatch, the sum of the square

deviation between experimental data and modelling results is usually used in accordance with equation (4)

$$R = \sum_{k=1}^K \sum_{s=1}^S \left( X_{k,s}^{(c)} - X_{k,s}^{(exp)} \right)^2 = R(\mathbf{u}_p) \quad (4)$$

where k –index time point on the kinetics curve;

s- index measured state variable in the kinetics experiment;

c- calculated data;

exp –experimental data;

K–number of experimental points on the kinetics curve;

S –number of measured state variables in the mathematical model;

$\mathbf{u}_p$  – required kinetics parameters (pre-exponential factors, activation energies, and reaction orders).

For the extremum search method, different variants of nonlinear programming methods are used. Values of calculated data state variables usually result from the numeric solution of mathematical model equations with different variants of the Runge-Kutta method or the LSODA method [13,14].

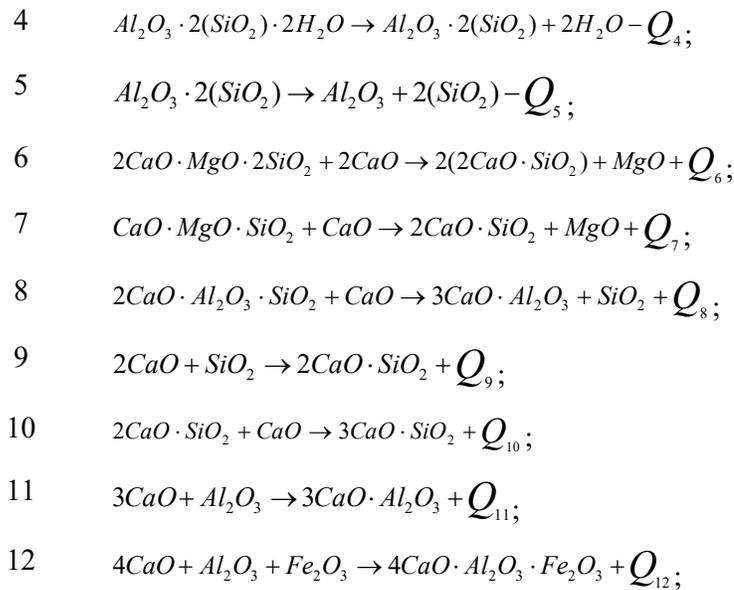
## RESULTS

The first objective of this study was to use a proposed approach to kinetics investigation in the process of cement clinker production in a tubular rotary kiln.

Experimental studies have been performed using a differential scanning calorimeter from NETSCH. The current sample mass and rate of heat generation were obtained as experimental responses. To formulate kinetics equations, chemical reactions that occur at the sintering cement charge were used [10,11]:

Table 1. The sequence of chemical reactions that occur when firing the raw mix to produce cement clinker.

No	Chemical reaction for producing cement clinker
1	$H_2O_1 \rightarrow H_2O - Q_1;$
2	$CaCO_3 \Leftrightarrow CaO + CO_2 - Q_2;$
3	$MgCO_3 \Leftrightarrow MgO + CO_2 - Q_3;$



With the solution reverse task in accordance with equation (4) in the ReactOp Program package [13,14], the kinetics parameters were determined.

The searched values of the thermal effects, activation energy and pre-exponential factors of the logarithms of the rate constants are presented in Table 2.

**Table 2.** The values of searched kinetics parameters of the kinetics model cement clinker production.

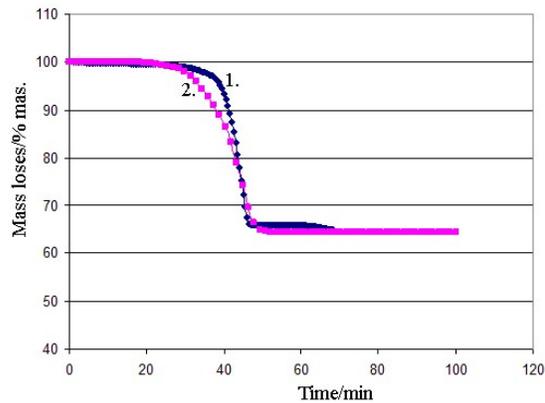
	Mineral of charge	Kinetics parameters value
1	CaCO <sub>3</sub>	
	ln(Ko)/min <sup>-1</sup>	13.37
	E/kJ·mol <sup>-1</sup>	102.17
	ln(Keo)/min <sup>-1</sup>	15.01
	Ee/kJ·mol <sup>-1</sup>	60
2	MgCO <sub>3</sub>	
	ln(Ko)/min <sup>-1</sup>	2.61
	E/kJ·mol <sup>-1</sup>	89.63
	ln(Keo)/min <sup>-1</sup>	93.18
	Ee/kJ·mol <sup>-1</sup>	187.06
	(-H)/kJ·kmol <sup>-1</sup>	-68819,37
3	Al <sub>2</sub> O <sub>3</sub> (SiO <sub>2</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub>	

	$\ln(K_o)/\text{min}^{-1}$	4.9
	$E/\text{kJ}\cdot\text{mol}^{-1}$	48.35
	$(-H)/\text{kJ}\cdot\text{kmol}^{-1}$	-237744
4	$\text{NaAlO}_2(\text{SiO}_2)_6(\text{H}_2\text{O})_2$	
	$\ln(K_o)/\text{min}^{-1}$	9.86
	$E/\text{kJ}\cdot\text{mol}^{-1}$	20.84
	$(-H)/\text{kJ}\cdot\text{kmol}^{-1}$	-66948
5	$\text{Al}_2\text{O}_3(\text{H}_2\text{O})_3$	
	$\ln(K_o)/\text{min}^{-1}$	10.47
	$E/\text{kJ}\cdot\text{mol}^{-1}$	11.22
	$(-H)/\text{kJ}\cdot\text{kmol}^{-1}$	-52891
6	$\text{NaAlO}_2(\text{SiO}_2)_6(\text{H}_2\text{O})_2$	
	$\ln(K_o)/\text{min}^{-1}$	2.19
	$E/\text{kJ}\cdot\text{mol}^{-1}$	48.84
	$(-H)/\text{kJ}\cdot\text{kmol}^{-1}$	-102920
7	$\text{Fe}(\text{OH})_3$	
	$\ln(K_o)/\text{min}^{-1}$	4.73
	$E/\text{kJ}\cdot\text{mol}^{-1}$	36.16
	$(-H)/\text{kJ}\cdot\text{kmol}^{-1}$	10292
8	$\text{Al}_2\text{O}_3(\text{SiO}_2)_2$	
	$\ln(K_o)/\text{min}^{-1}$	20,32
	$E/\text{kJ}\cdot\text{mol}^{-1}$	150,3
	$(-H), \text{kJ}/\text{kmol}$	-66948
9	$(\text{CaO})_2\text{MgO}(\text{SiO}_2)_2$	
	$\ln(K_o)/\text{min}^{-1}$	13,2
	$E/\text{kJ}\cdot\text{mol}^{-1}$	150,1
	$\ln(K_{eo})/\text{min}^{-1}$	103823
10	$(\text{CaO})_2\text{Al}_2\text{O}_3\text{SiO}_2$	
	$\ln(K_o)/\text{min}^{-1}$	23,21
	$E/\text{kJ}\cdot\text{mol}^{-1}$	250,34
	$(-H)/\text{kJ}\cdot\text{kmol}^{-1}$	10292

In Fig. 2, comparison modelling results with experimental data are shown.

The modelling results that have been calculated with identified kinetics parameters are shown in Table 2.

a)

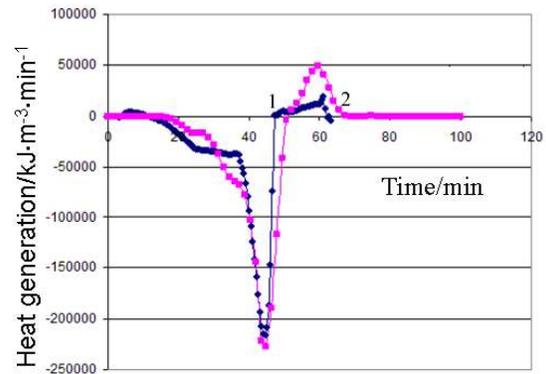


**Fig.2 a).** Mass losses as a function of time

1-experimental data

2- modelling results

b)



**Fig.2 b).** Heat generation as a function of time

1-experimental data

2- modelling results

As seen in Fig. 2, the kinetics model appropriately describes the experimental data and may be used for modelling the process of cement clinker production under industrial conditions. If the developed model is too complicated to identify optimal conditions, it may be simplified using the planning experiments method. Such a model requires less time to solve and has some advantages over the model obtained with passive experiments because in such a model, the coefficients of the equation of linear regression do not contain joint coefficients and every coefficient conveys action for the corresponding variable. Additionally, because the model was produced from the determined model, this model has substantial prognosis ability, even after the limits of linearization.

When using the described approach, the mathematical model of the sintering process for the cement charge in a rotary tubular kiln was developed [8]. The model represents a differential equation system describing the change in the concentrations of components in gas and solid phases on the length of the tubular kiln:

$$\begin{aligned} \frac{dc_i}{dl} &= \frac{1}{u_s} \sum_{j=1}^M w_{ij}; \\ \frac{dT_s}{dl} &= \frac{1}{u_s} \sum_{j=1}^M w_{i,j} \cdot Q_j - B_x(T_s - T_0) - K_v \cdot F_v \left( \frac{T_s^3}{100} - \frac{T_g^3}{100} \right) \pm K_{ch}(T_s - T_g) \pm K_{cep}(T_s - T_g); \\ \frac{dT_g}{dl} &= \frac{1}{u_g} K_{iF}(T_s - T_g) \pm K_{ch}(T_s - T_g) + K_{iF} \left( \frac{T_s^3}{100} - \frac{T_g^3}{100} \right); \\ \frac{dc_{gasdust}}{dl} &= G_s \frac{z + z'}{100}; \quad K_{con} = K_{ch}, \text{ if } l \leq l_{ch}; \quad K_{con} = K_{iF}, \text{ if } l \geq l_{ch} \end{aligned} \quad (5)$$

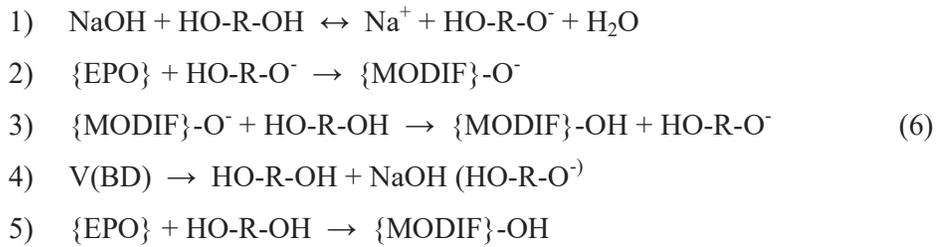
where  $l/m$  is the current kiln length;  $L/m$  is the total kiln length;  $c/kmol \cdot m^{-3}$  is the concentration of the  $i$ -th component in the reaction mixture;  $u_s/m \cdot s^{-1}$  is the linear velocity of a moving solid material;  $w_{i,j}/kmol \cdot m^{-3} \cdot s^{-1}$  is the rate of change of the concentration of the  $i$ -th component in the  $j$ -th reaction;  $T_g$  and  $T_s/K$  are the temperatures of the gas and solid phases, respectively;  $z' / \%$  is the dust level circulating in the kiln;  $z / \%$  is the dust level removed from the kiln;  $T_0/K$  is the temperature inside the kiln;  $B_x/m^{-1}$  is the heat exchange parameter;  $K_{ch}/W \cdot m^{-2} \cdot K$  is the heat transfer coefficient in the chain curtain zone of the kiln;  $l_{ch}/m$  is the chain curtain zone length;  $M$  is the number of chemical reactions;  $Q_j/kJ \cdot kmol^{-1}$  is the heat effect of the  $j$ -th reaction;  $K_{iF}/W \cdot m^{-2} \cdot K^{-1}$  is the heat transfer coefficient in the zone free from the chain curtain;  $c_{ngasdust}/kg \cdot m^{-3}$  is the dust concentration in the gas phase;  $G_s/kg \cdot kg^{-1}$  is the dust mass fraction inside the kiln;  $K_{con}/m^{-1}$  is the parameter of convective heat exchange; and  $F_v/m^2 \cdot m^{-3}$  is the specific radiation surface.

The counter current of the moving gas and solid phases in the kiln mathematical model represents the boundary problem, with boundary conditions given on different ends of the integration interval. To solve this model, the method of successive iterations has been used.

### **Modelling process for modifying chlorine-containing epoxy resins by 1,4-butanediol.**

The other example using the proposed approach is the process of modification of epoxy resins by 1,4-butanediol to expand the functionality and improve the physical and mechanical characteristics of the polymers. Investigations into the kinetics modification of chlorine-containing epoxy resins have been performed using heat flux calorimetry. A Setaram C80 was used as the main instrument. As experimental responses, heat generation curves were used. To

develop kinetics models of the modification process, the following elementary steps have been proposed:



Based on kinetics investigations, a mathematical model has been developed as described in the following differential equations:

- 1)  $\frac{dC_j}{dt} = -C_j(w/V_r) + r_j$
- 2)  $\frac{dC_{\text{EPO}}}{dt} = -C_{\text{EPO}}(w/V_r) + J_m/w + r_{\text{EPO}}$
- 3)  $\frac{dV_r}{dt} = w$
- 4)  $\frac{dV_{\text{EPO}}}{dt} = -w$  (7)
- 5)  $\frac{dH}{dt} = H_{\text{EPO}} \cdot \frac{dV_{\text{EPO}}}{dt}$
- 6)  $J_m = k_m \cdot 6 \cdot V_{0,\text{EPO}}^{(1/3)} \cdot V_{t,\text{EPO}}^{(2/3)} \cdot (C_s - C_{\text{EPO}}) / d_{k0}$
- 7)  $w = J_m$

where  $C_i/\text{kmol}\cdot\text{m}^{-3}$  – concentrations of all components in the reaction mixture, except the concentration of epoxy groups;

$C_{\text{EPO}}/\text{kmol}\cdot\text{m}^{-3}$  – epoxy group concentration in the reaction zone;

$V_r/\text{m}^3$  – volume of the reaction zone;

$V_{\text{EPO}}/\text{m}^3$  – volume of the epoxy resin in the reactor;

$J_m/\text{kmol}\cdot\text{m}^{-3}$  – mol flow epoxy group in reaction zone;

$w/\text{m}^3\cdot\text{s}^{-1}$  – volume flow in the reaction zone;

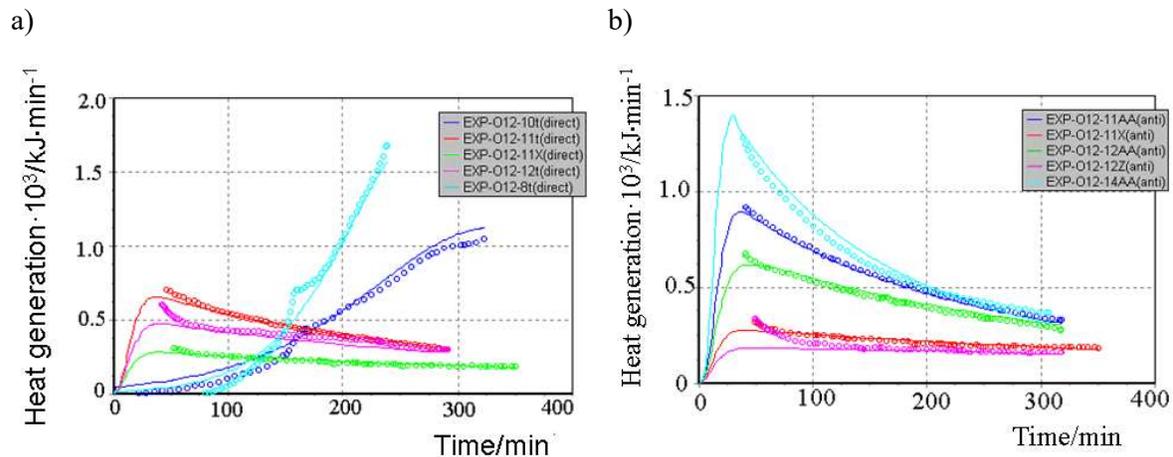
$d_{\text{dr},0}/\text{m}$  – drop volume of the dissolving phase at the initial time;

$d_{\text{EPO}}/\text{kmol}\cdot\text{m}^{-3}$  – mol density epoxy group.

All generated heat is uniformly distributed between phases, and heat exchange is not considered.

To solve the inverse task and define the kinetics parameters, special “ReactOp” software was used [13,14]

In Fig. 3, a comparison of the experimental data and modelling results is shown.



**Fig.3 a.** Comparison of the experimental data and modelling results under different conditions:

Mol relation «epoxy- group - butane diol-1,4»:  
~1:1.0;

Catalyst concentration (NaOH): ~0.10-0.12%  
mas.

Linear heating mode:

85-165°C;  $\beta=0.50^\circ\text{C}/\text{min}$  (**O12-8t**, 0.10%

NaOH)

75-165°C;  $\beta=0.30^\circ\text{C}/\text{min}$  (**O12-10t**, 0.12%

NaOH)

Isothermal mode:

128°C - (O12-11t, 0.12% NaOH); (O12-11X,

0% NaOH)

118°C - (O12-12t, 0.13% NaOH))

**Fig.3 b.** Comparison of the experimental data and modelling results under different conditions:

Mol relation «epoxy- group - butane diol-1,4»:  
~1:1.0;

Catalyst concentration (alcoholate NaO-R-OH):  
~0.34-0.38% mas.

(it corresponds to ~0.10-0.12% mas. NaOH)

Isothermal mode:

138°C - (**O12-14AA**, 0.34% NaO-R-OH)

128°C - (**O12-11AA**, 0.34% NaO-R-OH);

(**O12-11X**, 0% NaO-R-OH)

118°C - (**O12-12AA**, 0.38% NaO-R-OH):

(**O12-12Z**, 0% NaO-R-OH)

In this way, we developed a mathematical model with five chemical stages and one mass transfer stage.

## DISCUSSION

The definition of the optimal temperature profile has been formulated and solved based on the developed mathematical model.

We consider the temperature change profile along the length of the oven as a running control variable:

$$u = T(l), \quad (8)$$

In this case, the optimization criterion is the functional value expressed by the value of the tricalcium silicate concentration exiting the kiln.

$$C_{\text{tricalcium silicate}} = \int_0^l C_{\text{tricalcium silicate}}(l, T(l)) dl \Rightarrow \max, \quad (9)$$

This formulation of the optimization task is a variational calculus problem, and the control function of  $T(l)$  is the control variable. If we represent the desired optimum temperature profile as a piecewise linear approximation of the control function on length, we can proceed from the variational problem to the usual problem of finding the extremum of the function of several variables.

$$C_{\text{tricalcium silicate}}(L) = F(T_1, \dots, T_N, l_1, \dots, l_N) \Rightarrow \max, \quad (10)$$

$$T_{i \min} \leq T_i \leq T_{i \max}$$

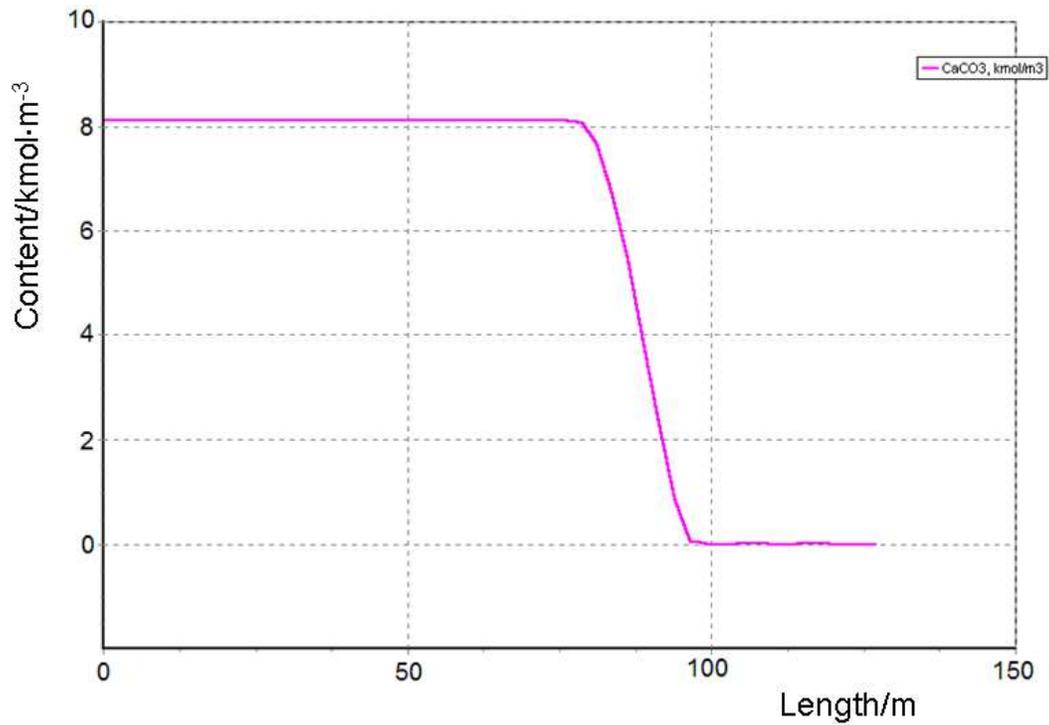
where  $L$  is the full length of the kiln.

In this case, the controls (certain points and temperature values in these certain points) will be found in an allowable control region. For each section of the temperature profile, the restrictions may be separately set. This is a typical problem for an extremum with inequality constraints. To solve such a problem, the method of nonlinear programming, which is implemented in ReactOp, may be used [13,14].

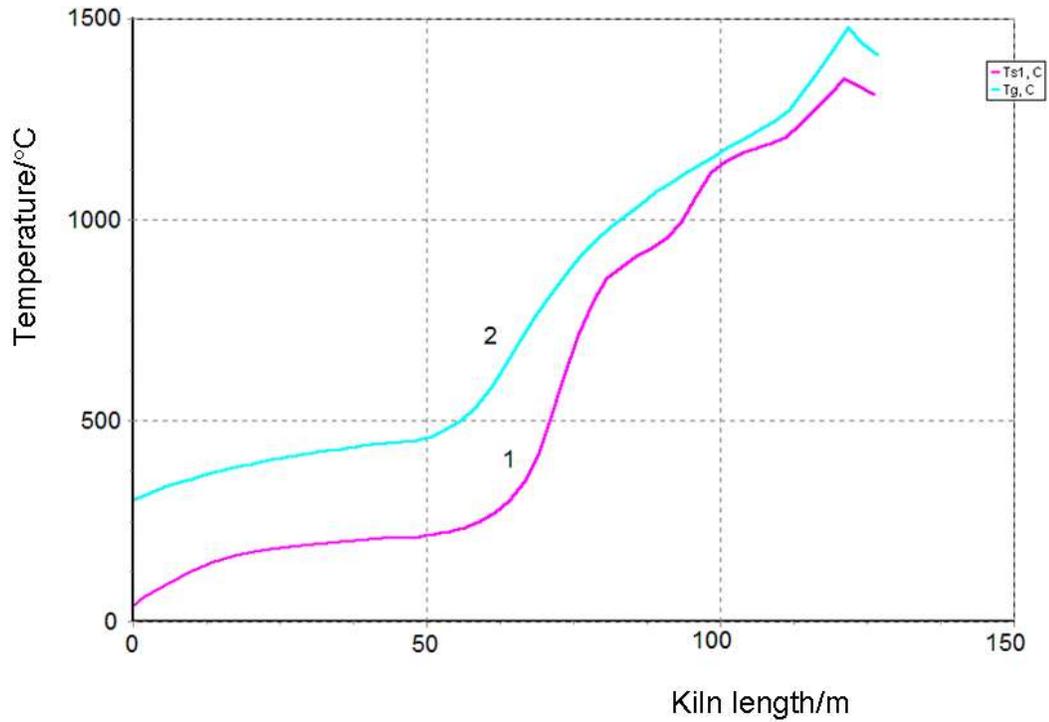
As a mathematical model, we have used a simplified model with equations that describe chemical reactions in the solid phase and the concentration of oxygen in the solid phase. The

equations of heat transfer between the phases and the equation for the temperature of the solid and gas phases cannot be used because the temperature of the solid phase is a control variable that must be solved in the optimization problem.

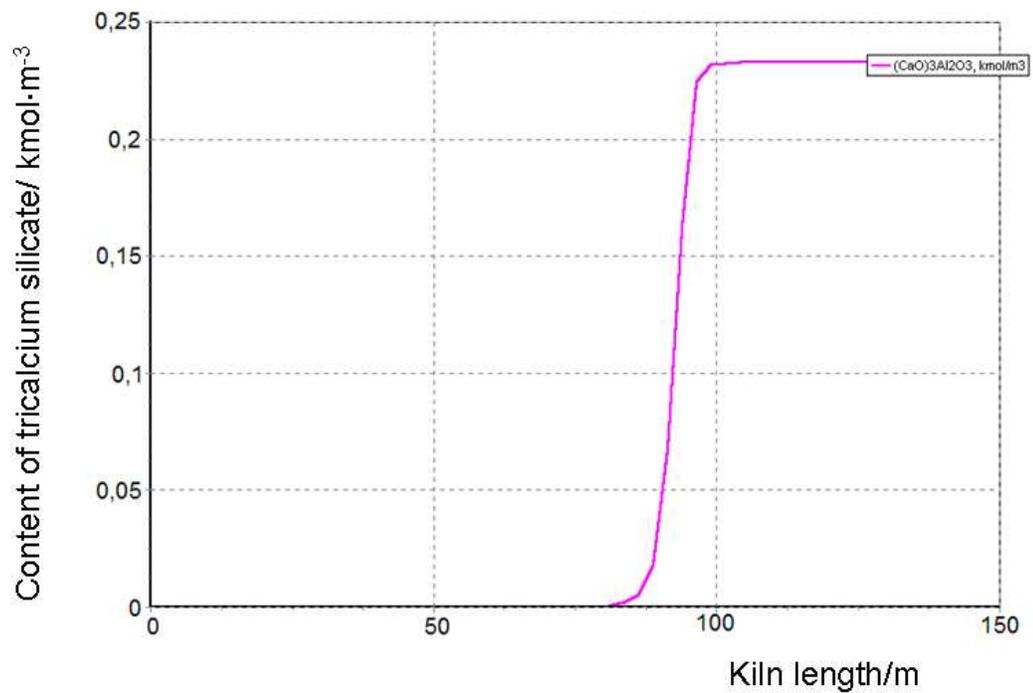
Below are graphs of the main concentrations of substances found in the temperature change profile.



**Fig.4.** Changes in the calcium carbonate content along the kiln during firing of the raw mix for producing cement clinker.



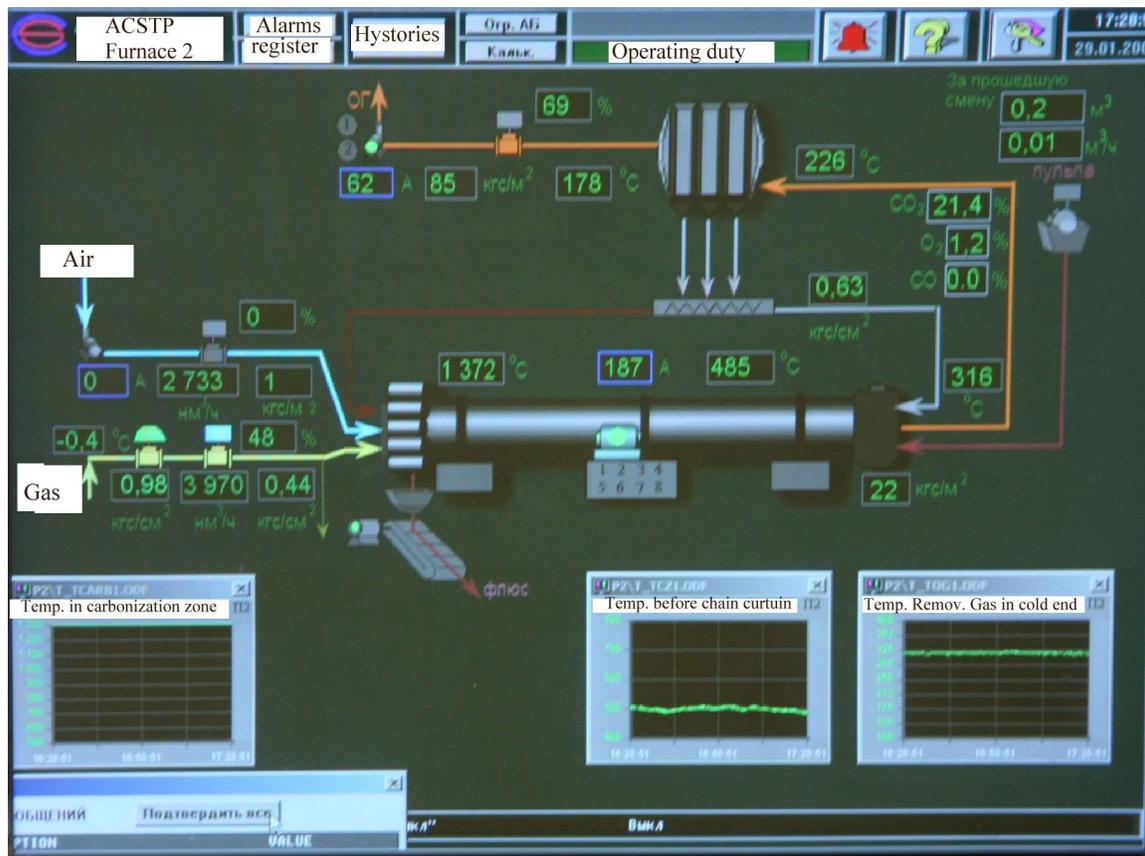
**Fig.5.** Profile temperatures of the gas (1) and solid (2) phases at the optimal profile temperature of the solid phase inside the kiln.



**Fig.6.** Changes in the content of tricalcium silicate (objective) with kiln length during raw material firing when producing a cement clinker at the optimal temperature profile.

The value objective at optimal conditions is more on 12 % in comparison with the commonly used operating duty.

The obtained results show the effectiveness of using mathematical modelling to determine the optimum process conditions in tubular rotary kilns during heat treatment processes. To develop a mathematical model of this unit with known chemical properties of the raw material, it is necessary to study the kinetics of chemical reactions with TG-DSC calorimetry. In the study of kinetics, we use the quasi-homogeneous model of heterogeneous processes and the numerical values of the kinetic parameters, which, especially the pre-exponential factors, depend on the dispersion of the solid phase and method for preparing the charge. The developed algorithm defined the optimal temperature profile used in the control system of cement clinker production on one industrial plant of the Russian Federation. The technological scheme and control loop of this process are shown in Fig. 7.



**Fig.7.** Technological scheme and control system of the unit for producing cement clinker.

The values calculated in the temperatures profile have been used as set points for the control system effects of the temperature on the kiln length. Control actions have been used for flows of natural gas and air.

Based on the work presented here, the next strategy of optimal control is as follows:

We establish the productivity of the final product. We select available compositions for the charge.

X-ray analysis of the phase composition of the charge was performed to determine the mineralogical composition and to write chemical reactions.

We completed the kinetic study of a charged sample in the heat flux calorimeter. The kinetics parameters of the mathematical model are identified in accordance with the above-described procedure.

The optimal temperature profile is estimated.

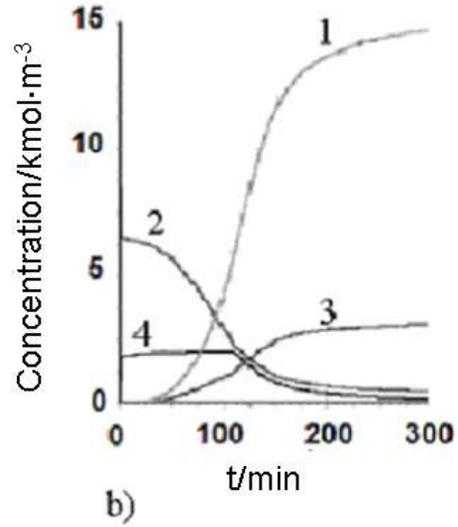
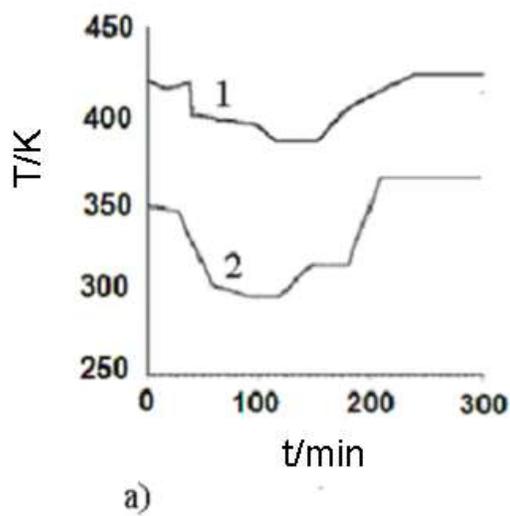
The heat balance of the process is evaluated by solving the direct task kinetics model at the optimal temperature profile.

The solution of the mathematical model is fulfilled, selecting the consumption of natural gas and air at which the optimal temperature profile is realized.

In this way, the strategy of optimal control is completed by defining parameters of the mathematical model for a given concrete charge and defining parameters in the technological system that satisfy the sintering process at optimal conditions.

### **Optimization of the modification process of chlorine-containing epoxy resins.**

The optimal temperature profile for this process has to provide maximal concentrations of the products (modified epoxy groups) at the end of the process. As control actions, the temperatures of heat exchange facilities were selected (temperature of cooling water and heating steam). These control actions demonstrate the optimal temperature profile while considering disturbances. In Fig. 8, the values of optimal control actions, calculated in the mathematical model in the control loop (in block ComD Fig. 1), are shown. These control actions are transferred into the controller, which is controlled by the process. This control scheme is shown in Fig. 9.



**Fig.8a.** Optimal control actions for the modification process of epoxy resins as a function of time. 1 – temperature of the steam jacket  
2- Temperature of cooling water in the coil.

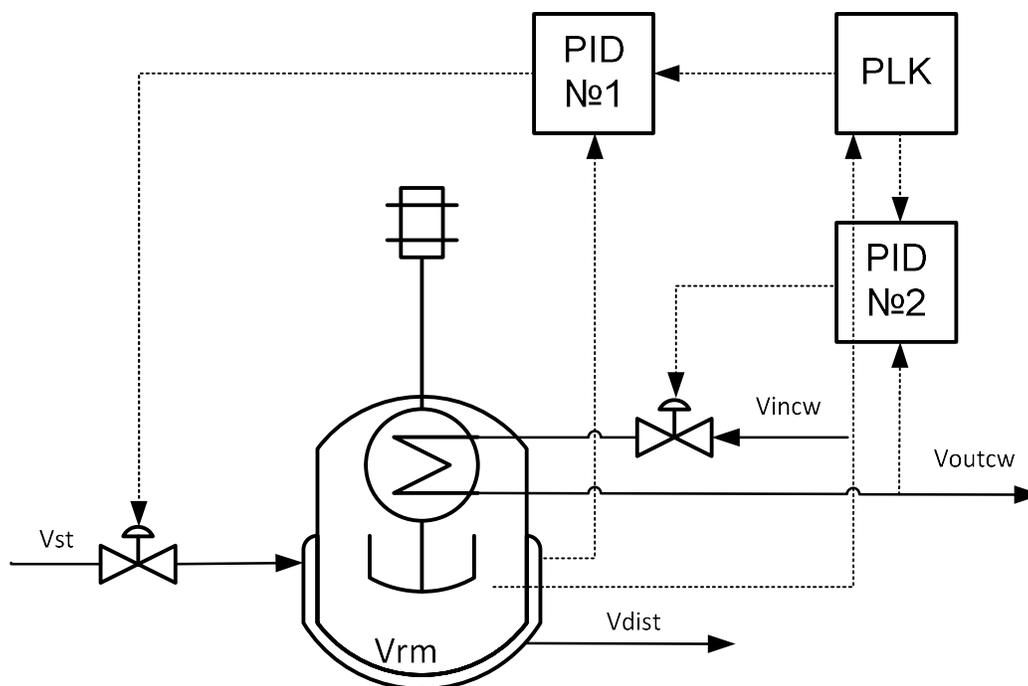
**Fig.8b.** Change state variable in the optimal control actions versus time.

1- $Q/kJ \cdot g^{-1}$  – total heat generation, proportional to the concentration of the aims component

2- $HO-R-OH/kmol \cdot m^{-3}$  – butanediol;

3- $Na^+/ kmol \cdot m^{-3}$  – sodium ion

4- $EPO/ kmol \cdot m^{-3}$  – epoxy resin



**Fig.9.** Scheme of the optimal control of the process of modification epoxy resins by 1,4-butanediol

Vrm – modification reactor; Vst – input of heating steam in the jacket; Vdist – distillate output from the jacket; Vincw – input cooling water in the coil; Voutcw – output cooling water from the coil; PID №1 – regulator of the temperature in the steam jacket; PID №2 – regulator of the temperature in the cooling coil; PLK – programmed logic controller.

## CONCLUSIONS

1. Analysis of the control by complicated technological processes has been performed.
2. It has been shown that heat flux calorimetry promotes the development of mathematical models of technological processes with high predictive ability.
3. Such kinetics models, in connection with hydrodynamics models, allow for consideration of the physicochemical and mass transfer features of the processes while obtaining optimal conditions that account for the mechanism of the processes.
4. The proposed approach has been illustrated in examples and detailed mathematical models, which were evaluated based on a study of heat flux calorimetry to define optimal control of the objects while considering disturbances to the industrial processes.

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