Virtual and analogue model of a continuous stirred tank reactor

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Abstract
This paper presents an analogue model of an exothermic stirred reactor developed at author's workplace. The comparison both models – analogue and virtual one is a main part of the paper. The tests of the both models include the steady states and dynamical responses of models. Briefly a further Research direction is mentioned.

Key words: Reactor analogue model, virtual technological process model.

Introduction

The first part of the paper is an analogue model of an exothermic reactor presented. The next part is devoted to brief description of virtual model of exothermic reactor. That is more detailed in (Kuník *et al*. 2006). The both models, the virtual and analogue ones, use the same mathematical model. The main part of the paper consists a comparison between the both models.

Merits of the both approaches primarily are economical operation, cost decreasing on operator training's and using them for education. The next advantage is a possibility of repeated simulation of critical states of controlled technology and a possibility of use an objective metric of operators.

The both types of models have their advantages. The virtual model is economical advantageous, robust and easily useable in distance education or in e-learning. The analogue model is more realistic, primarily its advantage is, that it can be connected direct to programmable controller through standard voltage inputs and outputs respectively.

Mathematical model

The mathematical model of reactor (Kuník *et al*. 2006) neglects thermal capacity of reactor wall and its thermal resistance. We assume constant density and thermal capacity of the reactive composite. Feed volume flow and output one are constant. The reactor is ideal stirred; therefore concentration and temperature of reactor and its output are equal.

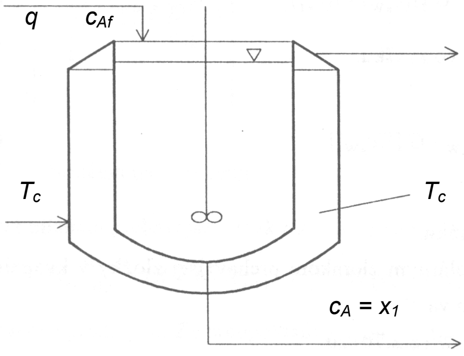

Fig.1 Continuous stirred tank reactor

The mathematical model of exothermic reactor simulates a process of exothermic reaction in a stirred reactor (Fig. 1). Dynamical process is described by non linear system if differential equations (1) and (2).

$$\frac{dx_1}{dt} = k_1\left(c_{Af} - x_1\right) - y \tag{1}$$

$$\frac{dx_2}{dt} = k_1 T_f + k_4 T_c - \left(k_1 + k_4\right)x_2 - k_3 y \tag{2}$$

where

$$y = x_1 k_0 e^{-\frac{k_2}{x_2}} \qquad x_1 = c_A \qquad x_2 = T$$

$$k_1 = \frac{q}{V} \qquad k_2 = \frac{E}{R} \qquad k_3 = \frac{\Delta H}{\rho C_p} \qquad k_4 = \frac{UA}{V\rho C_p}$$

Analogue model

The analogue model (Fig. 2) was developed at author's workplace. Dynamical process is described by non linear system if differential equations (1) and (2), which have been used implementing the virtual model (Kuník *et al*. 2006).

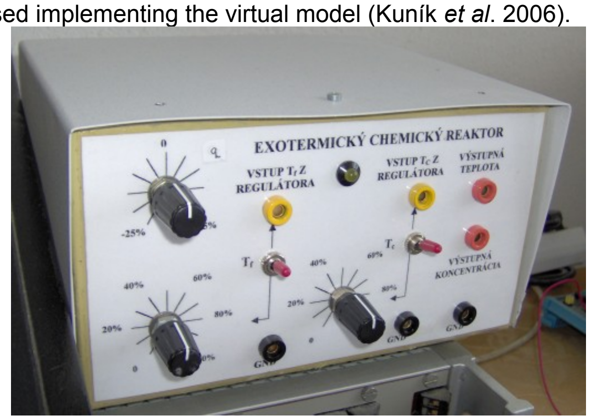

Fig.2 The analogue model

The analogue model has implemented the all input/output signal as the virtual one. Control action is thus realised by change of cooling temperature T_c or input temperature of feed T_f. As a disturbance variable is feed flow rate q. Controlled variables are reactor temperature T and concentration of reactor contents c_A.

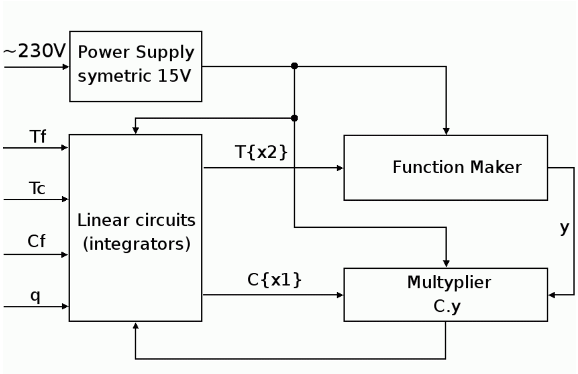

Fig.3 Block diagram of the analogue model

Fig. 3 gives the block diagram of the analogue model. Mathematical functions are simulated by operational amplifiers.

The steady state of the analogue model is given by values in Tab. 1. There are input and output ranges in the second column. The remainder parameters are the same as in virtual model (Kuník *et al.* 2006).

	Ranges	Steady state
c_{Af} [mol/l]	1 = counts.	1
q [l/min]	75 – 125	100
T_c [K]	273 – 400	311
T_f [K]	273 – 400	349
c_A [mol/l]	0 – 1,1	0,1
T [K]	273 – 400	378

Tab.1 Parameters of analogue model

Virtual model

The virtual model of the continuous stirred reactor is in detail described in (Kuník *et al.* 2006). The given technological process described by differential equations (1) and (2) is simulated by numeric integration method Runge – Kutta of 4th order. The variable ranges and steady state values are in Tab. 2.

	Ranges	Steady state
c_{Af} [mol/l]	0,9 – 1,1	1
q [l/min]	75 – 100	100
T_c [K]	273 – 373	311
T_f [K]	300 – 400	350
c_A [mol/l]	0 – 1,1	0,094
T [K]	273 – 473	385

Tab.2 Parameters of virtual model

Comparison of the models

As mentioned above, both the virtual and the analogue model represent the same technological process. Thus a comparison can be performed between these two types of model.

The goal of this comparison is a validation of the analogue model based on evaluation some quantitative static and dynamic parameters of the both models. The virtual model has been validated by model implemented in MATLAB.

The comparison of the models has been made under change of feed temperature and coolant temperature and feed flow rate. The results evaluation of the experiments follows.

Feed temperature change response

During the first experiments set have been followed the response of the models to stepwise change to feed temperature T_f in the steady states given by Tab. 1 and Tab. 2. The steady state values are identical practically in the whole tested range 300 – 400 °K. Likewise the dynamic responses are identical sufficiently. Deviations can be observed in the lower band of the range. The reactor temperature of the analogue model is physically limited by value 400 °K. The output temperature and concentration steady state values are collected in Tab. 3 for various values of the feed temperature T_f.

T_f [°K]	Model	300	340	360	400
T [°K]	Virt.	310	Osc.	390	405
	Anal.	320	Osc.	385	—
C_A [mol/l]	Virt.	0,96	Osc.	0,073	0,037
	Anal.	0,803	Osc.	0,077	—

Tab.3 Feed temperature change

The time responses of reactor temperature *T(t)* of the analogue reactor for step wise change of the feed temperature T_f are depicted in Fig. 4. The initial value of T_f is given by its operational value (see Tab. 1). The time responses correspond to 200 sec. Y - axis is in °K.

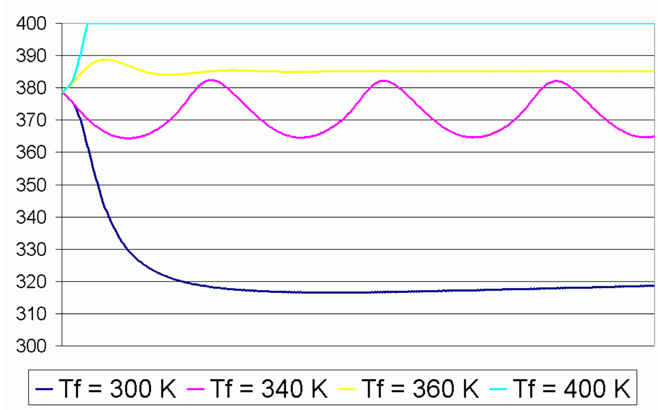

Fig.4 Time response *T* to the change T_f

A conformity evidence of the analogue model is an oscillation occurrence at T_f = 340 °K, that is characteristic for virtual model. The processes at lower and upper values of feed temperature are identically without any oscillations.

The following Fig. 5 – 7 show dynamic behaviour of virtual model.

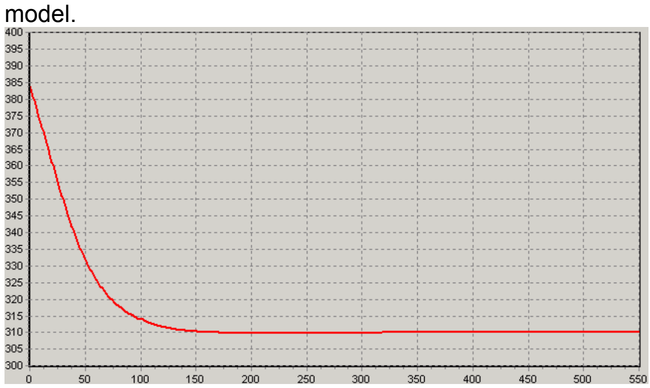

Fig.5 Time response *T(t)* for T_f = 300 °K

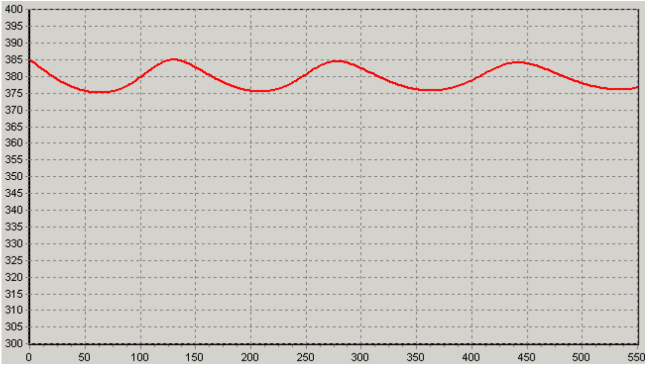

Fig.6 Time response *T(t)* for T_f = 340 °K

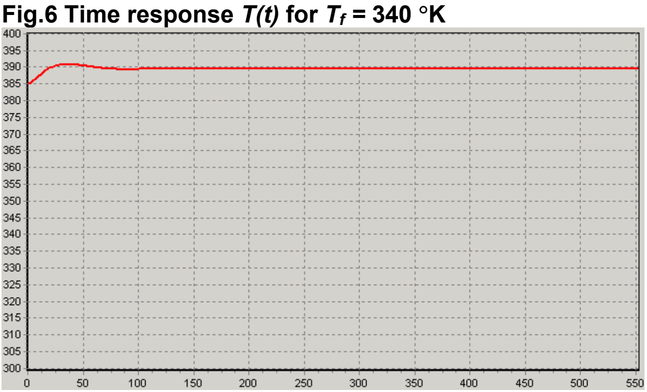

Fig.7 Time response *T(t)* for T_f = 360 °K

Coolant temperature change response

The test of coolant temperature has been similar to previous one; just during this test, coolant temperature has changed in the range 273 – 373 °K. The results of the steady state conformity are collected in Tab. 4.

T_c [K]	Model	298	305	324	337
T [K]	Virt.	321	384	397	407
	Anal.	Osc.	375	386	394
c_A [mol/l]	Virt.	0,902	0,16	0,05	0,03
	Anal.	Osc.	0,121	0,07	0,044

Tab.4 Coolant temperature change

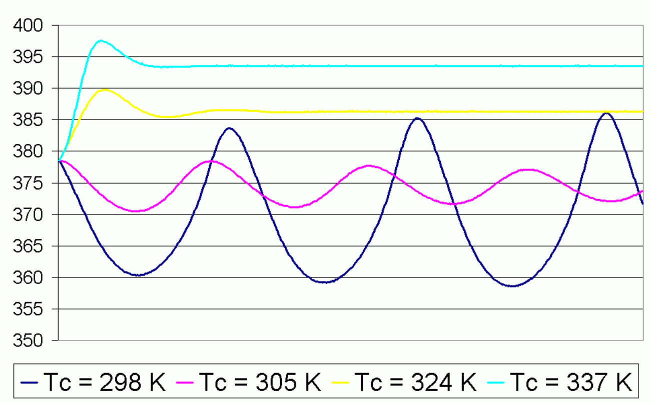

Fig.8 Time response T(t) for change Tc

The time responses of reactor temperature T for step wise change of coolant temperature Tc are depicted in Fig. 8. The initial value of Tc is given in Tab. 1. The time responses are in °K.

Fig. 9 – 11 show time responses of reactor temperature of the virtual model.

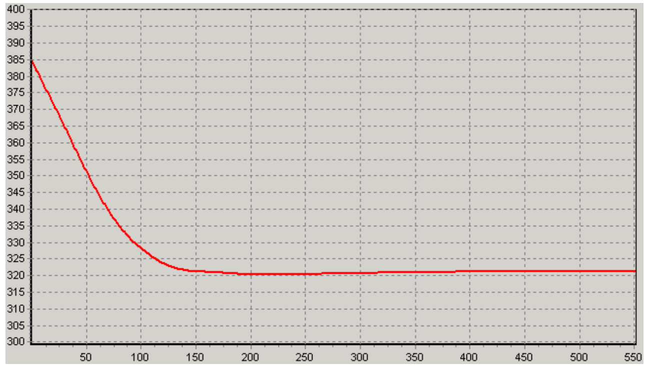

Fig.9 Time response *T(t)* for T_c = 298 °K

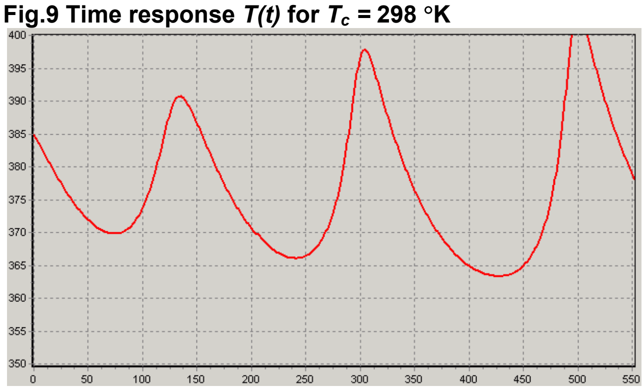

Fig.10 Time response *T(t)* for T_c = 305 °K

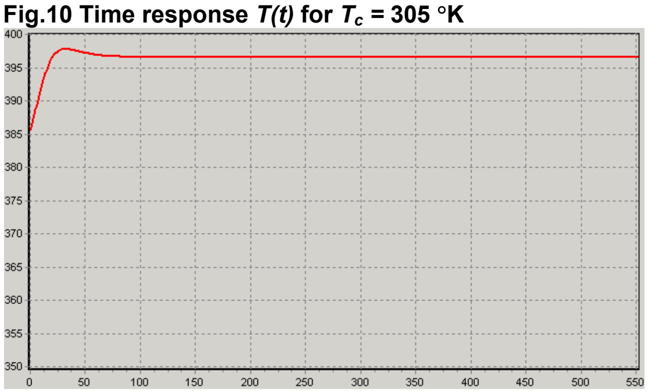

Fig.11 Time response *T(t)* for T_c = 324 °K

We can state, that the tested analogue model corresponds to virtual one in the range cca. 305 – 340 °K. Under the limit 305 °K the analogue model oscillates permanent.

Flow rate change response

The last testing has been made under feed flow rate *q* change. The steady state values are in Tab. 5.

q [l/min]	Model	90	95	100	105
T [K]	Virt.	377,8	381,5	385	—
	Anal.	373	376	379	381
c_A [mol/l]	Virt.	0,126	0,108	0,094	—
	Anal.	0,11	0,1	0,1	0,095

Tab.5 Feed flow rate change

As can be observed from Tab. 5, in the *q* range 90 – 100 l/min both the models correspond quite good. For lower values of flow, analogue model oscillates.

Conclusions

The tests have also been performed for higher values of the feed flow rate *q*. According experience this flow increasing stabilises the reaction processes. That validates the analogue model sufficient.

The difference in behaviour of the models at lower bounds of technological variables causes a technical realisation of analogue model. A gain of the non linearity block increases drastically for those operational bands and the dynamic behaviour of the analogue model depends on precise selection of the construct elements, resistors for example.

The virtual models are wide used in education and there are evident their above mentioned advantages in contrast to real equipment. The virtual models can be connected to virtual controllers or via proper interfaces to real industrial programmable controller, too. In present, we use the virtual exotermic reactor controlled by virtual programmable controller KRGN 90 and Honeywell UDC 3000/3300. (Kuník *et al.* 2006). Following research is focused to control of analogue model of exotermic continuous stirred reactor by real programmable controller (KRGN 90, Honeywell, Simatic...). There will also be developed analogue models other types of technological processes (synchronous generator and large scale power system follows).

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References

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Abstract

This contribution presents the analogue model of an unstable continuous stirred tank reactor developed on Department of Information Technology and Automation. The model is represented by two first-order nonlinear differential equations, there describes also the virtual model (presented also on Process Control conferences).

The virtual model is briefly presented too. Following section compares the new analogue model with the existing virtual one. The non-linear dynamic model of a continuous stirred tank reactor was also implemented on Department of Information Technology and Automation. As mentioned above, the dynamic non-linear model is represented by two first-order non-linear differential equations. The dynamic model of the reactor is non-linear, thus a suitable method of a numeric integration has to be chosen. From the accuracy, rate and convergence points of view, the Runge-Kutta method of 4^{th} order has been chosen.

Both models simulate the same technological process and those are based on the same dynamic non-linear model. Thus it is useful to compare them together, but each variant has characteristic advantages and disadvantages. The goal of this contribution is therefore the verification of the analogue model upon comparing his behaviour with virtual model behaviour. The virtual model has been already verified in collaboration with Faculty of Chemical and Food Technology STU.

Presented experiments regards steady-state output levels of models, time-response characteristics and influence of varied material flow *q*. Mentioned are also the analysis of the performed tests and direction of next research.

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