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# Self-tuning temperature control of an industrial PVC batch reactor

by

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The paper presents a case study of a successful implementation of self-tuning temperature control for an industrial polivinyl chloride (PVC) batch reactor. In particular it considers the preliminary stages involving on-line system identification, model testing, choice of sampling interval and controller structure selection. The performance of the implemented self-tuning controller is discussed and compared with the performance of a PI/PID cascade controller.

## 1. Introduction

Vinyl chloride batch polymerization is an important process of the plastic industry, resulting in a much demanded product with many applications. It is most often produced via a suspension process carried out in a stirred-tank batch reactor with a heating /cooling jacket. The raw materials used are vinyl chloride monomer (VCM), demineralized water and certain additives including e.g. a suspension stabilizer which determines the mean size of the monomer clusters and a suspension modificator which determines the internal friction of monomer clusters in water. The polymerization of VCM is a free radical type of chain reaction . It is started by heating the batch to a certain threshold temperature. This initiates the polymerization chain reaction which becomes self-sustaining and strongly exothermic. It takes 8—14 hours to achieve the desired 86—92% monomer conversion. During this time the reaction temperature must be precisely stabilized by heat removal through the jacket in order to achieve the desidered product quality. This constitutes

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a difficult control problem, discussed at length in the literature (see Nakagawa (1970), Amrehn (1977), Hoogendoorn-Shaw (1980), Kiparissides-Shah (1983)). The essence of the difficulties are:

a) nonstationary process dynamics caused mainly by decrease of the heat transfer coefficient between the bulk and jacket during the polymerization reaction. The heat transfer coefficient may decrease as much as 50%. Another source of nonstationarity is the change of cooling water temperature;

b) rapid change of the main disturbance which is the heat generation rate. At conversions of circa 65—75% the rate is subject to an auto-acceleration resulting in a quick increase followed by a quick decrease due to the decrease of monomer concentration;

c) process dynamics changes from batch to batch due to ageing phenomena (e.g. reactor scaling) or to different production targets.

This makes conventional analog P/PID or PI/PID cascade temperature control rather unsatisfactory and suggests a self-tuning approach. A recent simulation study (Kiparissides-Shah (1983)) based on a detailed phenomenological model of the process, entirely confirmed the suitability of this approach. As contrasted with the latter, the present paper advocates a purely "grey box" input-output approach, starting from on-line model identification for simulation purposes and controller structure selection. This was caused as much by financial- and time-constraints and the need to quickly produce implementable results as by the authors' preferences and previous experience. To the best of the authors knowledge the present paper seems to be the first reported implementiation of self-tuning techniques to an industrial PVC batch reactor.

## 2. The system and its preliminary identification

The polimerization batch reactor is one of many at the Polimerization Plant of the Zakłady Azotowe in Tarnów. Its main technological data are presented in Tab. 1.

Table 1. Stirred-tank batch reactor technological data

| |
|---|
| Volume 10 cu. m. |
| Height 4.5 m |
| Diameter 1.8 m |
| Mixer RPM 130 |
| Mixer power 35 KW |
| Maximum pressure 1.6 MPa |
| Maximum temperature 100°C |

The jacket is supplied through a split-range two-input one-output mixing valve with steam (temperature 140—180°C, pressure 0,32 MPa, flow rate 0—5,4 t/h) or cooling water (temperature 10—25°C, pressure 02—0,28 MPa, flow rate 0— 100 $m^3$/h).

The bulk temperature $\Theta_b$ is measured by a resistor themometer inserted in the tank bottom. The cooling water temperature $\Theta_c$ is measured at the inlet and outlet of the jacket also by resistor thermometers. The reactor is provided with an analog electronic PI/PID cascade temperature controller (see Fig. 1) which needs occasional

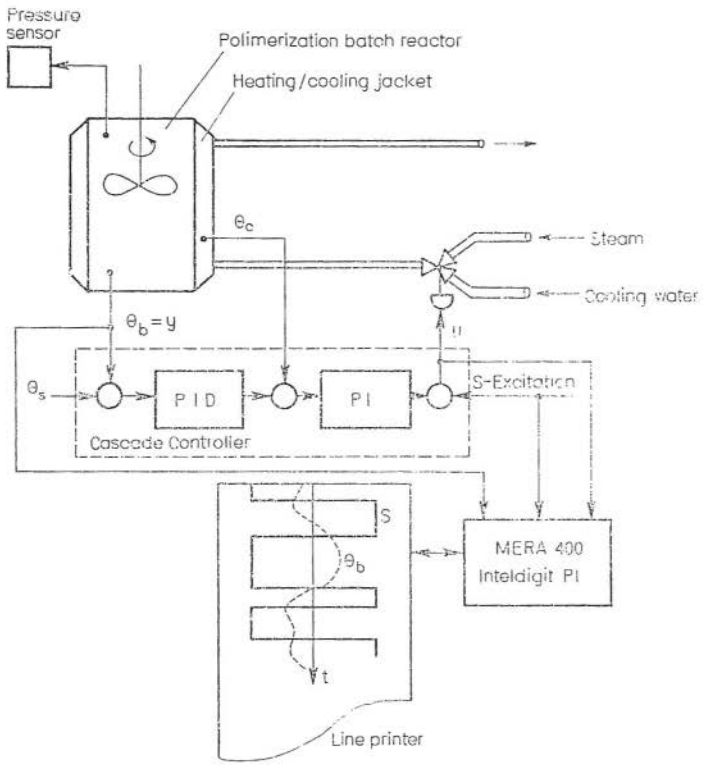


Fig. 1. Polimerization batch reactor with standard control system and the identification arrangement

retuning performed by the process operator. On the top of the tank is a pressure sensor whose output signal is registered.

Because the open-loop batch reactor may be in the polimerization phase very near to the stability limit and a model is necessary for small perturbations around the operating point, it was decided to perform a preliminary direct identification with both temperature controllers on-line. The reactor was interfaced through the INTELDIGIT PI System with a MERA-400 minicomputer system having a disc storage, a mosaic printer, a teletype and CRT alphanumeric display. The identification arrangement is presented in Fig. 1. To excite the system an additional input signal S was introduced after the main temperature controller. This signal and the bulk temperature signal were displayed and printed to guide the operator performing the identification experiment by choosing the switching times of the S signal having a constant, ex-

perimentally determined amplitude. The decision to leave the input signal generation entirely to the discretion of the operator is justified mainly by the lack of any prior knowledge about system dynamics necessary to generate typical pseudorandom sequences, and the necessity not to disturb unduly the reactor, which at the same time was processing a normal commercial charge. The temperature signal was sampled with the sampling interval 6 min which was slightly greater from the system dead time equal to about 5 min. This choice of sampling as much interval was mainly determined by the desire to simplify as possible the structure of the self-tuning controller: as will be shown in the sequel, it minimizes the number of controller parameters to be tuned. In view of the limited time available for controller tuning this was the most important constraint imposed upon the sampling interval. A check on the resonant frequency of the analog temperature control system and an a posteriori test of the disturbance model spectral density confirmed that this choice of sampling interval satisfies with an ample margin the constraints imposed by the Shannon-Kotelnikov sampling theorem.

The operator changed the input signal S at integer multiples of the sampling interval. Because the perturbations introduced by S about the normal operating point of 52°C had to be constrained to ±2°C, the analog input subsystem was effectively generating data having no more than 2 significant figures. This fact turned out to be of considerable importance for the model and controller structures.

The aim of preliminary identification was to get some ideas about the temperature control channel structure and parameter nonstationarity for the entire 12 hour long polimerization phase. In order to get information about the system nonstationarity, the entire batch period was divided into four equal subintervals, for each of which a stationary linear discrete-time model was identified. This model was assumed to have the difference equation form

$$y_i = z^{-k} \frac{B(z^{-1})}{A(z^{-1})} u_i + d_i \tag{1}$$

where $y_i$ is the bulk temperature at the $i$-th sampling instant, $u_i$ is the control variable between the $i$-th and $(i+1)$-st control instant, $d_i$ is the disturbance at the output at the $i$-th sampling instant, $k$ is the discrete-time delay, and

$$A(z^{-1}) = 1 + a_1 z^{-1} + \ldots + a_m z^{-m} \tag{2}$$

$$B(z^{-1}) = b_0 + b_1 z^{-1} + \ldots + b_n z^{-n} \tag{3}$$

are relative prime polynomials in the unit delay operator $z^{-1}$. It can be demonstrated (see Niederliński (1984)) that the model takes account of the two important pecularities of real-life discrete time systems:

1) the existence of a continuous time-delay not being an integer multiple of the sampling period,
2) the existence of a time shift between the $i$-th control instant and the $i$-th sampling instant, the former to be considered to occur not later than the latter.

The identification was performed using three different methods. It was considered reasonable to start with the simplest identification method — Least Squares (LS), where it is assumed that

$$d_i=\frac{1}{A(z^{-1})}e_i \tag{4}$$

$e_i$ being $N(0, \lambda^2)$ white noise. To remove the influence of the disturbance channel structure on the LS identification results, the Instrumental Variable (IV) method was used. The idea underlying the IV method can be explained in several ways. Writing the model (1) as

$$y_i=\Phi_{i-1}^{T}\Theta+v_i \tag{5}$$

where

$$\theta^T=[a_1 \dots a_m\ b_0 \dots b_n] \tag{6}$$

is the parameter vector, and

$$\Phi_{i-1}^{T}=[-y_{i-1} \dots -y_{i-m}\ u_{i-k} \dots u_{i-k-n}] \tag{7}$$

is the measurement vector, assume that $h_{i-1}$ is a $2n+1$ — vector whose elements are uncorrelated with the disturbance $v_i$. Then it is possible to estimate the parameter vector $\theta$ by exploiting this property, because for a sufficiently large number of data $N$

$$\frac{1}{N}\sum_{i=1}^{N}h_{i-1}v_i=\frac{1}{N}\sum_{i=1}^{N}h_{i-1}(y_i-\Phi_{i-1}^{T}\theta)=0 \tag{8}$$

which results in the IV estimate

$$\theta=\left(\sum_{i=1}^{N}h_{i-1}\Phi_i^{T}\right)^{-1}\left(\sum_{i=1}^{N}h_{i-1}y_i\right) \tag{9}$$

The elements of the instrumental variable vector $h_{i-1}$ are usually determined (see Mańczak and Nahorski (1983)) as

$$h_{i-1}^{T}=[-w_{i-1} \dots -w_{i-m}\ u_{i-k} \dots u_{i-k-n}] \tag{10}$$

where the signal $w_i$ is obtained by filtering the input $u_i$ with the best model so far, i.e.

$$w_i=z^{-k}\frac{B_j(z^{-1})}{A_j(z^{-1})}u_i \tag{11}$$

In (11) $A_j(z^{-1}), B_j(z^{-1})$ is the model obtained by the LS method for $j=0$ or the IV method for $j>0$, in the last case for the $w_i$ signal generated by the $(j-1)$-st model. After a few iterations the estimate can be shown to converge, provided the system

is stable. If the model structure corresponds to the system structure and the system is stable, the consistency of the IV estimate can be proved (see Söderström and Stoica (1983)).

The Maximum Likelihood method identifies the model

$$y_i = z^{-k}\frac{B(z_1^{-1})}{A(z^{-1})}u_i + \frac{C(z^{-1})}{A(z^{-1})}e_i \tag{12}$$

with

$$C(z^{-1}) = 1 + c_1 z^{-1} + \ldots + c_p z^{-p} \tag{13}$$

and $e_i$ being $N(0, \lambda^2)$ white noise.

The identification results for three experiments are presented in Tab. 2. For all models $k=1$. The model order was determined by using the prediction variance test and the covariance matrix determinant ratio test (see Van den Boom, van den Enden (1973)) as $m=2$, $n=1$, $p=0$. The results of the tests for $m$ for some of the models are presented in Fig. 2. The results from Tab. 2 demonstrate that the system model changes from batch to batch as well as during the various phases of the same batch. The $c_i$ coefficients identified by ML turned out not to possess any significant figures and therefore were omitted. The number of iterations for the IV method was generally low but sometimes the method resulted in an unstable model which was caused by the fact that the system could be near to the stability limit. This fact was confirmed by an independent physico-chemical investigation.

Table 2. Results of preliminary identification: BS — Batch Subinterval, hours, IM — Identification Method, s — residual standard deviation, +) model unstable after the first iteration, 1) — result after three iterations, 2) — result after four iterations.

| BS [h] | IM | Results of I-st experiment | | | | Results of II-nd experiment | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | $a_1$ | $a_2$ | $b_0$ | $s^2$ | $a_1$ | $a_2$ | $b_0$ | $s^2$ |
| 0 ÷ 3 | LS | −1,30 | 0.50 | 0.073 | 0.015 | −1.43 | 0.52 | 0.071 | 0.077 |
| | IV | −1.42 | 0.38 | 0.094+ | 0.018 | −1.26 | 0.40 | 0.066[2] | 0.114 |
| | ML | −1.35 | 0.48 | 0.058 | 0.006 | −1.60 | 0.63 | 0.068 | 0.066 |
| 3 ÷ 6 | LS | −1.45 | 0.68 | 0.084 | 0.055 | −1.60 | 0.66 | 0.087 | 0.066 |
| | IV | −1.56 | 0.71 | 0.108[1] | 0.062 | −1.76 | 0.81 | 0.059[1] | 0.092 |
| | ML | −1.43 | 0.64 | 0.098 | 0.047 | −1.13 | 0.21 | 0.085 | 0.017 |
| 6 ÷ 9 | LS | −1.30 | 0.62 | 0.034 | 0.036 | −1.42 | 0.69 | 0.004 | 0.045 |
| | IV | −1.45 | 0.72 | 0.050[1] | 0.043 | −1.55 | 0.77 | 0.041[1] | 0.088 |
| | ML | −1.77 | 0.93 | 0.041 | 0.016 | −1.78 | 0.90 | 0.050 | 0.025 |
| 9 ÷ 12 | LS | −1.42 | 0.74 | 0.059 | 0.036 | −1.46 | 0.62 | 0.054 | 0.011 |
| | IV | −1.50 | 0.65 | 0.071[1] | 0.044 | −1.48 | 0.61 | 0.062[1] | 0.012 |
| | ML | −0.88 | 0.127 | 0.065 | 0.009 | −1.00 | 0.19 | 0.057 | 0.005 |

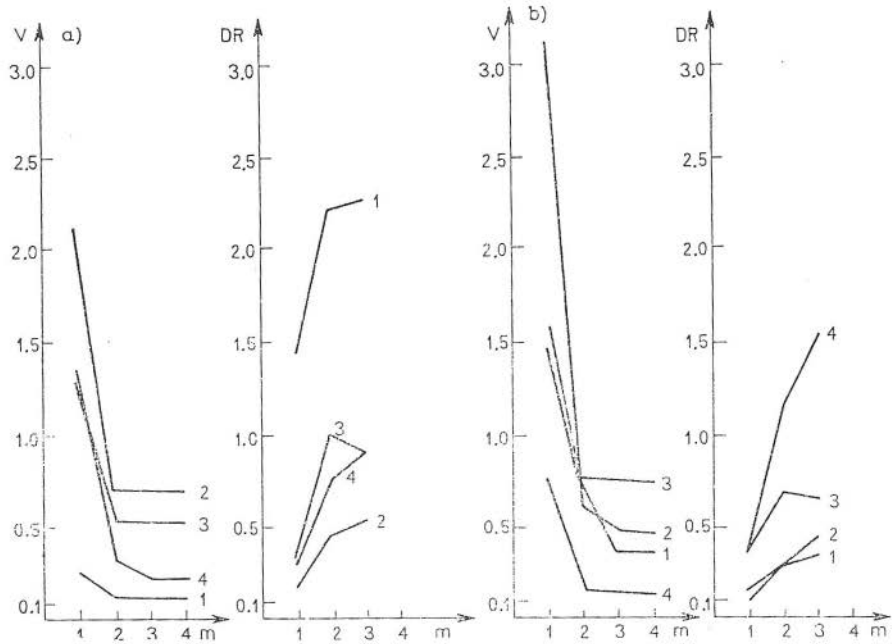


Fig. 2. Results of model denominator order testing using the prediction variance V and covariance determinant ratio order DR test. The numerator order is for these tests equal 1. a) I-st experiment, b) II-nd experiment, 1) BS=0—3, 2) BS=3—6, 3) BS=6—9, 4) BS=9—12.

### 3. Self-tuning temperature control

The self-tuning control concept, presented first by Kalman (1958), stimulated by Peterka (1970), extended by Åström and Wittenmark (1973) and developed further by Clarke and Gawthrop (1975) and Grimble (1982) has matured rapidly resulting in a large number of reported industrial applications. The entire field of theory and applications was recently reviewed by Isermann (1982) and Åström (1983).

Self-tuning control algorithms can be roughly divided into explicit which identify the system parameters and compute the appropriate controller parameters, and implicit which identify directly the controller parameters. For the discussed application the implicit approach for a minimum-variance control algorithm was chosen.

Although it needs the identification of a slightly larger number of parameters, it has the great advantage of easy implementation. The particular form of self-tuning controller chosen should minimize the performance index.

$$\min_{t} \left[E\{y_{i+K}^2\} + w\, u_i^2\right] \tag{14}$$

where $w>0$ is a weighting factor, $K=k+1$ is the overall loop time delay and $y_i$ is the deviation of the output from the setpoint. The system was assumed to be described by

$$y_i=z^{-K}\frac{B(z^{-1})}{A(z^{-1})}u_i+\frac{C(z^{-1})}{A(z^{-1})}e_i+d \tag{15}$$

where the plant time delay $k$ was increased by the controller time delay to give total delay $K$, and $d$ is a constant disturbance to be estimated along with the controller parameters. The minimum-variance control algorithm for this case is given by (see Niederliński (1985))

$$G(z^{-1})\,y_i+\left[B(z^{-1})\,F(z^{-1})+C(z^{-1})\frac{w}{b_0}\right]u_i+d'=0 \tag{16}$$

where

$$F(z^{-1})=1+f_1\,z^{-1}+\ldots+f_{K-1}\,z^{-(K-1)} \tag{17}$$

$$G(z^{-1})=g_0+g_1\,z^{-1}+\ldots+g_{m-1}\,z^{-(m-1)} \tag{18}$$

$$C(z^{-1})=A(z^{-1})\,F(z^{-1})+z^{-K}\,G(z^{-1}) \tag{19}$$

$$d'=A(1)\,F(1)\,d \tag{20}$$

The optimum output and control signal fulfill the relation

$$y_{i+K}+\frac{w}{b_0}u_i=F(z^{-1})\,e_{i+K} \tag{21}$$

The corresponding self-tuning algorithm follows immediately from the prediction model, which can be derived (see Niederliński (1985)) in the following way: introducing the auxiliary variable

$$\Phi_{i+K}=y_{i+K}+\frac{w}{b_0}u_i \tag{22}$$

it is seen from (15) and (19) that

$$C(z^{-1})\,\Phi_{i+K}-\left[B(z^{-1})\,F(z^{-1})+C(z^{-1})\frac{w}{b_0}\right]u_i-G(z^{-1})\,y_i-d'= =C(z^{-1})\,F(z^{-1})\,e_{i+K} \tag{23}$$

which can be written in the predictive model form as

$$\Phi_{i+K}-\left[B(z^{-1})\,F(z^{-1})+C(z^{-1})\frac{w}{b_0}\right]u_i-G(z^{-1})\,y_i-d'= =\left[1-C(z^{-1})\right]\left[\Phi_{i+K}-F(z^{-1})\,e_{i+K}\right]+F(z^{-1})\,e_{i+K} \tag{24}$$

The l.h.s. of (24) is a linear function of all unknown controller parameters and the overall weighting coefficient $w/b_0$; it may therefore be considered as the identification

error $\varepsilon_{i+K}$. The r.h.s. of (24) reduces to $F(z^{-1})\, e_{i+K}$ when either $C(z^{-1})=1$ (which is fairly often) or if during the identification the system is controlled by the controller (16) which assures (21). Introducing the notation

$$B(z^{-1})\,F(z^{-1})+C(z^{-1})\,\frac{w}{b_0}=M(z^{-1})=m_0+m_1\,z^{-1}+\ldots$$
$$\ldots+m_{n+K-1}\,z^{-(n+K-1)} \tag{25}$$

the identification error $\varepsilon_i$ can be expressed as

$$\varepsilon_i=\Phi_i-\varphi_{i-K}^T\,\underline{w} \tag{26}$$

where the data vector

$$\varphi_{i-K}^T=[u_{i-K}\ldots u_{i-n-2K+1}\ y_{i-K}\ldots y_{i-K-n+1}\ 1] \tag{27}$$

and the parameter vector

$$w^T=[m_0\ldots m_{n+K-1}\ g_0\ldots g_{n-1}\ d'] \tag{28}$$

The self-tuning algorithm can be expressed in the following way:

1. At each time step estimate the parameter vector $w$ using the LS recursive algorithm

$$\hat{w}_i=\hat{w}_{i-1}+k_i\,(\Phi_i-\varphi_{i-K}^T\,\hat{w}_i) \tag{29}$$

where

$$\hat{w}_i^T=[\hat{m}_{0,i}\ldots\hat{m}_{N-K-1,i}\ \hat{g}_{0,i}\ldots\hat{g}_{n-1,i}\ \hat{d}_i'] \tag{30}$$

$$k_i=\frac{P_{i-1}\,\varphi_{i-K}}{\alpha+\varphi_{i-K}^T\,P_{i-1}\,\varphi_{i-K}} \tag{31}$$

and

$$P_i=\frac{1}{\alpha}\left[P_{i-1}-\frac{P_{i-1}\,\varphi_{i-K}\,\varphi_{i-K}^T\,P_{i-1}}{\alpha+\varphi_{i-K}^T\,P_{i-1}\,\varphi_{i-K}}\right] \tag{32}$$

where $0\ll\alpha<1$ is the forgetting factor.

2. At each time step calculate the control signal $u_i$ using the estimated parameter vector $\hat{w}_i$ and the control algorithm (15) which for this purpose should be written as

$$u_i=-\frac{1}{m_{0,i}}\left[\sum_{j=1}^{n+K-1}\hat{m}_{j,i}\,u_{i-j}+\sum_{j=0}^{n-1}\hat{g}_{j,i}\,y_{i-j}+\hat{d}_i'\right] \tag{33}$$

To make the algorithm workable some additional points need closer attention:

1. To prevent an estimator blow-up in periods of no or low disturbances, the forgetting factor $\alpha$ must be adjusted so as to stop the least squares algorithm from forgetting information when the output changes are small. To achieve this the

forgetting factor is adjusted to the weighted sum of squared identification residuals defined by the expression (see Fortescue et al. (1981)):

$$S_i=\alpha_i S_{i-1}+(1-\varphi_{i-K}^T k_i)\,\varepsilon_i^2 \tag{34}$$

where

$$\varepsilon_i=\Phi_i-\varphi_{i-K}^T \hat{w}_i \tag{35}$$

is the latest residual. Considering $S_i$ as a measure of the information retained by the algorithm, it is reasonable to postulate that

$$S_i=S_{i-1}=\ldots=S_0 \tag{36}$$

This gives together with (34)

$$\alpha_i=1-\frac{1}{N_i} \tag{37}$$

where

$$N_i=\frac{S_0}{(1-\varphi_{i-K}^T k_i)\,\varepsilon_i^2} \tag{38}$$

is the time constant measured in sampling intervals with which old information is forgotten and $S_0$ is a constant for adjusting the adaptation speed: the speed increases with decreasing $S_0$, but to small value for $S_0$ may result in an unstable control system.

2. To improve the numerical stability of the algorithm, especially while using a short word computer, it is better not to propagate from step to step the $\boldsymbol{P}_i$ matrix, but its square root or inverse square root. This has the additional advantage of preventing the $\boldsymbol{P}_i$ matrix from becoming negative definite. A number of various so called square root filtering algorithms have been proposed (see Kaminski et. al. (1971)). For the discussed application the U-D covariance factorization filter was chosen, see Thornton (1978). It factorizes the $\boldsymbol{P}_i$ matrix as

$$\boldsymbol{P}_i=\boldsymbol{U}_i\,\boldsymbol{D}_i\,\boldsymbol{U}_i^T$$

where the $\boldsymbol{U}_i$ matrix is upper triangular and unitary (with ones along the diagonal) and the $\boldsymbol{D}_i$ matrix is diagonal. For this filter $\boldsymbol{U}_i\,\boldsymbol{D}^{1/2}$ can be interpreted as the square root of the $\boldsymbol{P}_i$ matrix.

For the pilot application the self tuning controller was replacing the master PID controller in the cascade control system from Fig. 1, the slave PI controller being implemented digitally. The system had two degrees of freedom, namely the weighting coefficient $w$ and the constant $S_0$ which had to be hand chosen during preliminary experiments. The self-tuner performance is illustrated by the time diagrams from Fig. 3a and 3b and contrasted with the best performance of a master PID controller, presented in Fig. 3c. For Fig. 3a and 3b the pressure decrease instant presents the end of the batch polimerization and the beginning of a noncritical cooling-off phase.

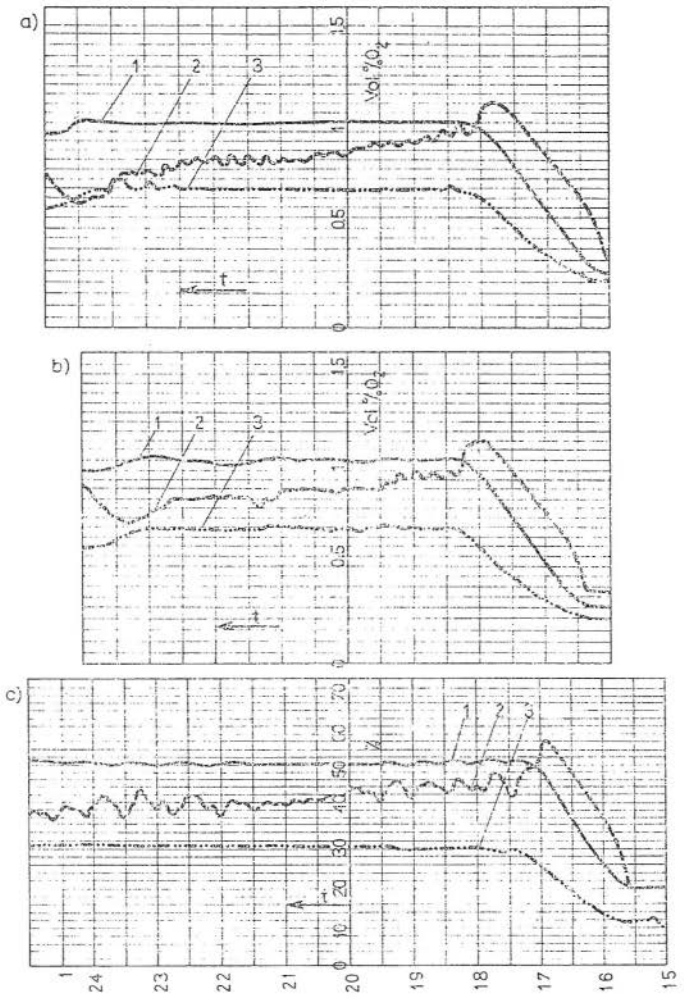


Fig. 3. Self-tuning versus PID/PI cascade temperature control: a), b) self-tuning control, c) PID/PI cascade control; 1) bulk temperature, 2) cooling jacket temperature, 3) reactor pressure.

The superior performance of the self-tuner as compared to the PID master controller is clearly evident. The oscillation of the bulk temperature under PID control can be removed only with a careful controller retuning.

## 4. Conclusions

The self-tuning approach proved once more to be a reliable way to cope with a difficult nonstationary and nonlinear control problem, clearly outside the reach of the conventional stationary PID controllers.

The system can be modelled by a low-order LS model leading — together with a proper choice of sampling interval — to a low-order self-tuner. Whilst no proof has been offered of the convergence of the self-tuner for the PVC batch reactor, the results demonstrate that rapid convergence can be obtained for a number of various operating conditions. They provide considerable encouragement and motivation for further implementation of self-tuners in the chemical industry.

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## Samonastrajające sterowanie temperaturą w przemysłowym wsadowym reaktorze PCW

W artykule przedstawiono opis udanego wdrożenia algorytmu samonastrajającego sterowania temperatury w przemysłowym wsadowym reaktorze polichlorku winylu PCW. W szczególności opisano wstępne etapy postępowania w których skład wchodzi identyfikacja na bieżąco, testowanie modelu, wybór kroku próbkowania i struktury regulatora. Przedyskutowano wyniki otrzymane przy sterowaniu za pomocą wdrożonego regulatora samonastrajającego i porównano je z wynikami otrzymanymi przy sterowaniu za pomocą kaskadowego regulatora PI/PID.

## Самонастраивающееся управление температурой в промышленном шихтовом реакторе поливинилхлорида

В статье представлено описание удачного внедрения алгоритма самонастраивающегося управления температурой в промышленном шихтовом реакторе поливинилхлорида. В частности описаны предварительные этапы, в состав которых входят: текущая идентификация, проверка модели, подбор шага выборки и структуры регулятора. Рассмотрены результаты, полученные при управлении с помощью внедренного самонастраивающегося регулятора и дается их сравнение с результатами, полученными при управлении с помощью каскадного регулятора ПИ/ПИД.