AN ADAPTIVE GMC ALGORITHM IN APPLICATION TO pH PROCESS

Krzysztof Stebel

Institute of Automatic Control, Silesian University of Technology
ul. Akademicka 16, 44-100 Gliwice, Poland
FAX: (+48) 32 237 21 27;
E-mail: kstebel@terminator.ia.polsl.gliwice.pl

Abstract: Key point of this paper is two-stage identification of block-oriented model and GMC control based on it. Important issue is that GMC algorithm is based on polynomial approximation of pH model. The main advantage of such solution is a simple form of GMC control law without loosing his functionality that has algorithms of this type. Three-segment polynomial approximations are used for static nonlinear characteristic. On-line identification allows fine-tuning of the model and robust control can be obtained. *Copyright © 2005 IFAC*

Key words: identification algorithms; algorithms; pH control; control applications; model approximation; adaptive algorithms.

1. INTRODUCTION

pH processes are frequently encountered in the chemical process industries and represent a significant challenge in terms of their identification and control. Additionally neutralization processes often exhibit nonstationary features. Because of that pH neutralization process is treated as benchmark for testing nonlinear controllers (Alvarez, et al., 2001). Many new algorithms are developed to solve this problem, see for example (Norquay, et al., 1999; Tadeo, et al., 2000). GMC algorithm was chosen as widely known and discussed in literature (Lee and Sullivan, 1988;). Input-output linearization algorithm comes from different assumptions but leads for affine type of model to the same control law (Isidori, 1995; Henson and Seborg, 1997). Most of algorithms are based on phenomenological models or models derived from phenomenological models. First mathematical model of pH in well-stirred tank was given by McAvoy (1972) and then variations of models are widely discussed in the literature, see for

example (Gustafsson et al., 1995; Kalafatis, et al., 2005). Most of these models are very complicated and in this sense not suitable for control purpose. In practice to obtain robust control in most cases some kind of on-line identification of internal model parameters is needed. Sensitivity is very important issue in case of such models. Even small changes in specific parameters have significant influence on model output. Controller is usually designed in two steps: First a system identification technique is used to obtain a suitable process model, followed by a model-based control design step. As the process model is always used an approximation of the plant dynamics, there has been increased interest in investigating the interrelation between system identification and control design (Ochs and Engell, 2000; Garrido et al., 1997). Block-oriented models are considered as a very good way of representing any non-linear dynamic systems. Wiener and Hammerstein models are most known and popular examples of this group (Kalafatis, et al., 2005). Discussed model is similar to Wiener type

with polynomial static part, dynamical part is bilinear which is not result of arbitrary assumption but is coming from phenomenological considerations. To obtain an accurate polynomial fit of given static nonlinearity may cause problems in some situations when only high order polynomials can approximate the non-linear characteristic adequately. Therefore, it may be reasonable, for such considerably asymmetric non-linear characteristic, to use description with two distinct maps (Voros, 2003) but in general more then one distinct maps can be used.

The main contribution of this paper is to present GMC based on polynomial approximation with on-line identification what allows to make control more robust.

2. GMC ALGORITHM FORMULATION

Polynomial approximation of strong non-linear processes can be used for process model based control (Metzger, 2001). Proposed pH model approximation (Stebel, 2001) consists of one bilinear differential equation which has following form (1)

$$\frac{V \cdot dx_h}{dt} = F_2 C_{2h} - F_1 C_{1h} - (F_1 + F_2) x_h \qquad (1)$$

Where:

x_h -is a difference between sum of acid and sum of base reagent concentrations in reactor.

C_{1h}, C_{2h} – hypothetical inlet concentrations of acid and base.

As a balance between high accuracy and simplicity of model for approximation of titration curve three simple polynomial functions were chosen, with restriction that in case of switching between them continuity of value and first derivative is assured (Stebel 2002). It is not possible to guarantee continuity of second derivative because of the method limitations. Controller depends on first derivative hence it is sufficient to eliminate rippling in the transition. Other basis functions (e.g., B-splines) can be used instead. First function responsible for low part of titration curve

$$pH_1 = a_0 + a_1 \cdot x_h + a_2 \cdot x_h^2 + a_3 \cdot x_h^3 \qquad (2a)$$

Second function responsible for part in the middle of titration curve

$$pH_2 = b_0 + b_1 \cdot x_h + b_2 \cdot x_h^2 + b_3 \cdot x_h^3 \qquad (2b)$$

Third function responsible for upper part of titration curve

$$pH_3 = c_0 + c_1 \cdot x_h + c_2 \cdot x_h^2 + c_3 \cdot x_h^3 \qquad (2c)$$

Proposed model is similar to Wiener model. The only difference is that presented model has bilinear dynamic part instead of linear as in Wiener models, additionally condition of reducing bilinear part to linear is not fulfilled (Kalafatis, et al., 2005). Presented above model was used to formulate GMC control algorithm according to Lee and Sullivan (1988).

$$\dot{y} = l \left(y_{sp} - y \right) + l_0 \int_0^t \left(y_{sp} - y \right) \qquad (3)$$

l, l_0 - Tuning algorithm parameters

Using equation (1, 2) and (3) control law (4) is obtained:

$$F_2 = \frac{\left(l \left(y_{sp} - y \right) + l_0 \int_0^t \left(y_{sp} - y \right) \right) \cdot V}{C_{2h} \cdot z(x_h) - w(x_h) - y} +$$

$$+ F_1 \cdot \frac{C_{1h} \cdot z(x_h) + w(x_h) + y}{C_{2h} \cdot z(x_h) - w(x_h) - y} \qquad (4)$$

Where of example:

$$w(x_h) = -b_0 + b_2 \cdot x_h^2 + 2 \cdot b_3 \cdot x_h^3$$

$$z(x_h) = b_1 + 2 \cdot b_2 \cdot x_h + 3 \cdot b_3 \cdot x_h^2$$

Coefficients of polynomial functions obtained via offline identification of phenomenological model (eq. 5-7) and can be found in previous work (Stebel, 2001).

To simulate process phenomenological model is used. It contains two main reagents acetic acid and potassium base. Addition of another two components makes obtained model more flexible. Addition of two hypothetical reagents to model does not make possible to model precisely every multi-component system, but such model can by treated as a kind of approximation allowing to observe main features of the process. Following form of model will be considered (Wright and Kravaris, 1991):

$$\frac{V d x_1}{dt} = F_1 C_1 - (F_1 + F_2) x_1 \qquad (5a)$$

$$\frac{V d x_3}{dt} = F_1 C_{31} + F_2 C_{32} - (F_1 + F_2) x_3 \qquad (5b)$$

$$\frac{V d x_2}{dt} = F_2 C_2 - (F_1 + F_2) x_2 \qquad (5c)$$

$$\frac{V d x_4}{dt} = F_1 C_{41} + F_2 C_{42} - (F_1 + F_2) x_4 \qquad (5d)$$

pH equation

$$[H^+]^5 + A \cdot [H^+]^4 + B \cdot [H^+]^3 + C \cdot [H^+]^2 + \\ + D \cdot [H^+] + E = 0 \qquad (6)$$

$$pH = -\log_{10}(H^+) \qquad (7)$$

Where:

$$A = x_2 + x_4 + K_a + K_c + \left(\frac{K_w}{K_b} \right)$$

$$B = \left(\frac{K_w}{K_b}\right) \cdot (x_2 + K_a + K_c - K_b) + K_a K_c +$$
$$+ (K_a + K_c) \cdot (x_2 + x_4) - K_a x_1 - K_c x_3$$

$$C = -\left(\frac{K_w}{K_b}\right) \cdot$$
$$((K_a + K_c) \cdot (x_2 - K_b) + K_a K_c - K_a x_1 - K_c x_3 - K_w) +$$
$$+ K_a K_c (x_2 + x_4 - x_1 - x_3)$$

$$D = \left(\frac{K_w}{K_b}\right)(K_a K_c (x_2 - x_1 - x_3 - K_b) - (K_a + K_c) K_w)$$

$$E = -\left(\frac{K_w}{K_b}\right) K_a K_c K_w$$

x_1- acetic acid concentration in reactor, x_2- potassium base concentration in reactor, x_3, x_4- concentration of hypothetical reagent in reactor, V – volume of reactor [l], $[H^+]$ – hydrogen ion concentration, K_a, K_b, K_w, K_c –equilibrium constants. C_{31}=0.0034[mole/l], C_{32}= 0.003[mole/l] - carbon acid or other weak acid inlet concentration in F_1 and F_2 stream. C_{41}=0.0035[mole/l], C_{42}=0.0025[mole/l] – calcium base or other weak base inlet concentration in F_1 and F_2 stream. Following coefficients were taken from pilot plant installation (CSCE group, Institute of Automatic Control, Silesian Technical University, Poland): acetic acid inlet concentration C_1= 0.0085 [mole/l], potassium base inlet concentration C_2= 0.0089 [mole/l], acetic acid inlet flow F_{10}= 0.5 [l/min]= const., range of potassium base inlet flow F_2= 0÷0.8 [l/min]. Proposed model and parameter ranges in most cases follow requirements for process benchmark (Alvarez, et al., 2001).

3. IDENTIFICATION FORMULATION

Different approaches to identification problem can be found in literature (Henson and Seborg, 1997; Voros, 2003). Basing on proposed polynomial model after rearrangement equations (8) and (9) are obtained. Using first-order backward difference approximation of first derivative discrete form is obtained (10).

$$\frac{V \cdot dx_h}{dt} = F_2 C_{2h} - F_1 C_{1h} - (F_1 + F_2) x_h \qquad (8)$$

$$V \frac{d(pH)}{dt} = -(pH + w(x_h)) \cdot (F_1 + F_2) + \qquad (9)$$
$$+ z(x_h) \cdot (F_2 \cdot C_{2h} - F_1 \cdot C_{1h})$$

In discrete form

$$V \frac{pH_i - pH_{i-1}}{dt} = -(pH_i + w(x_h)) \cdot (F_{1i} + F_{2i}) + \qquad (10)$$
$$+ z(x_h) \cdot (F_{2i} \cdot C_{2h} - F_{1i} \cdot C_{1h})$$

Equation (10) can be formulated by means of predictive model (11):

$$\eta(i) - \varphi^T(i-k)\Theta = \varepsilon(i) \qquad (11)$$

Where:

$$\eta(i) = V \frac{pH_i - pH_{i-1}}{\Delta t} +$$
$$+ (pH_i + w(x_h))(F_1 + F_2) - F_2 z(x_h) C_{2h}$$
$$\varphi(i-k) = -F_1 z(x_h)$$

Θ - is estimate of C_{1h} (hypothetical inlet acid concentration), $\varepsilon(i)$ - estimation error.

Model (11) is applicable for simple last squares method and concentration C_{1h} can be estimated. In case of identification it is assumed that used model is rich enough mainly by means of structure. In fact two step identification is carried out in this case. First step is offline estimation of a_* b_* c_* parameters based on data coming from real world experiment or simulation. Data for this stage of simulation should cover wide range of process changes to obtain possible general form of model because of that it has to be done offline. Second step of model identification is done by means of acid inlet concentration estimation where parameters a_* b_* c_* are assumed to be constant. This is a kind of retuning of model and accuracy for specific set point is significantly improved. Another advantage is that only one parameter needs to be estimated and excitation of the process does not have to be considered. Idea of proposed algorithm is shown on figure 1.
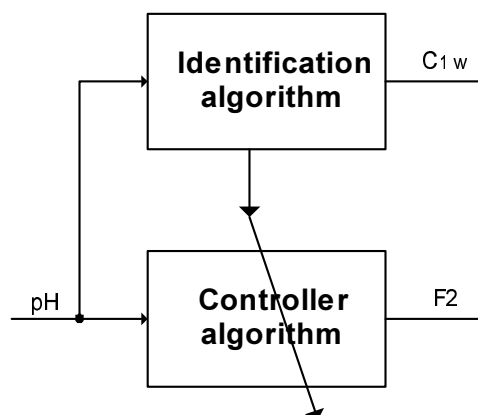

Fig. 1. Controller algorithm with adaptation.

4. SIMULATION RESULTS

Simulations were carried using phenomenological model (5-7). They were planed in this way that for time 0-15 [min] open loop system behaviour for step change of titration stream (F_2 0.45 to 0.50 [l/min]) is shown, then for time 15-30 [min] step change of acetic acid (C_1 0.0089 to 0.0091 [mole/l]) is applied. Finally for period of time 30-45 [min] as disturbance square wave of acid inlet flow described by equation (13) was applied where wave period is about 6.28 [min].

$$F_1 = F_{10} + 0.2 \cdot F_{10} \cdot sign(\sin(t)) \qquad (13)$$

t- time [min]

Square wave disturbance was applied to check suppressing capability of control algorithms. Experiments were repeated for three set points $pH_{sp}=6$, $pH_{sp}=7$ and $pH_{sp}=8$ and controllers had the same tuning parameters for each set point. Open loop response for all applied changes is shown on figure 2. This figure exhibits strongly non-linear character of the process and tracking ability of the polynomial model approximation. Inaccuracy at the beginning is connected with start-up of identification algorithm. Further changes of C_{1w} (fig. 3) are connected with compensation of inaccuracy of initial form of model (10). Although forgetting factor was chosen very conservatively (the value is 0.95) tracking ability is very good.
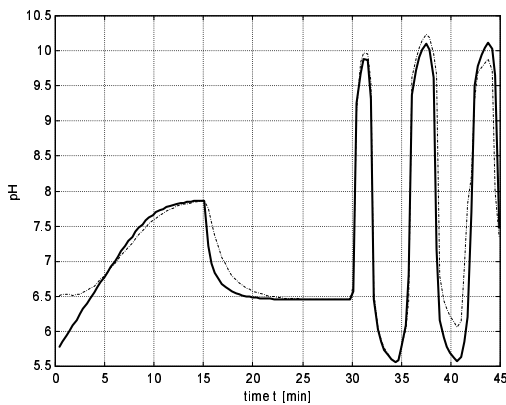
Fig. 2. pH open-loop response – solid line phenomenological model, dashed line polynomial approximation: for t=0÷15 step change of titration stream (F_2), for t=15÷30 step change of acid C_1, for t=30÷45 square wave disturbance.

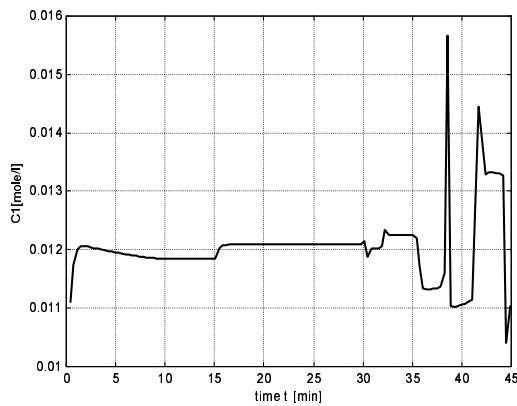

Fig. 3. Estimation of hypothetical inlet acid concentration (C_{1w}): for t=0÷15 step change of titration stream (F_2), for t=15÷30 step change of acid C_1, for t=30÷45 square wave disturbance.

Control performance for $pH_{sp}=7$ are shown on figures 4 and 5. GMC without estimation is worse then with C_{1w} estimation. Tuning parameters applied in experiments are listed in table 1. In controller without adaptation to compensate inaccuracy of internal model (visible on fig. 4.) integral part is used. Increase in controller gain leads to bigger overshoot.

Internal part allows eliminating steady state offset, but makes the controller slower. Similarly as in controller gain case integral part tuning parameter L_0 seems to be optimal by means of AES coefficient value. Although controller does not include internal limitations of output it is in range of boundaries for output signal 0-0.8 [l/min].

Table 1 Controllers tuning parameters and AES coefficient (absolute error sum divided by the time of integration).

	GMC$_1$	GMC$_2$ (adaptive)
$pH_{sp}=6$	l=10 l_0=2 AES=0.2604	l=10 AES=0.1985
$pH_{sp}=7$	l=10 l_0=2 AES=0.4458	l=10 AES=0.3654
$pH_{sp}=8$	l=10 l_0=2 AES=0.4938	l=10 AES=0.4590

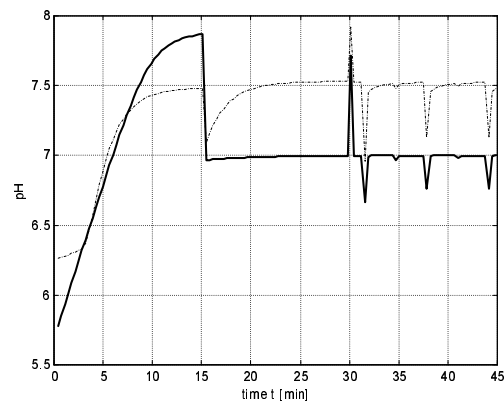Fig.4. pH value response – solid line GMC control ($pH_{sp}=7$) without C_{1w} estimation; dashed line - internal model: for t=0÷15 step change of titration stream (F_2) without control, for t=15÷30 step change of acid inlet concentration (C_1), for t=30÷45 square wave disturbance.

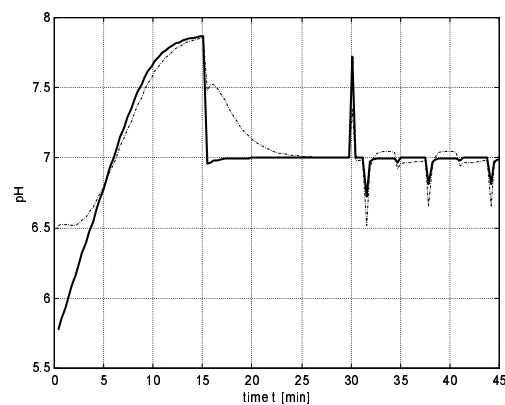Fig. 5. pH value response – solid line GMC control ($pH_{sp}=7$) with C_{1w} estimation, dashed line - internal model: for t=0÷15 step change of titration stream (F_2) without control, for t=15÷30 step change of acid inlet concentration (C_1), for t=30÷45 square wave disturbance.

Performance of GMC with estimation (fig. 5) visually is similar to GMC without estimation;

however by means of AES value it is distinguishable. The smaller AES, the better performance is obtained. Control is always an obstacle for model identification because this causes some level of correlation in data series for estimation. That is why forgetting factor in this case has to be more conservative than in case without control. Influence of forgetting factor is similar in case of adaptive algorithm to influence of integration part tuning parameter in nonadaptive case. From this stage of considerations can be found out that adaptive algorithm allows eliminating offset more efficiently. Change in estimated parameter C_{1h} is shown on figure 6. Initial stage of C_{1h} estimation is the same on the figure 3 and 6.
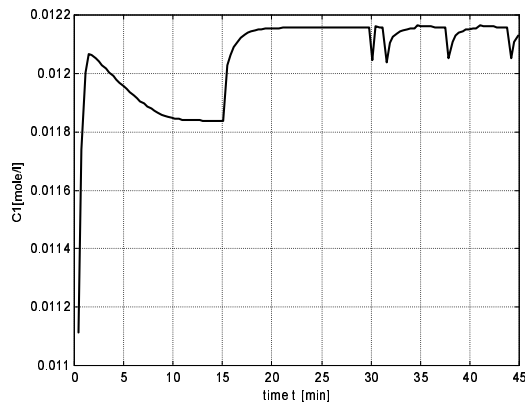

Fig. 6. Estimation of hypothetical inlet acid concentration (C_{1w}) in presence of control: for t=0÷15 step change of titration stream (F_2), for t=15÷30 step change of acid inlet concentration (C_1), for t=30÷45 square wave disturbance.
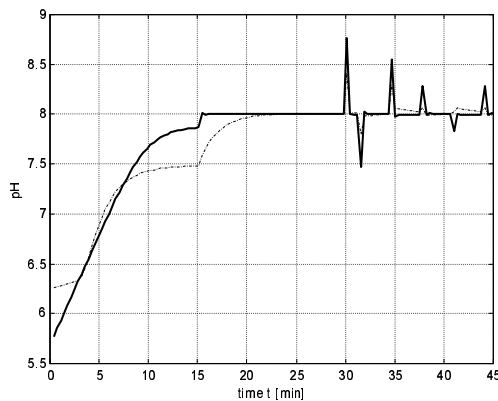

Fig. 7. pH value response – GMC control (pH_{sp}=8) without C_{1w} estimation dashed line - internal model: for t=0÷15 step change of titration stream (F_2) without control, for t=15÷30 step change of acid C_1, for t=30÷45 square wave disturbance.

Further evaluation was done for different set points (pH_{sp}=6 and pH_{sp}=8). pH process is strongly non-linear and significantly different performance can be observed mainly because of change in process gain. Control performance is similar and very good for adaptive and nonadaptive control considering AES value (table 1). For pH_{sp}=8 process gain is greater

than for pH_{sp}=6 because characteristic is not symmetric. For pH_{sp}=8 nonadaptive algorithm is better then adaptive one what might be surprise (results are not presented). Such situation can be explained by the fact that initial model without online identification is almost ideal for pH=8 (fig. 7). Hence parameter estimation is not needed and moreover makes the control slower. Although adaptive performance is worse by means of AES value but it is very close to nonadaptive shown on figure 7. In this point it could be concluded that in the case when process is stationary and initial model approximation is sufficiently good both algorithms adaptive and nonadaptive are comparable. One algorithm might exhibit superior behaviour in comparison with another depending on local model accuracy.

In practice of neutralisation process such conditions are not common and greater level of model mismatch should be considered. Main reagents were not changed in model, but hypothetical reagents concentrations were changed as follows C32=0.001 [mole/l], C41=0.0015 [mole/l], C42=0.0035 [mole/l]. Such parameter changes cause that initial model based on offline identification is very inaccurate what can be observed on figure 9. Model approximation (dashed line) is far from process response; hence model mismatch is really tremendous. Basis on that fact it could be expected that performance of nonadaptive algorithm would be very poor or even unstable. Even if tuning parameters are significantly decreased l=2 and l_0=0.8 the control algorithm is still unstable. When adaptive algorithm is considered performance is improved and for l=2 very good results are obtained (fig. 8).
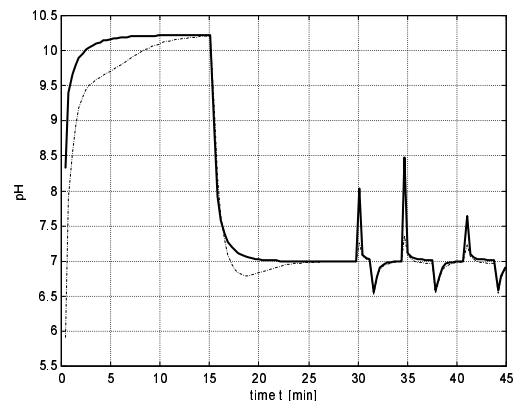

Fig. 8. pH value response – solid line GMC control (pH_{sp}=7) with C_{1w} estimation, dashed line - internal model: for t=0÷15 step change of titration stream (F_2) without control, for t=15÷30 step change of acid C_1, for t=30÷45 square wave disturbance.

It has to be stressed that model coefficients a_*, b_*, c_* were constant during all experiments. At the beginning model fit to process is good and adaptive and nonadaptive algorithms are comparable. Gradually process is hanged and because of initial model mismatch adaptive algorithm has superior

performance than nonadaptive what is well known fact, but the way of internal model identification is interesting approach.
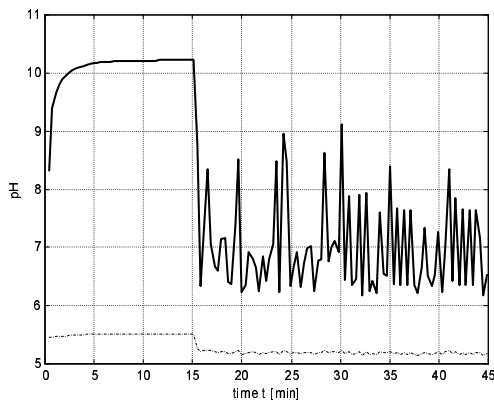

Fig. 9. pH value response – GMC control ($pH_{sp}=7$) without C_{1w} estimation, dashed line - internal model: for $t=0\div15$ step change of titration stream (F_2) without control, for $t=15\div30$ step change of acid C_1, for $t=30\div45$ square wave disturbance.

5. CONCLUSIONS

This paper presents the simulation study and comparison of GMC without adaptation and with adaptation. Non-linear model identification is considered to be difficult and proposed algorithms are very complicated. This is one of the reasons why such solutions are avoided in industrial practice. Proposed approach seems to be very promising. Both stages of identification can be done using standard estimation method. First offline stage of identification can be done periodically when important changes in process are assumed to assure general process fit. Second stage is on-line and allows obtaining local increment of model accuracy. On-line measurements accessible to both algorithms were the same. Performance of those algorithms is comparable when model used in both are close to real model. In case of significant model mismatch estimation still allows to control efficiently while controller without estimation becomes unstable. The results are confirmed only by deterministic simulation without the noise what is planed in next stage of researches.

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