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Stabilization of stochastic operating modes in the flow reactor

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Abstract. A conceptual multistable model of the flow reactor proposed by Volter and Salnikov is studied in the presence of random disturbances. A stochastic excitability of this system, even in a zone of stable equilibria, is explained by the high stochastic sensitivity. Such high stochastic sensitivity of the equilibrium can be a basic reason of the noise-induced destruction of the operating mode. For the stabilization of the stochastic flow reactor, a theory of the synthesis of the assigned low stochastic sensitivity is suggested. It is shown how to use this control approach and construct an appropriate regulator which suppresses unwanted large-amplitude stochastic oscillations and provide a proper operation of the flow reactor.

1. Introduction
Many manufacturing processes are described by nonlinear dynamic systems with equilibrium operating modes. Traditionally, a deterministic stability of the equilibrium is considered as a condition of the proper operation. However, such stability can be insufficient, especially in nonlinear systems. In excitable systems, even weak noise can destroy a stable operating mode, and cause unexpected consequences [1, 2]. In the study of the probabilistic reasons of noise-induced phenomena, the stochastic sensitivity analysis [3, 4] can be a useful tool.

Along with the analysis of nonlinear stochastic systems, control problems attract attention of many researchers [5-8]. A theory of the control based on the stochastic sensitivity synthesis was developed in [8-11].

Mathematical models of flow chemical reactors demonstrate a wide variety of the nonlinear dynamic regimes with complex oscillations [12-14]. In the present paper, we consider a conceptual dynamic model of the flow reactor proposed by Volter and Salnikov [15] in a presence of random disturbances.

In Section 2, dynamic regimes of the deterministic model are shortly discussed. In Section 3, an influence of the random noise on this model is studied. A stochastic excitability in a zone of stable equilibria is shown. For the stabilization of the stochastic flow reactor, a general mathematical approach based on the stochastic sensitivity synthesis is briefly presented in Section 4. In Section 5, it is shown how to apply this approach to the synthesis of the appropriate regulator which reduces the stochastic sensitivity and suppresses unwanted large-amplitude stochastic oscillations in the randomly forced flow reactor.
2. Deterministic model of the flow chemical reactor
Consider the following dynamic model of the thermochemical processes in the flow reactor [15] of ideal mixing:

\[
\begin{align*}
\dot{x} &= -x \exp \left(-\frac{1}{y}\right) + l(a - x), \\
\dot{y} &= x \exp \left(-\frac{1}{y}\right) + m(b - y). 
\end{align*}
\]  

(1)

Here, \(x\) is a concentration of the reagent, and \(y\) is a temperature in the reactor. Parameters \(a\) and \(b\) characterize the concentration and temperature at the reactor inlet; \(l, m\) are positive parameters.

Following [15] we fix \(l = 0.5, m = 0.25, b = 0.165\) and study the system dynamics under the variation of the parameter \(a \in [1.578, 1.584]\). In this zone, the system (1) exhibits three dynamic regimes: for \(a < a_1 = 1.580079\), the system is monostable with an equilibrium as a single attractor; for \(a_1 < a < a_2 = 1.582843\), the system is bistable with coexisting equilibrium and limit cycle; for \(a > a_2\), the system is monostable with a limit cycle as a single attractor. The critical point \(a_1\) corresponds to the saddle-node bifurcation, and \(a_2\) is a point of the subcritical Hopf bifurcation. In Fig. 1, \(y\)-coordinates of attractors and repellers of system (1) are presented.

![Figure 1. Bifurcation diagram of the deterministic system (1). Stable equilibria and cycles are plotted by solid lines, and unstable equilibria and cycles are shown by dashed lines.](image)

3. Model of the flow reactor with stochastic disturbances
To study an influence of noise on the dynamics of the reactor, we will use the following stochastic model:

\[
\begin{align*}
\dot{x} &= -x \exp \left(-\frac{1}{y}\right) + l(a - x) + \varepsilon_1 \xi_1(t), \\
\dot{y} &= x \exp \left(-\frac{1}{y}\right) + m(b - y) + \varepsilon_2 \xi_2(t). 
\end{align*}
\]

(2)

Here, \(\xi_{1,2}(t)\) are the standard Gaussian uncorrelated processes, and \(\varepsilon_{1,2}\) are the noise intensities. In what follows, we put \(\varepsilon_1 = \varepsilon_2 = \varepsilon\).

Random disturbances deform deterministic dynamics of the system and can destroy a required equilibrium operation mode of the chemical process.
In Fig. 2, a response of the system (2) to random disturbances is presented for two values of the parameter $a$ corresponding to the equilibrium ($a = 1.58$) and self-oscillations ($a = 1.583$) regimes.

As one can see in Fig. 2a, for $\varepsilon = 0.0001$, random trajectories are concentrated near the stable equilibrium, and the system exhibits the small-amplitude stochastic oscillations. Such inevitable small oscillations near the stable equilibrium are allowable. For $\varepsilon = 0.0005$, dynamics of the system (2) essentially changes. Indeed, for this noise intensity, the system begins to demonstrate a new excitable regime with the intermittency of small- and large-amplitude stochastic oscillations. Such breakdowns of the operating mode are impermissible, and require additional stabilization mechanisms.

Note that usually regulators are built for the stabilization of unstable equilibria. However, as we see in this system, a standard deterministic stability of the equilibrium is not enough. In the excitable case presented here, it is required to decrease the stochastic sensitivity of the equilibrium.

More expected reaction of the system in self-oscillation mode is shown in Fig. 2b for $\varepsilon = 0.0005$. Here, the large-amplitude stochastic oscillations are observed. In this case, a regulator has to solve two problems: to stabilize an unstable equilibrium, and provide a low level of its stochastic sensitivity.

Figure 2. Time series of the uncontrolled stochastic system with a) $a = 1.58$, $\varepsilon = 0.0001$ (black) and $\varepsilon = 0.0005$ (grey); b) $a = 1.583$, $\varepsilon = 0.0005$.

4. Controlling stochastic sensitivity
Consider a general stochastic system with control

$$\dot{x} = f(x, u(x)) + \varepsilon \sigma(x, u(x))\xi(t),$$

where $x$ is an $n$-dimensional state, $u$ is an $l$-dimensional control, $f(x, u)$ is an $n$-vector-function, $\xi(t)$ is an $m$-dimensional standard Gaussian process, and $\varepsilon$ is the noise intensity. The $n \times m$-matrix-function $\sigma(x, u)$ characterizes a dependence of disturbances on state and control.

It is supposed that the unforced and uncontrolled system (3) (with $\varepsilon = 0$, $u = 0$) has an equilibrium $\bar{x}$. The stability of $\bar{x}$ is not required.

Consider a set $\mathcal{U}$ of admissible feedbacks $u = u(x)$ satisfying the following conditions: (a) a function $u(x)$ is continuously differentiable and $u(\bar{x}) = 0$; (b) a feedback $u(x)$ provides an exponential stability of the equilibrium $\bar{x}$ for the closed-loop deterministic system

$$\dot{x} = f(x, u(x))$$
in some neighbourhood of \( \bar{x} \).
For deviations \( z(t) = x(t) - \bar{x} \) of states \( x(t) \) of system (4) from the equilibrium \( \bar{x} \), consider the following first approximation system:

\[
\dot{z} = (F + BK)z, \quad F = \frac{\partial f}{\partial x}(\bar{x}, 0), \quad B = \frac{\partial f}{\partial u}(\bar{x}, 0), \quad K = \frac{\partial u}{\partial x}(\bar{x}).
\] (5)

The second condition (b) is equivalent to the exponential stability of the trivial solution of system (3). Here, we consider the following linear feedback regulators:

\[
u(x) = K(x - \bar{x}).\] (6)

Denote by \( K \) a set of matrices \( K \) which provide an exponential stability of the trivial solution of system (5):

\[K = \{ K | \text{Re}\lambda_i(F + BK) < 0 \}.\]

Here, \( \lambda_i(F + BK) \) are the eigenvalues of the matrix \( F + BK \). Suppose that the pair \( (F, B) \) is stabilizable, so the set \( K \) and class \( \mathcal{U} \) are not empty.

Random trajectories \( x^\varepsilon(t) \) of the stochastic system (3) deviate from the equilibrium \( \bar{x} \). However, using the feedback (6) with a matrix \( K \in K \), one can provide an exponential stability of the equilibrium, localize random states of system (3) near the equilibrium \( \bar{x} \), and form a stationary distributed solution \( \bar{x}^\varepsilon(t) \).

For small deviations \( z(t) = x^\varepsilon(t) - \bar{x} \), the following first approximation stochastic system can be written

\[
\dot{\varepsilon} = (F + BK)z + \varepsilon G\xi(t), \quad G = \sigma(\bar{x}, 0).
\] (7)

The variable \( y = \frac{z}{\varepsilon} \) characterizes the sensitivity of the solution of system (7) to noise with the intensity \( \varepsilon \). For the covariance matrix \( V(t) = \text{cov}(y(t), y(t)) \), one can write the equation

\[
\dot{V} = (F + BK)V + V(F + BK)^\top + S, \quad S = GG^\top.
\] (8)

For any \( K \in K \), this equation has a unique stationary matrix solution \( W \) satisfying the following algebraic equation

\[
(F + BK)W + W(F + BK)^\top + S = 0.
\] (9)

For non-singular noises \( (\det S \neq 0) \), the solution \( W \) of equation (9) is positive definite.

Any solution \( V(t) \) of system (8) converges to the corresponding solution \( W \) of system (9)

\[
\lim_{t \to \infty} V(t) = W.
\]

It holds that

\[
\text{cov}(\bar{x}^\varepsilon(t), \bar{x}^\varepsilon(t)) \approx \varepsilon^2 W,
\]

where \( \text{cov}(\bar{x}^\varepsilon(t), \bar{x}^\varepsilon(t)) \) is a covariance matrix of solutions \( \bar{x}^\varepsilon \) of system (3). So, the matrix \( W \) is a simple quantitative characteristic of a response of the nonlinear system (3) to small noises. The matrix \( W \) is called a stochastic sensitivity matrix of the equilibrium \( \bar{x} \). The control of the dispersion of random states around the equilibrium can be realized as a synthesis of the assigned stochastic sensitivity matrix \( W \).

Denote by \( M \) a set of symmetric and positive definite \( n \times n \)-matrices. For any \( K \in K \), the regulator (6) forms a stable equilibrium of system (3) with the corresponding stochastic sensitivity matrix \( W_K \) which is a solution of the equation (9). Consider the following control problem.
Synthesis of stochastic sensitivity

For the assigned matrix $W \in \mathbf{M}$, it is necessary to find a matrix $K \in \mathbf{K}$ guaranteeing the equality $W_K = W$, where $W_K$ is a solution of equation (9).

Consider important notions of an attainability. The element $W \in \mathbf{M}$ is said to be attainable if the equality $W_K = W$ is true for some $K \in \mathbf{K}$. The attainability set

$$W = \{ W \in \mathbf{M} | \exists K \in \mathbf{K} \quad W_K = W \}$$

consists of all attainable elements.

An equilibrium $\bar{x}$ is completely stochastic controllable if

$$\forall W \in \mathbf{M} \quad \exists K \in \mathbf{K} : \quad W_K \equiv W.$$ 

So, the condition of the complete stochastic controllability of the equilibrium $\bar{x}$ can be written as $W = \mathbf{M}$.

To describe the attainability set, consider a connection between the assigned matrix $W$ and the feedback coefficient $K$:

$$BK W + WK^T B^T + H(W) = 0, H(W) = FW + WF^T + S.$$ (10)

The following Theorem gives a solution for the problem of the synthesis of the assigned stochastic sensitivity matrix $W$ [9].

**Theorem.**

Let the noise be non-singular $(\det S \neq 0)$.

(a) If the matrix $B$ is quadratic and non-singular then $W = \mathbf{M}$ and for any matrix $W \in \mathbf{M}$

$$K = \bar{K} + B^{-1}ZW^{-1} \in \mathbf{K}, \quad \bar{K} = -B^{-1} \left( \frac{1}{2} SW^{-1} + F \right),$$

where $Z$ is an arbitrary skew-symmetric $n \times n$-matrix.

(b) If rank($B$) < $n$ then the element $W \in \mathbf{M}$ is attainable if and only if the matrix $W$ is a solution of the equation

$$P_2 H(W) P_2 = 0.$$ (11)

Under these conditions for any matrix $W \in \mathbf{M}$

$$K = \bar{K} + C \in \mathbf{K}, \quad \bar{K} = B^+ H(W) \left( \frac{1}{2} P_1 - I \right) W^{-1},$$

where $C$ is an arbitrary $l \times n$-matrix satisfying the condition

$$BCW + WC^T B^T = 0.$$ 

Here, $P_1 = BB^+$ and $P_2 = I - P_1$ are projective matrices, an the sign ”$+$” means a pseudo-inversion.

Further, we apply this theory to the stabilization of operating mode for the stochastic flow reactor.
5. Stabilization of the stochastic flow reactor

As shown above, the system (4) is excitable, and the random noise can generate large-amplitude stochastic oscillations and destroy a normal operation of the system. So, it is important to suppress such oscillations and return the system to normal operating mode with acceptable small-amplitude oscillations around the equilibrium.

Consider now the system (4) with additional control inputs:
\[
\begin{align*}
\dot{x} &= -x \exp \left( -\frac{1}{y} \right) + l(a-x) + u_1 + \varepsilon_1 \xi_1(t), \\
\dot{y} &= x \exp \left( -\frac{1}{y} \right) + m(b-y) + u_2 + \varepsilon_2 \xi_2(t).
\end{align*}
\] (12)

A stochastic sensitivity of the equilibrium \((\bar{x}, \bar{y})\) of the uncontrolled system (2) is characterized by the \(2 \times 2\)-matrix \(W = \begin{pmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{pmatrix}\). This symmetric positive definite matrix is a unique solution of the matrix equation (9) with \(K = 0\), where for system (2) we have
\[
F = \begin{pmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{pmatrix}, \\
S = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},
\]
\[
f_{11} = -\exp \left( -\frac{1}{y} \right) - l, \\
f_{12} = -\bar{x} \exp \left( -\frac{1}{y} \right) \frac{1}{y^2}, \\
f_{21} = \exp \left( -\frac{1}{y} \right), \\
f_{22} = \bar{x} \exp \left( -\frac{1}{y} \right) \frac{1}{y^2} - m.
\]

For \(a = 1.58\) considered above, elements of the stochastic sensitivity matrix \(W\) are as follows:
\[
w_{11} = 1.0947 \cdot 10^4, \\
w_{12} = w_{21} = -2.2545 \cdot 10^3, \\
w_{22} = 5.2001 \cdot 10^2.
\]
The large values of elements of the matrix \(W\) are the main reason of the stochastic excitability with the generation of large-amplitude oscillations (see Fig. 2a).

To stabilize an operating mode of the stochastically forced reactor, we will use the regulator
\[
u_1 = k_{11}(x-\bar{x}) + k_{12}(y-\bar{y}), \\
u_2 = k_{21}(x-\bar{x}) + k_{22}(y-\bar{y}),
\] (13)
which provides much smaller values of the stochastic sensitivity. Here, for example, we restrict ourselves by the diagonal stochastic sensitivity matrices \(W = \begin{pmatrix} w & 0 \\ 0 & w \end{pmatrix}\).

As it follows from the Theorem, the coefficients of the regulator (13) which synthesizes such stochastic sensitivity matrix \(W\) with any assigned \(w > 0\) can be found explicitly. The results of the control based on this stochastic sensitivity synthesis are shown in Fig. 3.

For the value \(a = 1.58\), the time series of the controlled stochastic system with \(\varepsilon = 0.0005\) are shown in Fig. 3a. Here, the control providing \(w = 10\), is switched on at \(t = 5000\). As one can see, this regulator returns the system to the operating mode with small-amplitude oscillations. Analogous results are obtained for \(a = 1.583\) (see Fig. 3b).

Note that a decrease of the control parameter \(w\) allows us to decrease a dispersion of these small-amplitude oscillations (compare time series in Fig. 4 for \(w = 0.1\) and \(w = 10\)).

6. Conclusion

In the present paper, we have demonstrated how to stabilize stochastic operation modes of the flow reactor with the help of the appropriate feedback regulator. We have shown that the high stochastic sensitivity is a main reason for the destruction of the operation even for the weak noise. In order to avoid the unwanted large-amplitude oscillations and return the system to the proper operating mode, one has to use a regulator which reduces the stochastic sensitivity. On the basis of the presented theory of the synthesis of the assigned stochastic sensitivity, we have constructed a stabilizing regulator for the randomly forced flow reactor.
Figure 3. Time series of the controlled stochastic system with $\varepsilon = 0.0005$: a) $a = 1.58$; b) $a = 1.583$. The control is switched on at $t = 5000$, the regulator provides $w = 10$.

Figure 4. Time series of the controlled stochastic system for $\varepsilon = 0.0005$ with the regulator providing $w = 0.1$ (black) and $w = 10$ (grey). The control is switched on at $t = 0$.

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