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The following system of first-order ordinary nonlinear differential equations, which in certain approximations simulates the plasmochemical process of conversion of methane to acetylene in a hydrogen plasma jet, was examined in [1]:

$$\begin{aligned} \frac{dc_1(z)}{dz} &= -\frac{1}{v(z)} k_1(T) c_1(z), \\ \frac{dc_2(z)}{dz} &= \frac{1}{v(z)} \left[\frac{1}{2} \frac{\mu_2}{\mu_1} k_1(T) c_1(z) - k_2(T) c_2(z) \right], \\ \frac{dc_3(z)}{dz} &= \frac{1}{v(z)} \left[\frac{\mu_3}{\mu_2} k_2(T) c_2(z) - k_3(T) c_3(z) \right], \\ \frac{dc_4(z)}{dz} &= \frac{1}{v(z)} 2 \frac{\mu_4}{\mu_3} k_3(T) c_3(z), \\ \frac{dc_5(z)}{dz} &= \frac{1}{v(z)} \left[\frac{\mu_5}{\mu_1} k_1(T) c_1(z) + \frac{\mu_5}{\mu_2} k_2(T) c_2(z) + \frac{\mu_5}{\mu_3} k_3(T) c_3(z) \right], \\ \frac{dT(z)}{dz} &= -\frac{[N/M - 2v(z)] s_1 + v(z) RT(z) s_2}{[N/M - 2v(z)] s_3 + v(z) R s_4}, \\ \frac{dt}{dz} &= \frac{1}{v(z)}, \quad v(z) = N/2M - [(N/2M)^2 - RT(z) s_4]^{1/2}, \end{aligned} \quad (0.1)$$

where

$$\begin{aligned} s_1 &= \sum_{i=1}^5 \sum_{j=1}^8 \frac{dc_i(z)}{dz} [h_{ij} T^{j-1}(z) + h_i^0], & s_2 &= \sum_{i=1}^5 \frac{1}{\mu_i} \frac{dc_i(z)}{dz}, \\ s_3 &= \sum_{i=1}^5 \sum_{j=1}^8 c_i(z) h_{ij} T^{j-1}(z), & s_4 &= \sum_{i=1}^5 \frac{c_i(z)}{\mu_i}. \end{aligned}$$

Here, c_i is the mass concentration of the i -th substance ($i = 1-5$, 1-CH₄, 2-C₂H₄, 3-C₂H₂, 4-C, 5-H₂), h_{ij} is the coefficient in the expansion of the enthalpy of the i -th substance with respect to temperature T , h_i^0 is the heat of formation of the i -th substance, $k_i(T)$ is the rate constant for decomposition of the i -th substance, N and M are constants of integration determined from the initial conditions, R is the gas constant, and μ_i is the molecular weight of the i -th substance.

By means of a numerical integration of system (0.1)-(0.3) on a computer for various initial methane concentrations $c_1(0)$ ($c_5(0) = 1 - c_1(0)$, $c_2(0) = c_3(0) = c_4(0) = 0$), initial temperatures $T(0)$, and initial plasma jet velocities $v(0)$, it was shown that the variation of $c_1(0)$ and $T(0)$ has an important influence on the kinetics of the process, whereas the variation of $v(0)$ does not affect the kinetics of the chemical reactions, but merely changes the spatial scales of the process.

Since system (0.1)-(0.3) cannot be solved analytically, it is impossible to both establish directly a functional relationship between its solutions and the initial conditions and investigate the dependence of the solution on the initial conditions in general form.

However, it is possible to use the results of a numerical integration of system (0.1)-(0.3) with various initial conditions to establish approximate relations between the solutions and the initial conditions for a particular value of $z = z_m$. For z_m we can take the point at which the acetylene concentration obtained from solving system (0.1)-(0.3) reaches a maximum, which, as shown in [2], can be largely preserved by a suitable choice of the conditions and point of cooling.

In what follows, we establish the approximate functional dependence (at the point z_m) on the initial conditions $T(0)$ and $c_1(0)$ (the inputs) for the following four quantities (the outputs):

a) The length of the section from the beginning of the reactor ($z = 0$) to $z = z_m$. This section, through which the process of conversion of methane to acetylene chiefly takes place, will be denoted by L and, in accordance with the terminology of [3, 4], will be called the effective length of the plasmochemical reactor.

b) The reaction time τ_m , determined from Eq. (0.3),

$$\tau_m = \int_0^{z_m} \frac{d\xi}{v(\xi)}.$$

- c) The maximum acetylene concentration $c_3(z_m)$.
- d) The degree of decomposition of the methane

$$S = \frac{c_1(0) - c_1(z_m)}{c_1(0)}. \quad (0.4)$$

Two aspects of the problem will be considered. First, a method is proposed which makes it possible to treat the plasmochemical reactor described by a system of equations analogous to (0.1)-(0.3) as a nonlinear converter. Secondly, the effect of fluctuations of the initial conditions is examined.

1. **Dependence of L , τ_m , $c_3(z_m)$, and S on $c_1(0)$ and $T(0)$.** By numerically integrating system (0.1)-(0.3) for five variants of each of the inputs $c_1(0)$ or $T(0)$ with the other input fixed, we can construct graphs of all the outputs L , τ_m , $c_3(z_m)$, and S as functions of the inputs $c_1(0)$ and $T(0)$.

Curves 1-4 in Fig. 1 give the dependence of $c_3(z_m)$, L , τ_m , and S on $T(0)$ for fixed $c_1(0) = 0.95$ and $v(0) = 3 \cdot 10^4$ cm/sec (here and henceforth the concentrations are given in weight fractions).

Curves 1-4 in Fig. 2 give the dependence of $c_3(z_m)$, L , τ_m , and S on $c_1(0)$ for fixed $T(0) = 3.5 \cdot 10^3$ K and $v(0) = 3 \cdot 10^4$ cm/sec.

Using these graphs, it is possible to derive approximate linear quadratic analytical relations between the given outputs and inputs. The relations between the outputs $c_3(z_m)$, L , τ_m , and S and the inputs

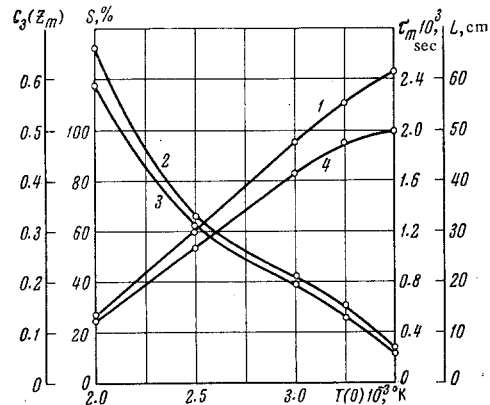


Fig. 1

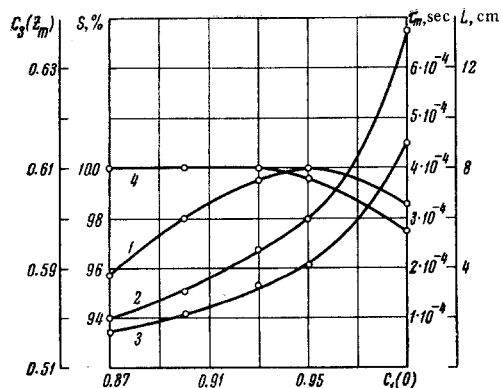


Fig. 2

$T(0)$ and $c_1(0)$ are represented by Eqs. (1.1)–(1.8), respectively:

$$c_3(z_m) = 0.125 + 3.5 \cdot 10^{-4} (T(0) - 2000^\circ),$$

$$2000 \leq T(0) \leq 3000^\circ \text{ K};$$

$$c_3(z_m) = 0.476 + 3.44 \cdot 10^{-4} (T(0) - 3000^\circ) -$$

$$- 1.6 \cdot 10^{-7} (T(0) - 3000^\circ)^2,$$

$$3000 \leq T(0) \leq 3500^\circ \text{ K}; \quad (1.1)$$

$$L = 67 - 9 \cdot 10^{-2} (T(0) - 2000^\circ) + 0.44 \cdot 10^{-4} (T(0) - 2000^\circ)^2,$$

$$2000 \leq T(0) \leq 3000^\circ \text{ K};$$

$$L = 21 - 2.6 \cdot 10^{-2} (T(0) - 3000^\circ) - 0.8 \cdot 10^{-5} (T(0) - 3000^\circ)^2,$$

$$3000 \leq T(0) \leq 3500^\circ \text{ K}; \quad (1.2)$$

$$\tau_m = 2.357 \cdot 10^{-3} - 2.99 \cdot 10^{-6} (T(0) - 2000^\circ) +$$

$$+ 1.44 \cdot 10^{-9} (T(0) - 2000^\circ)^2,$$

$$2000 \leq T(0) \leq 3000^\circ \text{ K};$$

$$\tau_m = 0.78 \cdot 10^{-3} - 0.113 \cdot 10^{-5} T(0) - 3000^\circ,$$

$$3000 \leq T(0) \leq 3500^\circ \text{ K}; \quad (1.3)$$

$$S = 24.7 + 5.83 \cdot 10^{-2} (T(0) - 2000^\circ),$$

$$2000 \leq T(0) \leq 3000^\circ \text{ K};$$

$$S = 83 + 0.558 \cdot 10^{-1} (T(0) - 3000^\circ) -$$

$$- 0.464 \cdot 10^{-4} (T(0) - 3000^\circ)^2,$$

$$3000 \leq T(0) \leq 3500^\circ \text{ K}; \quad (1.4)$$

$$c_3(z_m) = 0.5887 + 0.33 (c_1(0) - 0.87), \quad 0.87 \leq c_1(0) \leq 0.93$$

$$c_3(z_m) = 0.6085 + 0.1758 (c_1(0) - 0.93) - 4.29 (c_1(0) - 0.93)^2, \quad (1.5)$$

$$0.93 \leq c_1(0) \leq 0.99;$$

$$L = 2.0 + 21.7 (c_1(0) - 0.87) + 3.88 \cdot 10^2 (c_1(0) - 0.87)^2,$$

$$0.87 \leq c_1(0) \leq 0.93;$$

$$L = 4.7 + 24.17 (c_1(0) - 0.93) + 2.04 \cdot 10^3 (c_1(0) - 0.93)^2, \quad (1.6)$$

$$0.93 \leq c_1(0) \leq 0.99;$$

$$\tau_m = 0.277 \cdot 10^{-1} - 0.625 \cdot 10^{-1} c_1(0) + 0.353 \cdot 10^{-1} c_1^2(0),$$

$$0.87 \leq c_1(0) \leq 0.99; \quad (1.7)$$

$$S = 100, \quad 0.87 \leq c_1(0) \leq 0.93,$$

$$S = 100 - 0.391 \cdot 10^2 (c_1(0) - 0.93) - 0.417 (c_1(0) - 0.93)^2, \quad (1.8)$$

$$0.93 \leq c_1(0) \leq 0.99.$$

These relations show that with respect to the inputs $c_1(0)$ and $T(0)$ the plasmochemical reactor is a nonlinear converter and the graphs and corresponding approximate analytic expressions are its nonlinear characteristics.

2. Effect of fluctuating initial conditions on the solutions of system (0.1)–(0.3). Formulation of the problem. In the above calculations $c_1(0)$ and $T(0)$ were assumed to be independent of time. Thus the characteristics obtained for the reactor, regarded as a nonlinear converter, are its static characteristics.

In fact, the initial methane concentration and the initial temperature of the gas mixture experience random fluctuations in time.

We will describe the random fluctuations of $c_1(0)$ and $T(0)$ in terms of stationary random function [5, 6], assuming that $c_1(0)$ and $T(0)$ are absolutely continuous stationary normal random functions of time. In order to compare the results obtained with experimental data, it is obviously necessary to make the further assumption that the random functions are ergodic. For this assumption it is sufficient that their autocorrelation functions do not tend too slowly to zero [6].

Since the investigated random functions vary on a finite interval $[x_*, x^*]$ (here x represents either of the two functions $c_1(0)$ or $T(0)$), it is necessary to use truncated normal distributions [7].

The one-dimensional truncated normal distribution has the following form:

$$f_1(x_1) = D_1 \frac{1}{(2\pi\sigma_x^2)^{1/2}} \exp \left[-\frac{(x_1 - \langle x \rangle)^2}{2\sigma_x^2} \right] \text{ when } x_* \leq x_1 \leq x^*,$$

$$f_1(x_1) = 0 \text{ when } x_1 \leq x_*, \quad x_1 > x^*,$$

$$x_1 = x(t_1). \quad (2.1)$$

Here, σ_x is the standard deviation of the stationary random function.

The quantity D_1 is selected so that $f_1(x_1)$ is normalized to unity on the given interval of the random function.

If the inputs of the nonlinear converter are stationary random functions of time, its outputs L , τ_m , $c_3(z_m)$, and S will also be stationary random functions of time (we assume that the nonlinear converter has stationary characteristics). In order to determine the statistical properties of these random functions we use Eqs. (1.1)–(1.8), having assumed that the nonlinear converter is inertialess [8, 8, 9]; i.e., for a given time t , any output $y(t)$ is expressed as a function of some input $x(t)$ at the same moment of time:

$$y(t) = \varphi[x(t)], \quad (2.2)$$

3. Determination of the mathematical expectations and correlation functions of L , $c_3(z_m)$, and S . A knowledge of the correlation function and mathematical expectation of the random output function is of fundamental practical importance in the investigation and design of nonlinear systems.

The mathematical expectation $\langle y \rangle$ of the stationary random process $y(t)$ at the output of an inertialess nonlinear converter is defined as follows [10]:

$$\langle y \rangle = \langle y_1 \rangle + \langle y_2 \rangle, \quad (3.1)$$

where

$$\langle y_1 \rangle = D_1 \sum_{l=0}^2 A_{k1} \left\{ \sum_{l=1}^k \frac{k!}{l!(k-l)!} \sigma_x^l \langle x \rangle - \right.$$

$$\left. - x_*^{k-l} [Q_l(\xi_0) - Q_l(\xi_*)] \right\};$$

$$\langle y_2 \rangle = D_1 \sum_{l=0}^2 A_{l2} \left\{ \sum_{l=0}^k \frac{k!}{l!(k-l)!} \sigma_x^l \langle x \rangle - \right.$$

$$\left. - x_0^{k-l} [Q_l(\xi_0^*) - Q_l(\xi_0)] \right\}; \quad (3.2)$$

x_0 is a value of x dividing the region of variation $[x_*, x^*]$ into two parts;

$$Q_l(\xi) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\xi} \xi^l l^{-1/2} \xi^2 d\xi, \quad \xi = \frac{x - \langle x \rangle}{\sigma_x}. \quad (3.3)$$

Here, A_{k2} , A_{k1} are the constant coefficients in Eqs. (1.1)–(1.8).

The formula for the correlation function is written as follows [10]:

$$R_y(\theta) = \sum_{n=1}^{\infty} B_n^2 \langle x, \sigma_x \rangle \frac{r_x^n(\theta)}{n!}, \quad (\theta = t_2 - t_1); \quad (3.4)$$

$$B_n \langle x, \sigma_x \rangle = D_1 \sum_{k=0}^2 \sum_{l=0}^k A_{k1} \frac{k!}{l!(k-l)!} \sigma_x^l \langle x \rangle -$$

$$- x_*^{k-l} [M_{ln}(\xi_0) - M_{ln}(\xi_*)] +$$

$$+ D_1 \sum_{k=0}^2 \sum_{l=0}^k A_{l2} \frac{k!}{l!(k-l)!} \sigma_x^l \langle x \rangle -$$

$$- x_0^{k-l} [M_{ln}(\xi_0^*) - M_{ln}(\xi_0)]; \quad (3.5)$$

$$M_{ln}(\xi) = \int_{-\infty}^{\xi} \xi^l \frac{d^n \psi(\xi)}{d\xi^n} d\xi, \quad \psi(\xi) = \frac{1}{(2\pi)^{1/2}} e^{-\frac{1}{2} \xi^2}. \quad (3.6)$$

$r_x(\theta)$ is the normalized autocorrelation function of input x .

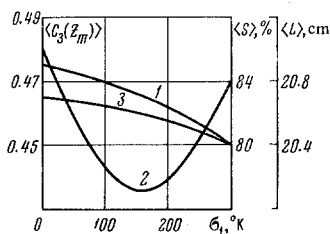


Fig. 3

In practical calculations, using (3.4) it is necessary to confine oneself to a finite number of terms of the series N . An estimate of the accuracy of the approximate determination of the correlation function $R_y(\theta)$ is given by the following expression [10]:

$$|R_y(\theta) - R_y'(\theta)| \leq \sigma_y^2 - \sigma_y'^2 \quad (3.7)$$

$$R_y'(\theta) = \sum_{n=1}^N B_n^2 \langle \langle x \rangle, \sigma_x \rangle \frac{r_{x^n}(\theta)}{n!},$$

$$\sigma_y'^2 = R_y'(0) = \sum_{n=1}^N \frac{B_n^2 \langle \langle x \rangle, \sigma_x \rangle}{n!} \quad (3.8)$$

The results of a calculation of the dependence of the mathematical expectations $\langle c_3(z_m) \rangle$, $\langle L \rangle$, and $\langle S \rangle$ on the standard deviation of the initial temperature σ_1 for a given mathematical expectation of the initial temperature $\langle T(0) \rangle = 3000^\circ \text{K}$ and a constant value of the initial methane concentration $c_1(0) = 0.95$ are represented by curves 1, 2, and 3 in Fig. 3, respectively. Similarly, in Fig. 4 curves 1, 2, and 3 represent the dependence of $\langle c_3(z_m) \rangle$, $\langle L \rangle$, and $\langle S \rangle$ on the standard deviation of the initial methane concentration σ_2 (mathematical expectation of the initial methane concentration $\langle c_1(0) \rangle = 0.95$ and the constant value of the initial temperature $T(0) = 3500^\circ \text{K}$).

On the basis of these graphs we constructed the following approximate analytic expressions:

$$\langle c_3(z_m) \rangle = 0.475 - 3.166 \cdot 10^{-6} \sigma_1 - 1.833 \cdot 10^{-7} \sigma_1^2;$$

$$\langle L \rangle = 21 - 1.135 \cdot 10^{-2} \sigma_1 + 0.355 \cdot 10^{-4} \sigma_1^2 \quad (0^{\circ} \leq \sigma_1 \leq 300^\circ \text{K}); \quad (3.9)$$

$$\langle S \rangle = 83 - 0.217 \cdot 10^{-2} \sigma_1 - 0.283 \cdot 10^{-4} \sigma_1^2; \quad (3.10)$$

$$\langle c_3(z_m) \rangle = 0.610 - 0.425 \sigma_2 + 9.5 \sigma_2^2;$$

$$\langle L \rangle = 6.0 + 15 \sigma_2 + 5 \cdot 10^2 \sigma_2^2 \quad (0 \leq \sigma_2 \leq 0.02);$$

$$\langle S \rangle = 99.2 - 40 \sigma_2 + 2 \cdot 10^3 \sigma_2^2.$$

Calculations based on Eqs. (3.4)–(3.6) gave the following formula for the correlation function of the output $c_3(z_m)$ $R_A'(\theta)$ (in the calculation $N = 3$, $\langle T(0) \rangle = 3000^\circ \text{K}$, $c_1(0) = 0.95$ and $\sigma_1 = 100^\circ \text{K}$):

$$R_A'(\theta) = 1.122 \cdot 10^{-8} r_T(\theta) + 1.62 \cdot 10^{-6} r_T^2(\theta) + 6.61 \cdot 10^{-8} r_T^3(\theta). \quad (3.11)$$

The relative error in determining the correlation function of the output $c_3(z_m)$ is on the order of 10%.

CONCLUSIONS

The approximate analytic expressions obtained make it possible to treat the plasmochemical reactor as a nonlinear converter with inputs $T(0)$ and $c_1(0)$ and outputs $c_3(z_m)$, L , τ_m , and S , and the graphs in Figs. 1 and 2 as its static characteristics.

From a comparison of the graphs in Figs. 1 and 2 it is clear that in the given region of variation of $T(0)$ and $c_1(0)$ the maximum of the acetylene concentration $c_3(z_m)$ is more sensitive to variation of the input $T(0)$, which obviously must be taken into account in controlling the output $c_3(z_m)$.

The static characteristics obtained make it possible to consider the problem when $T(0)$ and $c_1(0)$ are random functions of time.

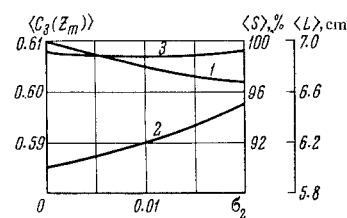


Fig. 4

We have found the mathematical expectations of the outputs $c_3(z_m)$, L , and S as functions of the standard deviations of the inputs $T(0)$ and $c_1(0)$.

The graphs in Figs. 3 and 4 show that in the presence of random fluctuations of the inputs $T(0)$ and $c_1(0)$ the mean value of the output of the acetylene target product $c_3(z_m)$ may be reduced by about 5.5%.

A method of calculating the correlation functions of the outputs has been demonstrated with reference to the output $c_3(z_m)$.

The static characteristics obtained for the plasmochemical reactor can be used in solving a number of problems:

- a) controlling the end state of the process, e.g., the maximum acetylene concentration, by varying the inputs $c_1(0)$ and $T(0)$;
- b) solving the more general problem of the choice of optimal (for a given optimality criterion) values of the inputs $T(0)$ and $c_1(0)$; etc.

The correlation functions of the inputs and outputs can be used to solve problems of predicting the behavior of the reactor outputs (in the presence of fluctuating inputs by means of the theory of stationary random functions).

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