Stochastic model for a wavelike exothermal reaction in condensed heterogeneous systems

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(Received 8 July 1991; revised manuscript received 29 April 1992)

The relationship between the stochastic and deterministic approaches to the description of the dynamic behavior for a nonlinear reacting system is studied. A self-propagating exothermal reaction in a heterogeneous medium has been chosen as an example. A stochastic model for this phenomenon is developed. The system is composed of cells characterized by temperature and degree of conversion, their transformation probability being dependent on temperature. Computer simulation showed that stochasticity reveals itself in the generation of disturbances that are absent in the deterministic model. For a well-developed steady-state regime, the distributions of the mean temperature and degree of conversion are close to those given by the deterministic model. Under the conditions of planar-wave-front instability, the stochastic model possesses a mechanism for spontaneous transfer to a stable regime from arbitrary initial conditions (temperature distribution, etc.) due to origination, propagation, and disintegration of disturbances. Such behavior agrees with experimental data and is not predicted by the deterministic model.

PACS number(s): 64.60.Ak, 05.50.+q

I. INTRODUCTION

At present the description of the dynamic behavior of nonlinear systems where the processes that are stochastic in nature take place is the subject of extensive investigations. Classical examples are the reaction-diffusion problems, processes in biological systems, etc. [1]. In such systems, diverse structural, phase, and chemical transformations proceed in isothermal and nonisothermal conditions, their velocities being dependent on temperature, reagent concentrations, and other factors. The changes in these spatially distributed parameters due to the transformations have, in turn, an inverse effect on the reaction rates, i.e., these systems possess a feedback mechanism. In a number of systems, a positive nonlinear feedback, coupled with diffusional instability, causes the origin of traveling waves. The systems with wavelike localization of chemical, phase, and/or structural transformations (e.g., reaction front in the case of a single reaction) are particularly interesting. The typical example for a comprehensively studied process of such a type is the combustion phenomenon in heterogeneous media [2].

Traditionally, the models for nonlinear reacting systems are expressed in terms of partial-differential equations using the mean-field approximation of the system parameters. Usually, such a deterministic approach enables one to describe the dynamic behavior, including steady-state regimes, bifurcations, instabilities, and oscillations, and even a transfer to chaos [1]. However, chemical reactions, structural transformations, and phase transformations are stochastic events by nature, and the mean-field approximation reveals only average values of the process velocities. Therefore, it is interesting to analyze the role of a stochastic factor in the models for systems with traveling waves, and to reveal its influence on the origin of instabilities and dynamic behavior. It seems reasonable to select a relatively simple well-studied nonlinear system for such an investigation.

For this purpose, in the present work we have chosen a solid-state wavelike self-propagating reaction in a heterogeneous medium [the so-called self-propagating high-temperature synthesis (SHS) or the combustion synthesis, of refractory borides, carbides, intermetallic compounds, etc., which is a promising energy-effective method for developing and producing advanced ceramic and composite materials [3]]. The regularities of this phenomenon have been comprehensively studied in numerous experimental works [4], as well as in theoretical investigations within the framework of the deterministic model [2], using both computer modeling [5,6] and analytical methods [7]. It has been demonstrated that variation of the system parameters changes the dynamic behavior from a steady-state wave-propagation regime into an unstable one with: (a) self-oscillating mode [5], (b) the so-called spin combus-

tion [6], when one or several hot foci follow a spiral trajectory along the specimen surface, and (c) transition to chaos [7].

Recently, a number of stochastic models for nonlinear reacting systems has been developed [8]. Nevertheless, the analysis of a relationship between the stochastic approach and the deterministic one has not yet been properly outlined. Therefore, the present work is aimed at developing a simple stochastic model for a self-propagating exothermal reaction in a heterogeneous medium, and to compare the results of computer simulation with those obtained within the deterministic approach, in order to reveal the principle similarities and differences between them.

II. DEVELOPMENT OF A STOCHASTIC MODEL

The heterogeneous wavelike exothermal reaction propagates through a powder mixture of initial solid substances (e.g., Ti + C to produce titanium carbide). Traditionally, the SHS processes are described by the deterministic model for thermal combustion consisting of the equations for heat transfer and chemical reaction kinetics [2]. Wherever the reagent particles are nonregularly spatially distributed and have a nonuniform surface structure, shape, size, etc., chemical reactions and structural transformations of the particles are stochastic in nature. The times of their transformations are randomly distributed around an average value. According to Ref. [3], the time scales for the interaction processes in the SHS wave are $10^{-4}-10^{-2}$ s. A relatively small number of particles situated in the region that is $1-100\mu$m wide can react during this time. The stochastic effects that are connected with the particles' heterogeneity influence on the processes in the combustion wave may prove to be noticeable, especially under unstable conditions. Therefore, it is rather important to take into account the effect of stochasticity on the system behavior.

We consider a two-dimensional problem for the reaction-front propagation along a semi-infinite strip or a cylindric shell. It is assumed that there is no reagent mass transfer along a sample, and thermophysical parameters are the same for both the initial substance and reaction product and are independent on temperature. Within the framework of the deterministic approach, the model is described by the following equations:

$$\frac{\partial T}{\partial T}=a\nabla^2 T+\frac{Q}{\rho c}\frac{\partial \xi}{\partial t},\ \frac{\partial \xi}{\partial t}=f(\xi,T) \tag{1}$$

where ξ is the conversion degree; T is temperature; a, Q, c, and ρ are the thermal diffusivity, heat release per unit volume, specific heat, and density, respectively.

In the stochastic model, the two-dimensional region is composed of square cells with a side h. Using cells is a simple way of introducing a scale of spatial inhomogeneity into the combustion model. A cell is characterized by temperature Θ and conversion degree η, both of which are random quantities. Their values are updated at a discrete moment of time with a time step τ. At the $(n+1)$th time step, a temperature of a cell with coordinates i,j is determined by the expression

$$\Theta(i,j,n+1)=\Theta(i,j,n)+\frac{Q}{\rho c}[\eta(i,j,n+1)-\eta(i,j,n)]+\frac{a\tau}{h^2}[\Theta(i-1,j,n)+\Theta(i+1,j,n)+\Theta(i,j-1,n)+\Theta(i,j+1,n)-4\Theta(i,j,n)]\ . \tag{2}$$

The second term on the right-hand side (rhs) of Eq. (2) denotes a heat release in the cell due to a chemical reaction, and the third term on the rhs denotes heat fluxes from the neighboring cells. Equation (2) is a discrete analog of heat transfer equation (1) for an average temperature $\langle\Theta\rangle$.

The reaction is ignited by a hot wall. For a striplike specimen, in the transverse direction (at the specimen edges), the adiabatic boundary conditions are used, while for a cylindrical shell, the periodic ones are used.

In the simplest model for chemical reaction, a cell is assumed to be burnt in a time τ. The conversion degree η attains two values: O, initial: and 1, burnt. Cell transformation during this time step is a random event, whose probability p is determined by the cell temperature.

In order to reveal a relationship between this model and the deterministic one [see the system of equations (1)], let us pass to average quantities and continuous time. Under isothermal conditions for the temperature Θ, the average portion of cells burnt to a temporal moment $n\tau$ is $\langle\eta\rangle(n)=1-(1-p)^n$, $p=p(\Theta)$. Passing to a continuous time, assuming the traditional conditions for the Poisson processes [9], and implying that the transformation probabilities for different cells in the time τ are independent, we obtain $p(\tau)=\lambda\tau+O(\tau)$ with $\lambda=\lim_{\tau\to 0} p/\tau$. Under these conditions, the portion of the cells that are burnt during the time t is $\langle\eta(t)\rangle=1-\exp(-\lambda t)$. This is consistent with the kinetics of the first-order reaction

$$\frac{\partial\langle\eta\rangle(t)}{\partial t}=[1-\langle\eta\rangle(t)]\lambda\ . \tag{3}$$

Within the framework of the deterministic approach [see Eq. (1)], the kinetic function used in the model that is considered is $f(\xi,t)=(1-\xi)\lambda(T)$, with $\xi=\langle\eta\rangle$. The reaction rate temperature dependence can be described by the Arrhenius law, $p(\Theta)=z\tau\exp[-E/(R\Theta)]$. The similarity of the expressions for the chemical transformation rate in the deterministic model and that in the stochastic one is violated in the nonisothermal case. For a domain S containing a relatively large number of cells N, we obtain the relation

$$\frac{\langle\eta\rangle(n+1)-\langle\eta\rangle(n)}{\tau}=\frac{1}{N\tau}\sum_{i,j\in S}\{1-\eta(i,j,n)p[\Theta(i,j,n)]\}\ . \tag{4}$$

Equation (4) reduces to a similar expression for the deterministic model, if we omit the correlations between $\eta(i,j,n)$ and $\Theta(i,j,n)$ and substitute $\langle p(\Theta)\rangle$ for $p(\langle\Theta\rangle)$. In this case we have $\langle\eta(n+1)-\eta\langle n\rangle\rangle=(1-\langle\eta\rangle)\lambda(\langle\Theta\rangle)\tau$.

The above considerations make clear the difference between the stochastic model and the deterministic one (considered as a system of equations for average quantities). The former takes into account the correlation between the cell temperature Θ and cell conversion degree η. This results in the continuous generation of disturbances, which are absent in the deterministic model.

III. NUMERICAL REALIZATION OF THE MODEL

In the proposed stochastic model, the combustion process is the result of the interaction of a great number of homogeneous elements obeying comparatively simple rules. For both the idea and implementation, the process is close to the cellular automata method, which is widely used in the modeling of crystal growth, reaction-diffusion processes, spin systems, hydrodynamic problems, etc. [10,11]. This method yields a convenient and computationally effective mechanism for constructing the models for dynamic systems in the cases when relatively simple regularities of cell interactions are known. It should be noted that in the framework of this method the proposed model can be easily modified to study different interaction mechanisms; e.g., the effect of adjacent cells on the transformation probability in a given cell (autocatalysis or self-deceleration by the reaction product), a random distribution of the activation energy for chemical reactions in different cells, a multistep reaction with a great number of cell states, etc.

In the computer-program realization of the proposed model, the temperature of each cell, Θ, is an integer parameter in the range 0–255. Equations (2) and (3) are rendered dimensionless to give

$$\Theta(i,j,n+1)=\Theta(i,j,n)+\left[[kN]\sum_{\substack{r,s\\ \text{neighbors of } i,j}}[\Theta(r,s,n)-\Theta(i,j,n)]/N\right]+\hat{Q}[\eta(i,j,n+1)-\eta(i,j,n)]\ ,$$

$$p(\Theta)=z\tau\exp\left[-\frac{ES_T}{R(\Theta+\Theta_0)}\right]\ ,$$

where $\Theta=(T-T_0)/S_T$, $k=a\tau/h^2$, $Q=QS_T/\rho c$, $\Theta_0=T_0/S_T$, S_T is the temperature scale, T_0 is the initial temperature of cells, N is the scaling coefficient, $N=256$, and the symbol [ ] means an integer part. The physical process is specified by the two traditional combustion parameters $\beta=RT_a/E$, $\gamma=\rho cRT_a^2/(EQ)$, with T_a being the final reaction temperature under adiabatic conditions, $T_a=Q/(\rho c)+T_0$.

Since an explicit finite-difference scheme is used to calculate the temperature field, the upper limit for the coefficient k is $k_m=0.25$ due to the loss of stability [6]. Therefore, the k value was fixed at 0.125. The specimen length used in the calculations was $\simeq 10L_M$, where L_M is the width of the combustion-wave preheated zone. The specimen was ignited by a hot wall with a constant temperature slightly higher than the adiabatic one. A computational grid was shifted along the sample, thus following the combustion front propagation.

IV. RESULTS AND DISCUSSION

A. Comparison of combustion wave velocities in the deterministic and stochastic models for a stable regime

Numerical calculations have been carried out for different values of the β and γ parameters and different cell sizes h. Stable and unstable wave-propagation regimes are studied. (Traditionally, in combustion theory these terms pertain to the stability of a planar combustion wave front [2]). The regime is called "stable" if the values of the parameters β and γ are within the range of stable combustion for the deterministic model [5,12]. In the deterministic model, a combustion wave velocity is merely the velocity of an isotherm propagation. In the stochastic model, the form of an isotherm fluctuates. Therefore, a velocity can be determined as a ratio of a cell number ΔN that is burnt in the time $\Delta t=n\tau$, to this time interval. For a short time interval, the combustion velocity is a random quantity. However, its mean value is constant for a rather great time interval under stable combustion conditions. The effect of a cell size on the thermal structure of the combustion wave is conveniently characterized by the parameter $M_h=h/l_r$, with $l_r\simeq u_z\tau_m$ being the reaction zone width, where $\tau_m=(1/z)\exp[E/(RT_a)]$ is the reaction completion time at the adiabatic temperature and u_z is the analytical estimate of the combustion wave velocity. The quantity u_z is determined from the following considerations. During the temperature mean time of the reaction completion $\bar{\tau}$, the wave propagates over a distance $u_z\bar{\tau}$, while the characteristic length of the preheated zone is of the order of $(a\bar{\tau})^{1/2}$. Since $L=(a\bar{\tau})^{1/2}=u_z\bar{\tau}$, where

$$1/\tau=[1/(T_a-T_0)]\int_{T_0}^{T_a}(1/z)\exp[-E/(RT)]dT \approx\gamma/\tau_m \quad \text{for } \gamma\ll 1\ ,$$

we obtain the estimation for a combustion wave velocity, $u_z\simeq(\gamma a/\tau_m)^{1/2}$. In Table I, the values of analytically estimated velocity (according to Ref. [2]), u_z, the mean velocity $\langle u\rangle$, calculated in the stochastic model, and the velocity obtained by computer calculation within the deterministic model, u_d, are compared on the natural scale, $u_S=(a/\tau_m)^{1/2}$. It is seen that for $M_h<2$ the values of u_z, $\langle u\rangle$, and u_d are rather close, i.e., the developed stochastic model demonstrates a good agreement of the combustion velocity with that received within the deterministic approach.

TABLE I. Combustion wave velocities obtained by the stochastic model $\langle u \rangle$ (computer calculation) and by the deterministic one (analytical estimation u_z and computer calculation u_d).

			Dimensionless velocity		
β	γ	M_h	$\langle u \rangle / u_s$	u_z / u_s	u_d / u_s
0.12	0.15	1	0.37	0.39	0.40
0.08	0.15	1	0.39	0.39	0.41
0.16	0.20	0.5	0.44	0.45	0.46
0.16	0.20	1	0.43	0.45	0.46
0.16	0.20	1.4	0.41	0.45	0.46
0.16	0.25	0.5	0.52	0.50	0.53
0.16	0.25	1	0.51	0.50	0.53
0.16	0.25	2	0.48	0.50	0.53
0.16	0.25	4	0.42	0.50	0.53

B. Analysis of two-dimensional instabilities

Figures 1 and 2 show the unrolling of a cylindrical shell with temperature fields at different time moments with temporal step $t_m = a/u_z^2$. The regime with $\beta = 0.08$ and $\gamma = 0.13$ (Fig. 1) is typical of the random focuses with elevated temperature that move together with a front, gradually spreading and interacting. This regime qualitatively corresponds to the experimentally observed autooscillating regime in the form of the pulsations of front sections [13]. Figure 2 corresponds to the regime with $\beta = 0.12$ and $\gamma = 0.12$. A hot focus appears at the moment $t^* = 4.46$ and moves along the spiral path. During three revolutions it has covered a distance of about 12 preheated zones, $L_M = a/u_z$. After having faced another focus it disintegrates into several small focuses and vanishes. This behavior is consistent with the observed transition to a spin regime [13].

Within the deterministic model, the linear theory of stability against small-magnitude perturbations has shown that one- and two-dimensional disturbances can develop when the following relations are satisfied, respectively [12]:

$$K_1 = \frac{9.19\gamma}{(1+3.1\beta+3.1\beta^2)} < 1, \quad K_2 = \frac{8.91\gamma}{(1+3.1\beta+3.1\beta^2)} < 1 .$$

In the stochastic model, one-dimensional disturbances are not observed. In the deterministic model, at $K_1 < 1$, under undisturbed initial conditions the constant-pattern wave-propagation regime changes into a self-oscillating one with a planar front [5] (i.e., with linear isotherms). For a low K_2 value, a spin combustion mode was observed [6] under a sufficiently great two-dimensional perturbation of temperature field.

To analyze the originating two-dimensional disturbances, it is convenient to use the amplitudes of the Fourier expansion of the value $N(y,t) = \sum_{x=0}^{x_{\max}} \eta(x,y,t)h$, which is the amount of burned substance in a longitudinal cross section. After summarizing along the sample length, the random shape of the "spotted" combustion front gives a function of transverse coordinate y and time t. The Fourier spectrum is calculated with a temporal step of the order of τ_m. After this, harmonic amplitudes are averaged in time. The thus obtained spectral function characterizes two-dimensional disturbances of the combustion front. Figure 3 shows spectral functions for the

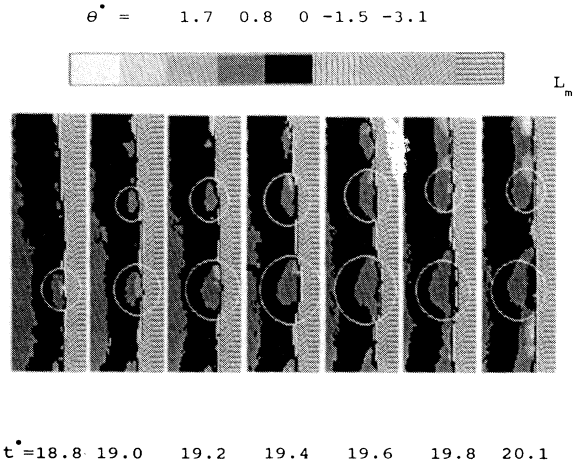

FIG. 1. Temperature charts for $\beta = 0.08$ and $\gamma = 0.13$; $L_m = a/u_z$ is the width of the preheated zone, $\Theta^* = (\Theta - T_a)/\Delta T$, $\Delta T = T_a^2 R/E$, $t^* = t/(L_m/u_z)$.

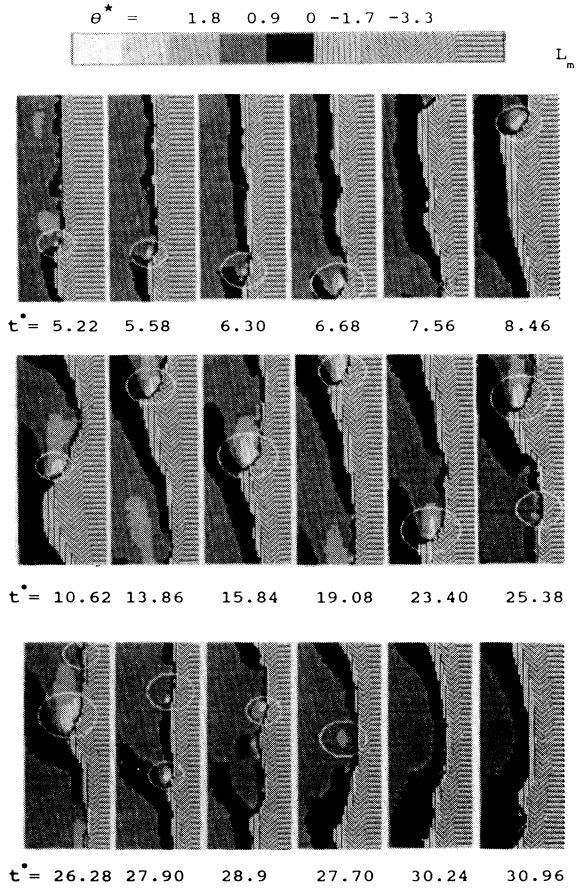

FIG. 2. Temperature charts for $\beta = 0.12$, $\gamma = 0.12$.

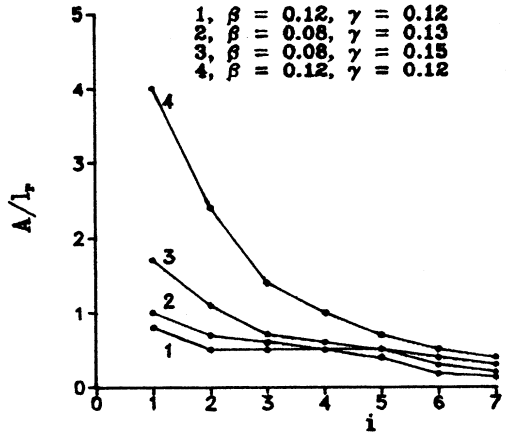

FIG. 3. Amplitudes $A(I)$ of low-frequency harmonics of the Fourier spectrum of the function $N(y)$ describing the front shape (I is the harmonic number): curve 1, $\beta=0.12$, $\gamma=0.12$, $K_2=0.75$; curve 2, $\beta=0.08$, $\gamma=0.13$, $K_2=0.91$; curve 3, $\beta=0.08$, $\gamma=0.15$, $K_2=1.05$; curve 4, $\beta=0.12$, $\gamma=0.20$, $K_2=1.26$.

different values of the β and γ parameters at $M_h=1$. The sample width is $128u_z\tau_m$.

Unlike the deterministic model, there is no clear boundary between stable and unstable regimes. Superheated sites randomly appear when several adjacent cells undergo transformation in a short interval of time. The criterion for wave stability against two-dimensional disturbances K_2 is somewhat lower than that for the case of one-dimensional disturbances K_1. Therefore, under unstable conditions this results in the predominant development of two-dimensional disturbances of the combustion front. Apparently, this throws light on the absence of a stable auto-oscillating regime, with a flat front in the stochastic model for the two-dimensional problem. Disturbances become more pronounced with a decrease in the K_2 value.

C. Effect of a cell size on the onset and development of two-dimensional instabilities

Let us study a mechanism of disturbance generation in the stochastic model. We should analyze a sufficiently small region S parallel to the combustion wave front, in which the temperature Θ is considered to be almost constant. In the direction of the wave propagation the size of this region is of the order of the reaction zone width, $l_r=(\gamma a\tau_m)^{1/2}$, while in the transverse direction its size is about $(a\tau_m)^{1/2}$. Region S having the square of $(1/\gamma)^{1/2}l_r^2$ contains N cells, $N=(1/\gamma)^{1/2}l_r^2/h^2=(1/\gamma)^{1/2}M_h^2$. At small cell sizes, the number N is rather great. The transformation probability for one cell during a given temporal step τ is $p=\tau z\exp[-E/(R\Theta)]=W(\Theta)\tau$. Within the region S, these probabilities are implied to be equal for all of the cells. If before the jth temporal step the degree of conversion in the region S equals η, then the amount of unreacted cells is $n=N(1-\eta)$. The probability that k cells would react during the jth step is determined by the expression $p(k|\eta)=C_n^k p^k(1-p)^{n-k}$. A mean value of k amounts to $\langle k\rangle=np$, and the variance is $D_k=np(1-p)$. It should be noted that at large N the distribution $p(k|\eta)$ approaches the normal one, with the same average value and variance. Since $p\ll 1$, it may be considered that

$$D_k np=N\tau W(\Theta)(1-\eta)\ . \tag{5}$$

In the stochastic model, a disturbance is generated by the deviation of the instantaneous number of burnt cells from a mean one. Since heat removal from the reaction zone corresponds to mean heat release, the excess heat remains in this region, thus resulting in the superheating of the latter. Increasing the temperature accelerates the chemical reaction, and a disturbance starts to grow. A magnitude of superheating may be estimated under the assumption that the deviation of k is of the order of its difference from the mean value, $|k-\langle k\rangle|$, in the domain S. As long as each cell under combustion can elevate the temperature of the region S containing N cells by a quantity of $(T_a-T_0)/N$, we obtain

$$\begin{aligned}\Delta\Theta&=\frac{(T_a-T_0)}{N}[N\tau W(\Theta)(1-\eta)]^{1/2}\\&=\frac{(T_a-T_0)}{N}\frac{M_h\tau}{2}[\gamma W(\Theta)(1-\eta)]^{1/2}\ .\end{aligned} \tag{6}$$

From Eqs. (5) and (6) it is easily seen that the maximum deviation of heat release from its mean value is attained in the region with maximum reaction rate $(1-\eta)W(\Theta)$. In this case, the value of a locally elevated temperature is proportional to cell size h.

The effect of cell size on the behavior of the stochastic model is demonstrated in Table I. Increasing the cell size decreases the combustion wave velocity. A difference becomes substantial at $M_h>2$. The distribution of temperature and degree of conversion in the combustion wave averaged across a sample are shown in Fig. 4 for different M_h. The curves are superimposed for spatial coincidence of the isotherm $\Theta=(T_a-T_0)/2$. As seen from Fig. 4, the decrease in the wave velocity due to increased cell size is bound up with the extending of the reaction zone.

The spectral functions for stable and unstable combustion regimes are shown in Fig. 5. The sample width is constant and equals $128l_r$. At different M_h values, the number of cells across the sample is different. For a stable combustion regime ($K_2=1.41$) the front distortion is caused by permanent generation of disturbances in the stochastic model. Therefore, the transverse long-wavelength distortions of the combustion front are noticeable only for rather large cell size. Under the conditions of the thermal instability of the combustion front ($K_2=0.82$), the parameters of long-wavelength disturbances are determined mainly by the thermophysical and macrokinetic properties of the medium and slightly depend on cell size (see Fig. 5). The origination of long-living hot foci moving along the combustion front is observed at all the M_h values. However, with increasing M_h the frequency of forming and decaying such foci grows, while both the lifetime and the distance covered

by these foci along the front decrease. Therefore, their behavior becomes more random. With increasing M_h, the difference in the spectrum of transverse disturbances for stable and unstable combustion conditions decreases.

In the stochastic model and in the deterministic one, the combustion wave velocity and the distribution type of $\langle\Theta\rangle(x)$, $\langle\eta\rangle(x)$ along the wave are close for the stable combustion regime and at small cell sizes. In both models, at small K_2 values two-dimensional disturbances may develop. The greatest difference in the properties of the models arises when the values of the β and γ parameters are in the transition region from stable to unstable combustion conditions. In the stochastic model, the cell size affects the system behavior, extending the combustion zone under the stable combustion mode and increasing the frequency of hot focus generation and disintegration under the unstable regime. These effects reveal themselves only at sufficiently large cell sizes.

D. Evolution of disturbances under unstable conditions

To study the regularities of the disturbance evolution both in the stochastic and deterministic models, the following computation experiment has been carried out un-

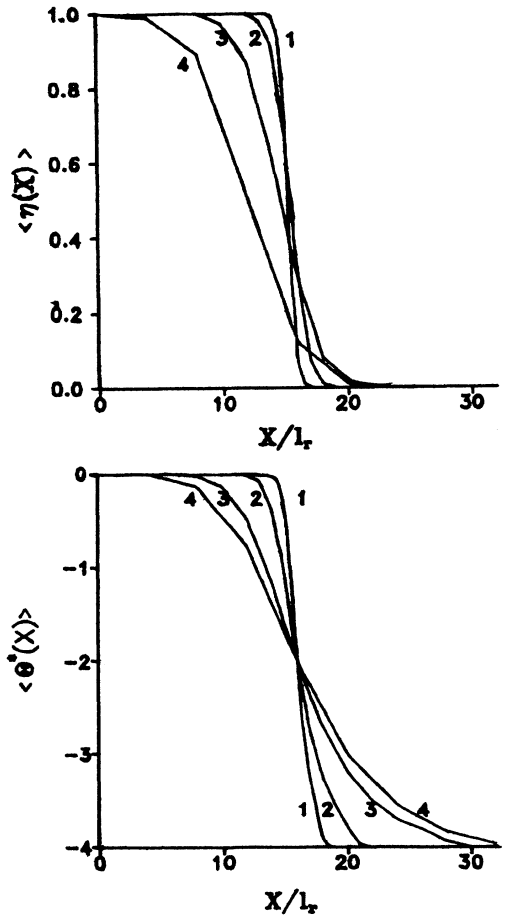

FIG. 4. Combustion wave structure for $\beta=0.16$ and $\gamma=0.25$: (a) averaged dimensionless temperature $\langle\Theta^*\rangle$, and (b) degree of conversion $\langle\eta\rangle$ (curve 1, $M_h=0.5$; curve 2, $M_h=1$; curve 3, $M_h=2$; curve 4, $M_h=4$).

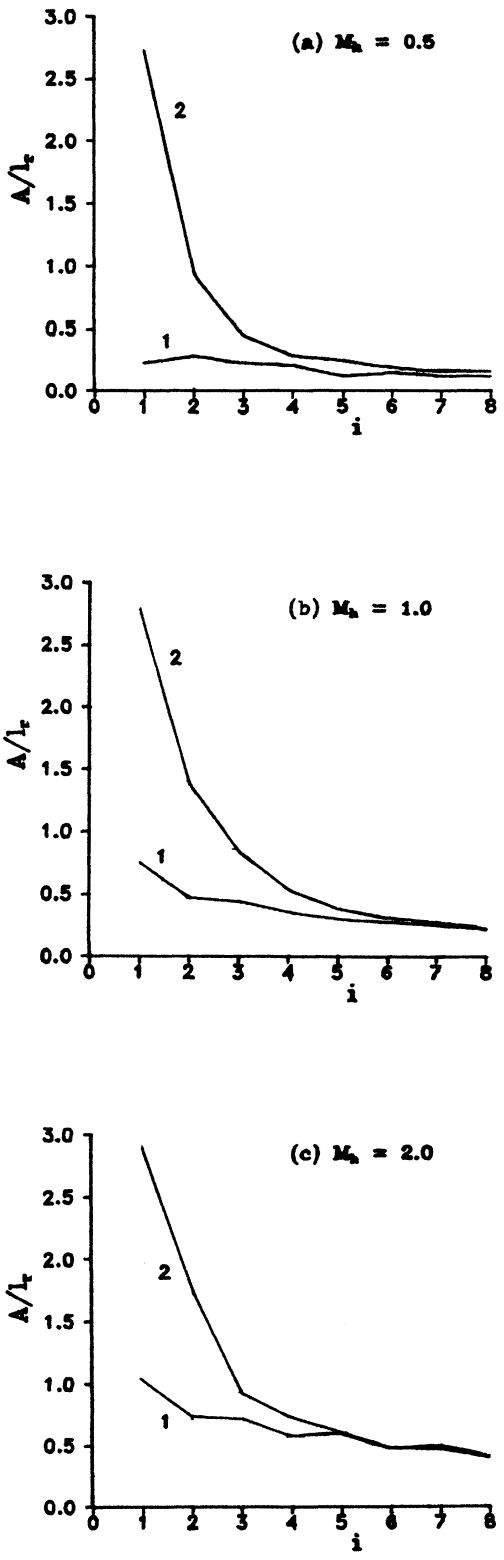

FIG. 5. Amplitudes of the low-frequency harmonics of Fourier spectrum of the $N(y)$ function at different values of the parameter M_h under stable (curve 1, $\beta=0.16$, $\gamma=0.25$, $K_2=1.41$) and unstable (curve 2, $\beta=0.12$, $\gamma=0.13$, $K_2=0.82$) combustion conditions (a) $M_h=0.5$, (b) $M_h=1$, (c) $M_h=2$, (d) $M_h=4$.

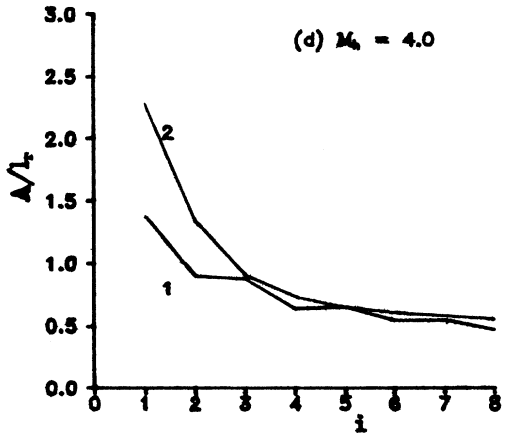

FIG. 5. (*Continued*).

der unstable conditions, $K_2 < 1$, for a relatively small cell size, $M_h \leq 1$. The temperature and degree of transformation fields calculated by the stochastic model have been used as initial data for the deterministic one. This permits us to trace the subsequent evolution of disturbances when their generation no loner operates. Also, it gives us an opportunity to compare the patterns of combustion waves obtained within the two models at a sufficiently long time, i.e., to reveal the effect of perturbations generated within the stochastic model upon the stability of a wave-propagation regime under various values of the β and γ parameters.

It is known that in the deterministic model the onset of a spin combustion mode is observed at $K_2 < 1$ only under a sufficiently great perturbation introduced "manually" into the temperature field [6]. For the values of $\beta = 0.12$ and $\gamma = 0.12$ ($K_2 = 0.75$) the stochastic model has demonstrated the spontaneous origination of the spin regime. During computer simulation, the rotating hot focus has been observed to disintegrate after several revolutions and then appear again at a random moment of time. This is connected with the self-generation of a disturbance great enough to destroy or to initiate the spin combustion regime.

After the temperature and degree of transformation fields corresponding to the well-developed spin regime have been introduced into the deterministic model, the latter demonstrates the further revolutions of the hot focus. The spin velocity and hot-spot temperature (about $1.5T_a$) are the same in both the models.

If the spin combustion regime has not already formed within the stochastic model, i.e., the temperature disturbance is still insufficiently great (e.g., under a relatively short time after the SHS initiation, or after spin disintegration), then this temperature field introduction into the deterministic model will never result in the spin-mode origination. In this case, the system demonstrates different kinds of behavior depending on the values of the parameters β and γ as well as the disturbance magnitude, for example, combustion decaying.

Therefore, the deterministic model only gives a proper picture of a well-developed regime of the spin combustion, while the stochastic one is able to demonstrate a transition to such a mode from initial undisturbed conditions due to continuous generation of perturbations.

For the K_2 value in the transient region from a self-oscillating mode with a planar front to a spin regime ($\beta = 0.12$, $\gamma = 0.14$, $K_2 = 0.88$), the two models demonstrate a rather different behavior. In the stochastic model, a hot focus (or several foci) originates sporadically, moves along the wave front with oscillating velocity, and vanishes, this process being repeated at random time intervals. The hot-spot lifetime is rather short, and the length covered by it is less than one revolution. Such a behavior is consistent with experimental observations for a number of systems [13,14].

After the insertion of the temperature field generated by the stochastic model in the deterministic one, the disturbance degenerates into a protuberance, and the latter splits into two parts moving in opposite directions along the wave front. Such a process is repeated at equal time intervals, combined with continuous-wave propagation in the longitudinal direction. In the case of an undisturbed temperature field, the deterministic model demonstrates a self-oscillating combustion regime with a planar wave front.

Therefore, in the region of planar front instability the wave behavior within the deterministic model depends not only on values of the β and γ parameters but also on the form and magnitude of the initial temperature field disturbance. In this region, every pattern of wave propagation has its own characteristic temporal scale, t_c (e.g., one revolution time in the spin mode, oscillation period in the self-oscillating mode). In the stochastic model two-dimensional perturbations are generated spontaneously; the greater the disturbance magnitude, the less its probability. If the time interval t_d between the origin of two disturbances that are sufficiently great to destroy the quasi-steady-state pattern exceeds the characteristic time of the latter ($t_d > t_c$), then the mean wave-propagation characteristics are close to those given by the deterministic model for a certain region of β and γ parameters. In the case when such disturbances are generated frequently, $t_d \leq t_c$, then the stochastic model demonstrates a chaotic change in wave-propagation regimes. In this situation, the deterministic model is not able to predict the system behavior. The results given by the stochastic model are close to experimental data [13,14].

V. CONCLUSION

The comparison of the deterministic model for the SHS phenomenon with the stochastic one shows that the former gives an adequate description of steady-state reaction propagation modes (e.g., constant-pattern wave propagation, self-oscillating regime, spin regime, etc.) and ensures the criteria for stability loss, i.e., for conversion of one mode into the other. But it does not provide the mechanism for the change of regimes nor the description of the system behavior in the transient region where the planar wave-front pattern is unstable.

Within the stochastic approach, the transformation probability introduced into the model reveals itself in continuous generation of disturbances, their pattern and

magnitude being dependent on the model parameters. This provides a mechanism for the transfer to different regimes from arbitrary initial conditions (for a certain value of the process parameters), thus providing an opportunity to trace the transition. Also, it makes possible a spontaneous transfer from one regime to the other by varying the system parameters (β and γ) due to origination, propagation, and disintegration of disturbances. The stochastic model gives us an opportunity to study the system behavior in the transient region.

The behavior similar to that observed in the SHS processes (constant-pattern wave propagation, self-oscillations, spin mode) is known in a great number of nonlinear phenomena (e.g., filtration, melting of a porous substance, solid surface ablation under laser irradiation, powder gasification, etc. [15]. We may expect that the above conclusion should also be valid for such systems.

ACKNOWLEDGMENTS

The authors are grateful to Professor G. I. Barenblatt for valuable discussion on the results of this work.

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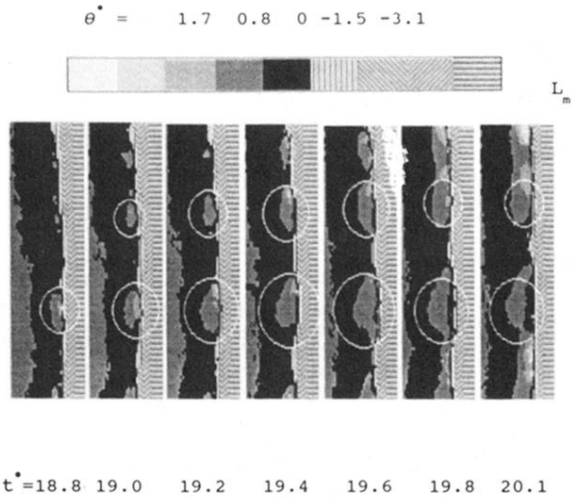

FIG. 1. Temperature charts for $\beta=0.08$ and $\gamma=0.13$; $L_m=a/u_z$ is the width of the preheated zone, $\Theta^*=(\Theta-T_a)/\Delta T$, $\Delta T=T_a^2R/E$, $t^*=t/(L_m/u_z)$.

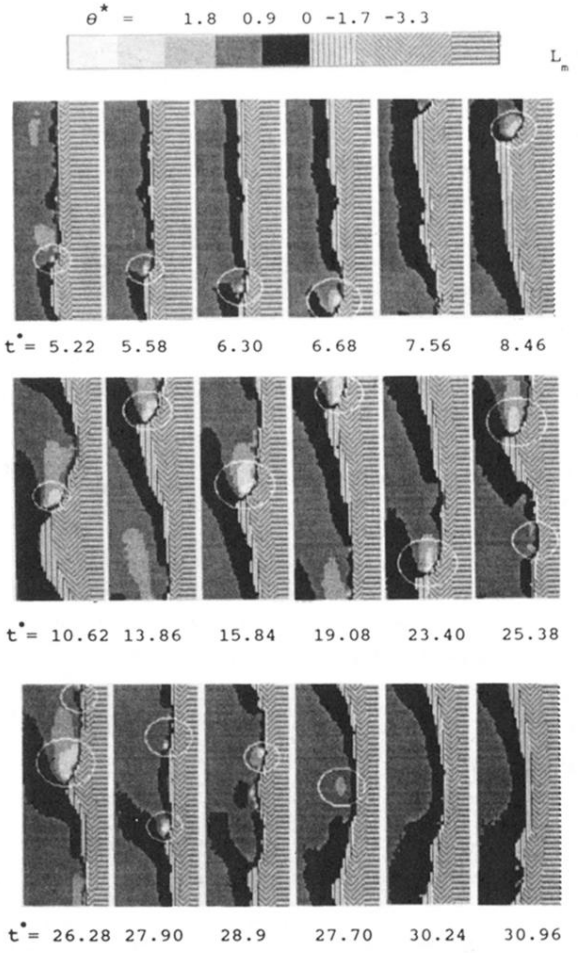

FIG. 2. Temperature charts for $\beta=0.12$, $\gamma=0.12$.