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Cell Size as the Main Geometric Parameter of a Multifront Detonation Wave

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The concept of the cell size of multifront gaseous detonation proposed about 40 years ago is used widely to estimate other detonation parameters: the critical initiation energy and critical diameters. In this paper the review of all known models for calculation of the cell size as the main detonation parameter is presented. Models were analyzed on their physical basis and basic assumptions. All models were checked also on their correctness to estimate the cell size for different mixtures. The calculated values of cell size were compared with available experimental data. On the basis of such comparison only some models are recommended for engineering calculations in practical applications. The formulas for estimating important detonation parameters with the dimension of length are proposed.

Nomenclature

A	=	preexponential factor, sec mol/cm^3
a, b	=	transverse and longitudinal cell sizes, respectively
c_1, P_1	=	sound velocity and pressure in the induction zone
D_0	=	Chapman–Jouguet detonation wave velocity (chemical equilibrium calculation)
D_2, $D_\perp$	=	velocities of shock wave and transverse wave at collision
E	=	effective activation energy, kcal/mol
E_0	=	collision energy
$[f]$, $[o]$, [in]	=	concentrations of fuel, oxidant, and inert; mol cm^{-3}
M	=	Mach number ($M = D_0/c_0$, $M_2 = D_2/c_0$, $M_\perp = D_\perp/c_0$)
P_0, c_0	=	initial pressure and sound speed
Q	=	specific chemical heat release
R, r	=	shock front radii from two neighboring microexplosions at a certain time instant ($R_0 = r_0$ at collision moment)
r	=	coordinate of shock front
r_2, t_2	=	shock wave radius and instant of transverse wave collision
r^*, t^*	=	shock wave radius and instant when the latest particle crosses the shock front, for the latest particle the ignition delay is over at instant of transverse wave collision
T	=	temperature
t	=	time
u	=	particle velocity in the laboratory frame of reference
x	=	r^*/b
y	=	$\lambda/2b$
α	=	parameter of the model of a strong point explosion
β	=	parameter of the model of a detonation wave with instantaneous chemical reaction behind the shock front
γ	=	adiabatic exponent of initial mixture
γ_e	=	equilibrium adiabatic exponent of detonation products
ε	=	$\sqrt{E_0/(4\alpha\rho_0 D_0^2 b^2)}$
λ	=	transverse wave size at collision moment
π_{ij}	=	P_i/P_j
ρ_0	=	initial mixture density
σ	=	ρ/ρ_0
$\hat{\tau}$	=	ignition delay

I. Introduction

THE classical Zel'dovich–von Neumann–Doering (ZND) concept (see, e.g., [1]) of a detonation wave (DW) as a stationary gasdynamic complex comprising an infinitely thin shock wave (SW) and one-dimensional (1-D) chemical induction and reaction zones is an idealized representation of an actual DW, which is a multifront pulsing complex (Fig. 1) of an essentially nonplanar shock wave at the lead front, transverse waves (TW) in the induction zone, triple collision points of TWs with the lead front, rarefaction waves (RFW), contact discontinuities, local zones of chemical activity, etc. (experimental investigations of multifront gaseous DWs in chronological ordering by, among others, Voitsekhovsky, Troshin, Strehlow, Mitrofanov, Edwards, Lee, Knystautas, Bull, Guirao, Benedick, Van Tiggelen, Borisov, Vasil'ev, Manzalei,

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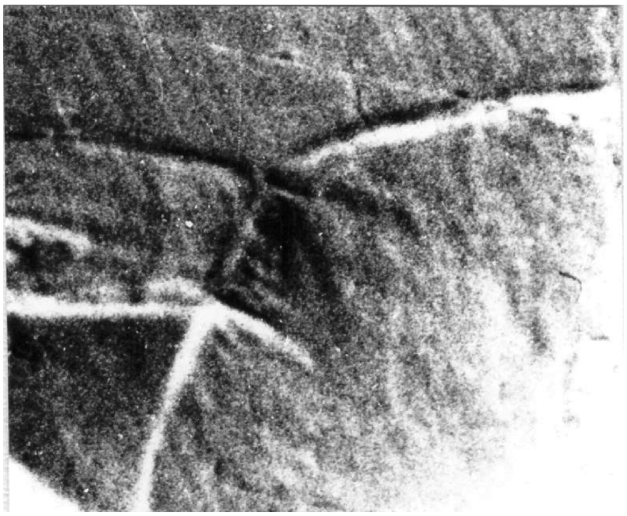

Fig. 1 Schlieren photograph of the complex structure of a gaseous DW in the vicinity of a triple point (DW propagates from the bottom to the top of the figure).

Kumar, Murray, Desbordes, Tieszen, Ciccarelli, Dorofeev have been reported elsewhere [2–20]).

The complex non-1-D and nonstationary structure of a DW front is inherent not only in gaseous systems, but also in some homogeneous liquid and solid high explosives (HE), as well as in heterogeneous explosive mixtures [21]. Such a structure is explained theoretically by instability of the coupled system of gasdynamic and kinetic equations for the majority of gaseous detonable systems (see, e.g., [22–26]). This means that even if a double-front classical ZND DW is created artificially, any small perturbation of an idealized planar reaction front will grow with time and the instability, sooner or later, will break a homogeneous and stationary structure of the DW. Such instability tends to destroy the 1-D structure of the DW and transform it to the multifront pulsing complex.

Despite the unsteady propagation of the realistic DW, its structure exhibits some periodicity: the propagation of triple points along the DW lead front in opposite directions results in a sort of self-organization and development of a cellular pattern of triple-point trajectories (Fig. 2). The individual rhombic imprint is referred to as the detonation cell, which is characterized by longitudinal b and transverse a sizes (along DW propagation and in normal direction).

The knowledge of physical aspects of combustion and detonation is important for explosion hazards evaluation. The consequences of large-scale accidental explosions of gaseous fuels depend directly on the characteristic modes of mixture burning: from low-speed (from cm/s to several m/s) laminar or turbulent flames up to high-speed (several km/s) detonation with a very wide range of dynamic and static parameters. There are numbers of gasdynamic, chemical, and physical parameters of chemically reactive systems, which are important for explosion hazard evaluation. The geometric shape of a fuel–air charge, mixture homogeneity, different obstacles, and other characteristics are among them. The comparative analysis of combustion and detonation regimes has become recently the main object of investigations in view of the development of detonation engines (with pulse-propagating or rotating waves). The higher efficiency of a pulse detonation engine (PDE) is realized only at detonation mode, and so the knowledge of conditions for stable initiation and propagation of a DW is very important. For example, for effective maneuvering of an airplane, the widest range of fuel/air equivalence ratios in an engine is required, and at any ratio the detonation mode must be stable from the point of view of not only DW initiation, but also DW propagation. Therefore, knowledge of cell sizes allows one to estimate correctly the required size of a detonation engine. Or, for a fixed size of an engine, the information about cells allows one to estimate the concentration limits for the detonation mode. Outside such a range, only the unsteady regime of combustion will be observed with a dramatic change of propulsion performance.

Cellular structure is an intrinsic feature of detonation. The cell size depends on the fuel and oxidizer types, fuel–air ratio, phase state, dilution with promoter, inhibitor (including radicals and ions, or inert gas), mean DW velocity, initial pressure, temperature, etc. The cells in different mixtures are characterized with several types of regularity as well (see, e.g., [27,28]). The regularity depends mostly on the activation energy: the higher the activation energy, the more irregular the cells. Nevertheless, a certain average size of detonation cells can be defined also for irregular cells, of course, with a wide-band distribution function. As a rule, the averaged cell size can be defined for any gaseous mixture if the experiments are performed over the wide range of conditions.

Based on the values of the cell size a, the other dynamic parameters of a multifront detonation (with the dimension of length) can be determined [12,29]. Among them are the critical diffraction diameter d^{**} (DW transition from a tube to a volume), geometric dimensions of channels relevant to limiting DW propagation, d_S, $l_{\lim}$, and $\delta^{\lim}$ (the tube diameter for a spinning DW and channel width and height for a marginal DW, respectively), critical diameters of free (unconfined) gaseous charges d^*, sizes of obstacles, and the way they are oriented in space in turbulence-enhancing devices for enhancement of deflagration to detonation transition, etc. Also, based on the known cell size a, the gas energy $E_{0\upsilon}$ in the region of TW collision, and the critical initiation energies, $E_{*\upsilon}$ can be determined for various cases of symmetry υ, as well as the diameters d_w of a high-velocity bullet (HVB) required for detonation initiation in a combustible mixture [30–33]. Knowledge of the previously mentioned parameters is useful for practical application of the detonation process in power engineering and technology, because it allows one to estimate correctly many specific features (for example, the PDE equipment sizes for a great range of fuel–air ratio, initial pressure, or initial temperature). During the last 40 years, the concept of the TWs as main elements of the quasistationary multifront DW structure and the cell size as the basic parameter of a detonable mixture were confirmed by many investigators. Moreover, it was shown that the TWs play an important role not only in multifront DW propagation, but especially in the initiation process.

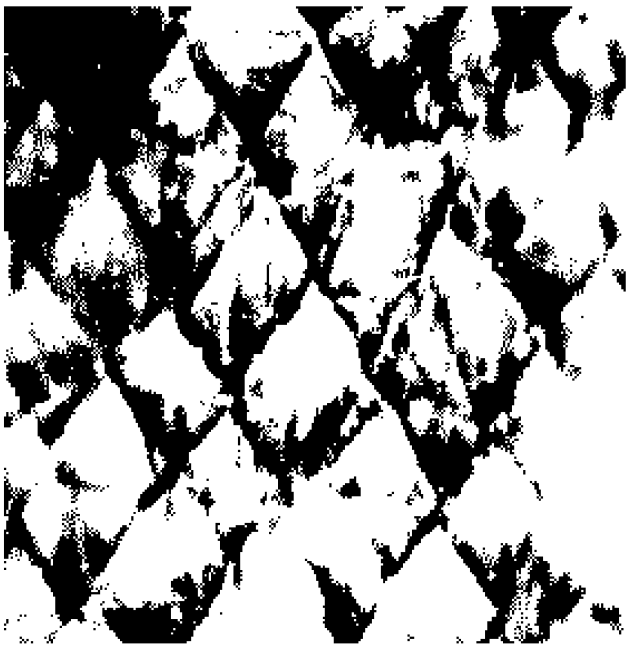

Fig. 2 Typical imprint of the cellular structure on a smoked foil. The structure is produced by the trajectories of triple points at DW and TW propagation.

II. Detonation-Cell Models

Despite much experimental evidence of deviations of realistic DW parameters from those predicted by the 1-D ZND model, there are still attempts to improve and save the idealized classical concept of a planar DW to describe some parameters of a multifront DW, in particular, the averaged parameters of the detonation process.

The review and analysis of the papers devoted to correlation of the cell size of a multifront DW with physical and chemical properties of an explosive mixture and to modeling of the cellular structures and elementary processes inside an individual cell allowed us to put forward the following classification of the available models in terms of their base postulates: 1) 1-D idealized models (based on considering a DW as a stationary double-front complex), 2) acoustic models (based on considering small perturbations of the DW front), 3) highly tailored models (based on modeling only some characteristic parameters of the cell), 4) approximate models taking into account the multifront DW structure, and 5) two-dimensional (2-D) and three-dimensional (3-D) models (accounting for planar DW instability numerically). Next, the cell models are considered in more detail.

A. One-Dimensional Idealized Models

The structure of the idealized planar DW can be determined formally by the solution of the coupled system of equations of flow dynamics and chemical kinetics with boundary conditions at the lead shock front. In the region between the lead shock front and the Chapman–Jouguet (CJ) sonic plane, a subsonic flow zone exists (in reference to the shock front). In this zone, all parameters depend only on the distance from the lead shock front and remain constant in any plane parallel to the lead front. Thus, determination of a as a function of some characteristic scale of the idealized DW model, for example, von Neumann spike length (induction-zone length λ plus chemical reaction zone length z) seems very attractive at a first glance. But new problems immediately appear at the next step: what are the lengths of the induction zone and chemical reaction zone in realistic multifront detonations? How do the averaged (in space and time) parameters of multifront detonation correspond to the 1-D model? What is the CJ surface in the multifront DW and where is it located?

The uncertainty in the magnitudes of λ and z in the conditions of realistic multifront detonations forced the followers of this approach to limit their theoretical estimations only by the induction-zone length λ_{10}:

$$\lambda_{10} = (D_0 - u_{10})\tau_{10} \tag{1}$$

where index 10 corresponds to the mixture state behind a planar steady SW of an ideal CJ detonation propagating at velocity D_0, τ is the ignition delay behind such a wave, and u is the fluid particle velocity in the laboratory frame of reference (see, e.g., [34,35]).

The ignition delay τ_{10} can be calculated by two widely used methods. The first is by using the average kinetics of an induction phase (Arrhenius-type formulas); the second is by using detailed kinetics of transformation of initial species to the products in a great number of elementary reactions. In both cases, the knowledge of kinetic constants of a combustible mixture is required in the range of parameters typical for detonation (that is not always fulfilled; see, e. g., [36–39]).

Detailed kinetic models and the calculations of induction zones for various explosive mixtures were reported in many papers: the number of elementary reactions taken into account can exceed several hundred (see, e.g., [34,35]). A comparison of calculated $(\lambda_{10})_i$ and experimental (a_i) results (for near-stoichiometric mixtures of hydrogen, acetylene, and ethylene with oxygen and air) gives the linear relation:

$$a = K\lambda_{10} \approx 29\lambda_{10} \tag{2}$$

but the values of the K factor differ for various fuels and equivalence ratios (see, e.g., [20,30]). The estimation of K is possible (for example, based on the shock compression ratio), however, the predictive capability of such estimations is questionable. Note that the linear relation between a and λ_{10} is confirmed only when the induction zone exceeds considerably the recombination zone (the energy release zone). If their lengths are comparable, the corresponding relation becomes more complicated. Nevertheless, such a procedure of estimating a is still used in studies dealing with kinetic modeling of chemical reactions at various pressures and temperatures. This approach is attractive due to its simple calculation of the induction-zone length λ_{10}, however, the physical relation of λ_{10} with a is questionable.

Another estimate [16] is based on the calculated value of the minimum diameter d_{limit} for the 1-D idealized model of DW propagation in a tube (with heat and momentum losses taken into account), and the assumption that the calculated value d_{limit} equals the spinning detonation diameter d_s, for which the experimental relation between a and d_s is defined as

$$a = \pi d_s \tag{3}$$

that is, $a = \pi d_{\text{limit}}$ in [16].

B. Acoustic Models

Historically, after development of the theory of an idealized 1-D DW, most attention was paid to the spinning detonation, that is, to the description of the gasdynamic structure of the spinning wave with a complex shock configuration and to theoretical explanation of rotary motion of the spinning DW. The hypothesis about the close correlation between the driving TW in the spinning configuration and acoustic oscillations of the detonation products was most successful among all explanations offered: the base frequency of axial oscillations of the detonation products coincided with the frequency of rotation of a TW [6,40–43]. At a first glance, attempts to assign acoustic properties to TWs in the multifront DW seem also natural.

One of the first estimates, based on considering the TW as an acoustic wave and on the instability criterion of a double-front detonation model with a planar SW and flame front, was reported in [5]. According to [5], the perturbation of the flame front (radial divergent motion with a sound speed across a steady induction zone with homogeneous parameters) expands in transverse direction (overtaking the SW front in time t') up to the magnitude

$$\Delta y = 2c_{10}t' = 2c_{10}\lambda_{10}/[c_{10} - (D_0 - u_{10})] \approx \beta D_0 \tau_{10} \tag{4}$$

The value of Δy is treated as the average size (cell size) of the DW structure in [5].

A series of theoretical studies based on the hypothesis on an acoustic character of TW was carried out under supervision of Strehlow [5,6,44–46]. In [44], the first estimate of the transverse scale in the DW structure differed only insignificantly from that proposed in [5]: instead of the sound speed c_{10} for the extending perturbation, the sound speed c_{00} in reaction products was selected; the extension time t' was estimated similarly to [5] as a propagation time of a longitudinal RFW (overtaking the lead SW) in the steady induction zone. The comparison between calculated cell sizes with experimental values for a hydrogen–oxygen–inert diluent mixture has shown their great discrepancy.

For decreasing such a discrepancy, it is suggested in [44] "to increase even more" the value of t' by adding to a steady induction zone a stage of movement of a longitudinal acoustic wave in the reaction zone [from some characteristic plane (CP) to the downstream boundary of the induction zone].

The CP concept, introduced first in [45], is interesting by the fact that the acoustic rays from a high-frequency (without dispersion) sound source (irrespective of its location relative to the reaction zone) becomes asymptotically parallel to the shock front. The acoustic ray in each point of the stream is determined as the vector sum of mass velocity v and sound speed c (from a source considered) and characterizes the direction of energy transfer in the given point. The

technique of explicit calculation of the CP coordinate inside the steady reaction zone (for the model reaction) is explained in [45].

Returning to [44], it must be noted that prolongation of t' at an expense of additional longitudinal movement of the acoustic wave in the reaction zone (from the CP to the induction zone) decreased a great discrepancy between calculated and experimental values only insignificantly.

A further step in acoustic modeling of TWs was made in [46]. The authors considered the behavior of acoustic rays not only in the CP (the coordinate of which represents the saddle point for all acoustic rays), but also in the entire steady 1-D (along the x coordinate) reaction zone [with variable $v(x)$ and $c(x)$]. In the variable velocity field in the reaction zone, the trajectory of any acoustic ray (not parallel to the x axis) is curved and, if it has not reached the CP, sooner or later, it should reach either the SW front or the CJ plane. In [46], the conditions of ray reflection from these boundaries were found explicitly: there exists a range of angles at which the acoustic rays are captured by the SW. In other words, after reflection from the SW and propagation in the homogeneous flow in the induction zone, the rays become curved in the reaction zone with variable (v, c) field in such a manner, that they return back to the shock front. Under certain conditions, such contacts of the acoustic ray with the SW will become cyclic. As a matter of fact, such a behavior means that the ray forgets the primary source and behaves as if the source was displaced from the reaction zone to the contact point at the shock front. Obviously, the distance between the contact points Δy_i for individual rays is determined not only by the size of the homogeneous induction zone and both mass velocity and sound speed values in it, but also depends strongly on the $v(x)$ and $c(x)$ profiles in the reaction zone, which are, in turn, determined by the models of chemical energy release in the 1-D steady DW used in the calculations. The authors [46] notice that the frequency of the contacts is mainly affected by the zone between the SW front and the CP, and the region from the CP down to the CJ surface has virtually no influence (the authors even suggest to discard the CJ plane as a major concept in 1-D detonations).

From a great number of acoustic rays captured by the SW, it is suggested in [46] to select the ray, which collides with the SW at the minimal time interval Δt (the analogue of the Fermat theorem in optics about a minimal propagation time of a light ray between two points), as a basic ray. The distance Δy between the points of contact of the basic acoustic ray is considered in [46] to be relevant to the transverse cell size in a realistic DW. In [2], the Δy values calculated in [46] were compared with a: in the authors' opinion "the calculated values were 30 to 180 times less than experimental" and "different dependence on the initial pressure" as compared with the experimental one. In particular, it was noted that within the framework of the adopted assumptions the distance between the contact points Δy depends on the lengths of both induction and energy release zones, and their relative contribution can vary with the initial pressure.

The new insight to the acoustic theory of TWs is given in [47,48]. The essence of the model is as follows. The sound source located between the SW front and the CP generates a great number of expanding acoustic rays, among which one can distinguish two characteristic sets. One set is represented by the rays moving at the beginning from the source plane $x = x_s$ toward the SW and then reflecting from the SW front and coming back to the x_s plane. The other is represented by the rays originally directed toward the CP and then, after distortion in the reaction zone coming back to the same x_s plane. The rays, coming back from two directions, should intersect somewhere. The ambiguity is eliminated in two stages: at the beginning, at every fixed x_s, the sets of pair rays are selected having identical times of propagation along the trajectories up to intersection at the x_s plane; then the principal pair of acoustic rays is selected from all pair rays of all sets, for which the propagation time is minimal. In [47], the point of collision of the principal pair of acoustic rays is called a hot spot. By virtue of symmetry (in respect to y), the sound source generates a pair of symmetrically located hot points, which in turn can be considered as new sources: two hot points will generate three hot points, etc.

Using the results of [44,45], the following formula for the half-cycle of acoustic ray motion (from the source plane x_s to the return point x_2 and backward motion) is suggested in [47,48]:

$$t_r = 2\int_{x_s}^{x_2} \frac{cw}{c^2 - v^2} \frac{1}{\sqrt{w^2 - (c^2 - v^2)}}\,\mathrm{d}x \tag{5}$$

The next formula obtained in [47,48] is for the distance between the source and the hot point

$$y_r = 2\int_{x_1}^{x_2} \frac{c}{\sqrt{w^2 - (c^2 - v^2)}}\,\mathrm{d}x \tag{6}$$

The value t_r is first minimized and then y_r is determined. The distance Z between two hot points is considered in [48] as a transverse cell size:

$$Z = 2y_r \tag{7}$$

Calculations for a hydrogen–oxygen mixture diluted with argon have shown that the value of Z for mixtures with 0, 40, and 70% Ar exceed by a factor of 1.7, 2.0, and 2.5 the experimental values of a. Comparing the latter result (based on considering the principal acoustic rays and the x_s plane) with the data of [2] (based on considering the collision of the basic ray with the SW front) one arrives at the conclusion that the coordinate of a sound source x_s affects greatly the final result.

A simplified version of the "acoustic model of hot spots" of [47,48] is put forward in [49]. When applied to high-pressure conditions, it neglects the reaction-zone length and only the propagation of acoustic rays in the induction zone is taken into account. Such a simplified model of sound perturbation behavior, when used in the calculations of cell sizes for the stoichiometric hydrogen–oxygen mixture diluted with 0, 40, and 70% Ar, predicted the values that are by a factor of 2.5, 2.0, and 1.5 below experimental values, respectively.

The common deficiency of the acoustic concept is the neglect of realistic SW interactions in the multifront detonation. Moreover, the concept of cell in the acoustic field is uncertain. As a matter of fact, in all of the previously mentioned models, some characteristic distance is calculated for the propagation of an acoustic wave during some time interval. As the number of sound sources and their spatial distribution in the models is not stipulated (more precisely, a single source located at the $y = 0$ axis is considered), it is incorrect to speak about a periodic structure: the induction zone and chemical-reaction zone are completely covered by a sound noise. The appearance of some ordered structure in the sound chaos is a typical task of the theory of dynamic systems.

The development of the acoustic models was initiated by the problem of instability of the 1-D detonation model, which was investigated thoroughly both analytically and numerically (see, e.g., [50–55]).

C. Semi-empirical Models

Significant underestimation of the calculated Δy values in the early acoustic models as compared with the measured cell sizes forced investigators to search for new approaches. One of the first attempts of combining the classical 1-D detonation model, the acoustic model of TWs, and the realistic structure of the multifront DW is reported in [56]. In this paper, the TW is considered as an element of the classical triple shock wave Mach configuration (reflected wave), and its intensity is considered in terms of the relative pressure differential:

$$s = \pi_{\mathrm{TW}} - 1 \tag{8}$$

In [57], using the experimental data on the structure of elementary cells of a multifront DW, the values of s at various time instants of triple configuration motion along the elementary cell were calculated (a flow pattern in the vicinity of a triple point was considered as steady at each instant and, besides, chemical reactions behind the shocks were not taken into account). Based on the assumption of an

acoustic character of the TW, the author of [56] uses the results of [45] on amplification of acoustic perturbations at TW propagation along the parallel plane inside the reaction zone:

$$S_e/s_i = \exp(Kt/2) \tag{9}$$

A half-cycle of wave motion in the cell was selected as a characteristic time of wave amplitude growth:

$$t \approx b/(2D_0) \tag{10}$$

where K is some function, depending on the energy release (see [45] for more detail). As a result, for a longitudinal cell size, the following formula was obtained:

$$b \approx 4M_0 c_0\, \ell_n(1+s)/\mathrm{K} \tag{11}$$

The author of [56] notes a poor predictive capability of this formula (the discrepancy with experimental data is on the level of the order of magnitude). It seems to the present author that the hypothesis on the acoustic character of the TW is one of the main reasons for such discrepancies. Calculations of the TW intensity in a triple configuration have shown that it noticeably exceeds the acoustic level. Elementary considerations give similar results: the TW velocity is close to the sound speed in the detonation products, and, as the sound speed in the induction zone is always lower, the Mach number of the TW and its intensity will be above the acoustic level.

The next attempt to combine the classical 1-D detonation model, acoustic model of TWs, and realistic structure of a multifront DW is made in [47]. A noticeable increase in t' for better correlation between the calculated cell size Δy and experimental values is obtained within the framework of the following model:

1) A particle, after crossing the front of a planar steady wave (the coordinate of the particle entrance is considered as the cell origin), self-ignites after the induction time τ at a distance $\lambda = (D-u)\tau$ from the SW front and, thus, generates a cylindrical compression wave (CCW).

2) The CCW catches up with the lead SW (in the origin of the cell axis).

3) The points of collision of the CCW with the SW front continue propagating along the front from the cell axis (similar to a TW).

In [47], the required time t' was selected as an instant when the CCW, spreading along the SW front, moves from the axis on a distance equal to a half of a transverse cell size of a multifront DW (in an actual cell, at this instant, the impact of opposite TWs or collision of Mach triple points occurs). Then within the assumption of steady propagation, the model DW passes exactly a half of a longitudinal cell size b to this instant:

$$b = 2\lambda_{10}\{\sigma_{10} + [(c_{10}/c_0)/(M_0\sqrt{1+\sigma_{10}^2 tg^2\varphi} - 1/\sigma_{10})]^{-1}\} \tag{12}$$

where s is the shock compression ratio and M_0 is the Mach number of the idealized DW. The calculated cell size (with the help of this model) for the $2H_2 + O2 + 7Ar$ mixture appeared to be 3 to 6 times less than the experimental value.

One of the first attempts of theoretical analysis of nonstationary propagation of a DW in an individual elementary cell was made in [58]. It became possible due to availability of a detailed theory of strong point explosion (see, e.g., [59,60]). The basic attention in [58] was paid to determining the induction-zone width (rather than a cell size) behind a nonstationary wave. The analysis was carried out without taking into account the energy release zone, and the profiles of all gasdynamic parameters in the DW were replaced by the corresponding profiles from the model of strong point explosion in the inert gas. It was shown that the experimental dependence of wave velocity on radius for the marginal detonation ($2H2 + O2 + 3N2$ mixture with one TW in the channel 25.4×38.1 mm size) can be simulated successfully by the profile of a decaying blast wave calculated in the assumption on the constant value of a decaying parameter $\alpha = d(\ell_n M^{-2})/d(\ell_n r)$, typical for inert media. Here, M is the Mach number of the SW and r is its radius. Successful correlation was obtained at $\alpha = 1.5$, which corresponds to intermediate (between planar and cylindrical) symmetry of a blast wave. The authors of [58] particularly noticed that at a Mach number of SW, close to the detonation value for a steady CJ DW, the calculations reveal a sharp increase of the induction time behind a nonstationary decaying wave as compared with the value, calculated for a steady SW (at identical velocities).

An attempt to represent the lead SW in the cell as the blast wave in an inert gas was considered also in [56]. The author obtained "the coincidence of the velocity profiles" only provided that the equivalent explosion was located rather far from the region of actual collision of triple configurations. Such an artificial location of the equivalent source led the author to make a conclusion on the necessity of taking into account the energy release in the wave in the course of its propagation along the cell.

Using the empirical law of velocity $D(r)$ decay along the cell

$$D(t) = 1.3D_0 \exp(-0.55t/t_0) \tag{13}$$

and the chemical kinetic equation for the induction period as

$$\mathrm{d}\,c/\,\mathrm{d}t = k\rho^l T^m \exp(-E/RT) \tag{14}$$

with the condition

$$\int_0^1 \mathrm{d}c = \int_{t_*}^{t_*+\tau} k\rho^l T^m \exp(-E/RT)\cdot\,\mathrm{d}t \tag{15}$$

the approximate formula for the ignition delay τ^* of the mixture at an instant of visible separation of the flame front from the SW was obtained in [61]:

$$\tau_* \approx t_0/4 = b/(4D_0) \tag{16}$$

Assuming some separation condition, for example, in the middle of the cell (or when the wave velocity passes through the D_0 value, or when the relation $\mathrm{d}\tau/\,\mathrm{d}t = 1$ is satisfied), it is possible to formally determine the values of $\tau*$, t_0, and, thus, the cell size as:

$$b = D_0 t_0 \tag{17}$$

It is worth referring also to paper [62], in which a longitudinal cell size b was suggested to be equal to the dynamic radius of strong point explosion:

$$b = R_{0\nu} = (E_{*\nu}/P_0)^{1/\nu} \tag{18}$$

In [50], the scale of longitudinal pulsations Δr, obtained in the solution of the 1-D nonstationary problem of detonation initiation, was suggested to consider as a cell size b. A similar suggestion was used later in [63,64] for the case of a 1-D model of detonation with longitudinal pulsations, when the governing mechanism involved flashes arising due to self-ignition of the reactive mixture in the shock-compressed gas. The formal correlation of the scale of 1-D pulsations with the cell size b was achieved in [65] with the help of a formal change in the activation energy E_a by a factor of three. It was emphasized in [65] that the lower the value of $E_a RT_{10}$, the more regular the cell.

The review given previously indicates that some (most physically justified) models of a detonation cell are capable of describing only qualitatively the behavior of some parameters of a cell (in general, the dependence of the cell size on the initial pressure and dilution ratio or the decaying profile of the wave velocity along the cell). The comprehensive approach to cell description and characteristic parameters of the cell are not provided by any of the models listed previously.

D. Closed-Cell Models

Description of a 2-D cell and its characteristic parameters was first obtained in [66]. Further developments and modifications of this model were reported in [11,29,67]. The essential features of the model are as follows: simultaneous account of the several phenomena that are inherent in gaseous detonation; multifront character of a DW; natural definition of an elementary cell as a

geometric object, the boundaries of which represent the trajectories of intersection points of contiguous microconvexities of the DW front; nonsteadiness of DW propagation in the elementary cell; and the account of chemical energy release in the wave at its propagation along the cell (in the approximate statement).

The basic stages of DW propagation in the individual cell look like the following sequence of events (Fig. 3): collision of TWs; nonstationary propagation of a blast wave with instantaneous chemical reaction at its front; termination of chemical energy release; separation of the shock wave and combustion front; accumulation of compressed and heated explosive mixture in the induction zone; and, finally, the next collision of TWs arriving from the neighboring cells followed by the repetition of a new cycle. The propagation of a multifront gaseous detonation is supported by such periodically repeated TW collisions.

For mathematical modeling of the detonation cell, the analogy between the collision of TWs and a local microexplosion is used. A solution for the wave velocity D was selected to be consistent with the self-similar solution for the linear explosion (2-D flow):

$$D = \sqrt{E_1/\rho_0}/(2r) \tag{19}$$

where the energy E_1 was represented as a linear combination of the internal gas energy E_I in the region I (see Fig. 3) of TW collision and the chemical energy $E_Q(r)$ behind the wave at its propagation:

$$E_1 = a_1 E_I + a_2 E_Q(r) \tag{20}$$

For determining the coefficients a_1 and a_2, two known asymptotic solutions of the similarity theory (see, e.g., [59,60]) were used: 1) the model of strong explosion in an inert medium during the stage when the chemical energy release is neglected and 2) the model of a stationary detonation with constant velocity during the stage of instantaneous energy release at the front.

The blast wave is highly overdriven in the vicinity of region I of TW collision, and the ignition delays of mixture are so short that it allows one to consider the chemical reaction in the mixture as instantaneous at the wave front at the initial stage of its propagation up to some radius r_* (or appropriate time instant t_*), and after r_*, to consider the reaction as terminated because of very fast increase of the ignition delays in the decaying wave. The size λ of the induction zone at the instant of the regular collision of TWs (the stage after r_*) determines the size of region I:

$$\lambda = \int_{t_*}^{T_b} (D - u) \cdot \mathrm{d}t \tag{21}$$

The longitudinal $D_\parallel$ and transverse $D_\perp$ components of the velocity vector of the colliding TWs determine the pressure P_I and the energy E_I in the collision area:

$$E_I = P_I h \lambda^2/(\gamma_I - 1) \tag{22}$$

where u is the mass velocity of the mixture in the induction zone, T_b is the total time of DW propagation in an individual cell, γ_I is the isentropic exponent, h is a constant ($h = \pi/4$ for region I with a circular cross section).

The average velocity of the DW on the cell length is defined as

$$\bar{D} = \frac{1}{T_b}\left\{\int_0^{t_*} D_Q(t) \cdot \mathrm{d}t + \int_{t_*}^{T_b} D(t) \cdot \mathrm{d}t\right\} = \frac{b}{T_b} \tag{23}$$

It characterizes the level of losses for the self-sustained regime or the overdrive degree of the wave at its external support, for example, with a moving piston. Its value can be defined formally as some constant, or obtained as a result of solution of the problem, simulating various external actions. The velocity D_0 of the idealized CJ detonation is usually taken for comparison.

Based on the dependence $D(t)$, the equations of wave propagation $r(t)$ in an individual cell (up to r^* and afterward) can be derived. From a combined solution of $r_i(t)$ for neighboring cells (with taking into account the repetition of all events with a time shift of $T_b/2$), the parametric dependencies $\xi(t)$ and $\eta(t)$ of the coordinates of TWs can be determined [as cross points of two cylindrical waves with radii $R(t)$ and $r(t)$]. See Fig. 3, where on Fig. 3a the idealized schema of the detonation cell is presented with the markings: I, region of TW collision; 1–2, shock fronts; 3, flame fronts; 4, induction zone; and 5, transverse waves. On the left graph of Fig. 3b, the induction times (solid curve) for different gas particles, crossing the front of a decaying blast wave of radius r and its squareform approximation are illustrated; on the right graph are trajectories of shock wave (solid curve) and reaction front in an arbitrary detonation cell. The velocities $D_\parallel$ and $D_\perp$ are determined by differentiation of ξ(t) and η(t). The value of P_I is calculated using the classical formulas of wave reflection from an ideal rigid wall.

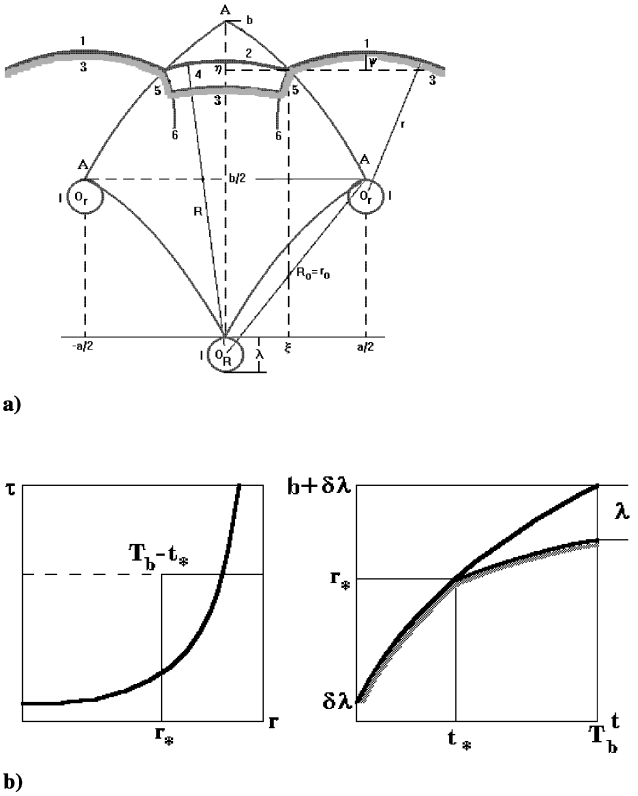

Fig. 3 Idealized schematic of the detonation cell.

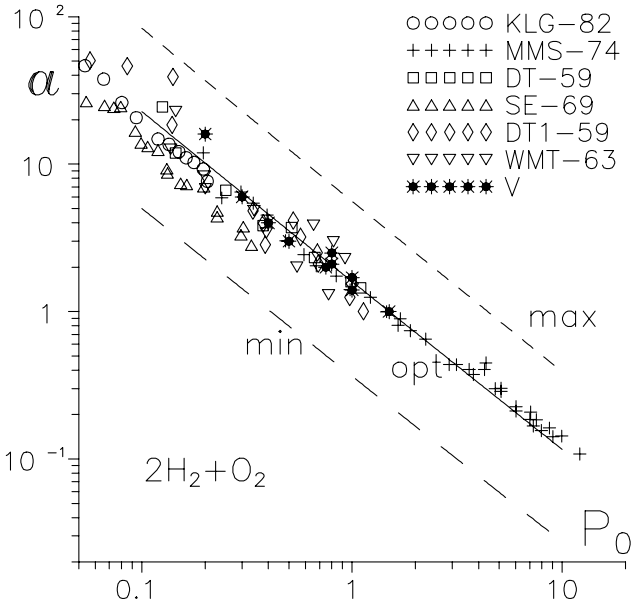

Fig. 4 Cell size a (mm) on P_0 (atm).

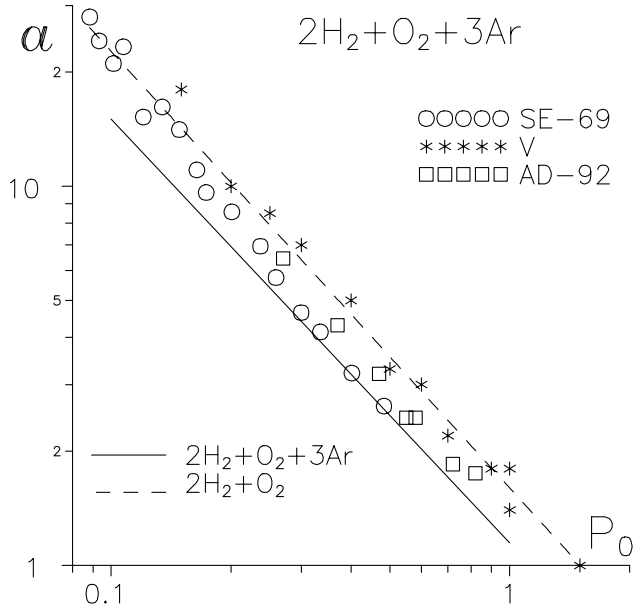

Fig. 5 Cell size a (mm) on P_0 (atm).

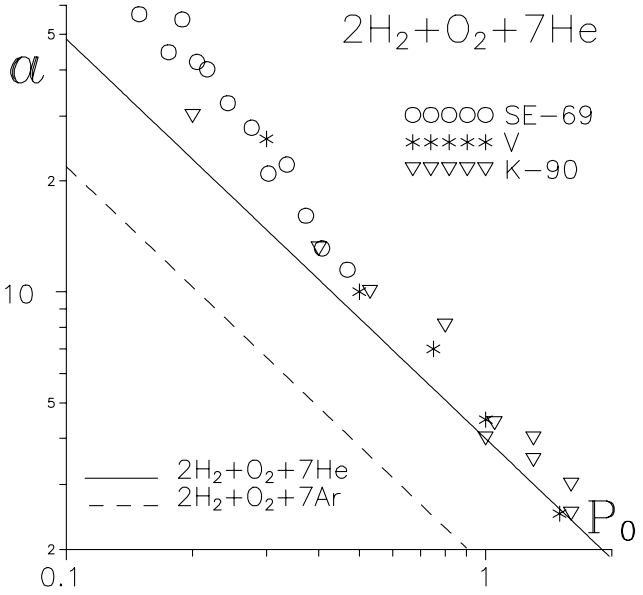

Fig. 7 Cell size a (mm) on P_0 (atm).

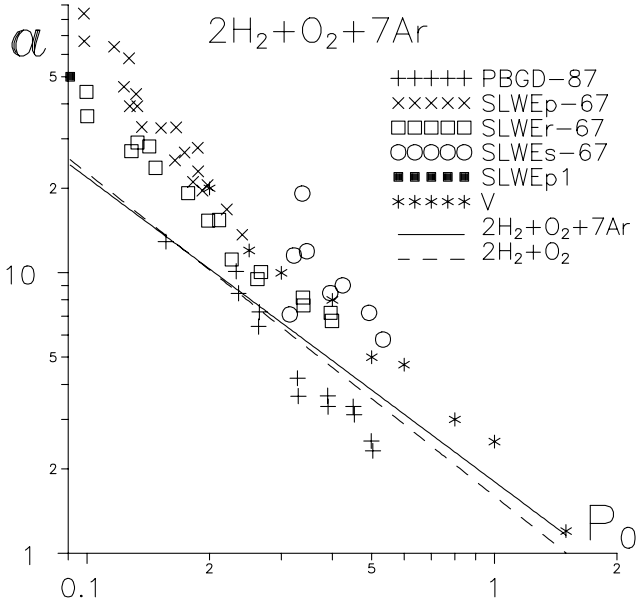

Fig. 6 Cell size a (mm) on P_0 (atm).

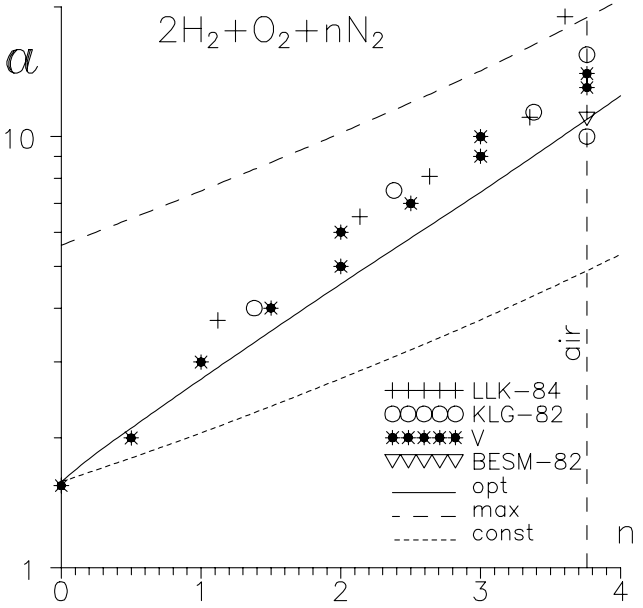

Fig. 8 Cell size a (mm), $P_0 = 1.0$ atm.

Self-ignition of a particle, crossing the wave front at an instant of termination of chemical reactions behind the front (r^* and t^*), at the instant of the next collision of TWs is the reliable mechanism of cellular structure generation. The induction time of this limiting particle is determined from the integral relationship:

$$1 = \int_{t_*}^{T_b} \frac{\mathrm{d}t}{\bar{\tau}} = \int_{r_*}^{b+\delta\lambda} \frac{\mathrm{d}r}{D \cdot \bar{\tau}} \tag{24}$$

with the integral taken along the trajectory of this particle. Here, $\tau = \tau_{\mathrm{st}}$ is the ignition delay at constant temperature and density. With the dimensionless variables $\zeta = r/b$, $x = r^*/b$, and $y = \delta\lambda/b$ a formula for the cell size can be obtained containing all physicochemical parameters of the explosive mixture:

$$b^{-1} = \int_x^{1+y} \frac{\mathrm{d}\zeta}{D(\zeta) \cdot \tau_{\mathrm{st}}(\zeta)} \tag{25}$$

Equation (25) may be used for determining τ_{st} and average kinetic constants in the induction zone as functions of the cell sizes b.

The approximate closed 2-D-model of a regular detonation cell is based on the concept of the governing role of microexplosions, arising due to collisions of TWs. It can be emphasized, especially, that only three parameters are required in this model as initial parameters for calculation of nondimensional characteristics of a detonation cell: the adiabatic indices of initial mixture and detonation products and the velocities of ideal DW (these parameters can be calculated with the help of any code for gaseous DW). The kinetic data for induction zone is required additionally for calculating the dimensional value of the detonation-cell size. The main difficulties with the application of the cell model for describing DW parameters are connected with the lack of knowledge on the kinetic data for a wide range of mixture compositions: from the lower to upper concentration limit, both for fuel–oxygen and fuel–air mixtures.

E. Numerical Modeling

Numerical 2-D and 3-D modeling of the detonation cell attracted the attention of investigators in many countries (see, e.g., [51–55,68–

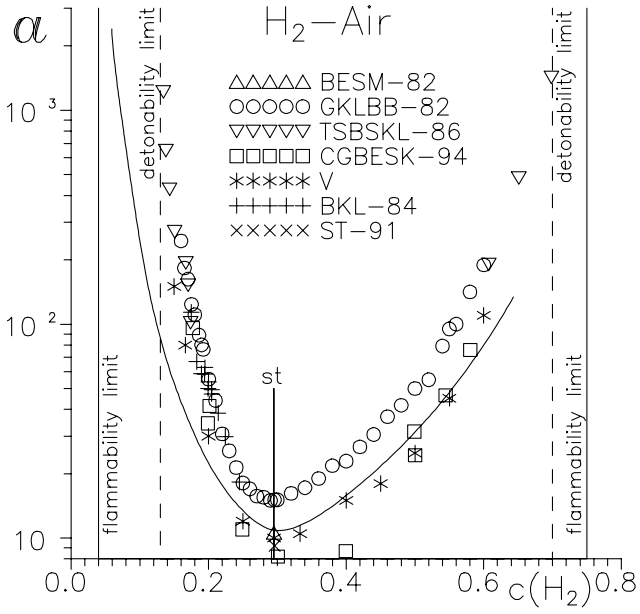

Fig. 9 Cell size a (mm), $P_0 = 1.0$ atm.

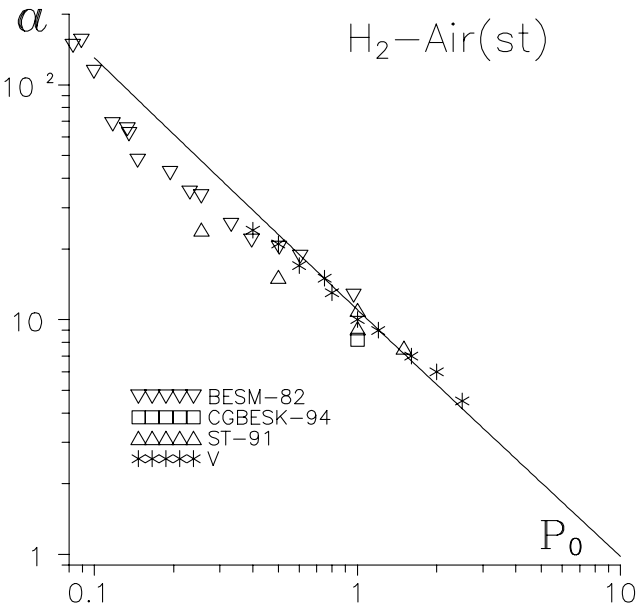

Fig. 10 Cell size a (mm) on P_0 (atm).

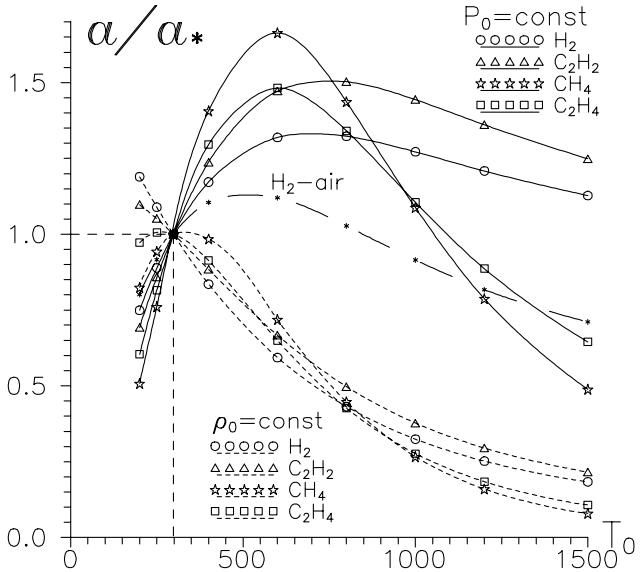

Fig. 11 T_0 (K), $P_0 = 1.0$ atm.

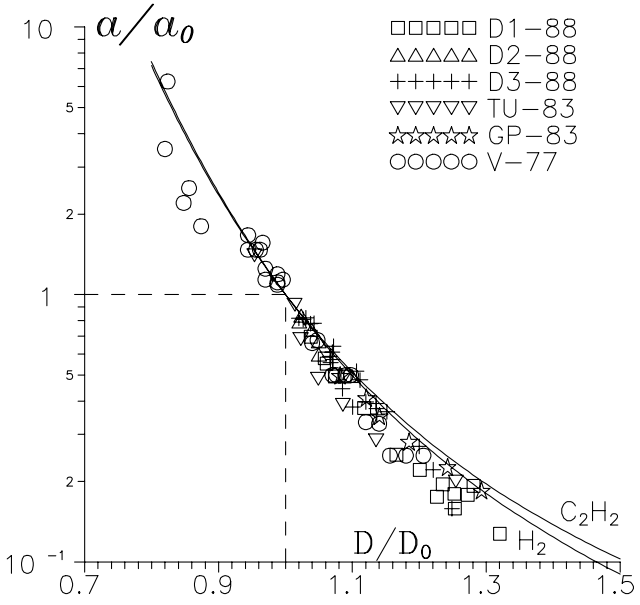

Fig. 12 Cell size on DW velocity.

85]). Traditionally, unsteady Euler or Navier–Stokes equations for the reactive flow coupled with some kinetic equations (Arrhenius type for the averaged case, or detailed kinetic mechanisms) are used for cell calculations. For Navier–Stokes equations, the k-ε model of turbulence, adapted to chemically reacting compressible media, was used as a rule. The k-ε model takes into account the development of turbulence (kinetic energy of oscillations) and its influence on the effective viscosity of the gas and other transport processes (diffusion and thermal conductivity). The critical issues are the numerical algorithm and mesh adaptation (spatial resolution of finite-difference schemes), as well as adequate kinetic models and data. The decay of velocity oscillations in the numerical models is caused by the numerical viscosity, which is often significantly higher than the actual viscosity. The Richtmyer–Meshkov [86,87] instability, turbulent combustion, pressure fluctuations, and compression waves are only a few real effects that must be included into consideration.

Through the numerical analysis of detonation processes on the basis of equations of hydrodynamics and chemical kinetics, it is possible to trace the dynamics of weak perturbation amplification, its interaction with a shock front, and formation of fractures on the front, as well as TWs, the origin of new and vanishing of old (decayed) waves, incipience of quasiperiodic regular or irregular structure, formation of unburned gas pockets, etc. The qualitative behavior of the wave and its characteristic structural elements appears similar to those observed in actual experiments. As to the quantitative agreement, it is determined by the adequacy of the chemical reactions and the kinetic coefficients used for the explosive mixture studied. For example, the steady transverse cell size in the $2H2 + O2 + 60\%Ar$ mixture calculated in [71] has virtually coincided with the experimental value ($a = 8.5$ cm at $P_0 = 65$ mm Hg), though the shape of the calculated cell differs noticeably from the measured one ($b/a = 2.3$ instead of the experimental value of 1.6).

Within the frame of the synergetic theory, a set of papers devoted to the nonlinear analysis of weak perturbation development in a nonequilibrium medium with relaxation is worth noting [88–90]. Using the evolution equation, the dynamics of nonlinearity growth was analyzed and the incipience of self-organized dissipative structures was obtained from the initial white-noise-type weak perturbations. The ordered structure obtained indicates that the transverse perturbations with a self-consistent wavelength move

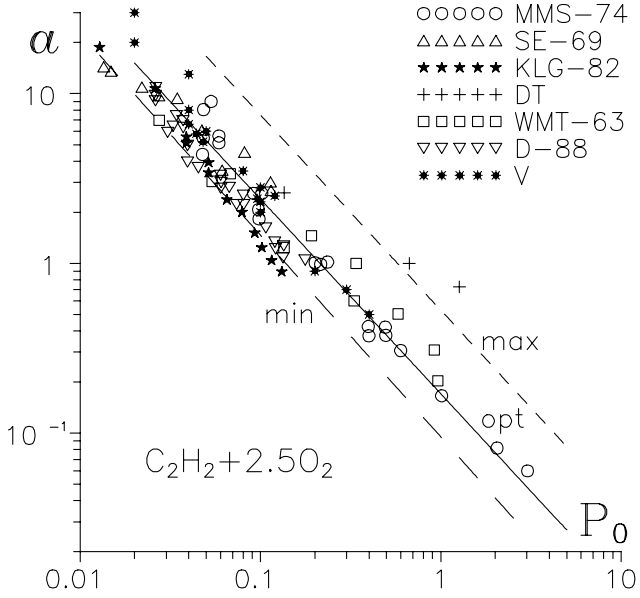

Fig. 13 Cell size a (mm) on P_0 (atm).

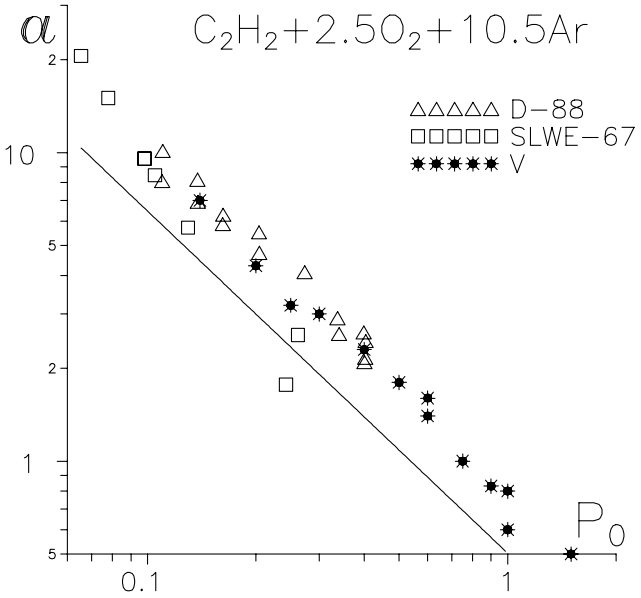

Fig. 15 Cell size a (mm) on P_0 (atm).

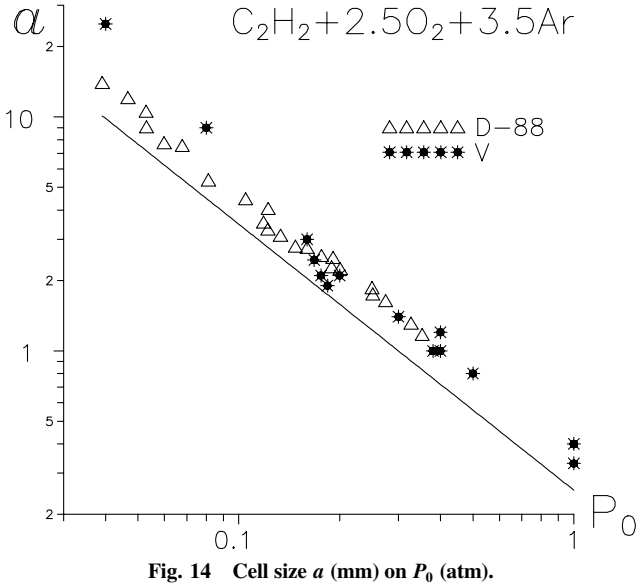

Fig. 14 Cell size a (mm) on P_0 (atm).

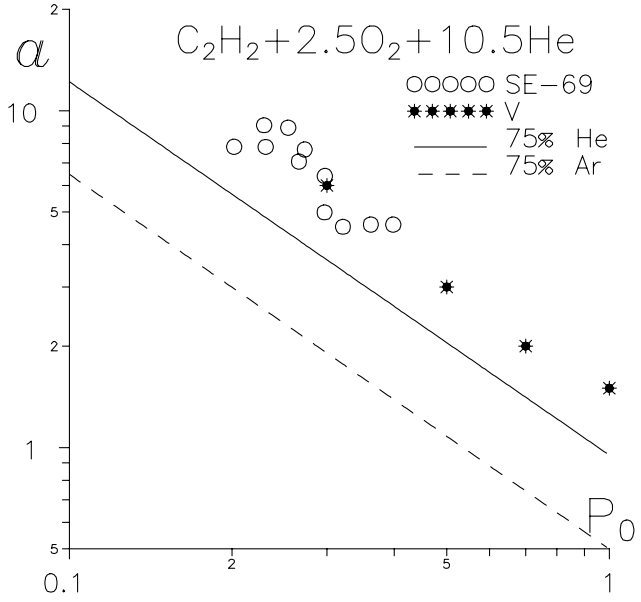

Fig. 16 Cell size a (mm) on P_0 (atm).

periodically along the DW front. Following the zero phases of the transverse perturbations, it is possible to obtain the trajectories of their motion, which represent a set of intersecting lines (due to propagation in opposite directions), forming a rhombic structure similar to a cellular structure on the imprints of a multifront detonation. Qualitatively, the result is the same, if instead of the zero phases one monitors the maxima of the perturbation amplitude or other characteristic points of the transverse perturbation. It is hardly possible to speak about the adequate correspondence of the multifront detonation cells and the idealized model [88–90], but some qualitative features (for example, modification of regularity of a calculated cellular structure at variation of the activation energy in the induction zone) appear rather interesting and promising. Note that the size of a characteristic structure calculated in [90] appeared to be "proportional to a virtual length of the reaction zone."

$$\lambda \approx 2\pi l' \tag{26}$$

which, in the authors' opinion, agrees qualitatively with the experimental data on the cell size a.

Despite high efficiency of modern computers, only a limiting number of mixtures (about ten and mainly for hydrogen as a fuel) were analyzed to determine the 2-D detonation-cell size. From the point of view of the explosion hazards or practical applications, much more mixtures must be analyzed (different fuels, oxidizers, fuel/oxygen ratios, diluents, pressure, temperature, etc.). Therefore, simple approximate models of the detonation cell play a very important role for quick estimations of the cell size in parallel with the numerical calculations. At present, the numerical calculations of the detonation cell are made with various codes that are not in the public domain, and the use of approximate models is currently the only feasible way for practical applications.

III. Relationships Between Cell Size and Other Length Scales

A. Critical Diameter of DW Diffraction

For detonation initiation by hot products, a self-sustained multifront DW propagates initially in the detonation tube with a constant cross section as a quasiplanar DW and then transitions into a volume filled with a reactive mixture. Once the DW reaches the tube exit section, it is diffracted and transformed to a spherical (or

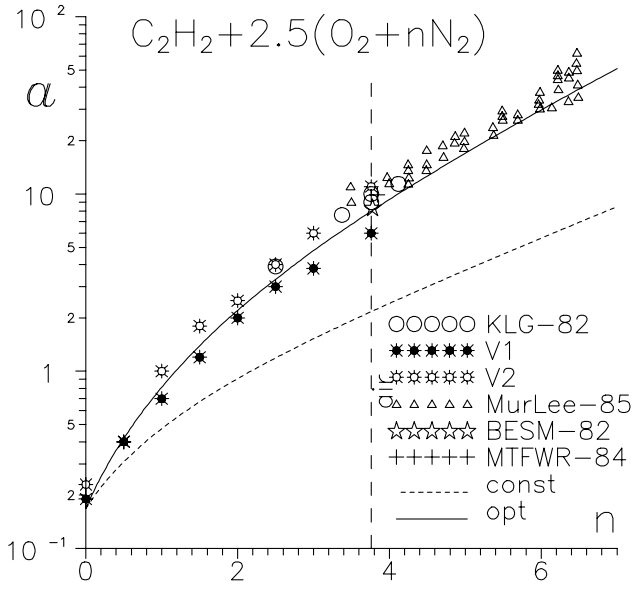

Fig. 17 Cell size a (mm), $P_0 = 1.0$ atm.

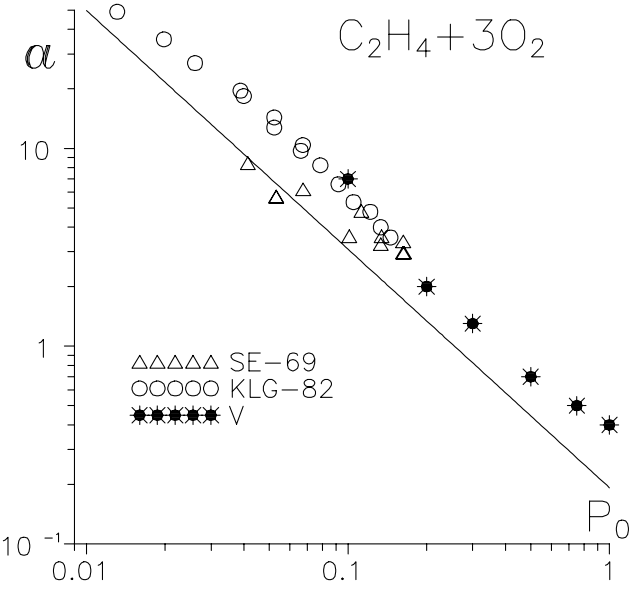

Fig. 19 Cell size a (mm) on P_0 (atm).

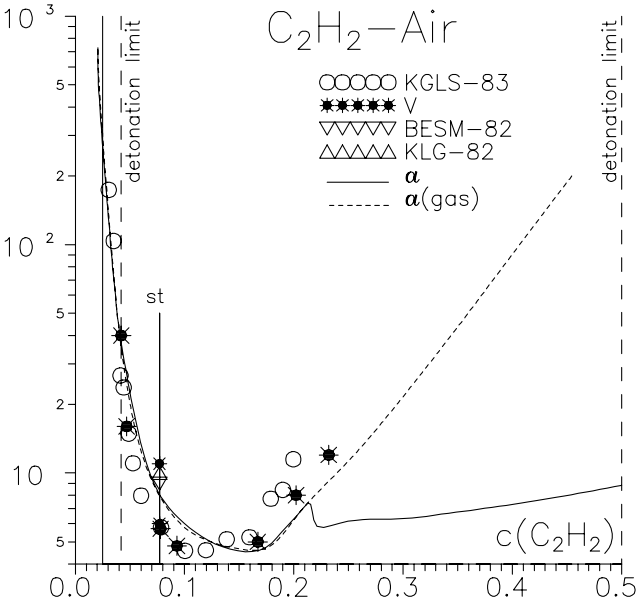

Fig. 18 Cell size a (mm), $P_0 = 1.0$ atm.

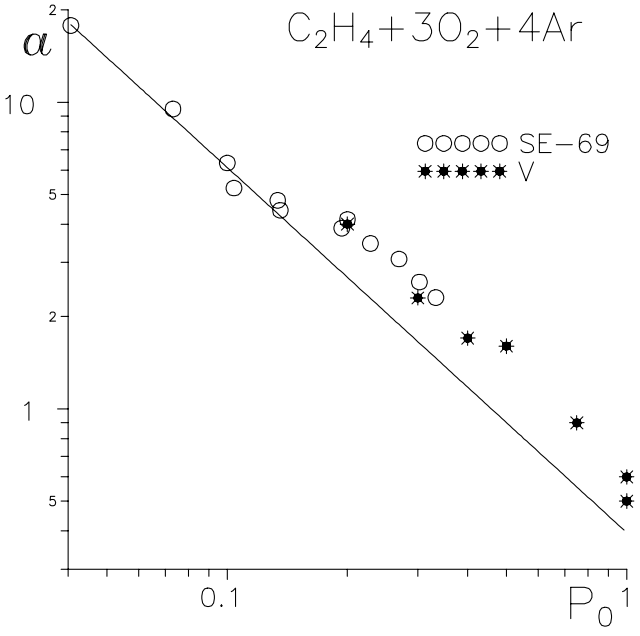

Fig. 20 Cell size a (mm) on P_0 (atm).

cylindrical) wave. The reinitiation of the detonation process at diffraction is traditionally characterized by such a critical size as the tube diameter d^{**} for the spherical case, or the channel width l^{**} for the cylindrical case. The empirical criterion of DW reinitiation at diffraction is usually formulated as

$$d^{**}/a = 13(\nu = 3) \quad \text{and} \quad l^{**}/a = 10(\nu = 2) \qquad (27)$$

(see, e.g., [91–95]). The assumption of $d^{**}/a = \text{const}$ for different mixtures is widely used for calculating the main dynamic parameter of a DW [34,35,95]. This assumption, however, may be used only for approximate estimations [96–100]. The associated errors may be considerable, in particular, for fuel–air mixtures and for marginally detonable reactive mixtures.

B. Critical Diameter of Free Charge for DW Propagation

A critical charge diameter d^* is defined as the minimum diameter of a free (without any confining wall) cylindrical charge for stationary propagation of a DW [101] at any charge length. If $d < d^*$, the detonation decays and only unsteady high-velocity deflagration is observed regardless of the initiator power. There also exists a critical thickness of a planar HE layer. The values of d^* for condensed HE and gases vary from some hundredth fractions of millimeters to tens of centimeters. At near-critical diameters, the heterogeneous charges exhibit several propagation regimes with different velocities, depending on the initiation conditions. The so-called low-velocity detonation regime is also included. The detonation propagation velocity D and other parameters depend in general on the HE structure, density, charge diameter, and properties of charge shell.

If the diameter d of a free gaseous charge exceeds the critical value d^* for the mixture under study, then the DW propagates along the charge axis in the self-sustaining regime. Such gaseous charges (jets) may appear in many accidental situations and must be taken into account in the explosion hazard evaluation. An approximate relationship based on experimental investigations [102,103] has been proposed for relevant estimates:

$$d^* \approx 2.5 d^{**} \qquad (28)$$

where d^{**} is the critical diameter of DW reinitiation at diffraction. The value of the proportionality coefficient was recommended to be taken in the range of 1–6 [104].

C. Critical Size of Experimental Equipment for Detonation Limits

Cellular structures usually form at a DW front if the tube or channel perimeter is greater than or equal to the transverse cell size. The cell size a is determined experimentally as the distance between the lines in the same direction on the smoked foil imprint on the tube walls (Fig. 2). As a rule, the cell size increases with decreasing initial pressure, so that the number of TWs in the channel decreases with decreasing pressure.

Spinning detonation with a single TW is a limiting case of stationary DW propagation in a circular tube, therefore

$$d_s \cong a/\pi \tag{29}$$

For a rectangular channel of size $l \times \delta$, the limiting regime of DW propagation is defined by the relationship

$$l_s = (k+1)a/2\pi \tag{30}$$

where $k = l/\delta$ [31].

For *galloping* detonation, a quasistationary regime in a long channel, powerful longitudinal pulsations of a DW are observed. At the first stage, a strongly overdriven DW continuously decays, and, as a result, the combustion front lags behind the leading shock front and the induction zone grows rapidly. Then, at the second stage, a flash ("explosion in the explosion") arises in the compressed unreacted gas behind the SW, which transforms to detonation in the induction zone. This secondary DW catches up with the leading SW and forms a new overdriven DW. The process repeats again [43,105]. A spatial pitch of 1-D oscillations attains hundreds of the channel diameter. The average value of the velocity oscillation is 10–30% lower than the CJ detonation velocity and remains constant. An approximate analytical model of the process was developed, which postulated that the oscillations are regular, their mean velocity equals the experimentally established value, and that the deflagration transforms to detonation immediately after the induction period in the gas compressed by the decaying SW [105]. The model provides a satisfactory description of the galloping detonation.

The so-called *low-velocity* detonation was registered experimentally below the galloping regime. It is a supersonic regime with the average propagation velocity approximately equal to one half of the CJ detonation velocity. The galloping DW is a self-oscillatory process intermediate between the low-velocity and multifront detonation regimes, outside the ranges of their existence. The low-velocity detonation can exist, for instance, in tubes with comparatively large obstacles or in narrow smooth tubes such as glass capillaries [106,107]. The formation of the wave structure of a low-velocity detonation is caused by transport processes near the flame surface rather than by accumulation of active spots in the induction zone behind the SW. The flame is located at a distance of 3–8 channel diameters from the SW and has a shape of an almost flat disk in the flow core with an adjacent oblique flame in the boundary layer. Twofold oscillations of the flame velocity have a length equal to 160 capillary diameters, which is many times the distance between the flame and SW.

Detonation in tubes with porous walls is sensitive to the presence of pores only in the near-critical regime of propagation [108]. The limiting criteria for galloping and low-velocity detonations may be presented in the following form:

$$d_g \approx 2\lambda_{10}, \qquad d_{lv} = \lambda_{10} \tag{31}$$

for galloping DW and low-velocity regime, respectively.

D. Critical Diameter of Bullet for DW Initiation

Based on the aerodynamics hypothesis known as the planar-section hypothesis (see, e.g., [109,110]), a criterion of detonation initiation by a high-velocity bullet is suggested in [30]. The work by

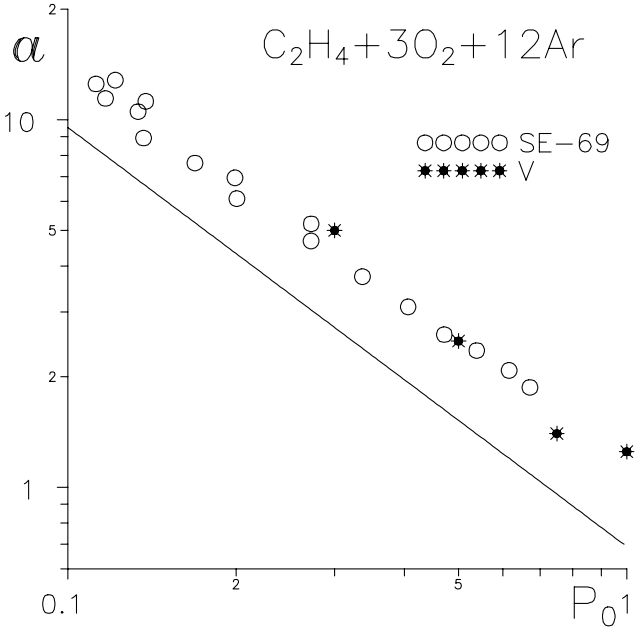

Fig. 21 Cell size a (mm) on P_0 (atm).

the aerodynamic drag on a unit length of the HVB trajectory in an explosive mixture should exceed the minimal initiation energy of a cylindrical multifront detonation:

$$c_x \cdot \rho_0 w^2 \cdot \pi d^2/8 \geq \beta E_{2^*} \equiv \beta \cdot A_2 \rho_0 D_0^2 b^2 \tag{32}$$

where c_x is the aerodynamic drag coefficient of the HVB, w is the relative velocity between the HVB and mixture, d is the HVB midsection diameter (the maximum cross section of HVB in a plane normal to the flight direction), β is the effectiveness ratio of spatial initiation, $A_2 = f(\lambda, E_{\text{act}}/Q, \epsilon, \alpha_2)$ is the coefficient from the multipoint initiation model (see, e.g., [30,32,33,96,111,112]). After some straightforward manipulations, the following expression can be obtained:

$$d/b \geq \sqrt{8A_2\beta/(\pi c_x)} \cdot D_0/w \tag{33}$$

Equation (33) gives the relationship between the HVB aerodynamic characteristics and physicochemical parameters of the explosive mixture. For a specific mixture at a fixed pressure, the values of D_0, A_2, and b are constant. Therefore, if the HVB does not change its

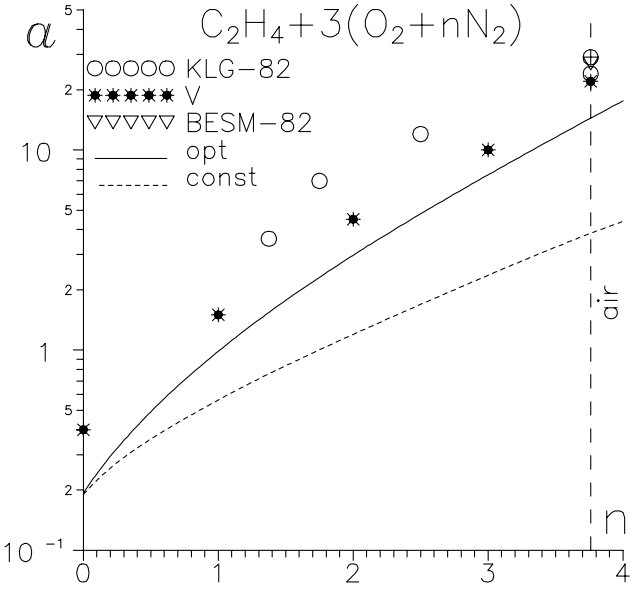

Fig. 22 Cell size a (mm), $P_0 = 1.0$ atm.

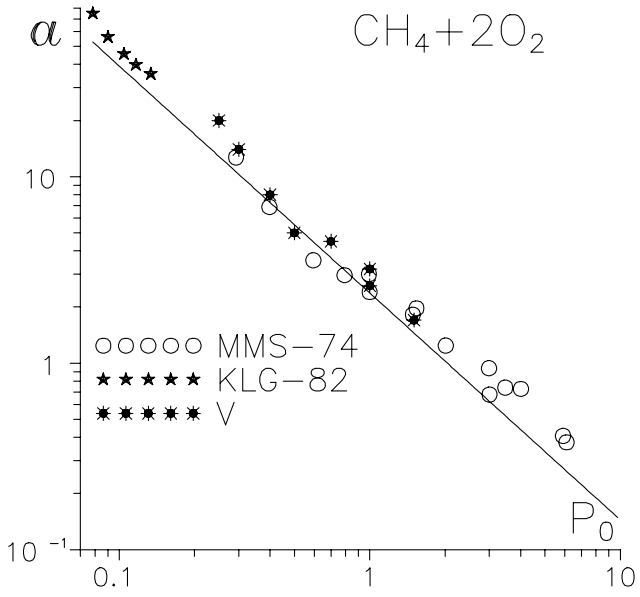

Fig. 23 Cell size a (mm) on P_0 (atm).

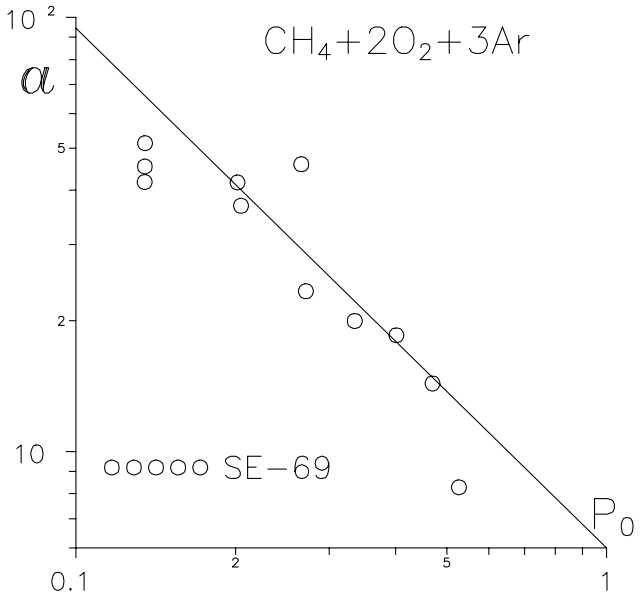

Fig. 24 Cell size a (mm) on P_0 (atm).

shape and orientation ($c_x = \text{const}$) during the flight, the criterion of detonation initiation has a simple form:

$$d \cdot w \geq \text{const} \tag{34}$$

Experiments have demonstrated that in the ranges of the HVB diameter of 5–250 mm and speed of 800-3500 m/s and for different explosive mixtures (from sensitive fuel–oxygen to less sensitive fuel–air mixtures), this criterion reliably predicts the parameters of HVB leading to detonation initiation in chemically active mixtures [30,113–115].

E. Critical Initiation Energy

The initiation problem was carefully analyzed in several studies by the author [14,30,32,33,96,99,111,112,116–125]. The critical initiation energy E^* was used as the basic parameter for comparing explosion and detonation hazards of combustible mixtures. It is defined as the minimum energy of an initiator that ensures propagation of deflagration or detonation in a given mixture. If the critical energy is small, then the mixture becomes especially dangerous.

IV. Computational Results and Comparison with Experiments

The most interesting and important parameters of multifront DWs can be calculated, for example, using the SAFETY code, whose details are published in [116–125]. The code contains the following three data libraries: 1) thermodynamic data for pure substances, including chemical formula, state, molecular weight, enthalpy, entropy, formation heat, etc., 2) kinetic data for mixtures, including coefficients in the Arrhenius formula for the induction period τ, expressed in the following form:

$$\tau = \frac{A \cdot \exp(E/RT)}{[f]^{k_f}[o]^{k_{ox}}[\text{in}]^{k_{in}}} \tag{35}$$

and 3) experimental data about main parameters of detonation and combustion regimes. In addition, several subroutines calculate 1) parameters for instantaneous explosion at constant volume, 2) constant-pressure combustion, 3) main characteristics of the CJ detonation, 4) main characteristics of the CJ deflagration, 5) parameters of shock waves (and von Neumann spike in the DW), 6) normal and inclined collisions of DWs, 7) elementary cell a and associated parameters, 8) critical initiation energies for various geometric configurations, 9) main geometric parameters of a multifront DW, and 10) kinetic constants based on the known cell size (reverse task).

Calculations are performed based on an ideal gas equation of state and the assumption of chemical equilibrium of combustion products (including ions and condensed components). For liquid fuels under standard conditions, the effect of liquid phase is taken into consideration within the framework of the ideal-gas model under the assumptions that the liquid phase is present in the form of a poorly dispersed droplet cloud in which one can ignore all physical relaxation processes (drop acceleration, fragmentation, etc.). The entropy and enthalpy of the initial propellant are fitted to the values that correspond to the liquid–gas phase transition (at a given temperature). With such a formulation, a certain portion of chemical energy is spent for the phase transition, resulting in variation of the basic combustion and detonation parameters.

Calculated results include the DW velocity, pressure, temperature, density, velocity, and sound speed in the combustion products, as well as their equilibrium composition, induction-zone parameters,

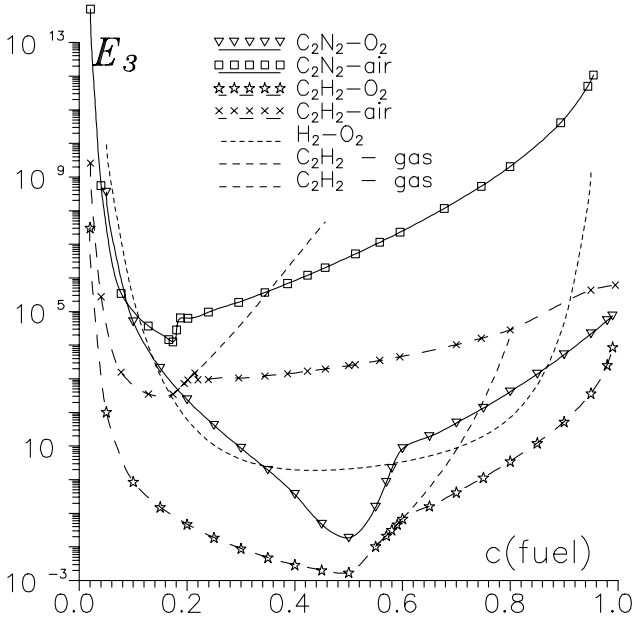

Fig. 25 E_3 (J), $P_0 = 1.0$ atm.

cell size, critical energy of DW initiation for planar, cylindrical and spherical geometries, critical parameters of DW reinitiation at diffraction, HVB parameters, geometric limits for DW propagation in channels of any cross section, etc.

A special feature of the SAFETY code is its well-established procedures and subroutines, which have been widely used for calculations of chemically active gasdynamic systems. The code determines the cell size and critical initiation energy using all known models. Results from different models are then compared among themselves and validated against experimental data. The best model can thus be recommended for engineering applications. For example, for a stoichiometric hydrogen–oxygen mixture at $P_0 = 1.0$ atm and $T_0 = 298$ K, the analysis gives the specific heat ratios of $\gamma_0 = 1.3971$, $\gamma_e = 1.2213$, and $D_0 = 2836.7$ m/s. Based on the kinetic data from [126] ($A = 5.38 \times 10^{-5}$ μs mol/cm^3, $E = 17,150$ cal/mol, $k_{ox} = 1$, $k_f = 0$, and $k_{in} = 0$), the cell size is $a = 1.59$ mm and the critical initiation energy of a spherical DW is $E_3 = 4.2$ J. It should be mentioned, especially, that the calculated cell size depends strongly on the kinetic data for the induction zone. In Fig. 4, the lower and upper dotted lines correspond to the experimental kinetic data for this mixture, where the lowest and highest values of ignition delays were observed. Note that the scatter of the kinetic data greatly exceeds the corresponding scatter of experimental cell size, in addition to cell irregularity.

It is impossible to show all calculated and experimental results within the present paper. Only selected data on the cell size are demonstrated herein. Figures 4–24 show the comparison of all available experimental data (symbols) with calculated results (lines) for some mixtures of hydrogen, acetylene (triple bond), ethylene (double bond), and methane (saturated hydrocarbon), where a and P_0 are in mm and atm, respectively, and c is the molar concentration. These figures demonstrate the dependence of the cell size on the initial pressure [see Figs. 4–7, 10, 13–16, 19–21, 23, and 24 for mixtures with different diluents (including argon and helium)]. Figs. 8, 17, and 22 show the effects of molar ratios of nitrogen at $P_0 = 1.0$ atm. The dependencies of the cell size on the initial temperature at constant pressure or density are shown in Fig. 11, where the cell size is normalized by the corresponding value at $T_0 = 298$ K. Figures 9 and 18 demonstrate the effects of molar fuel concentration at $P_0 = 1.0$ atm. The effect of the average detonation velocity, normalized by the idealized CJ velocity, on the cell size is shown in Fig. 12. Similar figures were obtained for many other fuels and oxidizers.

As an example for the PDE application, the minimum cell size for kerosene–air mixtures is measured to be 36 mm for $P_0 = 1.0$ atm, and so the diameter of an individual PDE tube must be greater than 12 mm [Eq. (29)] for this case.

Figure 25 shows the critical initiation energy E_3^* of a spherical DW, demonstrating the important role of the cell size in determining the parameters of multifront detonation. The situation with cylindrical and planar cases is qualitatively similar. The results given herein are important for comparing detonation hazards of different combustible mixtures. The data for hydrogen, acetylene, and cyanogens is presented for various fuel concentrations. Moreover, for acetylene and cyanogens, the soot formation in the products is taken into account in the calculations.

V. Conclusions

A comparative analysis of different detonation-cell models, along with validation against experimental data, has been conducted for fuels with different chemical structures and sensitivity in mixtures with oxygen or air. A wide range of governing parameters (pressure, temperature, equivalence ratio, fuel concentration, inert diluents, and overdrive extent) were considered. The results have shown that the approximate cell model [29,30] describes quite adequately the available experimental observations. The approximate model offers sufficient accuracy at simplicity of calculations, rendering itself a preferred alternative to 2-D or 3-D computer simulations for practical estimations of detonation parameters. Furthermore, the model opens new opportunities. It allows the effective activation energy E and other kinetic constants of the induction phase to be determined using the detonation-cell data (inverse task), which can be readily obtained experimentally under conditions relevant to detonation temperatures and densities.

Replacement of the induction time τ, whose value often involves uncertainties and may not be even unique, by a more precisely determined cell size a is of principal importance, because the measurement of a (in contrast to τ) has no limitations in terms of explosive mixture compositions. The cell size a can be used effectively for determining the other important parameters of a multifront detonation wave. These include the critical diffraction diameter d^{**}, limiting geometric characteristics of channels for DW propagation (i.e., the tube diameter for a spinning DW and the channel width and height for a marginal DW), critical diameters of free gaseous charges d^*, etc. Based on the known value of a and gas energy $E_{0,\upsilon}$ in the regions of TW collision, the critical initiation energies $E_{*,\upsilon}$ can be determined for various geometric configurations determined by the symmetry index υ. The critical diameter d_w of HVB for detonation initiation in a combustible mixture can be determined based on the cell size as well. Thus, the cell size can be considered as the basic detonation parameter, which can be used for determining other dynamic parameters of multifront detonations.

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