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# STUDIES IN PREMIXED COMBUSTION

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Summary for Annual Report on Activities Under the U.S. Department of Energy Grant #DEF-G02-88ER13822

# Studies in Premixed Combustion

Gregory I. Sivashinsky - Principal Investigator

November 1, 1992 - October 31, 1993

**Summary**

During the period under review, significant progress has been made in studying the intrinsic dynamics of premixed flames and the problems of flame-flow interaction. Specifically:

1. A weakly nonlinear model for Bunsen burner stabilized flames was proposed and employed for the simulation of three-dimensional polyhedral flames - one of the most graphic manifestations of thermal-diffusive instability in premixed combustion.

2. A high-precision large-scale numerical simulation of Bunsen burner tip structure is conducted. The results obtained supported the earlier conjecture that the tip opening observed in low Lewis number systems is a purely optical effect not involving either flame extinction or leakage of unburned fuel.

3. A one-dimensional model describing a reaction wave moving through a unidirectional periodic flow field is proposed and studied numerically. For long-wavelength fields the system exhibits a peculiar non-uniqueness of possible propagation regimes. The transition from one regime to another occurs in a manner of hysteresis.

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# STUDIES IN PREMIXED COMBUSTION

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During the period under review a significant progress has been made along the principal lines of the project. A brief account of the results obtained follows.

## 1. Flame Quenching by Periodic Flow-Field.

This study is motivated by the numerous experimental observations that the premixed flame propagating through a turbulent flow-field is quenched, provided the intensity of turbulence is strong enough. To elucidate the underlying mechanism of the phenomenon a simple flame-flow interaction scheme is proposed. In this model a time-independent spatially periodic flame is sustained by the underlying unidirectional periodic flow-field. The previous analytical study of this problem. based on Slowly - Varying - Flame formulation showed that for any wavelength of the underlying periodic flow, there exists a critical flow amplitude (intensity) above which the pertinent equilibrium solution ceases to exist (Berestycki & Sivashinsky, SIAM J. Appl. Math. (1991) **51**, 329-335 ). Shorter wave configurations quench at lower amplitudes than the lower ones. Being time-independent in nature. the above picture. unfortunately does not say much about what happens to the flame beyond the quenching point. Does the flame indeed go out or is the matter more involved? To answer this question a direct numerical simulation of the pertinent reaction-diffusion-advection system was undertaken.

In order to capture the essence of the phenomenon the simplest case of gasless combustion was considered. Setting the velocity profile to be a stepwise periodic function.

the system may then be associated with the reaction wave moving through a pile of alternating sliding layers of solid fuel (Figure 1). Unlike the gaseous case, such a system is quite feasible experimentally. The system also appears to be advantageous from the modeling point of view. It is well known that the main features of flame extinction in cooled ducts are successfully described within the framework of a one-dimensional formulation where heat exchange with the environment is perceived as a volumetric heat loss. This approach proves effective in the description of gasless combustion of the above layered system as well. The pertinent one-dimensional formulation is clearly much more tractable both analytically and numerically.

The numerical simulations show that at slow sliding, combustion waves in both layers move in tandem. However, if the sliding speed exceeds a certain critical value the overall picture undergoes a dramatic change. The flame is, as it were, torn apart by the flow. In the layers moving in the direction of the flame spreading combustion quenches, but survives in oppositely moving layers. Thus, the periodic flow-field indeed promotes extinction – at least partial.

At long wavelengths the transition between the two combustion regimes has the typical nature of a hysteresis. There is an upper threshold $A_+$ (Figure 2) corresponding to the passage from the complete burning to the partial extinction and the lower threshold $A_-$ where the reacting front catches up with the nonreacting one and lights it up.

"On Flame Quenching by Periodic Flow Field" by I. Brailovsky and G.I. Sivashinsky, Combustion Science and Technology (1992), submitted.

## 2. On Opening of the Bunsen Flame Tip.

It is well known that the structure of the Bunsen flame is strongly sensitive to the deficient reactant's Lewis number ($Le$). If thermal diffusivity of the premixture sufficiently exceeds the molecular diffusivity ($Le > 1$), the flame assumes a continuous luminous conical shape. However, in the opposite case, when molecular diffusivity is high enough ($Le < 1$), the flame appears "open" near its tip (e.g. Lewis & von Elbe, 1961).

The analytical description based on high activation energy asymptotics succeeded in capturing many basic features of the phenomenon (Sivashinsky, J. Chem. Phys. 1975, 62, 638). At ($Le < 1$), the temperature, reaction rate and flame speed were found to suffer a dramatic drop as the reaction zone approaches the tip. In order to maintain the flame at the tip its speed should be equal to that of the oncoming gas flow. In light of the observed tendencies it was plausible to expect that near the tip the flame simply goes out. Further analytical studies of the problem seemed to support this assertion.

For all that, the previous theories being asymptotic in nature were, strictly speaking, not valid at the extremity of the tip. To obtain a comprehensive picture it was therefore very instructive to undertake a direct numerical simulation of the phenomenon.

A detailed numerical study of the Bunsen burner flame is presented. It is shown that for the Lewis numbers exceeding unity the reaction rate and the flame speed gradually increase towards the flame tip. For small Lewis numbers the picture is quite different. The reaction rate drops near the tip (Figure 3). In spite of this the flame survives and, moreover, manages to consume all the fuel supplied to the reaction zone. There is no leakage of the fuel through the front. The flame speed varies nonmonotonously along the front from a gradual reduction to a steep increase near the tip.

The numerical simulations were conducted using an adaptive approach where the non-uniform grids have different density in different parts of the computational domain as dictated by the demands of the accuracy of the numerical method. Because the flame front shape is not known in advance the refined area continually changes its location as the computational process proceeds (Figure 4).

"On Open and Closed Tips of Bunsen Burner Flames" by G. Kozlovsky and G.I. Sivashinsky, Theoretical and Computational Fluid Dynamics (1993), submitted.

## 3. On Burner Stabilized Polyhedral Flames.

Bunsen burner polyhedral flames are one of the most graphic manifestations of cellular instability in premixed combustion. Vast experimental data have been accumulated on this both striking and elegant phenomenon. While the basic mechanisms underlying the cellular flame instability are believed to be understood reasonably well, progress in the actual description of the three-dimensional polyhedral flames remains rather limited. There are still many questions concerning the sensitivity of polyhedral instability to the composition of the mixture and to the burner rim aerodynamics. As a first step, clearly, it is important to examine the potential of the inherent front dynamics when the upstream flow-field is regarded as unidirectional and uniform, while the role of the burner rim is reduced merely to keeping the flame above the prescribed border. The present study provides numerical simulations of burner stabilized premixed flames within the framework of a weakly nonlinear model for flame interface dynamics (Figure 5). In a qualitative agreement with experimental observations, the results obtained show that the occurrence of the polyhedrals is largely controlled by the conditions at the burner rim.

"On Burner Stabilized Polyhedral Flames" by S.M. Gutman, R.L. Axelbaum, C.K. Law and G.I. Sivashinsky, Combustion Science and Technology (1992), submitted.

## 4. Tulip Flame Formation in Closed Channel.

The problem of laminar flame propagation in a closed channel is studied by means of a numerical integration of the pertinent dynamical model for reacting gas. Possible mechanisms of "tulip" flame formation are explored. It is argued that the tulip flame phenomenon is induced by the hydrodynamic flame instability in accordance with the classical Darrieus–Landau theory. The influence of initial and boundary conditions as well as various physico-chemical parameters of the system are discussed.

"Tulip Flame Formation in a Closed Channel" by G.M. Makviladze. V.I. Melikhov and G.I. Sivashinsky. Dynamics of Explosion and Reactive systems (A.L. Kuhl and J.-C. Leyer Eds. ) (1993), to appear.

## 5. Finite Dimensional Dynamical Systems Modeling Thermal Instabilities.

Using the collocation method, we derive a finite-dimensional (3-D) dynamical system to simulate a free boundary problem for the heat equation. This problem has been studied recently as a model of the thermal instabilities observed in combustion and some phase transitions and has been shown to produce complex dynamical patterns such as infinite period bifurcations, sequences of period doubling leading to chaotic oscillations, period doubling sequences followed by "Silnikov type" orbits etc. The 3-D dynamical system turns out to be a remarkably accurate qualitative approximation of the free boundary problem capable of generating all of its behavior patterns. We further simplify the system and present results of numerical solution which show a variety of dynamical scenarios depending on boundary kinetics functions inherited from the original problem. This multitude of nontrivial dynamical features as well as remarkable robustness of the system make it intersting in its own right.

**"Finite-Dimensional System Modeling Thermal Instabilities" by M. Frankel and V. Roytburd, (1993), submitted for publication.**

**"Dynamical Portrait of a Model of Thermal Instability: Cascades, Chaos, Reversed Cascades and Infinite Period Bifurcations" by M. Frankel and V. Roytburd (1993), submitted for publication.**

## 6. Work in Progress.

We are currently working on the following four projects.

The first one deals with the problem of renormalization of Markstein's length in premixed flames moving through a turbulent flow-field.

As is well known, normal speed $U_F$ of a weakly distorted laminar flame moving through a motionless gas depends on the local curvature of the flame front $R^{-1}$, according to the relation

$$U_F = U_0 \left(1 - \ell_M R^{-1}\right) \tag{1}$$

where $U_0$ is the speed of a planar laminar flame and $\ell_M$ is the characteristic (Markstein's) length controlled by the physico-chemical properties of the mixture. In the presence of the turbulent flow-field Eq. (1) undergoes modification, $R^{-1}$ being replaced by the so-called flame stretch $\mathcal{K}$, which reflects the combined effect of the local flame curvature and the strain imposed by the underlying flow. However, as we show in the present study, if the largest length-scale associated with the curved flame markedly exceeds the integral scale of the turbulent flow-field (assumed to be isotropic and homogeneous) the functional dependence expressed by Eq. (1) still holds provided $\ell_M$ is replaced by some effective Markstein's length, while $U_0$ and $U_F$ are regarded as speeds of 'planar' and 'curved' turbulent flames correspondingly.

The second project deals with the analytical and numerical investigation of Bunsen flame tip structure accounting for the radiative heat losses. This study should clarify the question whether the effect of nonadiabaticity in low Lewis number Bunsen flames may lead to the flame tip extinction or at least to the fuel leakage, which does not seem to happen under adiabatic conditions.

The third project concerns the problem of flame propagation through porous media when the effect of barodiffusion dominates over the thermal and molecular diffusivities of the system. It transpires that in this limit one may identify two modes of flame propagation. The first one is the deflagration, where the combustion wave is driven by the effective thermal diffusivity of the system while the pressure is instantaneously equalized throughout the system. In the second regime, which may be regarded as a "creeping detonation", the combustion wave is driven by the slowly advancing pressure wave which, in turn, is supported by the adiabatic compression induced by the reaction heat release.

The fourth project deals with the computer simulations of reaction waves employing random-walk technique. This approach proved to be very efficient in studying related physical systems (e.g. crystal growth) but somehow did not enjoy enough attention in modeling of reaction-diffusion systems. Specifically, we are currently involved in random-walk simulations of (i) propagability limits of autocatalytic chain reactions spreading through narrow ducts, whose walls act as the chain terminators (Figure 6 ) and (ii) cellular instability in autocatalytic reactions where mobility of the limiting species is high enough.

The self-sustained autocatalytic reaction waves have many common features with conventional premixed gas flames, but, due to the extended reaction zone, are much more convenient for numerical simulations.

We aim to complete these studies within the next six months in order to bring the present program to a successful conclusion.

## FIGURES

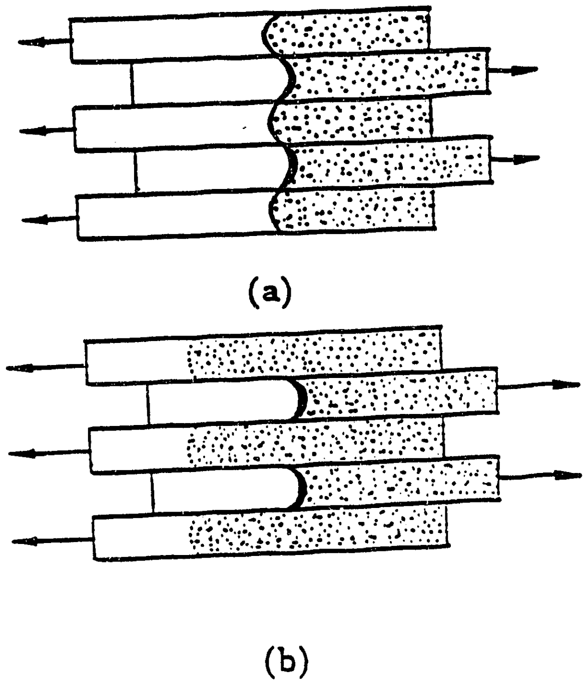


Figure 1. Diagrams illustrating gasless combustion wave moving through alternatingly sliding layers of solid fuel. Arrows indicate the direction of motion of the layers. Dotted area corresponds to the burned material. Bold line corresponds to the reaction zone.

(a) regime of complete combustion.

(b) regime of partial extinction.

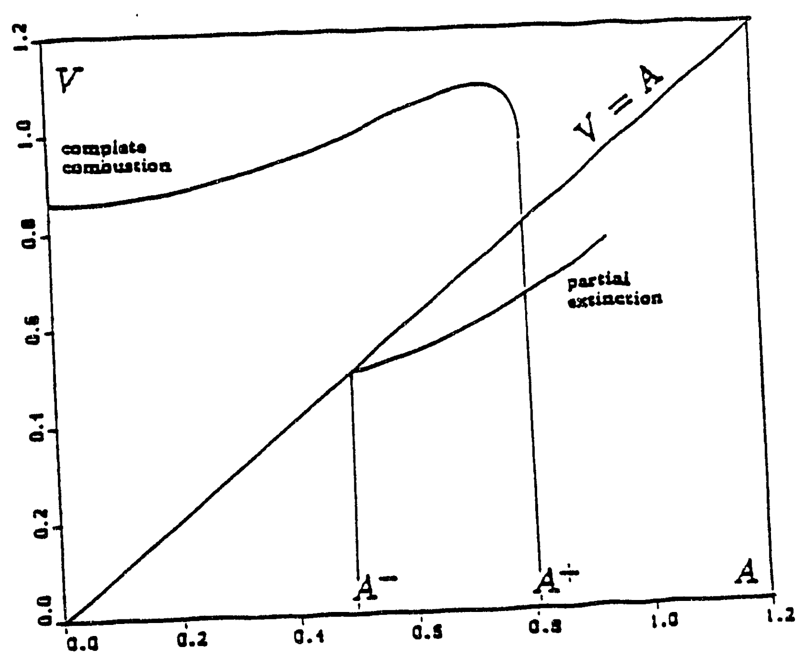


Figure 2. Speed ($V$) of the reaction wave moving through alternatingly sliding layers of solid fuel versus the intensity of the relative sliding speed ($A$).
($k = 0.3$)

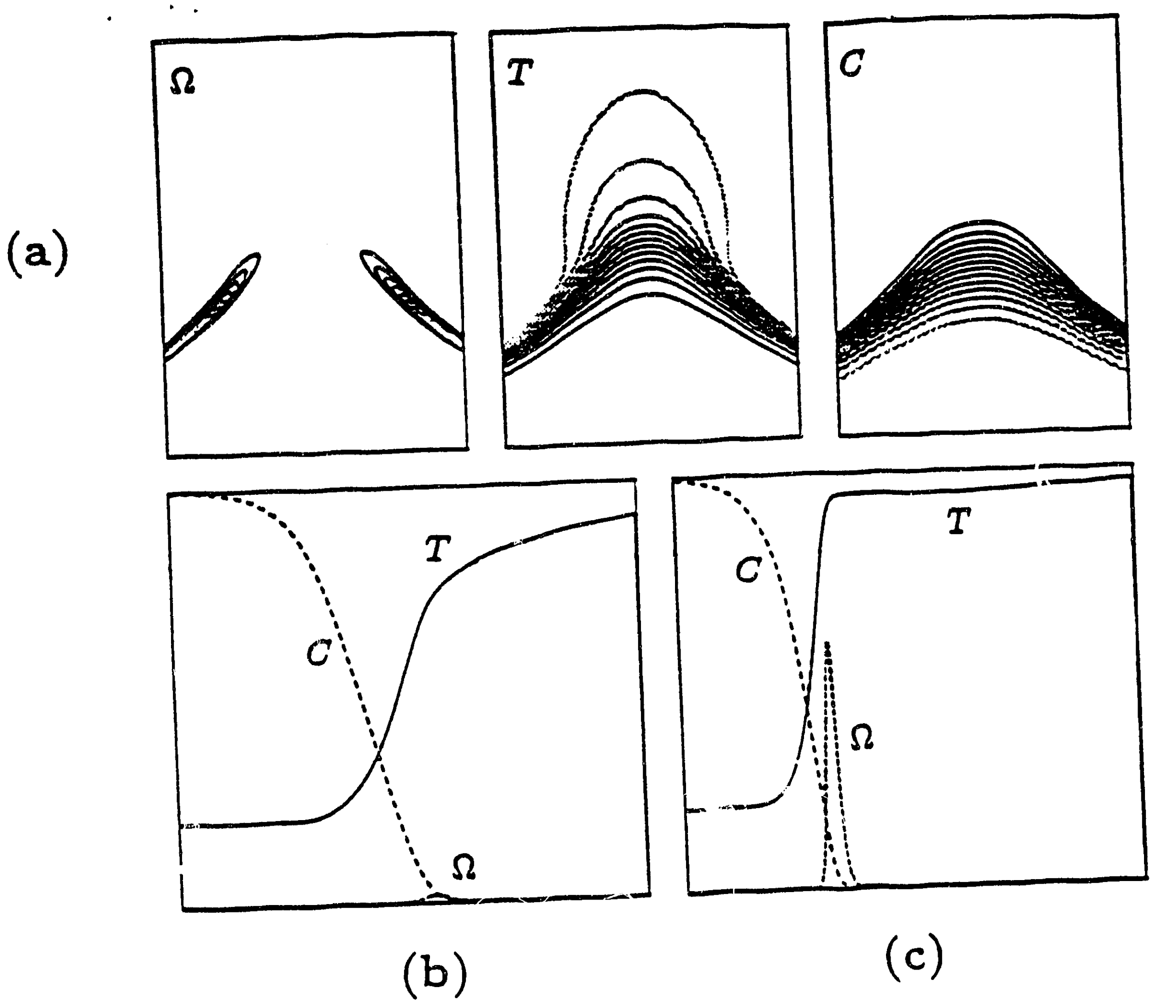


Figure 3. Numerical simulation of the circular burner Bunsen flame described by the model

$$\frac{1}{\sin\alpha}\frac{\partial T}{\partial z} = \frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} + (1-\sigma)\Omega$$

$$\frac{1}{\sin\alpha}\frac{\partial C}{\partial z} = \frac{1}{Le}\left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2}\right) - \Omega$$

$$\Omega = \frac{(1-\sigma)^2\beta^2}{2Le} C \exp\left[\beta\left(1 - \frac{1}{T}\right)\right]$$

$\alpha$ is the angle of inclination of the flame interface to the symmetry axis at large $r$. $Le, \beta$ are the Lewis and Zeldovich numbers, correspondingly. $\sigma$ is the cold/burned gas temperature ratio.

(a): Reaction rate ($\Omega$), temperature ($T$), and concentration ($C$) distribution in the $(r, z)$ plane for $\alpha = \pi/6$, $Le = 0.5$, $\beta = 10$, $\sigma = 0.2$, $0 < r < 10$.

(b)(c): Reaction rate ($\Omega$), temperature ($T$) and concentration ($C$) profiles at $r = 0$ (b) and $r = 7.5$ (c).

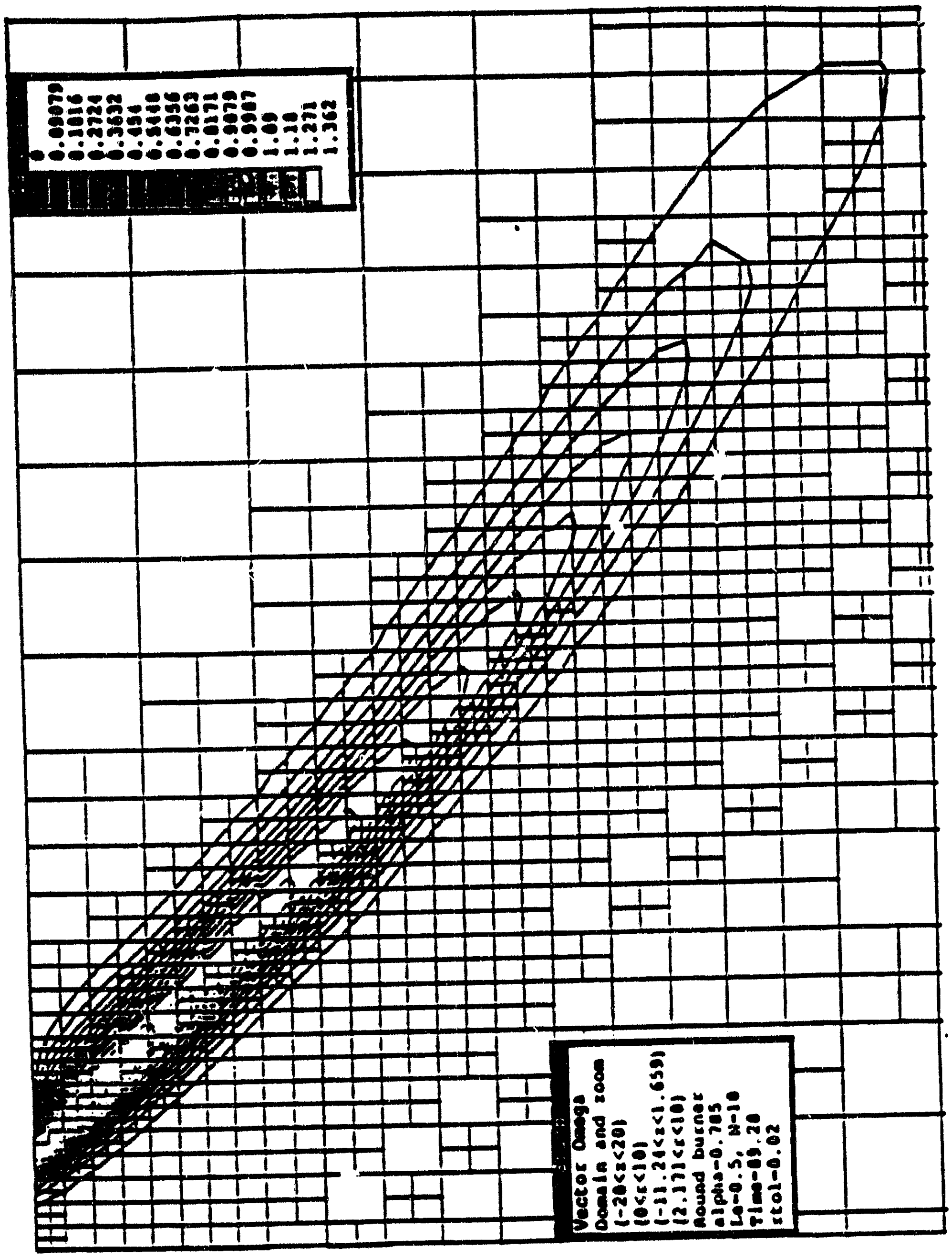


**Figure 4. Part of automatically generated grid for $\alpha = \pi/6$, $Le = 0.5$, $\beta = 10$, $\sigma = 0.2$, $0 < r < 10$, superimposed over the iso-contours of reaction rate distribution.**

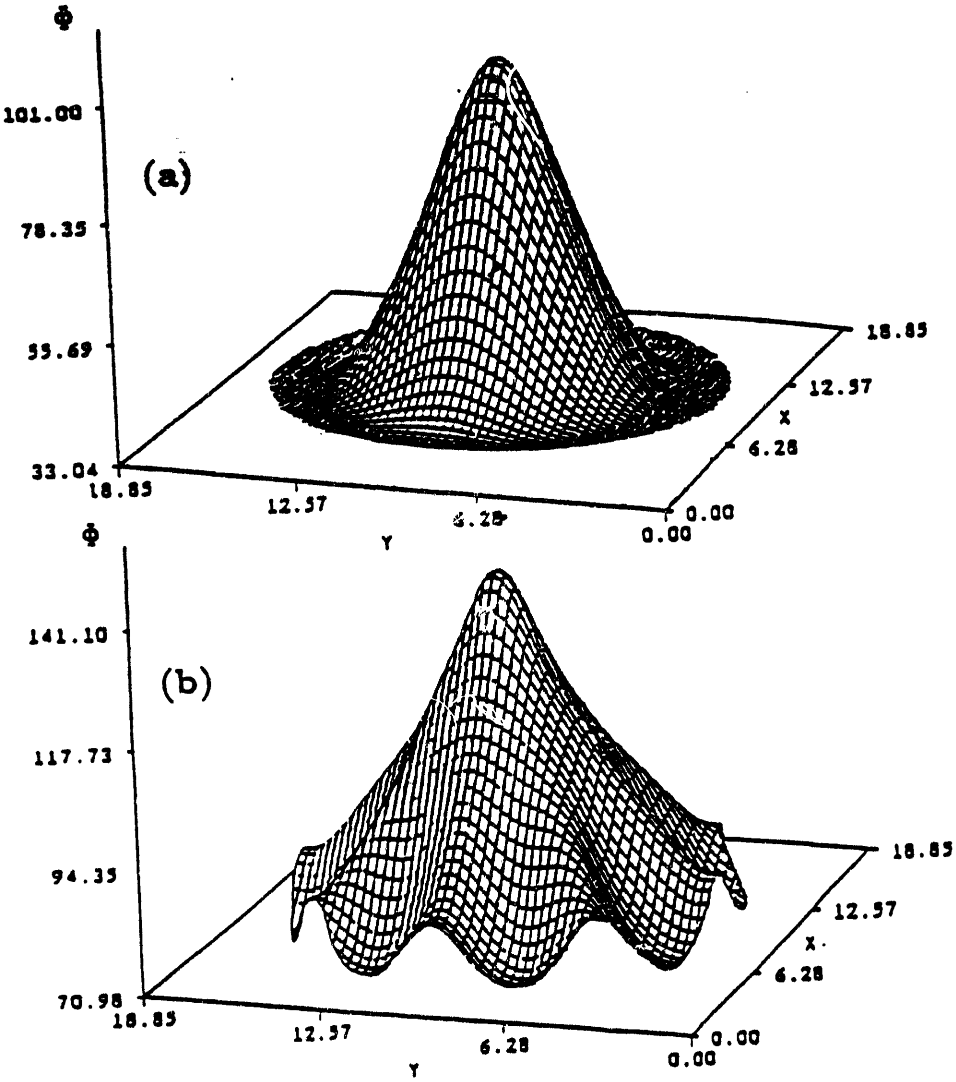


Figure 5. Numerical simulation of polyhedral Bunsen flames described by the flame interface equation

$$\Phi_t + \frac{1}{2}(\nabla\Phi)^2 + 2\nabla^2\Phi + \nabla^4\Phi + \beta K \Phi = Q \ .$$

Here $z = \Phi(x, y, t)$ is the flame interface; $Q$ is the reduced flow-rate parameter; $\beta K \Phi$ is a flame-holder term introduced to ensure the attraction of the flame to the burner rim: $\beta$ is the coefficient characterizing the intensity of the flame-holder effect. $K$ is the normalized flame-holder function, which is set to be unity in a narrow strip along the rim and zero over the rest of the burner cross section.

(a) Cellularly stable round-burner flame ($Q = 50$, $\beta = 30/\pi$, $K = 0$ at $0 < r < 2\pi$ and $K = 1$ at $2\pi < r < 2.5\pi$).

(b) Polyhedral round-burner flame ($Q = 50$, $\beta = 5/\pi$)

(a)

(b)

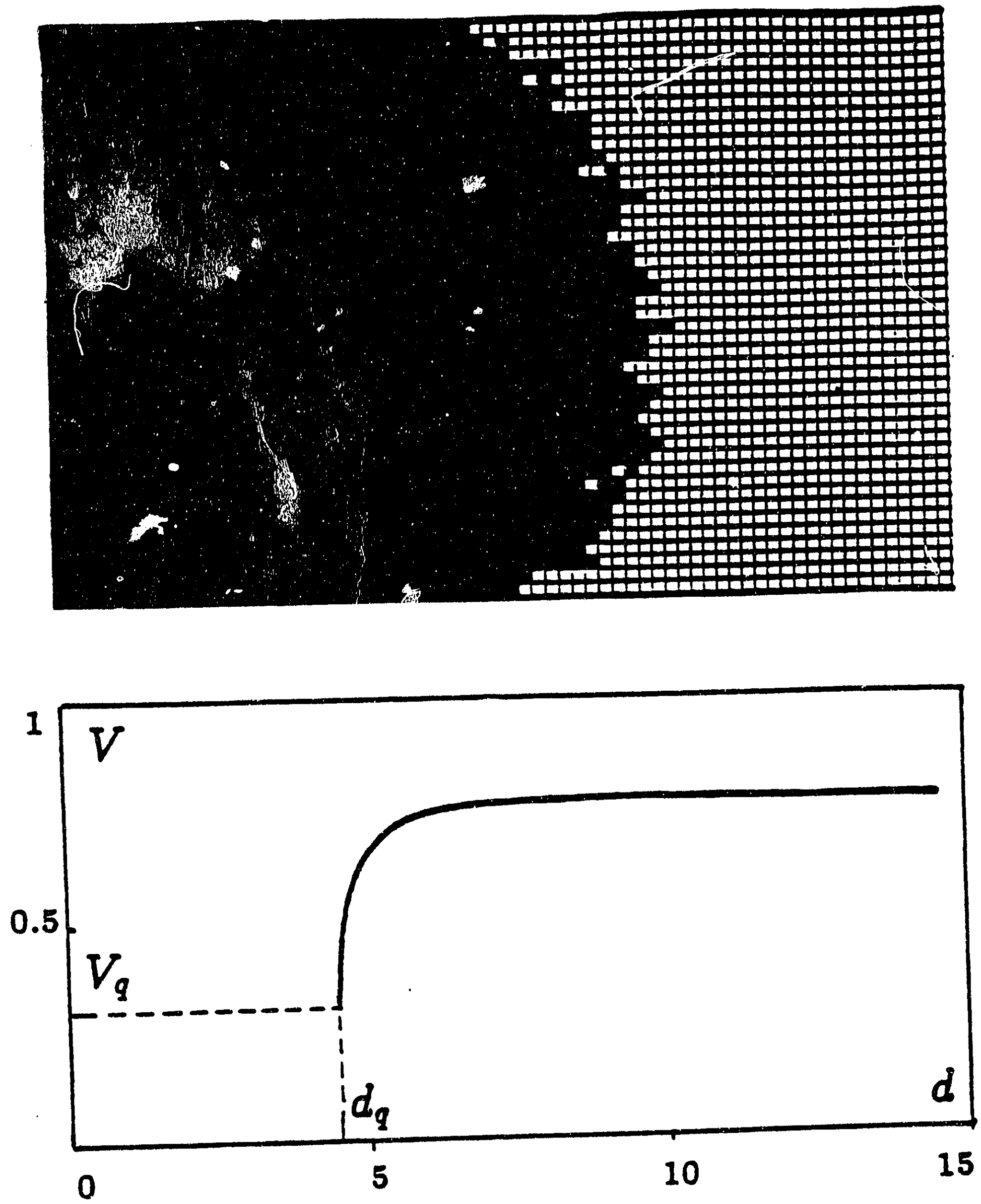


Figure 6. (a) Random-walk simulation of autocatalytic chain reaction $2A + B \rightarrow 3A$, propagating through a narrow duct. The walls of the duct act at the chain terminators. Dark and light squares correspond to the reactants $A$ and $B$ correspondingly. (b) Flame propagation speed, $V$, vs. the duct diameter, $d$.

As happens in premixed flames in sufficiently narrow ducts ($d < d_q$) the equilibrium between the production of $A$ in the reaction zone and its absorption by the walls becomes impossible and, as a result, the reaction wave quenches at some finite speed $V_q$.

# END

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