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Numerical Simulation of Ignition of Premixed Air/Fuel Mixtures by Microwave Streamer Discharge

Mikhail Bulat, Pavel Bulat, Petr Denissenko, Igor Esakov, Lev Grachev, Konstantin Volkov, Igor Volobuev

Abstract—A subcritical microwave streamer discharge is used to initiate ignition of premixed air/fuel mixture. The streamer is arising on the internal surface of the dielectric tube using a passive vibrator in a single pulse regime at atmospheric pressure and temperature. The propagation speed of the combustion front in the quartz cylindrical tube filled by the air/propane mixture is analyzed numerically. The performed studies showed that the streamer discharge, which creates a multitude of ignition points, provides practically instantaneous ignition of the mixture in the entire volume of the tube, where the streamers reach. The results of numerical simulation are compared with the experimental data. Increasing the length of streamer discharge leads to increasing the flame propagation speed.

Index Terms—streamer discharge, plasma applications, microwave technology, ignition, combustion, air/fuel mixture.

I. INTRODUCTION

THE ignition system has always posed problems in commercial applications. Many experimental, theoretical and numerical studies have been performed for the past years, and various ignition systems (e.g., electric discharge, microwave discharge, laser radiation) have been tested. Extensive efforts have been applied to circumvent several challenging engineering problems associated with the development of ignition system. These include fuel injection and mixing, repetitive detonation initiation, integration of detonation tubes with inlets and nozzles, and overall system optimization [1], [2], [3].

Plasma igniters are the most developed units for short term operation (up to several minutes) [4], [5], [6]. Plasma pilots and flame sustainers provide ignition and continuous flame control [7], [8], [9], [10], [11]. The main obstacle on the way of the full-scale gasification technologies is absence of the energy efficient plasma sources with affordable lifetime and operation costs [12].

Ignition in air/methane mixtures has been achieved using low energy seed laser pulses and an overlapping subcritical microwave pulse [13]. It was shown that an extremely weak ionization by a laser localizes the microwave energy deposition and leads to rapid heating, high temperatures, and

ignition. Multiple simultaneous localized regions of ignition were also achieved using the same microwave pulse. The developed microwave streamer discharge absorbs almost all the electromagnetic energy incident on it. The microwave streamer discharge grows into a region of the electromagnetic beam where the amplitude of the electric component of the initial field is substantially lower than the critical breakdown amplitude.

Mechanisms for the acceleration of combustion under the action of a non-equilibrium plasma are actively discussed including the generation of atomic oxygen and other chemical radicals, development of molecules of singlet delta-oxygen, chain ion-molecular reactions with intermediate radicals [14], [15]. The main active particle responsible for accelerating the burning of hydrocarbon fuels in the air is atomic oxygen. The most important source of atomic oxygen in the plasma is the dissociation of oxygen molecules in collisions with excited nitrogen molecules and a direct electron impact [14]. Then, oxygen atoms enter into rapid chemical reactions with hydrocarbons. The possibility of a non-equilibrium electric discharge was experimentally demonstrated under conditions of heat engines [16], [17].

The use of nanosecond pulsed high frequency discharges has been suggested to maintain high electron density in a discharge for relatively long periods of time (or continuously) without the large power requirements of direct-current discharges [18]. The development time of the ignition event is reduced by increasing the number of pulses beyond the minimum required to ignite the mixture. There have been a number of following studies exploring the physics of the discharge [19], [20], [21] or the interaction of flames or combustion chemistry with the discharge at low pressure [22], [23].

In [24], nanosecond pulsed high frequency discharges are applied to a mixture of methane and air to examine the effects of the plasma characteristics on ignition. The probability of ignition and ignition kernel growth rate were monitored, and the influence of inter-pulse coupling was determined. In inter-pulse coupling the heat and radicals produced in one discharge could not fully diffuse or recombine before the following discharge pulse, leading to a build-up in both temperature and radical concentration [25]. The effect of increased energy deposition via the application of additional discharge pulses led to higher ignition probability and faster kernel growth rate. The numerical model proposed in [26] is an effective model using drift-diffusion equations for charged species coupled with Poisson equation. This model has been widely used in

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simulations of streamer propagation in plane-plane and point-to-plane geometry for many purposes [27], [28].

The resolution of the Boltzmann equation using particle techniques validates the fluid approach for streamer simulations [29]. Recent developments in experimental diagnostics and simulation tools make it possible to carry out challenging thorough comparison studies on discharge dynamics and structure [30], [31]. This enables the understanding of important properties of discharges for the application of interest.

Numerical simulation of the streamer discharge, including the transition from avalanche to streamer and streamer propagation, was carried out in [32]. Some important characteristics such as distributions of electrons, ions and electric field which almost can not be obtained by theoretical or experimental method were computed. The propagation mechanism of streamers in weak external fields (below the breakdown field) was studied in [33]. The growing, decaying and stable propagation of streamers was demonstrated to be controlled not solely by the external field but also by the physical dimensions of streamers.

The presence of seed electrons in front of the propagating streamer head plays a critical role for the propagation of streamers. In some conditions these seed electrons are present in the gas, the gas can be efficiently pre-ionized by the previous discharge [34]. However, when the pre-ionization of the gas is too low, the photo-ionization mechanism has been found to be essential to accurately model the streamer propagation.

In this study, possibilities of the use of microwave radiation to initiate combustion of premixed air/fuel mixtures in the quartz cylindrical tube are investigated numerically. The streamer discharge is formed by a field with the electrical field strength which is smaller than the minimum pulse intensity leading to the air breakdown. Electromagnetic beam has sizes about tens of wavelength of microwave radiation along its propagation and about some units of a wavelength in the radial direction. The discharge is ignited in a space far away elements forming electromagnetic beam.

II. NUMERICAL ANALYSIS

Streamers are non-thermal filamentary plasmas developing in insulating mediums under the influence of strong external electric fields.

A. Assumptions and simplifications

The streamer model consists of the drift-diffusion equations for charged species to account for the development of the space-charge coupled with Poisson equation to account for the modification of the electric field due to space charge. These equations are hyperbolic (excluding Poisson equation) and complexity of their numerical solution is comparable with Euler or Navier–Stokes equations.

Viscous and thermal conductivity effects as well as turbulence effects are taken into account in simulation of phenomena in practical combustion systems. However, the ignition by a streamer discharge changes the nature of combustion. The rate of combustion and combustion efficiency increase

by times, and no soot is formed. The indirect evidence from experiments suggests that the ignition by the microwave discharge is of the non-thermal nature. The advantages of igniting the fuel mixture by streamer discharge are attributed to the ultraviolet radiation emitted by oxygen atoms subjected to the discharge. The ultraviolet radiation generation causes formation of the non-equilibrium cold plasma with avalanche increase in the number of free electrons. The presence of seed electrons in front of the propagating streamer head plays a critical role for the propagation of streamers. In some conditions, these seed electrons are present in the gas, the gas can be efficiently pre-ionized by the previous discharge [34]. However, when the pre-ionization of the gas is too low, the photo-ionization mechanism has been found to be essential to accurately model the streamer propagation. The photo-ionization is responsible for the main dynamics of streamer propagation in low external field when $E < E_c$, where E_c is the conventional breakdown field [27].

The dominant mechanism of the effect of non-equilibrium plasma on ignition and combustion is associated with the generation of active particles in the discharge plasma. Numerical simulation of discharge processes is based on the solution of the Boltzmann equation for electrons and of the balance equations for active particles. The input data are electron–molecule cross sections and rate constants for reactions with excited and charged particles. Numerical simulation of the streamer discharge, including the transition from avalanche to streamer and streamer propagation, is too challenging from the computational point of view. To accelerate the simulation of streamers, different approximations have been proposed to reduce the computation time spent on calculations. In the developed model, plasma is treated as ideal gas.

A streamer discharge in air at atmospheric pressure is a thin plasma filament with a bright streamer head which propagates rapidly (streamer velocity is of the order of 10^7 – 10^8 cm/s). Time development of streamers is much shorter than time of microwave pulse and typical time of the process. In the model, process development of plasma filaments is treated as instantaneous (from the mathematical point of view, it is based on delta-function). To simulate the energy deposition in perfect ideal gas, a step energy distribution in a finite volume depending on the size of metallic net covering internal surface of the tube is taken for an initial condition. In calculations for a perfect ideal gas, a simplified model of energy deposition is used. It ignores ionization, dissociation and chemical reactions going in a real gas at high temperatures.

One step chemical reaction between propane and oxygen is the resultant reaction of stoichiometric combustion and cannot describe the processes of ignition. To describe the ignition processes, it is necessary to use multistage mechanisms with intermediate compounds, including charged particles. The developed model includes a heat release from stoichiometric chemical reaction. Ignition of the mixture is described with energy deposition from the streamer discharge which is calculated with a simple unsteady model. In the model, source term in the energy equation is other than zero and specific energy (energy per unit mass) deposited in a given volume is found from experimental data. The applicability of the

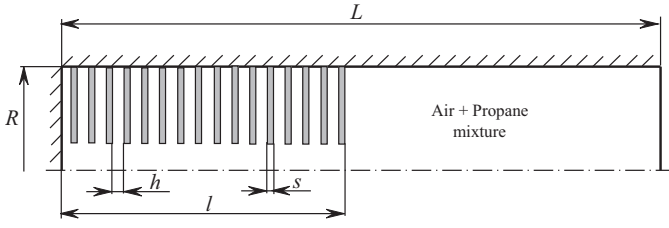


Fig. 1. Cylindrical tube filled by premixed air/propane mixture.

model is validated by comparing the simulation results with experimental data. The model has a free parameter — width of an individual plasma filament (width of energy deposition region). In calculations, it depends on the size of the metallic net (discharge initiator) covering internal surface of the quartz tube. The variation of the gas-dynamic structure and flow parameters near an energy deposition zone developing in a quiescent medium is analyzed for different energy deposition powers.

B. Geometry and domain

The numerical simulation of streamer propagation is usually based on a gas dynamic approach, in which the motion of electrons, ions and excited molecules is governed by continuity equations coupled to Poisson equation [35]. Open boundary conditions are used in all simulations [36]. The photo-ionization process is taken into account through a source term which is added to the continuity equations of electrons and ions. The simplest model for the photo-ionization term considers a uniform neutral background ionization of the gas.

To simplify streamer plasma calculations, plasma is treated as an ideal gas. Geometrical model is shown in the Figure 1. A closed circular tube is filled with a premixed air/propane mixture. The length of the tube is $L = 500$ mm, and its radius is $R = 15$ mm. The width of energy release zone is $s = 1$ mm. The distance between two zones of energy release is $h = 8$ mm, and the width of the thread is 3 mm. Numerical calculations are performed for different lengths of surface streamer discharge ($l = 8, 16, 32, 64, 128$ and 144 mm). During the microwave discharge, the convective motion of the plasma is small compared to the characteristic size of the problem (radius of tube). In the numerical simulations it is assumed that energy is released instantaneously.

C. Governing equations

The mathematical model takes into account the convective transport, the chemical reaction kinetics and the reaction mechanism of propane and air solving the Euler equations in a cylindrical geometry.

Simulation of flame propagation through a cylindrical tube involves solution of gas dynamics equations written in the axisymmetric form. Since the characteristic times of the process are rather small, there is no need to take into account viscosity and heat transfer. Therefore, the model includes conservative equations of mass, momentum, energy and species for a mixture of ideal multi-component non-viscous and non-conducting

components (Euler equations). In the Cartesian coordinates, these equations are written in the form

$$\frac{\partial y U}{\partial t} + \frac{\partial y F_x}{\partial x} + \frac{\partial y F_y}{\partial y} = H. \quad (1)$$

The vector of conservative variables, U , the flux vectors, F_x and F_y , and the source term H have the form

$$U = \begin{pmatrix} \rho \\ \rho v_x \\ \rho v_y \\ \rho e \\ \rho Y_i \end{pmatrix}, \quad F_x = \begin{pmatrix} \rho u \\ \rho v_x v_x + p \\ \rho v_x v_y \\ (\rho e + p)v_x \\ \rho Y_i v_x \end{pmatrix},$$

$$G = \begin{pmatrix} \rho v_y \\ \rho v_x v_y \\ \rho v_y v_y + p \\ (\rho e + p)v_y \\ \rho Y_i v_y \end{pmatrix}, \quad H = \begin{pmatrix} 0 \\ 0 \\ 0 \\ Q \\ W_i \end{pmatrix}.$$

Here, t is the time, x and y are the axial and radial coordinates, ρ is the density, v_x and v_y are the velocity components in the coordinate directions x and y , p is the pressure, e is the total energy per unit mass, Y_i is the mass fraction of i th component of the mixture, W_i is the rate of formation/consumption of i th component, Q is the rate of heat release by the chemical reactions. The mixture consists of N_c components.

The three-dimensional reacting flow simulation in a tube with fine mesh resolution involving the chemical reaction model requires massive computing resources. In order to reduce the massive calculation load to the computing resources, 2D analysis is used. For simplicity, a single-step irreversible chemical reaction between propane and oxygen is chosen to investigate the influence of ignition area on the subsequent propagation of a premixed flame.

The specific total energy of the gas is given by

$$e = u + \frac{1}{2} (v_x^2 + v_y^2),$$

where u is the specific internal energy of the gas. The equation of state of an ideal gas is

$$p = \rho RT \sum_{i=1}^{N_c} \frac{Y_i}{\mu_i},$$

where μ_i is the molecular weight of the i th component and R is the universal gas constant. The specific internal energy and equation of state are used to find the thermodynamic properties of the mixture, its temperature and pressure. The temperature dependence of the specific heat capacities of the components are presented in the form of a fourth-order polynomial (JANAF tables).

The chemical transformations are described with a set of N_r irreversible chemical reactions

$$\sum_{i=1}^{N_c} \nu'_{ik} A_{ik} \rightarrow \sum_{j=1}^{N_c} \nu''_{jk} B_{jk},$$

where A_{ik} are the initial reactants, B_{jk} are the gaseous products of the k th reaction, ν'_{ik} and ν''_{jk} are the stoichiometric

coefficients ($k = 1, \dots, N_r$). The rate of the k th reaction is based on the Arrhenius type equation

$$w_k = A_k T^{n_k} \left(\frac{p}{p_0} \right)^{m_k} \exp \left(-\frac{E_k}{RT} \right) \prod_{i=1}^{N_c} \left(\frac{\rho Y_i}{\mu_i} \right) \text{sgn}(\nu'_{ik}),$$

where A_k is the pre-exponential factor, E_k is the activation energy, n_k is the effective reaction order, m_k is a parameter describing the pressure dependence of the reaction rate, and p_0 is the reference pressure. The sign function is an odd mathematical function that extracts the sign of a real number. Using reaction rates, quantities Q and W_i are presented as

$$Q = \sum_{k=1}^{N_r} w_k Q_k;$$

$$Q_k = \sum_{k=1}^{N_c} (\nu'_{ik} - \nu''_{ik}) \Delta T_i^0;$$

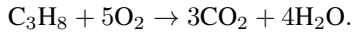
$$W_i = \sum_{k=1}^{N_r} (\nu''_{ik} - \nu'_{ik}) \mu_i w_k.$$

Here, Q_k is the heat effect of the k th reaction and ΔH_i^0 are the standard enthalpies of formation of the substances.

D. Chemical kinetics

The actual reaction of the propane oxidation is a multiple-step reversible reaction which is composed of many elementary steps. A large amount of efforts have been devoted to the development of detailed and reduced kinetic mechanisms for hydrocarbon combustion [37]. The overall reaction order and overall activation energy are important to characterize from kinetic point of view the dependency of the burning velocity on pressure and temperature of air/fuel mixtures.

The chemical reaction is assumed to be an irreversible single step reaction between oxygen and propane, and the chemical species are C_3H_8 , O_2 , N_2 , CO_2 and H_2O . The reaction rate of a single-step reaction is estimated using an Arrhenius-type of formulation [38]



To calibrate the model, the laminar flame velocity and the minimum ignition energy were calculated for various air/propane mixtures. The effective rate of the reaction was then adjusted to achieve a good fitting with published data. The reaction rate is calculated for a bimolecular reaction of propane with oxygen. The kinetic parameters are $A_1 = 7 \times 10^8 \text{ m}^3/(\text{mol s})$ and $E_1 = 191 \text{ kJ/mol}$ ($n_1 = 0$, $m_1 = -0.2264$). The heat effect of the reaction calculated from the enthalpies of formation of the reactants and products of reaction is 46.6 MJ per kg of propane.

E. Energy release

The plasma filaments propagate toward the microwave source at the order of km/s velocity, and the distance between each filament is about one-quarter of the incident microwave wavelength. The filamentary arrays are driven toward the

microwave source at the atmospheric pressure, and the distance between each filament is one-fifth of the microwave wavelength. An energy absorption rate by the plasma is estimated from the empirical expressions, and the absorbed energy is deposited as a source term of a two-dimensional Euler equations.

The streamer discharge forms a uniform grid with rectangle cells. To find amount of heat delivered by each filament, it is assumed that a uniform heat supply takes place over internal surface of the tube. Heat flux is calculated as a ratio of heat release from each elementary streamer channel by the surface area. The maximum heat release takes place in the middle point of the streamer, where induced current has a maximum value. The heat release is found from the expression

$$q(t, x, y) = q_0 f_1(t) f_2(x, y).$$

Function $f_1(t)$ takes into account energy of the pulse in time

$$f_1(t) = \begin{cases} 1, & \text{if } 0 \leq t \leq \tau, \\ 0, & \text{if } t > \tau, \end{cases}$$

where τ is the time of pulse. Function $f_2(x, y)$ defines change of the pulse shape in space. The distance between each filament is one-tenth of the wavelength of the incident microwave. This distance corresponds to that used in [39] to reproduce propagation of electromagnetic wave, ionization process of plasma, and shock wave formation in atmospheric microwave discharge.

F. Computational procedure

The unstructured computational mesh consisting of about 1 million of cells is generated. At the initial time moment, the channel is uniformly filled with stoichiometric air/propane mixture. The initial state of the mixture is set to 101,325 Pa and 300 K. The concentration of each chemical species is set so that the equivalence ratio between oxygen and propane could be 1. No-penetration boundary conditions for velocity and zero flux for scalars such as temperature and mass fraction are used at the walls. Axisymmetric boundary conditions are specified for the physical quantities on the centreline. Neumann outflow boundary conditions are applied to the outlet boundary.

The governing equations are solved numerically with the finite volume method using the principle of separation of physical processes (splitting scheme). At each time step, the effects of convective transfer and pressure work are first treated, then the effects of chemical transformations are taken into account. At the first step, the source term is zero, and Godunov-type method is used. The explicit Runge–Kutta scheme of the third order is used for time discretization, and MUSCL scheme is exploited for space discretization. The time step size is chosen from the Courant condition. At the second step, the system of differential equations describing the gas composition change and the energy release by the chemical transformations is solved.

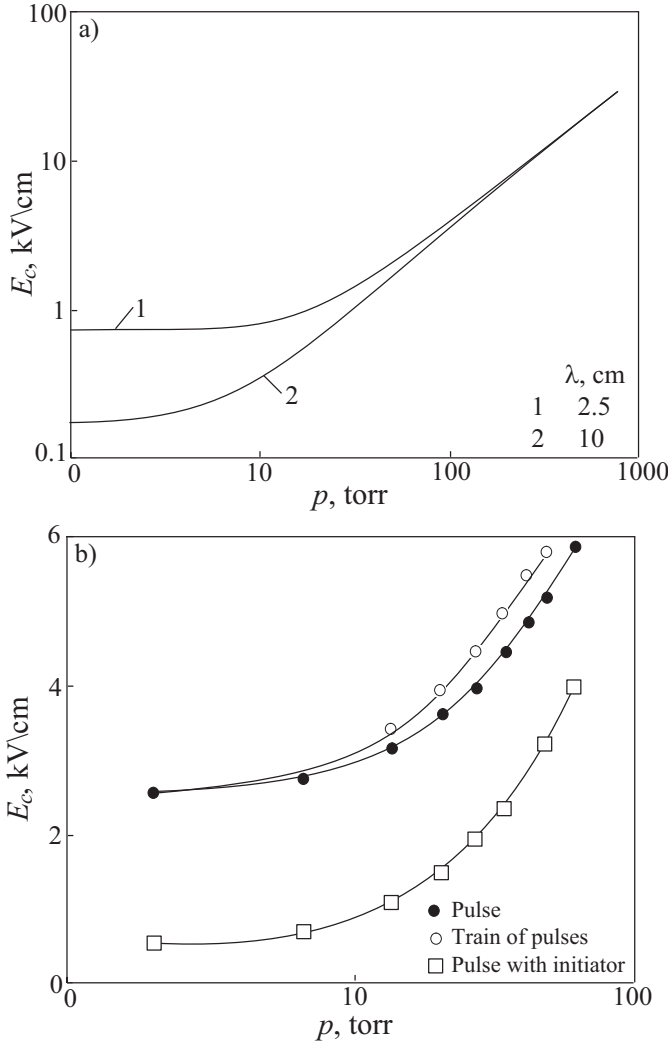


Fig. 2. Dependence of threshold of air breakdown on pressure for continuous (a) and pulsed (b) radiation.

III. RESULTS AND DISCUSSION

The critical strength of the electric field is found from the semi-empirical equation [40]

$$E_c = 42p_{\text{torr}} \left[1 + \left(\frac{\omega}{\nu_c} \right)^2 \right]^{1/2} \quad [\text{W/cm}],$$

where ν_c is the frequency of collisions of electrons with molecules ($\nu_c = 4 \times 10^9 p_{\text{torr}}$ for air), ω is the cyclic frequency of the electric field, p_{torr} is the pressure. A linear dependence of energy threshold on air pressure takes place at high pressures. For continuous microwave radiation this dependance is shown in the Figure 2a. For a pulsed microwave radiation, a probability of air breakdown depends on the presence of free electrons in the focus region during the pulse. Figure 2b shows experimental values of critical strength of electric field for a single pulse (circles) and train of pulses with 1 Hz frequency (bullets). Placement of the source of electrons in the focus region of microwave beam leads to decrease of threshold of air breakdown (squares).

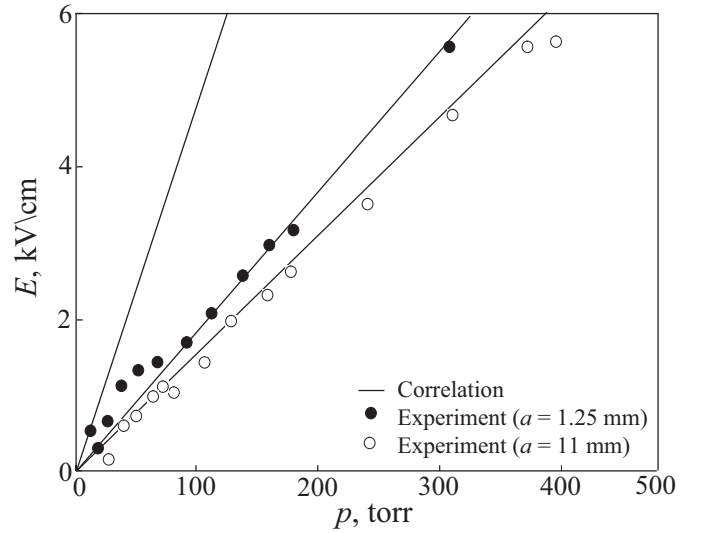


Fig. 3. Comparison of threshold of air breakdown (line 1) with threshold value in the presence of metallic sphere with radius $a = 1.25$ mm (line 2, ●) and radius $a = 11$ mm (line 3, ○).

Placing a conducting element in the region of microwave beam, for example, metallic sphere dimensions of which are compared to the wavelength, the electric field increases and breakdown energy decreases (Figure 3). The solid lines correspond to the calculations based on semi-empirical correlation, and bullets and circles correspond to the experimental measurements, where a is the radius of metal sphere used as initiator.

Direct measurements of the gas temperature in the streamer are difficult. The analysis of the temperature using numerical simulations complements the investigation of streamer discharges and allows to interpret the experimental findings. The effect of ignition area on the propagation of a premixed laminar flame in axisymmetric channel has been obtained with the numerical model. Figure 4 shows comparison of experimental (symbols ○) and computational (symbols ●) results for stoichiometric mixture. The simulation results fit well the experimentally measured quantities.

The time needed to burn the whole amount of gas is dependent on the amount of electrical energy released into the gas. Ignition is promoted by thinner plasma channels, where the energy density is higher. The ability of the discharge to ignite air/propane mixtures, even at low equivalence ratios, is strongly correlated to the energy density that the discharge is able to release into the gas.

The density and the temperature gradients are steep across the flame, allowing to define the flame front as the fixed isothermal surface. Figure 5 shows development and deformation of flame front in time. The fragments corresponds to non-dimensional time moments tu_L/R , where u_L is the laminar burning speed.

Figure 6 shows the dependence of burning velocity on initial pressure (stoichiometric mixtures) for different initial temperatures (300, 325 and 350 K). Increase in initial pressure has a significant effect on the burning velocity of air/propane mixture.

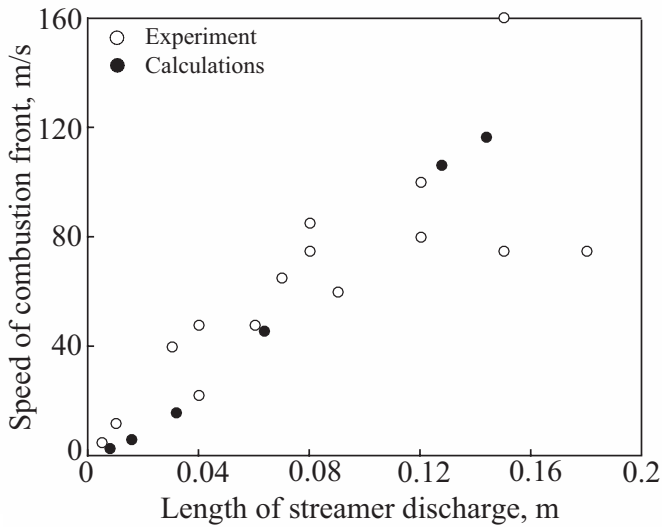


Fig. 4. Comparison of experimental and computational results for stoichiometric mixture.

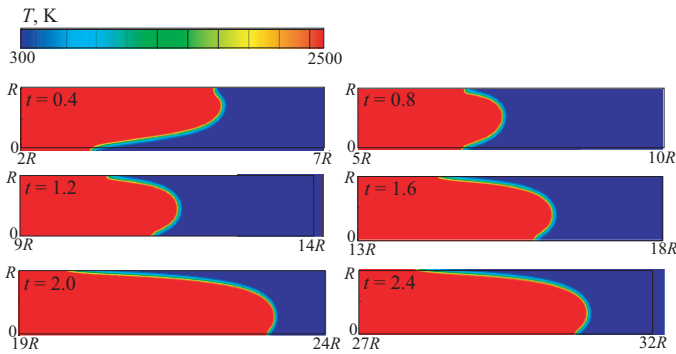


Fig. 5. Temperature contours at different time moments. The length of streamer discharge is 64 mm.

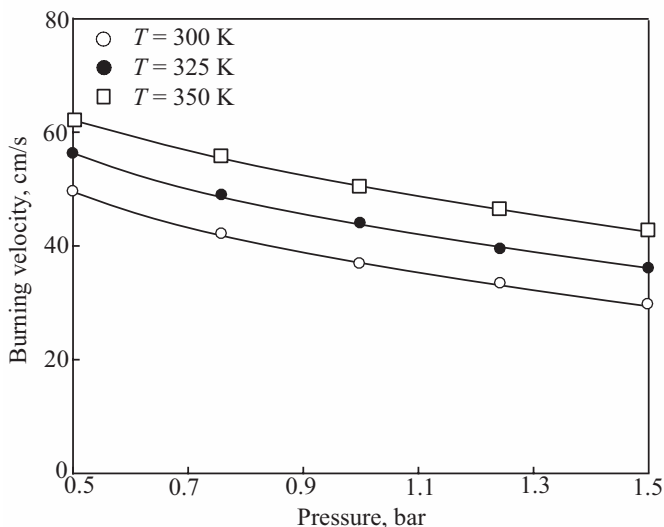


Fig. 6. Effect of pressure on burning velocity for different initial temperatures.

The higher propagation speed is the result of the higher flame surface area evolved from the larger ignition areas.

The flame propagation speed becomes very high due to the enlargement of flame surface area caused by the larger ignition area, and consequently, flame propagation time in the channel is reduced.

IV. CONCLUSION

Understanding of streamer propagation mechanism is of essential importance for the studies of electrical breakdown phenomena and their related applications. Streamers understanding involves many scales from the microscopic scale of collisions of electrons with neutral molecules to macroscopic scales ranging from thin space charge layers within each streamer finger up to the streamer tree with possibly thousands of branches.

Ignitable area becomes one of the key parameters in addition to minimum ignition energy. The streamer discharge produces multiple filaments that can initiate ignition along the plasma channels, providing a volumetric ignition process as the streamers sweep a much larger volume compared to the conventional spark ignition. The effect of ignition surface area on the propagation of a premixed flame is investigated numerically in an axisymmetric channel. The microwave streamer discharge is able to ignite air/propane mixtures at a low initial temperature and atmospheric pressure.

The more rapid combustion with streamer discharges could be exploited in practical combustion devices. Increase in flame surface, caused by the large ignition area, is one of the potential methods in improving combustion efficiency by reducing the burning time in the propulsion systems. These results suggest improved ignition devices for internal combustion engines, premixed gas turbines and pulse detonation engines. Dilution of combustible mixtures with excess air or exhaust gas provides lower NO_x emissions due to lower flame temperatures.

The model demonstrates the potential of using the Euler equations to numerically simulate the evolution of localized/distributed energy deposition zones in a channel (quartz cylindrical tube). The developed model makes it possible to analyze the influence of a continuous, pulsed and pulsed-periodic energy deposition of different duration and frequency. A more sophisticated mathematical model of the energy source should take into account the absorption, reflection and radiation of energy by the resulting extended plasma region and also for ionization, dissociation, and non-equilibrium chemical kinetics.

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