Experimental and theoretical investigation of the mechanism of flame propagation above the surface of combustible liquid moving under the action of an oxidant in microchannels

Yu O Kabova\textsuperscript{1,2}, V V Kuznetsov\textsuperscript{3,4}, V V Zamashchikov\textsuperscript{4,5}, E A Chinnov\textsuperscript{1,4} and O A Kabov\textsuperscript{1,4}

\textsuperscript{1}Kutateladze Institute of Thermophysics, SB RAS, 630090, 1 Lavrentiev prosp., Novosibirsk, Russia
\textsuperscript{2}Novosibirsk State University of Architecture and Civil Engineering, 630008, 113 Leningradskaya Str., Novosibirsk, Russia
\textsuperscript{3}Lavrentyev Institute of Hydrodynamics, SB RAS, 630090, 15 Lavrentiev prosp., Novosibirsk, Russia
\textsuperscript{4}Novosibirsk State University, 630090, 2 Pirogov str, Novosibirsk, Russia
\textsuperscript{5}Voevodsky Institute of Chemical Kinetics and Combustion, SB RAS, 630090, 3 Institutskaya, Novosibirsk, Russia

E-mail: kabova@itp.nsc.ru

Abstract. Flames propagating above the surface of n-butanol in mini and microchannels have been investigated experimentally. It was determined that when oxygen is used as an oxidant, the critical channel size is about 0.3 mm, and according to the estimates this corresponds to the critical size for a premixed homogeneous gas mixture. In order to understand the mechanism of flame propagation above the surface of liquid, in this study, we attempted to simulate the processes, occurring in liquid. The problem of “thermal wave” propagation in a horizontal rectangular channel, when the liquid film moves under the action of gas flow, was studied theoretically. The analysis was carried out taking into account evaporation, specific heat release, and radiation and absorption processes in the gas and on the free surface, as well as the formed zone of strong heating above the liquid film surface for low oxidant velocities in the channel. Based on data obtained, it can be concluded that at high concentration of oxygen and low oxidant velocities, the experimental value of velocity coincides with the calculated value with satisfactory accuracy.

1. Introduction
The tendency to reduce the characteristic sizes of devices in various fields of technology determines the development of fluid mechanics and heat transfer studies in mini and microchannels. Recently, there are many papers on combustion of gaseous fuels in narrow channels of various configurations. This relates to the great practical interest in the miniature power sources, sources of heat and mechanical energy [1], caused by the high energy density of hydrocarbon fuels relative to conventional accumulators of electric energy.

With a decrease in the height of flat channels, the ratio of surface to volume of the channel increases inversely proportional to its minimal transverse dimension, and this causes high intensity of
heat transfer in the microsystems. From the point of view of processes taking place in the reacting systems, for instance, combustion of flammable liquids in the small channels, an increase in heat transfer intensity leads, as a rule, to a decrease in the mass burning rate. Finally, at a certain size, the limit of flame propagation comes [2]. The magnitude of the critical size is an important characteristic widely used in practice. On the other hand, high intensity of heat transfer in micro and mini channels allows the creation of the efficient heat exchangers, which can be also useful from the point of view, for example, of thermoelectric converters. In addition, under the certain conditions, high intensity of heat transfer with the walls of microsystem leads to a return of a significant amount of heat released due to the chemical transformation into the initial mixture, which makes it possible to burn even when the characteristic size of the system is less than the critical one. Therefore, investigation of combustion processes in such systems is important for the development of new applications and increasing the energy efficiency of existing engineering solutions.

Most works dealt with investigation of diffusion combustion of liquid, whose saturated vapor pressure at the initial temperature is lower than the limiting one, were performed in large volumes [3]. At diffusion combustion in a limited volume, there is an important feature - impossibility of flame propagation over the liquid surface in the absence of an oxidant flow [4–7]. Experiments [5–7] have shown that the rate of flame propagation in such systems depends on the oxidant flow. In a cylindrical channel, when air is used as an oxidant, the flame moves with pulsations [5]. In a rectangular channel with the height less than 4 mm, flame propagation is possible only when air is enriched with oxygen. Papers [5–7] also show that the flame velocity can vary in a wide range from millimeters per second to several meters per second. The flame propagation velocities obtained under such conditions are comparable with the normal velocities for carbon-oxygen gas mixtures. These facts make us think about the mechanism of flame propagation above the liquid surface. The currently accepted thermocapillary mechanism is reasonably criticized in [7]. The authors point out that the flow of heated liquid from the area with the combustion products to the pre-flame zone due to the capillary forces requires a considerable amount of time. There is no such a process, when the flame propagates in a premixed gaseous mixture; therefore, in order to obtain the velocities close to the normal velocities of carbon-oxygen gas flames, formation of combustible mixture in the pre-flame region should be substantially accelerated. To understand the mechanism of flame propagation above the liquid surface, in this paper we attempted to simulate the processes taking place in the film of a combustible liquid; the model is based on the previously developed mathematical model [8, 9]. To simplify the problem, we consider small oxidant velocities in the channel, whose height was chosen much less than its width and this corresponds to the parameters of flat compact heat exchangers. This was also done in order to create a two-dimensional structure of the flow and flame front, which facilitates process simulation. According to the data available to the authors, there are no theoretical studies on the mechanism of flame propagation above the surface of combustible liquid moving under the action of an oxidant in microchannel.

2. Mathematical model

As a first step, “thermal wave” propagation in a horizontal rectangular channel at the liquid film motion under the action of a gas flow was studied theoretically taking into account evaporation (figure 1). The model is based on the previously developed model of thermocapillary flow of the locally heated liquid film moving under the action of a gas flow in a microchannel. The model takes into account the dynamic effect of gas flow on the liquid as well as diffusion and convective mechanisms of heat and mass transfer in liquid and gas and through the deformable gas-liquid interface [8, 9]. It is assumed that the gas flow consists of oxygen-enriched air and liquid is n-butanol.

The problem is solved in two-dimensional formulation, when the conditions of thin layer approximation are satisfied, taking into account specific heat release and processes of radiation and absorption in gas and at the free interface, as well as the formed zone of strong heating above the liquid film surface. The mathematical model is based on the systems of Navier-Stokes, continuity, energy and diffusion equations (1)–(2).
The unknown functions are \( \vec{v} = (u,v), \vec{\gamma} = (u, v_g), T(t,x,y), T_g(t,x,y), C(t,x,y) \), whose functions define correspondingly the velocity and temperature fields in liquid and gas, and distribution of evaporated matter in gas (everywhere, index \( g \) indicates that the value belongs to the gas phase). Function \( z = H(t,x) \) that specifies the free interface is also unknown. We obtain the system of equations in liquid

\[
\rho (dv/dt - g) = -\nabla p + 2 \text{div} (\mu W), \quad \nabla \cdot v = 0, \quad \rho c_p dT/dt = \kappa \Delta T, \tag{1}
\]

and in gas:

\[
\rho_g (dv/dt - g) = -\nabla p_g + 2 \text{div} (\mu_g W_g), \quad \nabla \cdot v_g = 0, \quad \rho_g c_p dT_g/dt = \kappa_g \Delta T + Q - \alpha (T^4 - \bar{T}^4), \quad dC/dt = D \Delta C - \gamma / \rho_g, \tag{2}
\]

the components \( W_{ij} \) and \( W_{gij} \) (\( i,j = 1,2,3 \)) of rate of strain tensors \( W \) and \( W_g \) are defined as follows:

\[
W_{11} = u_x, \quad W_{12} = u_y + v_x/2, \quad W_{13} = (u_z + w_x)/2, \quad W_{11} = u_x, \quad W_{12} = u_y + v_x/2, \quad W_{13} = (u_z + w_x)/2, \quad W_{22} = v_y, \quad W_{23} = v_g + w_z, \quad W_{33} = w_z, \quad W_{33} = w_g.
\]

Here \( p \)—pressure, \( g \)—vector of gravitational acceleration, \( D \)—diffusion coefficient, \( \kappa \)—thermal conductivity, \( c_p \)—heat capacity, \( \mu = \mu(T) \)—dynamic liquid viscosity, \( \rho \)—liquid density, \( \sigma = \sigma(T) \)—surface tension. Subscripts in the paper have the following meaning: 0—initial parameters of the flow (at initial temperature \( T = T_0 \)), \( x, y, t, z \)—derivatives on \( x, y, t \) and \( z \).

With the initial conditions, specifying an undisturbed flow and appeared zone of strong heating (ignition):

\[
\vec{v} = \vec{v}_0, \quad \vec{\gamma} = \vec{\gamma}_0, \quad T = T_0, \quad T_g = T_{g0}, \quad C = C_0, \quad H = H_0, \quad T_{g0} = \begin{cases} T_0, & x < x_0, \\ T_0', & x > x_0, \end{cases} \tag{3}
\]

boundary conditions on the channel bottom:

\[
\vec{v} = 0, \quad T = T_0, \tag{4}
\]

conditions on the free interface:

\[
\vec{v} - \hat{n}(\vec{v} \cdot \hat{n}) = \vec{v}_g - \hat{n} (\vec{v}_g \cdot \hat{n}), \quad \rho (\vec{v} - \hat{n} - V_g) = \rho_g (\vec{v}_g - \hat{n} - V_g), \quad \rho (\vec{v} - \hat{n} - V_g) = -D \hat{n} \cdot \nabla (C \rho_g), \tag{5}
\]

\[
(P - P_g) \cdot \hat{n} = 2 \sigma K \hat{n} + \nabla \cdot \sigma + \rho_g (\vec{v}_g - \hat{n} - V_g) \left( \frac{\rho}{\rho} - 1 \right) \hat{n}, \quad \kappa \frac{\partial T}{\partial n} + \kappa_g \frac{\partial T_g}{\partial n} = \frac{\rho \lambda D}{1 - C} \frac{\partial C}{\partial n} + \omega_c E, \quad T = T_g, \quad C = C_c(T).
\]

and conditions on the upper wall of the channel:

\[
\vec{v}_g = 0, T = T_0'. \tag{6}
\]
Here, $T'$ is the ignition temperature of combustible mixture, $\bar{T}$ is the average temperature of heat release zone in gas, $\gamma$ is the burning rate, $Q$ is a specific heat release, $\omega$, $\omega_0$ are the radiation and the absorption coefficients.

The problem was transformed to specially developed new variables, so that continuity equations in the liquid and in the gas retain their form in new variables but kinematic condition at the free interface simplifies and become linear. We employ the lubrication theory to derive reduced set of equations, so we assume that the characteristic film thickness and the characteristic film thickness variation are much smaller than the characteristic length scale of the film in streamwise and spanwise directions, thereby the film aspect ratio is taken asymptotically small $\varepsilon = H_0/l << 1$. Considering inertial terms to be negligible, the system of equations with boundary conditions was rewritten in dimensionless form.

Numerical solution of the problem is implemented by the finite difference method. The alternating directions implicit (ADI) method is used to solve the system of grid equations with boundary conditions. To solve the problem on each fractional grid step the Thomas algorithm is used. For more details refer to [8, 9]. The numerical algorithm based on the developed mathematical model allowing theoretical and numerical investigation of the joint nonisothermal liquid and gas motion in the microchannel, as well as heat and mass transfer on the free surface of the liquid film, of the problem was developed. When developing the numerical algorithm, the method of approximation by the mesh functions was used. Herewith the computational domain is divided by the surfaces of constant coordinate’s value in equal steps, and the values of calculated functions are determined at all nodal points. The problem was solved numerically using the finite-difference method. The solution algorithm consists of the blocks allowing calculating the temperature, position of the gas-liquid interface, and velocity and pressure fields. The temperature is calculated by the method of alternating directions by introducing the fractional steps, and at each time step, calculations along the longitudinal and transverse directions are performed in turn. Since the temperature is continuous at the interface, calculations in liquid and gas are performed simultaneously, and the heat balance condition plays the role of the missing equation on the layer containing the boundary. This method ensures that the boundary conditions are met exactly. Evolution of the interface is calculated using a two-layer implicit difference scheme for parabolic equations of the fourth order. The velocity and pressure fields are calculated according to the analytical quadrature formulas obtained for the given problem when developing the numerical algorithm. The numerical code is written in Fortran. Each block-procedure in the program code allows independent testing on the check tasks. The corresponding check of the program blocks was carried out, and results give a good match to the tests. The check was made by deriving the solutions with the help of separate blocks of the code for quasilinear parabolic equations of the second and fourth orders for comparison with the known solutions. Totally, the discrepancy does not exceed 1% for all blocks. Stability of calculations was set using the implicit difference schemes with a second order of time approximation and the second and third order of approximation with respect to spatial variables when calculating the temperature and free interface position, respectively. It is known that approximation and stability together guarantee the convergence of numerical solution of the problem. Numerically it was shown that combustion of oxygen-enriched air leads to formation of a “thermal wave” rapidly moving towards the gas flow with the velocity close to constant. In figure 2 one can see evolution of the temperature field in the microchannel at different time moments. Here, all values are given in the dimensionless form: temperature $T = T - T_0$ and time $\tau = lt/U$. Zone of strong heating moving upstream may be treated as a combustion wave. The velocity of this zone in this case of calculations is equal to 2.7 m/s.
Figure 2. The process of combustion front propagation in time across the channel ($x$). Temperature in the channel at different moments of time $t$ (all values are in dimensionless form). Channel height is 500 $\mu$m, channel length is 30 cm, Reynolds number in gas is $Re_g=10$, liquid film thickness is 90 $\mu$m. Temperature of self-ignition is $T'=340 ^\circ$C, initial temperature is $T_0=20 ^\circ$C.

3. Experimental results

New experimental results on investigation of flames propagating over the surface of n-butanol in mini and microchannels are obtained. The channel height was varied from 0.23 to 0.5 mm. The description of experimental setup is given in [7]. Propagation at a change in oxidant composition was studied experimentally. Experiments showed that the average velocity of flame propagation increases with increasing proportion of oxygen in the oxygen-nitrogen mixture. Therefore, for the channels with low height, pure oxygen was chosen as the oxidizing mixture. Experimental results for oxygen were obtained in the channels 0.3 and 0.5 mm in height. The comparison showed that an increase in the average velocity of oxygen, as in the channel with the height of 0.5 mm, leads to a decrease in the flame velocity. However, if the flame velocity changes significantly with a decrease in the channel height from 1 to 0.5 mm, then with a decrease in the channel height from 0.5 to 0.3 mm, it changes insignificantly at low oxidant velocities with a tendency towards increasing velocity difference with an increase in the oxidant velocity, figure 3.

![Figure 3](image)

Figure 3. Flame velocities vs. average oxygen velocity for different channel heights

It is determined that in a channel with the height of 0.3 mm, the flame can propagate if pure oxygen is used as an oxidant. The photographs of the flame front moving in this channel are presented in figure 4. Flame extinction in the channel is determined by heat losses to the wall, which depend on the channel height. According to theoretical estimates, the limiting condition is determined by Peclet number $Pe = U_n d/a = const$. Where $U_n$ is normal velocity (velocity of flame propagation along the normal to its surface relative to the fresh mixture), $d$ is hydraulic diameter of the channel, $a$ is thermal...
diffusivity coefficient. Experiments of other researchers showed that for hydrocarbon-air mixtures the critical channel height is about 2 mm. Since, according to the critical condition, the size is inversely proportional to the normal velocity and normal velocities for carbon-air and carbon-oxygen mixtures differ approximately by the factor of 10, the critical size for the mixture of n-butanol with oxygen, used in our experiments, should be of the order of 0.2 mm. For the channel of 0.3 mm height, if we take into account that there is a liquid film on the surface, the actual size of the channel will be even smaller, so it is expected that this size is close to the size of extinction. However, experiments showed that this channel is not critical; moreover, the flame velocities with a decrease in the channel height from 0.5 to 0.3 mm vary insignificantly. The result requires further investigation.

Figure 4. Flame front moving towards the oxidant flow in the channel with the height of 0.3 mm. a: V(oxygen)=1 m/s, b: V(oxygen)=3.8 m/s.

4. Conclusion

New experimental results on investigation of flames propagating over the surface of n-butanol in mini and microchannels are obtained. The height of the channel was varied from 0.23 to 0.5 mm.

It is found that if oxygen is used as an oxidant, the critical channel size is about 0.3 mm, and according to the estimates, this corresponds to the critical size for a premixed homogeneous gas mixture.

The problem of “thermal wave” propagation in a horizontal rectangular microchannel at the liquid film motion under the action of a gas flow at high oxygen concentration and low oxidant velocities was studied theoretically. When developing the model, evaporation, specific heat generation, and radiation and absorption processes in gas and at the free interface, as well as the zone of strong heating above the liquid film were taken into account. It can be concluded that at high oxygen concentration and low oxidant velocities, the experimental value of velocity coincides with the calculated value satisfactorily.

Acknowledgments

The study was financially supported by the Russian Science Foundation, project no. 15–19–30038.

References

[1] Maruta K 2011 Proc. of the Combustion Institute 33 125–150
[2] Zeldovich B Ya, Barenblatt G I, Librovich V B and Makhviladze G M 1980 Mathematical theory of combustion (ed R I Soloukhin, Moscow: Nauka) 478
[3] Ross H D and Miller F J 1996 Proc. of the Combustion Institute 26 1327–34
[4] Bieri J A, Kurdyumov V N and Matalon M 2011 Proc. of the Combustion Institute 33 1227–34
[5] Zamashchikov V V 2009 Combustion Sci. and Technology 181 1 176–189
[6] Zamashchikov V V, Korzhavin A A and Chinnov E A 2014 Combustion, Explosion and Shock Waves 50 4 381–386
[7] Zamashchikov V V, Korzhavin A A and Chinnov E A 2016 Int. J. Heat and Mass Transf. 102 470–478
[8] Kabova Yu, Kuznetsov V V, Kabov O, Gambaryan-Roisman T and Stephan P 2014 Int. J. Heat and Mass Transf. 68 527–541
[9] Kabova Yu, Kuznetsov V V and Kabov O 2014 Interfacial Phenomena and Heat Transfer 2 85–102