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Hydrogen Flame Propagation from a Variable Volume Combustion Chamber in a Narrow Moving Annular Gap

Revaz Kavtaradze*, and Yi-Chun Wang****

* *Rafiel Dvali Institute of Machine Mechanics, Tbilisi, Georgia*
** *School of Mechanical Engineering, Beijing Institute of Technology, Beijing, China*

(Presented by Academy Member Tamaz Natriashvili)

We have considered the use of a 3D mathematical model based on fundamental Navier-Stokes differential equations describing the turbulent motion of a chemically reacting gas, the flame propagation process and the associated problem of local unsteady heat transfer in a narrow gap located between the piston and the cylinder above the upper compression ring. The conditions of extinguishing and flame propagation in the gap has been established, which significantly affects the thermal boundary condition used to simulate the heat-stressed state of the piston and cylinder liner. This task is especially relevant when converting serial, traditional internal combustion engines (ICE) into a hydrogen engine. It is shown that by changing the composition of the combustible mixture (hydrogen-air), it is possible to control the process of hydrogen flame propagation in the gap, thereby reducing heat losses in a hydrogen engine. *© 2024 Bull. Georg. Natl. Acad. Sci.*

hydrogen engine, flame propagation, annular gap, heat losses

The features of modeling homogeneous gas flows in narrow flow sections of various shapes, in particular the issues of hydraulic resistance and intensification of heat exchange occurring during the flow of bodies are analyzed in [1-3]. The processes of flame propagation and extinguishing in limited volumes (in combustion chambers, pipes and gaps of various shapes and sizes), in contrast to these flows, are accompanied by heat release and displacement of the flame front surface separating the cold combustible mixture from high-temperature combustion products. Processes, especially in narrow gaps, become so complicated that they prefer the use of traditional stroboscopic or other methods of visualizing flame propagation using high-speed video [4]. The use of similar methods for our purpose requires not only the creation of a single-cylinder experimental hydrogen engine with a transparent combustion chamber, but also the introduction of observation and simultaneous registration of processes both in the chamber and in a small gap that is hard to reach on the running engine. The use of approximations of a plane or spherical flame, usually used in the classical (analytical) theory of combustion [4], requires the introduction of simplifications and assumptions that can lead to results that are very different from the real ones. In this regard, mathematical modeling using verified and reliable 3D models is the most reliable and cheapest way to solve the problem.

A Brief Description of the Mathematical Model Used

The combustion chamber, the variable volume of which is limited by the heat-sensing surfaces of the moving piston and stationary parts: the cylinder and its head (Fig. 1), is filled with a homogeneous hydrogen-air mixture, the composition of which is characterized by the excess air ratio α_{air}. The piston is connected to the crankshaft with the help of a crank mechanism, and each of its positions is fixed by the angle $\varphi = \omega\tau$ of rotation of the crank relative to the vertical axis of the cylinder (ω is the angular speed of rotation of the crankshaft, τ – current time), i.e. at a given frequency of rotation of the crankshaft, φ essentially represents the current time τ. After the mixture is ignited by an electric spark from the spark plug located in the cylinder head in the central part of the chamber, a flame front is formed separating the cold combustible mixture from the combustion products. A pressure drop is formed between the mixture and the combustion products, which moves the flame front. Moving from the ignition source towards the periphery of the chamber, it reaches the annular gap, which moves together with the piston along the surface of the cylinder. In Fig. 1, the gap is marked with a circle.

Depending on various factors (fuel type, mixture composition, pressure, temperature, gap size), which are analyzed below, there are two scenarios for the further behavior of the flame:

1. The flame penetrates into the annular gap, limited from three sides by the surfaces of the piston FSFK, cylinder FSFZ and piston ring FOFR, spreads in it and goes out after reaching the ring surface (Fig. 1). It is obvious that the process of flame propagation in the gap is accompanied by heat release and intensive heat exchange with the walls of the gap;
2. When entering the gap, the flame goes out, the heat release in the gap stops and intensity of the heat exchange with the walls of the gap is significantly reduced. After extinguishing the flame, the unburned hydrogen-air mixture flows back into the combustion chamber.

The task is as follows: depending on the conditions of penetration and extinguishing of the flame into the noted annular gap, to simulate the processes of flame propagation and heat exchange with the walls of the gap and conduct a comparative analysis of heat losses in cases of penetration and extinguishing of the flame, depending on the composition of the mixture.

Figure 1 shows the axial (diametral) cross-section of the 3-dimensional design of the piston engine cylinder. The thermophysical processes (move-

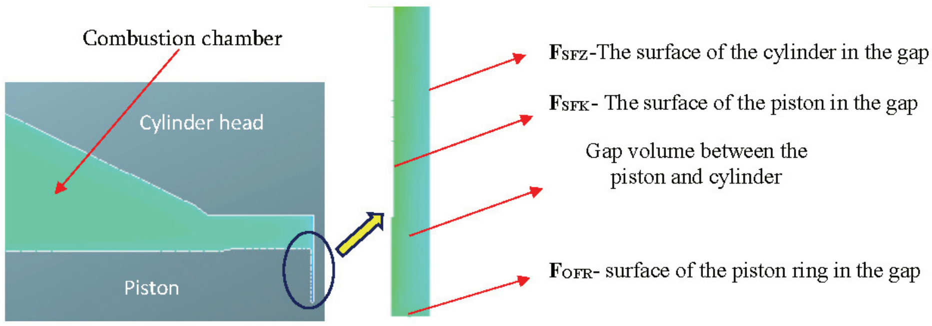

Fig. 1. The annular gap between the piston and the cylinder above the upper ring of the piston and the corresponding heat exchange surfaces (axial section).

ment, ignition and combustion of the mixture, as well as heat generation, formation of nitrogen oxides and heat exchange with the walls) occurring in the combustion chamber and adjacent gap are investigated using a 3D mathematical model. The model is based on the fundamental equations of momentum (Navier-Stokes equations), energy (Fourier-Kirchhoff equation), diffusion (Fick equation) and continuity equation. These equations, after averaging by the Favre method, take the form of Reynolds and form an open system, to which are added the models of turbulence (k-ζ-f – Hanjalich model), combustion (CFM-Coherent Flame Model), formation of nitrogen oxides NOx (the thermal mechanism of Zeldovich) and the model of heat exchange in the boundary layer (Wall functions of Spalding–Patankar). The augmented system of equations is solved by the numerical control volume method (CVM).

The description of these models and their features related to the specifics of processes in piston engines, as well as numerical solution procedures are described in [5-7]. The 3D mathematical model of processes, used both in, the combustion chamber and the gap is implemented using the AVL FIRE CRFD program [8].

The Condition of Extinguishing the Flame in the Gap

The surface over which the flame spreads is usually called the fiery surface. The total fiery surface of the piston, on which heat transfer from the burning gas (from the flame) occurs, has an area F_{GFK}. This area is equal to the sum of the areas of the upper fiery surface of the piston F_{OFK} and the side fiery surface (surface of the fiery belt) of the piston F_{SFK}, i.e. $F_{GFK} = F_{OFK} + F_{SFK}$. The upper fiery surface of the piston with an area of F_{OFK} is the upper surface of the piston, which at the same time is the movable boundary of the combustion chamber F_{OFK}. The piston fiery belt is a side surface of the piston above the first (compression) ring, having an area of F_{SFK}. If the flame does not penetrate into the gap, it is obvious that the F_{SFK} is not a fiery surface and heat exchange between the unburned mixture (hydrogen-air) and the piston occurs on it. The fiery belt of the cylinder liner is the side surface of the cylinder liner above the first (compression) ring F_{SFZ}. Unlike other fiery surfaces, it varies depending on the movements of the piston. Earlier, for a basic gasoline engine, it was experimentally established that with a cylinder diameter of D_Z=86 mm and the height of the piston fiery belt h=5.5 mm, the radial width of the annular gap is equal to $\ell_h = D_Z - D_P = 0.2$ mm in the hot state of the engine (at maximum load mode at $\alpha_{air}=1$), and in the cold state $\ell_c = D_Z - D_P = 0.8$ mm (on the engine not running) [9].

According to the theory of Ya. B. Zeldovich, the extinguishing of the flame in the combustion chamber (Fig. 1) occurs when its front is cooled, when the rate of convective heat removal by cold walls becomes equal to or greater than the rate of heat release (the rate of self-heating of the flame). At the same time, a constant value of the Prandtl number P_r=const is indicated at the flame extinguishing limit [10]. In [11], under the condition P_r =const, the limits of the change in the critical gap size for a gasoline flame are established. Subsequent experimental studies, the analysis of which is described in review articles [12, 13], have shown that a flame in a fuel-air mixture with specified values of temperature, pressure and composition (aair) cannot pass through a gap smaller than a certain minimum size ℓ_{kr}, called the critical size or flame extinguishing distance (FED). The real value of ℓ_{kr} depends on the configuration of the volume in which the flame spreads. For example, the FED may be the minimum inner diameter of the pipe d_{kr}, or the minimum distance between parallel plates ℓ_{kr}, in which the flame passes (does not go out).

The higher the speed of movement of the flame front, the pressure and temperature of the mixture, the lower the FED. Other things being the same, in particular, at $\alpha_{air}=1$: for a hydrogen flame, the FED ℓ_{krH2} is 4-4.5 times less than the FED $\ell_{kr\ gesoline}$ for a gasoline flame, and replacing the oxidizer (air) with oxygen reduces the ℓ_{krH2} from 0.52 mm to 0.19 mm in the case of parallel plates. The value of the FED is also affected by the geometric shape of the gap itself, for example, according to [14], in the case of parallel walls, ℓ_{kr} is 65% of the d_{kr} for a cylindrical pipe.

In the case of a piston engine, for an annular gap (Fig. 1), the FED is defined as the distance between the side surface of the piston and the inner surface of the cylinder, whose value coincides with the hydraulic diameter of the annular gap Dhydr, i.e. $\ell_{kr}=D_Z-D_P\equiv D_{hydr}$. In [9], based on the analysis carried out as well as extrapolation the known dependences $\ell_{krH2}=f(p, T, \alpha_{air})$ [12], the following values of FED were established for stoichiometric mixtures for the ranges of pressure p, temperature T and excess air ratio α_{air}, typical for the combustion process in a piston engine: air with gasoline $\ell_{kr\ gesoline}$= 0.5 mm and air with hydrogen ℓ_{krH2}=0.125 mm. The low value of ℓ_{krH2} compared to $\ell_{kr\ gesoline}$ is explained, among other things, by the relatively high speed of the hydrogen flame compared to gasoline one.

Then, taking into account the experimentally determined value ℓ_h=0.2 mm for the engine under study in the hot state, we write down the condition

$$\ell_{kr\ gesoline} > \ell_h > \ell_{krH2}, \qquad (1)$$

previously introduced in [9].

It means that when the experimental engine is running on stoichiometric mixtures, the flame penetrates and burns out in the gap ℓ_h=0.2 mm if hydrogen is used as fuel, and vice versa: in the case of gasoline, the flame cannot penetrate into the gap ℓ_h=0.2 mm and goes out. It follows from this that in a gasoline engine on the inner surface of the gap, the heat exchange process with an unburned gasoline-air mixture is less intense than in a hydrogen engine, in the gap of which there are high-temperature combustion products, and the gap surface itself is the surface of intense heat exchange.

The Influence of the Composition of the Combustible Mixture

Leaning the mixture significantly affects, of course, the indicator pressure in the cylinder, and as a result, the effective (power, torque) and environmental (nitrogen oxide emission) indicators of a hydrogen engine. Figure 2 shows pressure changes in the combustion chamber depending on the excess air ratio α_{air} at a gap ℓ_h=0.2 mm (φ=0° – Upper Dead Center). It can be seen that with a stoichiometric mixture (α_{air}=1.0), the maximum cycle pressure reaches the highest value p_z=6.21 MPa. Depletion of the hydrogen-air mixture to the value α_{air}=1.64, reduces the maximum cycle pressure to p_z=41.8 bar and, accordingly, when the mixture is depleted to α_{air}=2.0, we have p_z=26.3 bar.

In addition, it is noticeable that the higher α_{air}, the further away from upper dead center (UDC) is the moment of reaching the maximum value pz, which indicates a deterioration in the efficiency of the working cycle. The latter can be explained by the fact that the depletion of the mixture leads to a decrease in the rates of combustion and heat release.

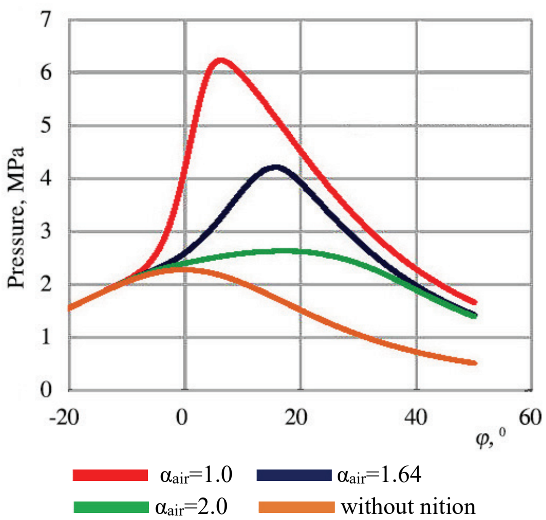

Fig. 2. Pressure changes in the combustion chamber depending on the excess air coefficient α_{air} (ℓ_h=0.2 mm).

The numerical experiments also showed that increase in the gap to ℓ_h=0.35 mm, practically does not affect either the nature of the change in pressure p(φ) in the combustion chamber or the value pz shown in Fig. 2. It should also be noted that the indicator diagrams p(φ) obtained by mathematical modeling, as well as the heat release rates dQx/dφ calculated on their basis, are in good agreement with their experimental values recorded on the experimental hydrogen engine in laboratory conditions.

Influence of the Gap. Size on the Heat Transfer Process

The intensity of heat transfer from the gas to the walls of the gap significantly depends on the composition of the hydrogen-air mixture. It can be seen from Fig. 3 that with a stoichiometric mixture (α_{air}=1), the value of the instantaneous heat transfer coefficient on the fiery zone of the piston reaches its maximum value α=6158 W/(m^{2}K) at φ=230 after UDC. In the case of lean mixtures α_{air}=1.64 and α_{air}=2, it decreases to α=5028 W/(m^{2}K) and α=4712 W/(m^{2}K), respectively. This is due to the fact that when α_{air}=1, the hydrogen flame penetrates into the gap and while the piston is moving down, the hydrogen continues to burn in the gap.

The leaning of the hydrogen-air mixture helps to prevent the spread of the flame into the gap. By modelling the heat transfer process, it was also established that:

1. An increase in the size of the gap ℓ_h from 0.2 mm to 0.35 mm (i.e. by 42%) leads to a decrease in the maximum instantaneous value of the heat transfer coefficient on the surface of the piston fiery zone αwp max from 6158 W/(m^{2}K) to 4407 W/(m^{2}K), i.e. by 28%. This corresponds to the theoretical result of Ya. B. Zeldovich, according to which, by increasing the linear size of the gap ℓ_h, one can achieve arbitrarily small heat losses [10];
2. On the surface of the cylinder related to the gap, the maximum instantaneous value of the non-stationary heat transfer coefficient at ℓ_h=0.2 mm takes the value $\alpha_{wz\ max}$=5586 W/(m^{2}K), which is approximately 10% less than on the surface of the fiery zone of the piston $\alpha_{wp\ max}$.

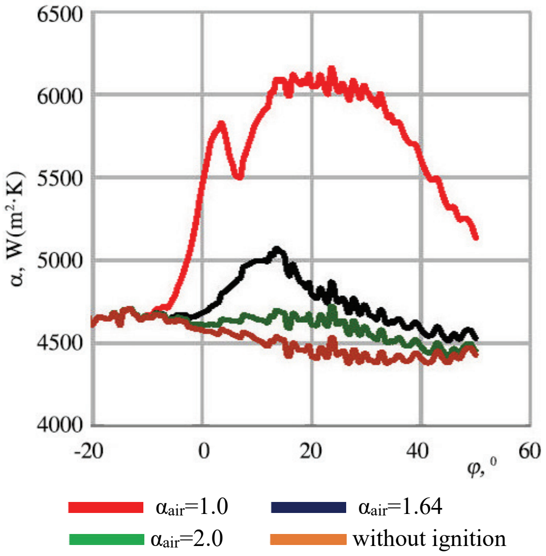

Fig. 3. Change in the heat transfer coefficient of the piston surface in the gap at l_h=0.2 mm, under the operating mode of the hydrogen engine n=3000 min^{-1} depending on the excess air coefficient.

The results obtained explain the phenomenon of increasing heat losses in hydrogen engines, observed in experimental studies by a number of authors: T. Shudo and H. Suzuki [14, 15], as well as J. Demuynck et al. [16]. The above-mentioned authors believe that the reason for the existence of this phenomenon is an increase in the intensity of convective heat exchange between the burning gas and the wall, due to the high speed of propagation of the hydrogen flame. Without denying the influence of this factor, the obtained results (Fig. 3) prove that the penetration of a hydrogen flame into the gap has a significant effect on the increase in heat losses, which was not paid attention to in previous studies.

Simulation Results of the Hydrogen Flame Propagation in the Gap

The propagation of a flame in a volume is usually studied on the basis of an analysis of the movement

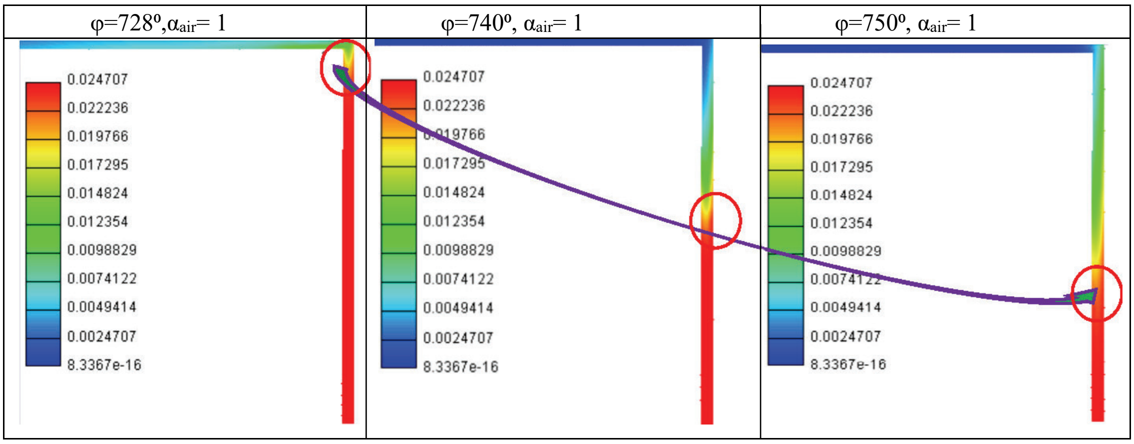

Fig. 4. Change in the mass fraction of hydrogen $\overline{m}_{H2}$ in the gap at ℓ_h = 0,2 mm; α_{air}=var.

of the flame front, which is a thin layer in which the processes of chemical transformation of a combustible mixture into combustion products take place. At numerical experiments, flame propagation can be observed from the results of modeling the changes in instantaneous local temperatures T(x, y, z, τ), as well as instantaneous local mass fractions of unburned hydrogen $\overline{m}_{H2}$(x, y, z, τ) in the gap volume (Fig. 4 and 5).

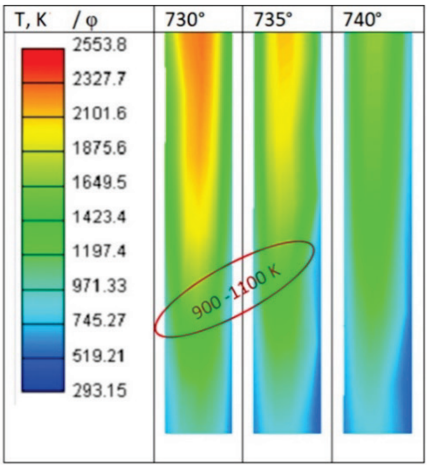

Fig. 5. Instantaneous temperature fields during hydrogen combustion in the gap for different time points φ at ℓ_h=0.2 mm and α_{air} = 1.

Analysis of the results of modelling the process of changing $\overline{m}_{H2}$(x, y, z, τ), given in Fig. 4 in the form of enlarged fragments of the gap sections, shows that when a hydrogen flame penetrates into the gap, the combustion process in it clearly lags behind combustion in the chamber volume, i.e. it is essentially the last phase of combustion: after burning in the cylinder. In addition, with a stoichiometric mixture (α_{air}= 1), hydrogen starts to burn in the inlet part of the gap at the time φ=728⁰ and by the time φ=770⁰ it almost completely burns out.

In the case of a lean mixture (α_{air}=1.64 and α_{air}=2), a small flash of the hydrogen is observed only at a shallow depth of the inlet part of the gap, and in the main part of the gap volume, the proportion of hydrogen in the mixture remains unchanged and is maximum for the corresponding excess air coefficients, i.e. the flame goes out and the hydrogen in the gap does not burn out.

When the piston approaches the bottom dead center, the hydrogen-air mixture remaining in the gap flows into the combustion chamber and burns out there. However, this delayed heat release does not contribute to an increase in the efficiency of the engine's working cycle, but an increase in exhaust gas temperature can positively affect operation of the nitrogen oxide neutralizer. It is known that the possibility of raising the first piston ring upwards, usually used in the case of conventional engines, reduces the emission of unburned hydrocarbons CH. In hydrogen engines, however, the problem of CH emissions is absent. Nevertheless, the reduction in the surface area of the piston fiery zone rises the efficiency of the operating cycle, as it helps to reduce heat losses.

It has also been established that the propagation of the hydrogen flame over the volume of the annular gap at a stoichiometric mixture (α_{air}=1) occurs the faster, the larger the gap size ℓ_h is. This, as mentioned above, is associated with a decrease in heat transfer at an increase in ℓ_h.

Observations of the change in the mass fraction of hydrogen $\overline{m}_{H2}(x, y, z, \tau)$ and the gas temperature $T(x, y, z, \tau)$ in the annular gap also showed that hydrogen burns out faster in the central (axial) part of the annular gap, rather than near the walls of the piston and cylinder, i.e., flame elongation is achieved faster than expansion. This is due to cooling from the respective walls of the gap. It is also noticeable that due to more intense cooling in the near-wall areas near the cylinder surface, the temperature drops faster than near the piston surface (Fig. 5). In addition, it is noticeable that by the time φ=760° (i.e. at 40° after TDC) the flame reaches the bottom of the gap, i.e. to the surface of the compression ring and hydrogen burns out almost completely.

The temperature of the hydrogen-air mixture ahead of the flame front, as can be seen from Fig. 5 can take on values of 900-1100 K (circled), exceeding the self-ignition temperature of hydrogen (858 K). This indicates the possibility of the appearance of the Mach effect, for the proof of which a separate study of the processes in the gap, including the vector fields of the flow velocity, should be carried out.

Conclusions

In the theory of reciprocating engines, the problem of the non-stationary propagation of a hydrogen flame in the gap between the piston and the cylinder, above the upper piston ring, in a 3-dimensional formulation is solved. The obtained results are of both scientific-theoretical and practical significance, since: 1. They explain the phenomenon of increasing heat losses in hydrogen engines, previously observed in experimental studies by a number of authors [14-16], but a full theoretical explanation of this phenomenon is not given. 2. They confirm that the thermal boundary conditions on the internal surfaces of the gap for the cases of penetration and extinguishing of a hydrogen flame in it, differ significantly from each other. Obviously, the heat losses in the combustion chamber and the heat loads on the main parts, primarily on the piston and on the cylinder liner, will also differ significantly. This should be taken into account in practice, especially when converting serial engines running on hydrocarbon fuel into a hydrogen engine. 3. They indicate the possibility of controlling the process of the flame propagation into the gap between the piston and the cylinder and reducing heat losses by adjusting the composition of the hydrogen-air mixture.

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ენერგეტიკა

წყალბადის ალის გავრცელება ცვლადი მოცულობის წვის კამერიდან ვიწრო რგოლურ ღრეჩოში

რ. ქავთარაძე*,** და იჩუნ ვანი**

* *რაფიელ დვალის მანქანათა მექანიკის ინსტიტუტი, თბოენერგეტიკული დანადგარების განყოფილება, თბილისი, საქართველო*
** *პეკინის ტექნოლოგიური ინსტიტუტი, მანქანათმშენებლობის ფაკულტეტი, პეკინი, ჩინეთი*

(წარმოდგენილია აკადემიის წევრის თ. ნატრიაშვილის მიერ)

ნავიე-სტოქსის ტიპის ფუნდამენტურ განტოლებებზე დაფუძნებული 3D მათემატიკური მოდელის გამოყენებით (რომელიც ქიმიურად რეაგირებადი აირის ტურბულენტურ მოძრაობას აღწერს), გამოკვლეულ იქნა წყალბადის ალის გავრცელების პროცესი დგუშსა და ცილინდრს შორის განთავსებულ ვიწრო, რგოლურ ღრეჩოში და გადაიჭრა არასტაციონარული თბოგადაცემის ამოცანა. დადგინდა ღრეჩოში წყალბადის ალის გავრცელება/ჩაქრობის პირობა, რომელიც მნიშვნელოვნად მოქმედებს დეტალების (დგუშის, ცილინდრის) თერმული დაძაბულობების განმსაზღვრავ სასაზღვრო პირობებზე. აღნიშნული ამოცანა განსაკუთრებით აქტუალურია წყალბადზე კონვერტირებული ტრადიციული, სერიული ძრავებისათვის. ნაჩვენებია, რომ ჰაერწყალბადის საწვავი ნარევის შედგენილობის ცვლილებით შესაძლებელია ალის გავრცელების პროცესის მართვა, შედეგად კი წყალბადის ძრავაში თბური დანაკარგების შემცირება.

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