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A NUMERICAL STUDY ON THE TRANSITION CHARACTERISTICS OF AN INVERSE MICRO-SCALE DIFFUSION FLAME TO MICRO-SCALE PREMIXED FLAME UNDER HEAT RECIRCULATION CONDITIONS

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Abstract

In this investigation, the gaseous hydrogen peroxide (H_2O_2) is issued at the inner port, and methane (CH_4) is injected at the outer port of the sub-millimeter scale burner in order to establish an inverse CH_4/H_2O_2 micro-scale diffusion flame numerically under heat recirculation conditions. The velocity of gaseous H_2O_2 is considered only as a *numerical parameter* in this study and the velocity of CH_4 is kept constant to examine the flame structure and the transition behavior of an inverse micro-scale diffusion flame. The numerical simulation has been conducted using ANSYS Fluent 14.5 based on Finite Volume Method (FVM) under normal gravity (1G) conditions with low thermally conductive burners. The semi-detailed reaction model, which consists of 58 chemical reactions and 17 chemical species, has been applied in this study. It is found that when the momentum of the gaseous H_2O_2 is high, then a CH_4/H_2O_2 inverse micro-scale diffusion flame is formed, and this flame is attached just on the top of the burner by which one can easily analysis an active flame-wall interaction phenomenon. On the other hand, when the momentum of the gaseous H_2O_2 has been reduced significantly, then H_2/O_2 micro-scale *premixed* flame is established entirely inside the micro-burner. Furthermore, it is found that when the momentum of H_2O_2 reduces remarkably, then CH_4 does not diffuse inside the micro-burner at the flame zone, and consequently only H_2/O_2 micro-scale *premixed* flame is established there as H_2O_2 is playing the role of a monopropellant, where no extra oxidizer is needed for the survival of flames. This type of *flame mode transition* phenomenon under micro-burner systems is the *first ever reported event* in the literature of reacting fluid dynamics (i.e., combustion dynamics). Besides, this is the primary findings of our ongoing research, and hence, the further numerical calculation adopting different pertinent parameters is now under progress with the aim of extracting more profound physical and chemical insights that are associated with the aforesaid transition phenomena.

Keywords: Micro-scale, Diffusion flame, Premixed flame, Flame transition, Inverse flame.

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Introduction

The developments of miniaturized devices such as micro-robots, micro-gas turbines, and other small-scale portable devices have dramatically been increased over the past few decades in Micro-Electro-Mechanical Systems (MEMS) (Fernandez-Pello, 2002; Maruta, 2011). As a result, these devices have been an essential part of our daily life because of being lighter and smaller than standard scale. So, the high-density micro-power source is necessary to operate these miniaturized devices smoothly over a longer period of time. It is well-known that the typical hydrocarbon fuels' energy density is around 100 times higher than that of the most widely used advanced electrochemical lithium ion-batteries (Chen, 2007). Consequently, the hydrocarbon-based micro-scale combustion system is treated as a potential alternative candidate to the traditional batteries in supplying power to the above-mentioned micro-devices. To establish such potential combustion systems, a comprehensive understanding about thermal, and chemical structure, and their associated complex physical processes involved in a micro scale flame is necessary (Cheng, 2006). However, in such portable small-scale power devices, due to an inherent existence of high surface-to-volume ratio (S/V), the thermal quenching at the wall due to an excessive heat loss to the wall, and the chemical quenching owing to the destruction of key radicals at the wall (Chou, 2011) are extremely dominant factors. Consequently, the establishment of the stable flames in micro-scale systems is a non-trivial event. Therefore, it is an extraordinarily difficult task to control the stability of the micro-flames in small scale burner (Fan, 2012), which is still remained to be investigated in detailed. Hence, it poses a great challenge to the researchers and scientists. To overcome this difficulty, several types of fundamental combustion researches such as heat recirculation (Ronney, 2003), Swiss-roll configuration (Kim, 2005), and so forth have been proposed and studied by researchers and scientists. Besides, there are many such attempts are available in the literature; however, among them *heat recirculating combustion* has received a lot of attention at the small scale as it is automatically occurred phenomena (Rana, 2014). The diffusion flames are well-known excellent candidate for safety performance, applicable for a wide range of operating conditions, and the most common and fundamental types of flames. As a result, it has received a huge research attention as a 'flame model' in extracting practical flame characteristics (i.e., flame extinction, pollutant formation, microscopic structure of turbulent flame and so on) due to its simple geometrical configuration (Cheng, 2006). Therefore, to address the flame stability problem encountered in the micro scales, the researchers and scientists have been investigated in detail for the deeper understanding about the interrelated flame parameters and their influences on flame stability over the last few decades. The characteristics of micro-scale diffusion flame has been studied by Ban et al. (Ban, 1994) at the first time in the literature of combustion research by employing three types of fuels subjected to three kinds of burner diameters. They have observed that the effect of buoyancy is disappeared as the flame size is reduced, and the fuel diffusive transport process is balanced with the convective transport process. Later on, Ida et al. (Ida, 2000), and Matta et al. (Matta, 2002) have studied the micro-diffusion flame physics, and they have found that heat loss has a great influence on flame extinction limit. Nakamura et al. (Namura, 2006) have accomplished numerous numbers of studies on the structure and stability events of micro-diffusion flames, and Cheng et al. (Cheng, 2006; Cheng, 2006; Cheng, 2005; Cheng, 2008) have also investigated on the stability phenomena of micro-diffusion flames. They have elucidated the corresponding flame structures over the wide range of pertinent conditions. Recently, Hossain and Nakamura (Hossain, 2015) and Gao et al. (Gao, 2017) have been studied the heat recirculation assisted micro-scale diffusion flame (or, micro- diffusion flame) stability employing detailed chemistry. They found that the heat recirculation between flame and loading fuel via the burner wall through the conduction affects the stability of micro-diffusion flames and its structures over the wide range of operating conditions.

As summarized above, all of the studies have been devoted on the stability mechanism of the normal micro-scale diffusion flame (NMSDF) and its associated physical processes in detail. However, an inverse micro-scale diffusion flame (IMSDF) is a kind of diffusion flame where an oxidizer is surrounded by the fuel, which has not been investigated due to the fact of inherent flame stability problems at the small-scale diffusion flame. To the best of the author's knowledge, this is the *first attempt* in the combustion literature to investigate

the structure of an inverse micro-scale diffusion flame (IMSDF) and its *transition characteristics* to another mode of flames. The normal scale (i.e., not micro-scale) inverse diffusion flames (NSIDF) have gained enormous research attention and therefore significant number of studies have been done for the clarification of associated physical processes. It is well-known that the pollutants such as soot inception and its growth, soot precursor (PAHs) and so on don't exist inherently in the normal micro-scale diffusion flames, and this scenario also valid for an inverse micro-scale diffusion flame (IMSDF) as it is basically a micro-scale diffusion flame. Nevertheless, in fundamental and theoretical viewpoints, the stability and structure (i.e., thermal and chemical) of an inverse micro-scale diffusion flame (IMSDF) are very important to enrich the literature of micro-combustion, the associated theoretical development as well as improving the basic understanding of an inverse micro-scale diffusion flame (IMSDF) and its transition processes to another mode of flame at the small scale. At the present time, it is well-known that the miniaturization techniques have dramatically been increased over the past several decades in MEMS regimes for the development of various portable power devices, heating devices and so on. Since we have started to investigate the stability mechanism, thermal and chemical structures and the transition process of an inverse micro-scale diffusion flame (IMSDF) over the sub-millimeter scale burner, the findings of this study are expected to assist us in designing an efficient eco-friendly (i.e., free from carbon dioxide and carbon monoxide) micro-scale heating device by the proper arrangement of several single micro-scale IMSDF and this heating device is anticipated to be a very useful device in the regimes of medical technology, bio-technology, environmental technology, energy conversion technology, and so forth. Therefore, the above stated issues (i.e., an improvement of theoretical understanding, and innovation of a new eco-friendly portable heating device) are the motivation of our study.

Mathematical model and Numerical Approach

A set of partial differential equations which governs the mass, momentum, heat and species transports with multi-steps chemical reactions under two-dimensional (2D), axisymmetric and steady conditions is written as follows and these equations are principally the same as our earlier model (Hossain, 2015). It is worthy to mention here that our previous study (Hossain, 2015) was concerned with *normal* micro-scale diffusion flame (NMSDF). But, our present investigation focuses on the characteristics of an *inverse* micro-scale diffusion flame (*IMSDF*), which is completely different from our earlier study (Hossain, 2015).

$$\nabla \cdot (\rho \vec{u}) = 0 \tag{1}$$

$$\nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot (\mu \nabla \vec{u}) + \rho g_x, \tag{2}$$

$$\nabla \cdot (\rho \vec{u} T) = \frac{1}{c_p} \nabla \cdot (\lambda \nabla T) - \frac{1}{c_p} \sum_{i=1}^{N} h_i \omega_i, \tag{3}$$

$$\nabla \cdot (\rho \vec{u} Y_i) = \nabla \cdot [\rho D_i \nabla Y_i + \rho D_i^T \nabla (ln\, T)] + \omega_i, \tag{4}$$

$$p = \rho R_0 T \sum_{i=1}^{N} \frac{Y_i}{M_i}, \tag{5}$$

where $\rho, p, T, c_p, \vec{u} = (u, v)$, λ , μ, R_0, N and g_x are the density, dynamics pressure, temperature, heat capacity, velocity vector, thermal conductivity, dynamic viscosity, universal gas constant, total number of species, gravitational acceleration in x-direction, respectively and Y_i, h_i, ω_i, D_i, D_i^T and M_i are the mass fraction, enthalpy, production rate, mass diffusion coefficient, thermo-diffusion coefficient and molecular weight of species i , respectively.

The governing equations (Fernandez-Pello, 2002; Maruta, 2011; Chen, 2007; Cheng, 2006; Chou, 2011) as described above have been solved subjected to following initial and boundary conditions over a two-dimensional axi-symmetric computational domain that is designed in the cylindrical coordinate (***r–z***) system as shown in Figure 1 by applying Finite Volume Method (FVM) incorporation with SIMPLE algorithm under the platform of a multi-scales and multi-purposes commercial CFD (Computational Fluid Dynamics) package: ANSYS Fluent 14.5. The physical dimensions of calculation domain, and adopted boundary conditions for this simulation have been demonstrated in Figure 1.

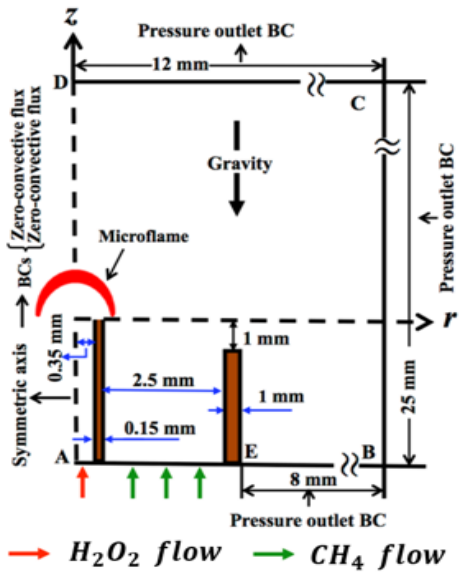

Figure 1. Schematic view of 2D, axi-symmetric calculation domain along with applied boundary conditions for numerical calculation.

As for the boundary conditions in detail, at the inner port and outer port, the inlet velocity boundary condition is applied. That is the gaseous hydrogen peroxide (H_2O_2) is ejected into the computational domain, filled with air (O_2: 21% and N_2: 79%) at atmospheric conditions (i. e., for this study, it is an initial condition), through the inner tube (i. e., burner) of diameter 0.75 mm and an outer diameter of 1.0 mm, and methane (CH_4) is injected at the outer port with inner diameter 5 mm and all other associated dimensions are shown in Figure 1. At the external port (EB), at the top of the burner (DC) and the external surface (BC) of burner wall, the pressure outlet boundary condition has been applied, and at the symmetric axis (AD), the zero-flux boundary condition is used for both velocity and scalars. At the bottom of the burner walls, the Dirichlet boundary condition for temperature field (T = 300 K) is used to allow the heat drainage from the domain. Also, the walls of the burner are treated chemically inert, and the conjugate thermal boundary condition is applied at the top-, outer- and inner-surface of the walls. No-slip condition for velocity field, and non-catalytic reaction scheme are applied on the surface of the inner-burner walls as well as outer-burner walls. The low conductivity burner (titanium) is considered here to enhance the heat recirculation (Ronney, 2003) between the flame and the loading of fresh fuel via the burner wall. A skeletal chemical reaction scheme, which is composed of 17 species and 58 elementary chemical reaction steps, is applied in the gas phase to carry out this study which was developed by Bilger *et. al* (Bilger, 1990). Each elementary reaction is of the type of the Chemkin formatted, which includes the value of the reaction rate constants of the Arrhenius equation (A, n and E). The thermodynamics data and transport data files are used from the database of the Chemkin package (Gao, 2017). Furthermore, the radiation effect has been neglected in this study as the radiation effect is found

to be non-dominating event for small-scale flames (Gao, 2017). The velocity of gaseous hydrogen peroxide (H_2O_2) at the inner port is considered as the numerical parameter while the velocity of methane (CH_4) at the outer port as presented in Figure 1 is kept fixed throughout this investigation under normal gravity condition. A minimum grid size of 0.025 mm is placed inside inner tube and also at the exit of inner tube, and the grid size is then gradually enlarged toward the outer boundaries of the computational domain. The flame transition phenomena that is the major findings of this study is found to be unaltered with respect to the decrease/increase of the grid size from 0.025 mm, and hence the grid size of 0.025 mm is emerged as an optimal size of the grid in terms of flame transition characteristics and computing resources of this study.

Results and Discussion

The structure and transition behavior of an inverse CH_4/H_2O_2 micro-scale diffusion flame, which is formed over a 2-D axisymmetric sub-millimeter burner (see Figure 1), has been investigated numerically by ANSYS Fluent 14.5 based on Finite Volume Method (FVM), adopting semi-detailed combustion chemistry subjected to heat recirculation condition. As shown in Figure 1, the gaseous H_2O_2 and CH_4 have been injected through the inner port and outer port of the burner, respectively, to establish an inverse micro-scale diffusion flame (IMSDF) over the sub-millimeter scale burner. At the extremely outer port, the chemically inert gas (N_2) is induced, due to the consideration of the normal gravity (1G) condition, automatically through the pressure outlet BC of length 8 mm at the bottom of Figure 1 by natural convection instead of issuing air to prevent the formation of the secondary flame between CH_4 flow and external flow of air. Consequently, the flow instability driven by the shear layer between H_2O_2 and CH_4 is suppressed up to a reasonable level so that the prime objective of this article is to the elucidation of flame transition characteristics can be done without any flow-induced difficulty. Due to the inclusion of semi-detailed chemistry, the current numerical simulation becomes extremely complex, too time-consuming and expensive in terms of computational resources. So, this simulation has been conducted using a high speed and parallel computing facility to reduce the physical computing time.

Figure 2 represents the thermal structure (white contours) and heat release rate for two different velocity conditions adopted in this study. It is found (see Figure 2a) that the CH_4/H_2O_2 inverse micro-scale diffusion flame is formed over the burner, which is attached just on the top of the micro-burner when the velocity of gaseous H_2O_2 at the inner port is 5 m/s. It is found in this case that both temperature contours and heat release rate (HRR) isopleths are attached to the top of the burner, which indicates the active burner wall and flame interaction are prevailed, and thus the heat recirculation process is enhanced. On the other hand, when the velocity gaseous of H_2O_2 is reduced to 0. 5 m/s, it is found that a tiny premixed micro-flame of H_2/O_2 is established entirely inside the burner (see Figure 2b). This H_2/O_2 premixed micro-flame is known as an *eco-friendly flame* as no harmful products (CO_2 and CO) are generated during combustion process. The temperature of this tiny flame is ~ 1588 K, which is seen on the white contours of the temperature located along the axis-symmetric line of the burner. It is worthwhile to state here that when the velocity of H_2O_2 is reduced to 0.5 m/s, then no mixing between CH_4 and H_2O_2 is occurred as CH_4 does not diffuse in the flame zone, which is located approximately 8 mm (see Figure 3) inside the burner as the pink colored curved indicates heat release rate (HRR) which is the location of tiny H_2/O_2 premixed flame zone. Thus, the potential readers may wonder that why this flame is termed as the small-scale H_2/O_2 *premixed flam*e, which is formed around 8 mm inside the burner from the burner tip? To the address this question, the readers have to pay their full attention on the chemical structures that formed at close vicinity of 8 mm (see Figure 3). It is obvious that the gaseous H_2O_2 is decomposed into the stable molecules: H_2, O_2, H_2O and unstable radical pools: O, H, OH, HO_2 at the vicinity of 8 mm and then they mix with others and consequently, the combustible gaseous mixture is produced at that location. Due to the presence of high temperature (> 1500 K), that is, under this favorable condition, H_2/O_2 micro-scale premixed flame is formed inside the burner (see Figure 3 for HHR and temperature profiles as the indicators of the location of H_2/O_2 micro-premixed flame) where as CH_4 is not

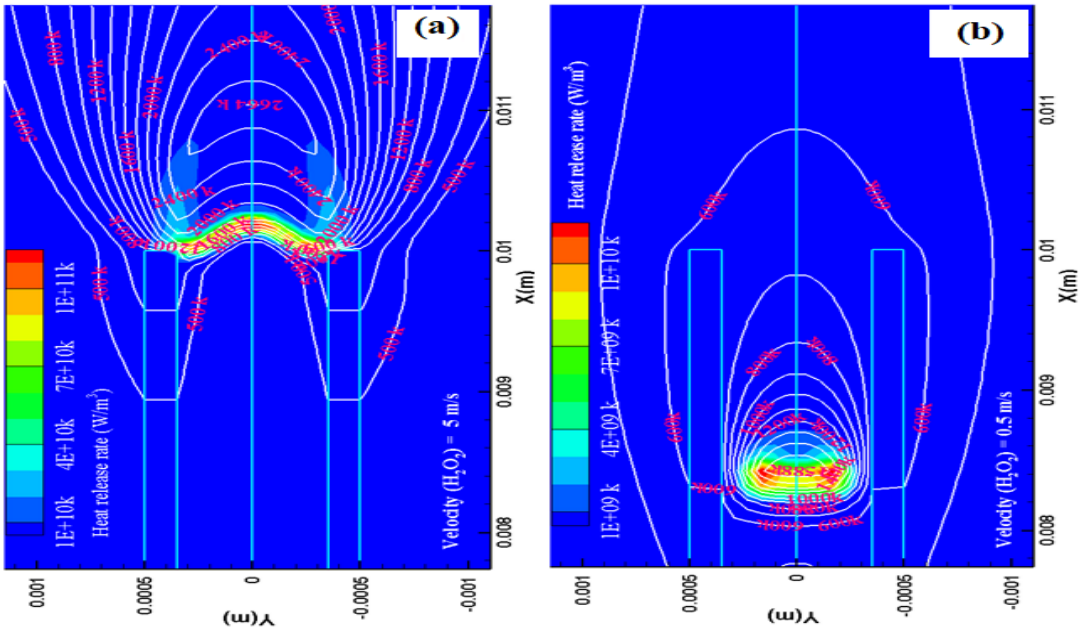

Figure 2. The distribution of temperature field (white contour) [K], and heat release rate [W/m^3]: (a) for velocity 5 m/s, and (b) 0.5 m/s.

available there, which is clearly seen in Figure 3. However, in Figure 3, it is seen that a slight amount of CH_4 is diffused inside the burner, but this small amount of CH_4 does not have chance to mix with products of H_2O_2 inside the burner (see Figure 3) as the location of the mass fraction H_2O_2 is far away from the mass fraction of CH_4. Therefore, H_2/O_2 micro-scale premixed flame is established inside the burner very easily as H_2O_2 is playing the role of a monopropellant, where no extra oxidizer is needed to establish this premixed micro-flame. Besides, it is evident in Figure 3 that the amount of H_2O_2 is reduced drastically at a location where the heat release rate (pink line) and temperature profiles are providing high peaks. These events prove the stable location of H_2/O_2 micro-scale premixed flame inside the burner 8 mm away from the tip of burner. This kind of transition phenomena (i.e., an inverse micro-scale diffusion flame to micro-scale premixed flame) and the establishment of a micro-scale premixed flame entirely in the burner are the *first-ever* reported phenomena in the literature of micro-combustion research and combustion research as well. In this study, when the injecting velocity of H_2O_2 is reduced from 5 m/s to 0.5 m/s, and then the corresponding the flame temperature is reduced from 2664 K to 1588 K (approximately).

However, this temperature, 1588 K at the velocity of 0.5 m/s is not a near extinction condition as this temperature is still pretty high regarding the extinction condition. It is believed that near extinction prevails under much lower temperature condition than that of 1588 K, which means that the velocity of H_2O_2 should be reduced further to reach the near extinction limiting condition. Therefore, a further investigation considering much lower velocity is now under progress in order to gain the profound insights of the aforestated transition phenomenon, its extinction limit and the elucidation of chemical reactions path analysis. Under such extraordinary lower of momentum of H_2O_2, where usually this type of tiny premixed flame is supposed to be experienced the extinction process. With the aim of the improvement of the fundamental theory as well as to identify the dominating chemical reactions for the survival of micro- scale H_2/O_2 premixed flame inside the micro-burner, further study is under progress now as the part of our whole targeted research.

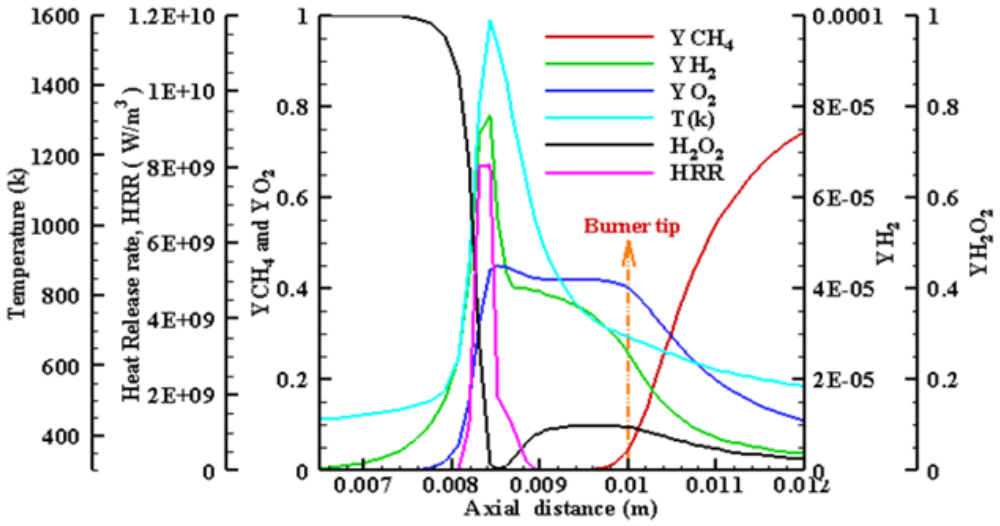

Figure 3. The distribution of temperature [K], different vital species, and heat release rate [W/m^3] for velocity = 0.5 m/s.

Hence, we are expecting that the outcomes of our ongoing research works will be reported elsewhere soon as the full journal article as well as the conference articles by selecting different pertinent parameters as appropriate.

Conclusions

In this work, a numerical study has been performed in order to elucidate the inverse micro-scale diffusion flame (IMSDF) of CH_4/H_2O_2, and its transition behavior to micro-scale H_2/O_2 premixed flame formed entirely inside the sub-millimeter micro conductive burner under 1G environment by employing a multi-scales and multi-purposes commercial CFD package: ANSYS Fluent 14.5 under heat recirculation mechanism. The combustion chemistry is modelled by the skeletal chemical reaction mechanism including 17 species and 58 elementary reaction steps. It is observed that CH_4/H_2O_2 inverse micro-scale diffusion flame is formed over the burner when the velocity of the gaseous H_2O_2 is high (i.e., 5 m/s), and in this case, the flame is anchored just on the top of the burner tip by which the flame-wall interaction phenomena can be promoted. Consequently, the heat recirculation process is accelerated which supports the flame stability process. In contrast, due to reduction of the velocity of gaseous H_2O_2 significantly up to 0.5 m/s, then H_2/O_2 micro-scale premixed flame is established entirely inside the micro-burner. It is notable to state here that when the velocity of H_2O_2 reduces, then CH_4 does not diffuse inside the micro-burner at the flame zone, and consequently H_2/O_2 micro-scale premixed flame is formed there as H_2O_2 is playing the role of a monopropellant, where no additional oxidizing agent for example air is needed for the survival of micro-scale premixed flames inside the burner. This flame mode transition phenomenon (TP) is the *first ever reported event* in the literature of reacting fluid dynamics (i.e., combustion).

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