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Research Article

Effects of the combustor size and the molecular diffusion on a methane air premixed microflame stability

S. Kenfack Lontsi†, O. T. Sosso Mayi ‡, M. B Obounou Akong† and S. Zekeng†

†Department of Physics, University of Yaoundé I, Cameroon, BP:812 Yaoundé, Cameroon
‡Department of Electrical Engineering, ENSET of the University of Douala, Cameroon.BP:1872 Douala, Cameroon

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Abstract

In this research work the effects of the cylindrical combustor size and the molecular diffusion on a methane air premixed microflame stability are investigated in order to highlight the parameters that most influence the given stability of the flame during microcombustion. A premixed methaneous–air microflame has been through a simulation-modelisation method was established as in a microreactor with a cylindrical configuration. Variable external diameters have been tested with a fixed thickness e = 200 µm and a length L = 10000 µm. The input dimensions of the micro-reactor considered are 2000 µm, 1000 µm, 500µm, 300µm and 200 µm. The results showed that the molecular diffusion coefficient influences the position, the formation and the shape of the flame along the micro reactor unpreviously. Indeed, when the inlet diameter of the reactants is reduced, the flame is shapely deflected from the inlet of the microreactor towards the inside of the reactor with a more bamboo appearance allowing a certain more or less intensive temperature redistribution along the micro-reactor walls. Nevertheless, the order of magnitude of the temperature does not suffer from any influence because of the stability of the coefficient of the molecular diffusion.

Keywords: *Micro reactor, microcombustion, molecular diffusion, combustion Size, flame stability.*

1. Introduction

The development of microtechnology has inevitably led consumers to a continuous miniaturization of the applications simultaneously with a growing of portable energy devices having a comfortable energetic autonomy. The various weight, autonomy and energy of batteries that met these needs have greatly favoured the development of microsystems for the production of energy using fossilic fuels. The demands for this new generation of micro-power sources of energy are increasing due to its higher energy density in comparison with conventional batteries (Rahaghi A. *et al*, 2010). Microcombustor is a key component of micro-power systems, which utilizes the oxidant-fuel mixture to release desired energy, which is fundamentally link to the quality and the intensity of the flame. Although recently, the development of micro power systems enable us to minimize the combustors size, the stability of the flame and the reduction of the dimensions of this type of device are not completely managed.

Unfortunately, the benefits arising at the microscale are overshadowed by major difficulties in creating working microburners (D.G. Norton *et al*, 2004). As a result of the reduced size of the combustors, combustion becomes less efficient due to the intensified heat loss from the flame to the combustor wall, radical destruction at the gaswall interface and reduced residence time, making the systems efficiency relatively low (A.C. Fernando-Pello et al, 2002; J. LI et al, 2009). Thermal quenching occurs when sufficient heat is removed through the walls, that combustion cannot be self-sustainable. Radical quenching occurs by adsorption of radicals on the system walls and subsequent recombination, which results with the lack of homogeneous chemical structure. The small scales of these systems make them significantly more suitable to both quenching mechanisms (D.G. Norton *et al*, 2003). In addition to this, the blowout can occur when the burner exit velocity exceeds the flame burning velocity (A. Linan *et al*, 1993) and all these disadvantages or challenges are due to the very small dimensions of the micro combustor, which leads to the establishment of a laminarly unstable regime. The small physical dimensions tend to lower the Reynolds number such that the flow is more likely to be laminar, implying that the beneficial effects of turbulent mixing may not be harnessed (Li Jun *et al*, 2009). All these listed difficulties, which weaken the stability of the micro-flame, show that several factors intervene, some of

*Corresponding author's ORCID ID: 0000-0001-9559-6123
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which have been identified, but others not yet elucidated nor determined.

Many efforts to investigate and propose the solutions to the problem of micro flame stability can be trace back to the previous works. (N. S. Kaisare *et al*, 2007) studied the stability of catalytic combustion of methane–air mixtures, focusing on the effect of an equivalence ratio and flow velocity of the thermal quenching. Ronney (P.D. Ronney, 2003) used a simplified model to study flame stability in heat recirculating Swiss-roll type burners. Sosso et al. investigated the effects of a simplified "one-step-overall-chemical-kinetic" equation on a microflame stability [8]. Raimondeau et al. studied the effect of the radical and thermal quenching of the flame propagation in microchannel. Norton and Vlachos (D.G. Norton *et al*, 2003; D.G. Norton *et al*, 2004). investigated the stability and thermal quenching of homogeneous premixed methane and propane flames in microchannels using a two-dimensional (2D) elliptic computational fluid dynamics (CFD) model. Leach and Cadou (T.T. Leach *et al*, 2006) used a simple heat resistor network analogy to obtain all the extinction limits of a microflame. (D.G. Norton *et al*, 2003) Shown that, overall heat management plays a critical role in determining homogeneous flame stability of the methane/air mixtures in microburner, all these studies and more (D.G. Norton *et al*, 2004 ; D.G. Norton *et al*, 2003 ; N.S. Kaisare *et al*, 2007 ; S. Karagiannidis *et al*, 2007 ; J.S. Hua *et al*, 2005) were focused globally on the effects of all design factors and operating conditions for the flame stability limits in micro-combustors. Despite the challenges solved in all aforementioned works, there are still a number of unanswered questions regarding flame stability at the microscale. While flame propagation at the microscale could be obtained, the interplay of kinetics and transport for what regards flame stability and combustion characteristics of these systems is still poorly understood (D.G. Norton *et al*, 2003).

If the flame propagation in such devices is now possible, it should be noted that the interaction between the kinetics and transport of the stability of the micro flame is weakly known (D.G. Norton *et al*, 2003), indeed the walls of micro burners react as destructive enthalpy in the homogeneous combustion zone, by lowering the temperature and thus delaying the kinetic mechanism, which may lead to the extinction of the flame (D.G. Norton *et al*, 2004) with the diminishing consequently the pressure and the heat content. On the other hand, with the very small dimensions (gap) of the device, the Reynolds number is low and the flow is essentially laminar, which eliminates the advantage of mixing the reactants through the turbulence process, then the diffusion becomes more difficult when the diffusion time increases, having a bad effect on the stability of the flame. These questions are of a great interest in this research work.

The aim of this work is to study the effects of molecular diffusion with the reduction of microburner's dimensions, taking in account operating conditions, the flame stability and others combustion characteristics. In order to understand how a microflame within different microreactors behaves when reducing more and more its dimensions, the recirculation of the heat, the flames form and its nature are also investigated.

2. Methodology

Fig. 1 shows the cross-sectional view of the micro-channel (cylindrical tube) in which a steady-state combustion of a CH_4–air mixture takes place. The origin is fixed at the center of the inlet plane. x depicts the axial or downstream distance, and r represents the radial distance or the distance from the centerline of the cylindrical tube or 2D parallel plates, respectively.

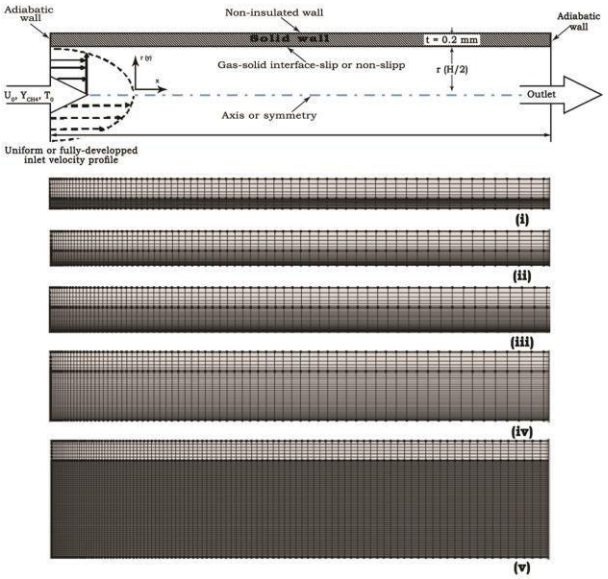


Fig.1 (a) computational domain along and (b) Mesh used in these simulations with different combustors sizes: (i) d=200 µm (2000 nodes), (ii) d=300 µm (2400 nodes), (iii) d=500 µm (3300 nodes), (iv) d=1000 µm (4200 nodes), (v) d=2000 µm (18900 nodes).

Premixed mixture methane/air feeds a cylindrical microreactor, whose dimensions vary between: 200 µm and 2000 µm for the size and a length of 10000 µm, as shown in Fig. 1 (a), with alumina walls of 200 µm thickness. The input velocity of the reactants is 0.5 m/s. All calculations are made using COMSOL 4.2a software (COMSOL Multiphysics, 2008). Since we assume that the component of the swirling velocity is zero, we can only study the centerline of the microreactor symmetrically. To reduce the computational time, only half of the reacting zone will be considered. Moreover, we consider that there is no Dufour effects (T. Mantel *et al*, 1996), no gas radiation (D.G. Norton *et al*, 2004 ; D.G. Norton *et al*, 2003), no

work done by- viscous forces and pressure, and steady state conditions are prescribed.

To study the reactive flow, we first use the COMSOL's module named reaction engineering, which sets the selected chemical mechanism and the analysis of combustion with the help of plugflow model of the reactor. During this step, all thermodynamic and transport data are required to achieve successful combustion processes as shown in Fig. 1. The second step consists of evaluating the transport species, heat transfered in the gazeous phase and solid walls, and in the optimal flow regime by using the multi-physical coupling of reaction engineering module with the transport and concentrated species, heat transfer and laminar flow modules.

2.1 Reaction Engineering module

Reaction Engineering Module is the module used to study chemical kinetics in different reactor models and sets up the chemical kinetics mechanism. Thermodynamic and transport parameters are calculated through the chemical equations and equations (1), (2). In our study, we have chosen an adapted single-step reaction rate of Mantel (C. Jensen *et al*, 2003) and five species namely hydrocarbon, oxygen, nitrogen, carbon dioxide and water. The chemical kinetic model that we use is:

(/) ( ) (1)

The source term is given by the following reaction rate equation:

1. ∏ (2)

2. (—) (3)

In the equations (1) and (2), (/ /) is the reaction rate of j gaseous species, in our work is methane, (/)the reaction rate is constant, (consistent unit) is the pre-exponential factor, (J/mol), is the activation energy (8.314 J/mol/K) is the constant universal gas , (K) is the temperature in Kelvin, c (/) is the molar concentration, a and b are the concentration exponents or the partial orders of the reaction. The Arrhenius parameters, , , are given by [13].

2.2 Numerical Modelisation

- The flow of the fluid along the wall during axial displacement in the reaction is described by the Laminar flow module with the equations of continuity and momentum (4-5). As Reynolds number is less than 2000, the flow regime is laminar,
- The Heat transfer module in the fluid is defined by the equation of energy (6). It evaluates the heat transfer through the fluid along the walls during the axial displacement in the reaction.
- Transport and Concentrated species Module determines the transport of species by defining the transport coefficients. Here, we study diffusion convection phenomena and manipulate the mass fractions. This module helps to solve the equation of conservation of transport species (7-8).

The 2D governing equations are defined as follows:

— ( ) (4)

— ( ) * (( ))

– ( )) (5)

— ( ) (6)

( ) (7)

(—— —) (8)

(9)

Σ (10)

(∑ —)

—

In these equations, ρ (kg/m^3) is the density of the reactants, μ the dynamic viscosity (Pa.s) , k(W/mK) the thermal conductivity, C_p (J/kgK) the specific heat , M_n (kg/mol) is the molar mass of each gaseous species, p (Pa) is the pressure. H_{sr} (J/mol) is the enthalpy of formation of species, the mass fraction w_i and D_{jk} (m^2/s) are the multi component Maxwell-Stefan diffusivity.

The 2D governing equations are discretized by the finite element method and solved by Comsol 4.2a (COMSOL Multiphysics, 2008). The equations are solved implicitly with a separate 2D solver using a method of relaxation, while computing the first equations of momentum and the continuity, all followed by an update of the pressure and mass flow, energy and transport species equations. For all equations, the criteria of convergence for residuals are fixed at……The gas density is calculated using the ideal gas law. The thermodynamic parameters are based on the average of the mass fraction of each of the gaseous species.

The boundary conditions are taken as follow: at the inlet a linear velocity of / , This velocity is choosen because it is close to the combustion speed of methane (0.40 m/s), it constitutes one of the parameters of the flame stability in a microreactor [26]. The inlet temperature is uniform and evaluate at 300 K. The mass fraction = 0.054, the equivalent ratio of the fuel is such that ϕ = 0.9, The composition of the mixture is choosen according to the fact that quenching distance for a stoichiometric composition is lower than that of lean mixtures (T. Takeno *et al*, 1993 ; J. Li *et al*, 2009), no-slip boundary condition is imposed to a solid-fluid interface where u = 0 m/s, the heat flux is

calculated from Fourier's law, the continuity of the temperature and the heat flux creates the link between the gas and the solid phase. A non-regular mesh is used in all our stimulations. More nodes are concentrated close to the inlet reactor and around the reactive zone. The computations were performed with 5400 nodes (Fig. 1(b)).

3. Results and discussion

In the present work, the effects of the combustor size and of the molecular diffusion on the micro-flame structure, central axis and wall temperature are simultaneously investigated numerically to explore the different characteristics of the flame stability at the micro-scale. The tests are done as follow; first of all the combustors sizes are reduced from 2000 µm to reach 200 µm with a constant molocular diffusion parameter, during these tests the behaviour of the flame is scrutinized and its different characteristics determined. Then the molecular diffusion parameter is changed and made varied between / , / , / , keeping the same dimensions of the micro combustor as below. The flame structure is monitored and compared to one of the flame taken as our reference case.

3.1 Reference case

In this section, two works J. Li *et al*. (J. Li *et al*, 2009) and D. G. Norton, D. G. Vlachos (D. G. Norton *et al*, 2003) (detailed and simplified kinetic mechanisms) on the microflame of the premixed methane-air mixtures for different gap are chosen as a framework to compare and assess with the relevant of our simulations results. D. G. Norton, D. G. Vlachos studied the flame characteristics within three rectangular microcombustors with 1000 µm, 600 µm, 400 µm. In our study we have chosen cylindrical microcombustors for our simulations, knowing that the relevant study of J. Li et al. has been chosen as a reference case as a bridge between the two works that mentioned above. The geometry is another important factor for microcombustors design. Cylindrical tubes and model of 2D parallel plates employed to represent the rectangular channels are the two commonly used geometries. In the simulation, the spacing (H) between the plates is taken to be the gap of the fuel entrance, same as the inner diameter.

The simulations done by D. G. Norton, D. G. Vlachos have been conducted for a few microburner dimensions (400 µm, 600 µm, 1000 µm, and 4000 µm). Here the authors compare the combustion characteristics in microburners by varying the separation distance between the two plates. For large separation distances, such as the 4 mm case, the reaction rate is observed to be low and spreaded out over approximately 5–6 mm of the burner. This is because at the walls of the microburner where ignition started towards the centerline we have a slow heat transfer due to the existence of unburned mixture. The reaction is more localized, with greater intensity, for smaller separation distances, such as the 600 µm case causing steeper temperature and higher composition gradients. When the distance was reduce (e.g., 400 µm), the transverse length scale of the fluid is reduce considerly such that the transverse heat transfer influence the centerline temperature hence the maximal fluid temperature. The maximal fluid temperature is significantly lowered for this case, as compared to larger separations. Consequently, incomplete conversion is observed. Combustion becomes difficult for diameters equal to 400 µm and less due to the increased transverse heat transfer until a point where combustion become impossible. A distance of the order of 100 µm was experimentally determined by Jensen et al. for materials that do not adsorb radicals. Here appears that an optimum plate separation, of approximately 600 µm, is the one that exhibits the shortest flame location. This distance permits to the wall to preheat the inlet fluid faster.

J. Li *et al*. showed that the flame temperatures in the cylindrical tube are higher than those in the 2D planar channel and justified it through the action of radial diffusion, heat recirculation and incomplete combustion. Their simulations done in the rectangular microreactor with gap H= 1mm presented higher flame temperature than the cylindrical microreactor with d = 1mm over the entire velocity range, owing to the difference of the hydrodynamic diameter. However, in the same logic, the cylindrical tube with d = 2mm which has the same hydrodynamic diameter, the 2D channel with H= 1mm also gives higher flame temperature. Joined to the factors discussed above, the difference in terms of heat loss area between the two geometries could be another reason. In addition to the latest statements, they showed that the quenching distance for the parallel plates is related to that of the cylindrical tube by a factor of 0.65. In other words, when H= 0.65 d, the heat loss condition of a cylindrical tube is identical to the one of a 2D planar channel. They concluded that the factor of 0.65 is applicable in micro-combustors sized up to 1mm diameter.

In view of all that proceeds, compared to the simulations that we carried out in cylindrical microreactor with diameters of 2000 µm, 1000 µm, 500 µm, 300 µm, 200 µm, we can deduce that the gaps of similar rectangular micro combustor are 4000 µm, 2000 µm, 1000 µm, 600 µm, 400 µm.

3.2 Structure of the microflame

Five micro cylindrical reactors with different diameters were tested using one-step global chemical kinetic models to simulate the resulting stable methane micro-flame. The realized simulations showed that; in all the microburners (2000 µm, 1000 µm, 500 µm, 300 µm, 200 µm) the flame shapes are completely different one from another as we can observed on the Fig. 2.

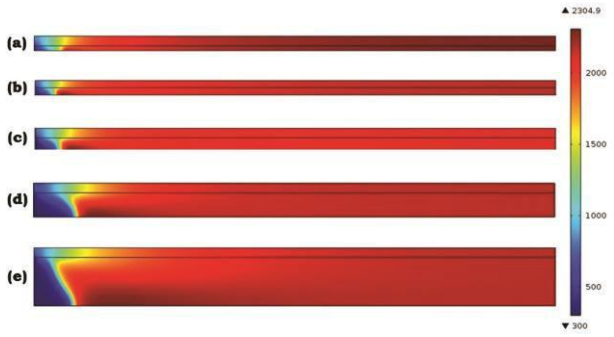


Fig. 1 Results of flame simulation giving heat distribution within the micro reactor with different combustors sizes; (a) d=200 µm, (b) d=300 µm, (c) d=5400 µm, (d) d=1000 µm, (e) d=2000 µm.

The micro-flame obtained with the micro reactor whose diameter is 2000 µm is shown in the fig. 2(c), the stable micro flame developed with a particularly so called " half bamboo shoot shape" is observed at the inlet after a cold fluid accumulation zone. *Hackert et al.* [15] investigated the flame shape and propagation speed in parallel plates and cylindrical ducts, and observed that the flame is a tulip-shaped one in the microchannel. However, the same convex micro-flame is found in the previous works of *Li et al.* (J. Li *et al*, 2009). The developed thickness of the micro-flame can be estimated arround 1.6 mm, which is in the same order of magnitude of the thickness value of the micro-flame produced with gaseous fuel. The mass fraction of methane is shown in fig. 5, and it is clear that entire methane is consumed in the combustion zone. The reaction rate of methane is 20000 kgmol/m^{3}at the inlet, and only after 1000 µm it becomes zero as observed on the fig. 4 while at the same time the mass fraction which is fixed 0.055 remains quite constant as sketched on the fig. 5 at the entrance of the micro reactor, as further as we go beyond the zone of accumulation of the cold fluid, its value drops drastically and becomes zero after the flame thickness. Among all the obtained flame, intensifies the delay in the flame generation is the most important in the microreactors with the highest diameters, although the temperature may be the highest one.

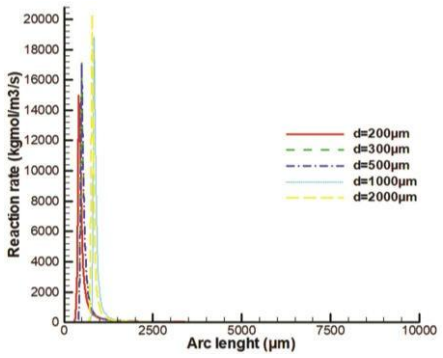


Fig. 4 Reaction rate profile along with the axial displacement of micro reactor with different combustor size

That flame may ensure the warming of the walls, and therefore the heat redistribution. Heat spread out in the microgenerator device plays a key role for the auto ignitions of cold penetrate gases. So, the dead zone observed at the entrance of a microreactor can be explained by the fact that, with the large gap of the micro reactor, the rate mass of fluid is important and absolutely needs an important quantity of heat to increase the average temperature of the fluid, what is obtained values higher than 700 µm. In fact, the concentration exponents meeting the reactive stoichiometric coefficients of the methane combustion, could explain the entire methane oxidation inside the reaction zone.

Others predicted flame obtained in the Fig. 2 have the same half bamboo shoot shape for the micro reactors with diameters equal to 1000 µm, 500 µm, 300 µm. All the particularities observed are quite the same; dead zone is observed at the inlet, before reaching the combustion zone where the fluid is consumed. The rest of the micro reactor or the post-combustional zone is warmed by the gases and the heat recirculation throughout the walls assuring the heating of incoming gases and their self depending ignition.

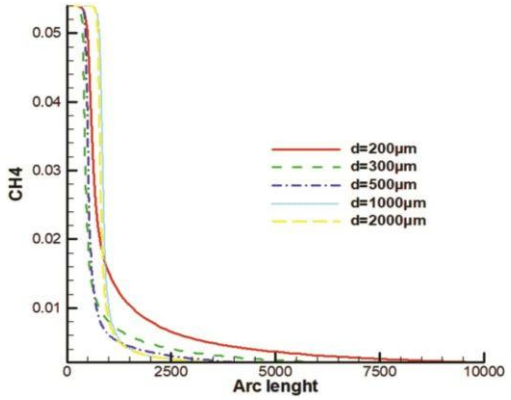


Fig. 5 Methane mass fraction profile along with the axial displacement of micro reactor with different combustors sizes

It's also possible to observe that: as the temperature decreases, the dead zone increases due to the lack of sufficient heat recirculation trough the walls. The thickness of the flame also drops as the diameter decreases and the flame formation is located in a restricted area. That phenomenon is highlighted in a smallest microreactor where the flame is quite represented by the very hot dot point. The combustion zone is extremely narrow and the so called blowout revealed by D. G. Norton, D. G. Vlachos (D. G. Norton *et al*, 2003) is observed within the post combustion zone. The temperature observed at the post combustion zone is upper than at the other two zones fact that means that the combustion still continues in the rest of the microreactor during the blowout phenomenon.

The redistribution of temperature and the shape of flames obtained in the microreactor are almost similar to the one established in previous works of Norton and Vlachos (D. G. Norton *et al*, 2003) who studied the structure of microflames within the rectangular microreactors with the gap dimensions L_w of (a) 4000 µm, 1000 µm (b) 600 µm, (c), and (d) 400 µm. With the link established by J. Li et al. (J. Li *et al*, 2009) between rectangular and cylindrical micro reactor, it's possible to compare the both flame's structures. We noticed that for a biggest rectangular microreactor the dead zone has the similar form like the one we obtained with a cylindrical microreactor, the preheated reactive zone is also quite the same, nevertheless if in the rectangular microreactor the boundering of the combustion zone hide the flame formation, it's quite the same thing which happened in the use of a cylindrical microreactor with a little difference because here the flame zone is visible. Within others microreactors, with a reactant gap equal to 1000 µm (b) 600 µm, (c), and (d) 400 µm corresponding for cylindrical microreactor to diameter equal to 500 µm, 300 µm and 200 µm the structure of the flames is quite similar, this fact means that, the form of the flame, the dead zone, the heat recirculation throughout the walls, the flashback and even the dot hot point in the smallest microreactor have same similarities. Furthermore this aspects shows that the link highlighted by J. Li *et al.* between the two types of commonly used microreactors as models by researchers is relevant.

It's important to note that all the predicted flames were simulated with a constant molecular diffusion coefficient equal to / , chosen in the literature as one of reliable one by using one step chemical kinetic models.

3.3 Effect on the central axis temperature

The sketched variation of the temperature profiles is presented at the Fig. 3 where are drawned five profiles of temperature linked with the simulated diameters of microreactors. The results illustrate the axial temperature of reactive evolution within the microreactor.

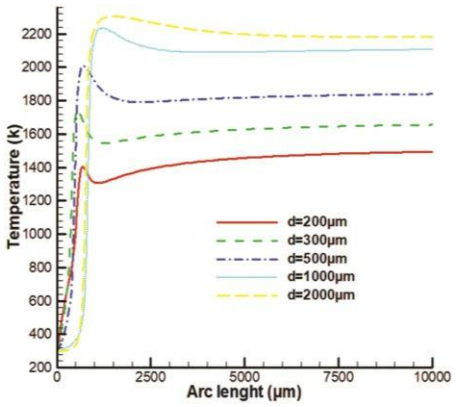


Fig. 2 Temperature profile along walls with the axial displacement of micro reactor with different combustors sizes

The temperature profile obtained with the biggest diameter equal to 2000 µm is shown on the Fig. 3 in a yellowish color, the initial inlet temperature of premixed methane-air mixtures is 300 K, and the temperature begins to increase with 0.5 mm of diameter. The temperature rapid growth in a narrow space, barely 0.25 mm, along walls preheats the reactant. Once the temperature of the reactant reaches approximately 950 K, the ignition switches on the reactive mixtures. Then, the micro-combustion occurs extremely rapidly, and the central axis of temperatures at x = 2.5 mm reaches an extreme point of 2300 K, which is greater than the CH_4 adiabatic flame temperature (about 2130 K for φ = 0.9). The heat propagates within microcombustor as well as along the walls, then the temperature drops to 2200 K at x = 4.5 mm then, stabilizes and remains quite constant until the outlet. The temperature profile obtained is almost similar to the previous works of Norton and Vlachos (D. G. Norton *et al*, 2003) which have first shown that the temperature remains at higher value.

The temperature along increase obtained with the microreactor with a diameter equal 1000 µm along the central axis and walls is shown in Fig. 3 with a lime green color. As observed, the temperature profiles show the slow ascendantal growth at the inlet, indicating a delay in the mixture's ignition and the temperatures of the incoming cold reactants are maintained at 300∼400 K over a diameter approaching 0.5 mm. Thereafter, the temperature rises up constantly to x = 0.5 mm and x = 0.750 mm, when the ignition occurs. The complete combustion occurs quite at x = 0.8 mm, here the flame temperature reaches a maximum of 2200 K. The position of the flame quenching is at x = 2.4 mm where the temperature a little bit decreases to reach 2100 K , while the temperature is still at 2100 K, its value is almost kept constant, we observe its mitigated increase at the outlet. But globally the two first profiles of temperature described present the same form with the dead zone located at the same dimension in comparison with the situation at the inlet, the flame occurs quite at the same area and despite an inflexion point appearing in the temperature profile of the microreactor with d=1000 µm the rest remains similar. It's important described to notice that, the above microreactors with this choosen dimensions are not often considered as microreactor.

The temperature increase obtained with the microreactor model with the diameter equal to 500 µm along the central axis is shown in Fig. 3 in the blue color. The mixture temperature at the inlet is 300 K, and it undergoes an abrupt change almost from the inlet. The maximum temperature value is reached quickly at 2000 K at 0.5mm from the entrance, that clearly prove that the rewarm of cold fluid is effective, barely reached, then the temperature drops to about 1800 K and remains almost constant until the outlet. The temperature is generally considered as one of the most significant features to characterize the combustion process and behavior. The micro-

combustion characteristics have been identified three major zones, i.e. pre-heating zone, combustion zone and post combustion zone (T. Mantel *et al*, 1996; COMSOL Multiphysics, 2008). In the present work, the aforementioned three zones can be observed in that case.

The temperature inside the micro reactor with a diameter equal to 300 µm plot with the green color in the Fig. 3 shows that the temperature of fluid increases to reach the maximum of 1750 K at the axial distance at 0.5 mm from the entrance, then decreases slightly to 1600 K. The profile of CH_4 reaction rate is shown in Fig. 4, which appears that the CH4 combustion is very rapid despite the small micro-flame thickness but when we observe the methane mass fraction in Fig. 5, we can notice that there is still the presence of the reactant after the reaction zone, what can easily explain why the combustion still continue to be maintained at the outlet of the microreactor with the contribution of the warm coming from the walls;

The temperature inside the smallest microreactor plot with the red color in the Fig. 3 shows that the temperature of fluid begins to evolve from the entrance of the microreactor and reach a maximum of 1400 K at the axial distance at 0.65 mm from the entrance, and then decreases slightly to 1300 K. Just After the release of the energy contained in the mixture characterized by the hyot dot point, in the context of micro-combu stion, it is necessary that understanding the flame temperature for the proper selection of wall materials to micro power system (Niazmand H. *et al*, 2008; Renksizbulut M. *et al*, 2006; Mlcak J. D. *et al*, 2008). After dot hot point we can observe the inflexion of the plot illustrating the rapid decrease of temperature and its sudden rise in temperature slightly closed to that of combustion, 1450 K which remains constant until the outlet of the microreactor. The profile of CH_4 reaction rate is shown in Fig. 4, where appears that the reaction rate of CH_4 is very limited about 8000 kgmol/m3 due to the small gap of cold fluids mixture entrance. Nevertheless when we observe the methane mass fraction in Fig. 5, we can notice that there is still an important quantity of reactant after the reaction zone, all the mixture is burnt so as at the bottom of the microreactor. In this case, the heat flashback risk is high, because the gaseous phase reactive zone is relatively narrow. The micro-flame obtained has the micro-flame has a shape's pic and the highest temperature zone is mainly located near the inlet. The mass fraction of methane is shown in Fig. 5, prove that the conversion of methane is partial and highly incomplete.

D. G. Norton, D. G. Vlachos did very early a relevant work where they studied the structure of the flame inside the rectangular microreactors with different gaps, 4000 µm, 2000 µm, 600 µm, 400 µm. Our study was realized in the cylindrical microreactors with also different diameters namely 2000 µm, 1000 µm, 500 µm, 300 µm, 200 µm, with the target to analyze if the two common used microreactors have a link as Li *et al.* show in a previous study (J. Li *et al*, 2009). We can assert from what clearly appeared in our study that there are several similitudes and the both micro reactors are crossed by almost the same magnitude of temperature, the structure and the location of the flame are the same, and the phenomena as blowout or flashback are distinguished in the phenomena as the blowout or the flashback are distinguished as the same in each respective microreactor.

3.3 Effect of molecular coefficient diffusion on flame structure and on the temperature.

The effects of the molecular diffusion are studied throughout two parameters, the structure of the flame and the temperature of the mixture following the central axis of the diffusion of the heat.

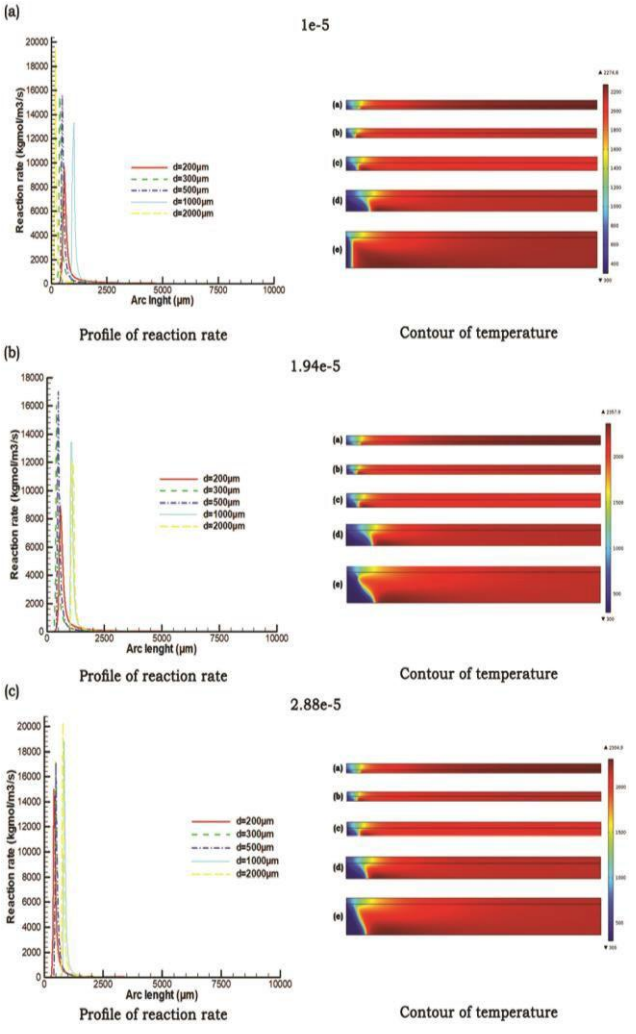


Fig. 6. Results of flame simulation giving heat distribution and reaction rate within the micro reactor with different diffusion parameters; (a) k=1e-10m2/s, (b) k=1.94e-5m2/s, (c) k=2.88e-5m2/s

Three coefficients of molecular diffusion are chosen and gradually change to simulate the flow of the reactants within the microreactors. These coefficient are / , / ,

/ . The last coefficient is recommended in the literature [28], the second is proposed by COMSOL software once you determined the modeling of your system and the first coefficient is chosen deliberately. The simulated micro flame are presented in the Fig. 6 composed of six figures showing the behavior of the flow reactants in the five different microreactors chosen during our work. Among all these figures, there are sketches of the reaction rate of the methane and of the different flame structures.

The Fig. 7 presents the axial temperature of the different microreactors for each molecular diffusion coefficient. The predicted flame with a molecular diffusion coefficient equal to / has already been presented, discussed and established basical for our work whose results have been compared with those of the reference cases. The two remaining predicted microflames have been compared using previous discussed results.

The predicted flame structure clearly shows that all the microflame zones namely, the preheated, the combustion and post combustion zones are broadened, and the dead zone in all the cases are shifted inside the microreactor except in the case of a larges diameter with the molecular diffusion coefficient equal to / . In this specific case an uncommon situation is observed: the flashback is established and the flame is stuck to the reactor inlet, that situation solely happen with a large reactor, unexpected in the case of mesocombustion. What concern for the combustion zone, we noticed the thickening of the microflame in all the cases while the molecular diffusion is decreasing. This fact makes possible to infer that, the molecular diffusion coefficient has an impact on the microflame especially in what concerning the flame form and the flame location. Indeed the decrease of the coefficient of molecular diffusion leads to the displacement of the combustion zones inside the microreactor and to the deformation of the microflame which is thickened. The nature of the microreactor walls could be chosen according to the molecular diffusion coefficient, chosen and to the reinforcement of the walls at the level of the potential combustion zone of the microflame.

Concerning the temperature of the reactants on the central axis, the results obtained are explicite and show that the molecular diffusion coefficient does not have any impact on that parameter. In all the predicted cases, the order of magnitude of the temperature hardly changes. In the five microreactor models, the plots obtained are quite similar and no particular point is observed, except the case of flashback highlighted previously which occurred in the mesoreactor with the diameter equal to 2000 µm when the molecular diffusion coefficient is minimal.

The contribution of the molecular diffusion coefficient was not yet fully understood in the case of micro-combustion, some studies in the field alluded about it, however it must be recognized that this parameter proposed in certain software has not really been a brake in the evolution research following in this domain. The study that we present here gives us a little more informations and makes it possible to understand that the order of the magnitude of the temperature which is one of the fundamental parameters in combustion does not suffer from any influence because of the coefficient of the molecular diffusion.

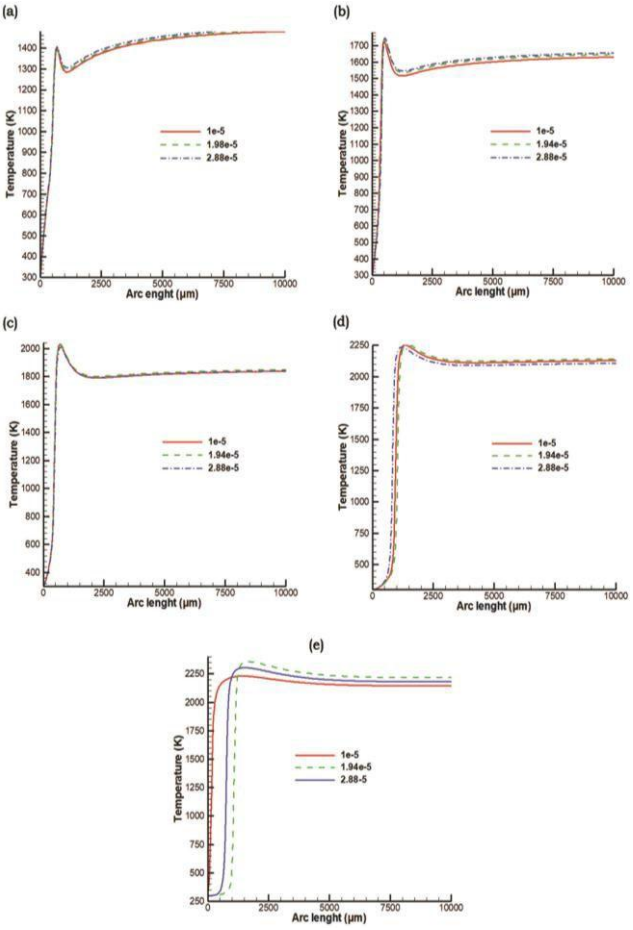


Fig. 7 Temperature profile along with the axial displacement of the micro reactor with various diffusion parameters in different cases of combustor size; (a) d=200, (b) d=300, (c) d=500, (d) d=1000, (e) d=2000. The diffusion parameter is k=2.88 e-5m2/s

Conclusions

Characterizing the combustion process, the flame temperature and structure are important parameters especially in the micro-combustion, they are the master tool for the flame location and the judicious choice of the walls material. Numerical investigations of the premixed methane-air flame were carried out to analyze the effect of the gap dimension in a circular microreactor and the impact of the molecular diffusion on both the flame temperature and its location. Five models of microreactors with different diameters 2000 µm, 1000 µm, 500 µm, 300 µm, 200 µm have been tested. In the same time three molecular diffusion coefficients / , / ,

/ have been applied in all the microreactors simulated. The micro-flame structure along the central axis and reactants temperature has been analyzed. A comparison study between rectangular and cylindrical microreactors has been done with the help of the existing results found in the literature. In the results it clearly appear that the molecular diffusion coefficient has a significant effect on the micro-flame shape, that the bamboo shoot shape can be observed, and that the flame location is also modified by using the different molecular diffusion coefficient. The micro-flame obtained by the smallest microreactor presented a very hot spot or an extreme hot dot point, consequently increasing a blowout risk. The different temperatures obtained confirmed that the decreasing of gap dimension leads to the lowering of the temperature. However, we noticed no impact of the molecular diffusion coefficient in all the cases studied. Our study also highlighted that the link between the rectangular and circular microreactor is relevant, all the predicted flames, their structure as well as their location are quite similar, even though the order of magnitude of the temperature is closed.

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Nomenclature

	Reaction rate of j species	(/ /)
	Reaction rate constant	(/)
	Pre-exponential factor	(consistent unit)
	Activation energy	(J/mol)
	Universal gas constant	(J/mol/K)
	Temperature	(K)
	Molar concentration	(/)
	concentration exponent	
n	Temperature exponent	
k	Thermal conductivity	(W/mK)
	Specific heat	(J/kgK)
	Molar mass	(kg/mol)
	Pressure	(Pa)
	Enthalpy of formation	(J/mol)
	Multi component Maxwell-Stefan diffusivity	(m^2/s)
	Mass fraction	
	Parts per million	ppm
	Cubic foot per minute	cfm

Greek letters

ρ	Density	(kg/m^3)
μ	Dynamic viscosity	(Pa.s)
ϕ	Equivalence ratio	
δ_r	Flame thickness	(m)

Subscripts

j	Specie

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