Micro Combustion Chambers for UAV propulsion

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Abstract

Recent developments in the fields of micro-technologies increased the interest on system miniaturisation. The main objective of this thesis is to study how a geometric parameter and two thermal parameters affect flame structure. A numerical study of a 2D laminar ($0.5 \text{ m/s}$), lean ($\phi=0.9$), CH$_4$–air premixed flame in a micro-channel is performed in the commercial software COMSOL Multiphysics®. The effect of channel’s height (0.4, 0.6 and 1 mm), solid wall thermal conductivity (adiabatic, 2, 10 and 50 W/(mK)) and a distributed power loss in the wall (5 and 20 W) are evaluated. Several quantities are analysed: temperature, velocity, methane mass fraction and reaction rate. A decrease in the channel’s height from the baseline case (1 mm) to the critical case (0.4 mm) induces a reduction of temperature and velocity of 36% and 45% respectively, which leads to lower values of methane conversion across the channel. A change in flame shape is observed with the increase of thermal conductivity, being that three types of flame shapes can be distinguished: concave, flat and convex. Besides this, it is possible to observe that the lowest thermal conductivity leads to localized temperature peaks. Imposing a distributed power loss of 20 W in the wall of the channel, it is observed a decrease of 45% and 27% in velocity and temperature respectively, when compared to the baseline case, translating into a maximum methane conversion of 52%.

Keywords: Micro-combustion, premixed flames, numeric analysis, fluid mechanics, methane.

1. Introduction

Recent developments in the fields of micro and nano technologies increased the interest on system miniaturisation, which is translated into the development of portable and multifunctional systems with applications in many areas. Traditional battery technology offers supply systems that are too heavy and have low functioning times. Compared to these, micro combustion-based devices present higher energy densities [1] as shown in Figure 1.

![Figure 1: Comparison of specific energy densities of lithium ion batteries with hydro-carbon and oxygenated hydrocarbon fuels as well as different engines [2].](image)

From an environmental perspective, these systems present flaws in the fabrication and disposal processes. In 2016, in Australia, no recycling of lithium-ion batteries was performed, and 98.3% of lithium-ion portable batteries ended up in landfill. Increasing the amount of waste requires more land area for disposal, and adds to the amount of harmful chemicals that eventually re-enter the environment [3].

Pollutant emissions are highly associated to the use of combustion. While accurate, given the small size of the devices considered, carbon dioxide (CO$_2$), water vapour (H$_2$O) and heat emissions are comparable to those of an human being. On a negative note, these micro-systems are likely to have smaller efficiency than the ones found for conventional devices. This is translated in a comparatively large fractional production of unburned hydrocarbons, as carbon monoxide (CO) and other product of incomplete combustion generating the need for post-combustion treatments.

Micro-combustion systems also gained interest when high-precision fabrication of devices in the centimetre-scale evolved. New micro-fabrication techniques appeared, such as Electro Discharge Machining (EDM), Laser Beam Machining (LBM) and Focused Ion Beam Machining (FIBM). Devices in the millimetre scale range are being fabricated using Micro-Electro-Mechanical Systems (MEMS), rapid prototyping and batch-manufacturing techniques [4].

In the aerospace industry, this technology is being considered to plan space missions and aerospace projects. In these projects the launch phase is highly
correlated to the mass budget and is one of the segments that has more impact when it comes to project cost. Taking this into consideration, it is extremely important to reduce system’s mass in order to optimise these processes. The development of these engines is attributed not only to aviation modellers, but also to be used on the production of micro turbojet engines for the propulsion of contemporary drones, the Unmanned Aerial Vehicles (UAV) or Unmanned Aerial Systems (UAS) [5]. Some examples of Micro Turbine Engines (MTEs) already produced are pictured in Figure 2.

2. Objectives

Micro-combustion has great advantages and follows the trends of system miniaturisation and multifunctionalisation. However, micro-scale combustion still has several practical limitations in its design and performance, reason why currently it is being subjected to extensive investigation, both numerically and experimentally. This work proposes to develop a numerical model to be applied on the study of micro-combustion for lean methane mixtures using a commercial software, COMSOL. The main objective of this work is to study how a geometric parameter (gap size), and two physical parameters (thermal conductivity of the walls and an imposed power loss to the walls) affect flame behaviour and structure at the small-scale combustion regime.

3. Bibliographic Review

Micro-combustion is defined differently depending on the bibliographic source considered. Some authors use a physical device scale to distinguish micro and mesoscale combustion, others use a physical dimension associated to the flame - the quenching distance.

Combustion at this scale involves a diversity of physical and chemical processes, such as the gas-phase and surface reactions, molecular transport, thermal and mass diffusion, convection and radiation phenomena. When entering this combustion regime, the burning on these combustors becomes less efficient due to intense heat loss from the flame to the walls, radical depletion on the gas-wall interface and reduced residence time. Given these, it is extremely difficult to stabilise a flame in an experimental environment, illustrating the importance of performing numerical studies in order to better understand the present behaviours. Different flame dynamics are observed, such as: weak flames, flameless combustion, non-stationary flame patterns and associated spinning and pulsating instabilities.

Efforts have been made to improve flame stability for this type of combustors. The heat-recirculation concept was discovered and is a great "ally" of flame stabilisation. "Swiss Roll" structures that allow the exploitation of heat released in the reaction to further use in the unburned gases pre-heating were developed. Also the use of catalytic combustion has been studied. Other methods of improving flame stability involve the change in chamber’s geometry introducing recirculation zones.

The origin of the interest for micro-power generation systems dates back to 1999 [6, 7]. Regarding numerical studies, small-scale combustion has been evaluated by various researchers, all focusing on a variety of parameters. Eriko Miyata et al. [8] studied, using Direct Numerical Simulation (DNS), micro-combustion in a narrow circular channel for a methane–air mixture focusing on the transient phenomena. Yiguang Ju et al. [9] analysed the effects of channel width and Lewis number on the propagation limits and flame transition between multiple flame regimes. The author focused on channels over the millimetre scale. Maruta et al. [10] studied the characteristics of premixed combustion in a heated channel with an inner diameter smaller than the conventional quenching distance, employing an 1D computation.

3.1. Small Scale Combustion

Due to the small characteristic dimensions of all the length and time scales, the coupling of the various magnitudes is evident, affecting all the phenomena observed. The Knudsen number helps to determine if continuum mechanics formulation of fluid dynamics can be considered to model a situation. For air at standard temperature and pressure flowing through a small channel $Kn$ is still smaller than that for free-molecule flow. Consequently, the standard assumptions regarding thermo-fluid will still apply. Nevertheless, the small size of the micro-devices causes particular characteristics. Two other relevant dimensionless parameters for the phenomena at this scale are: the Reynolds number $Re$ and the mass Peclet number $Pe$. As the characteristic length of the device is reduced, the Reynolds $Re$ and Peclet $Pe$ numbers decrease and fluid flow tends to be less turbulent, so the viscous effects and the diffusive transport of mass and heat become increasingly important.

The small height of the channels for the reactant intake, the product exhaust, and the actual combustion chamber constrain the flows in micro-devices to relatively small Reynolds number and hence, the majority of small-scale power systems are laminar and issues related to viscous drag and mixing of multiple streams become crucial. The small channels also result in high
velocity gradients in the fluid that lead to high wall frictional losses and high convective heat transfer coefficients. These can result in large pressure losses, high heat transfer to or from the fluid to the wall, as well as enhanced diffusive mixing [4].

4. Model Definition

A numerical study on flame structure in a micro-channel is performed using COMSOL Multiphysics as the chosen commercial software. This study uses an iterative method, the Newton’s method. A convergence test, often the solution’s residual, is specified in order to decide when a sufficiently accurate solution is achieved. All of the simulations were performed using an Intel Xeon. A two-dimensional (2D) steady-state model is considered. The reactive laminar flow to be evaluated is described mathematically by the energy conservation equations for a continuous, compressible and perfectly mixed Newtonian fluid. The following equations are considered: total mass conservation, mixture momentum, species’ mass fraction and mixture energy, given by Equations 1, 2, 3 and 4 respectively.

\[
\frac{\partial}{\partial t} \rho + \nabla (\rho u) = 0 \tag{1}
\]

\[
\frac{\partial}{\partial t} (\rho u) + \nabla (\rho u u + p I) = \nabla \tau + \rho g \tag{2}
\]

\[
\frac{\partial}{\partial t} (\rho Y_i) + \nabla (\rho u Y_i) = \nabla (\rho D_i Y_i) + \dot{\Omega}_i \tag{3}
\]

\[
\rho C_p \frac{\partial T}{\partial t} + \rho C_v \nabla T = -\nabla q - \rho \sum_{i=1}^{N} C_p Y_i D_i - \sum_{i=1}^{N} h_i \dot{\Omega}_i \tag{4}
\]

In these equations \(t\) [s] represents the time, \(\rho\) [kg/m\(^3\)] the mixture’s density, \(\rho\) the mixture’s pressure [Pa], \(u\) the mixture’s vectorial velocity [m/s], \(\tau\) the fluid stress tensor [Pa], \(g\) the gravitational acceleration vector [m/s\(^2\)], \(Y_i\) the \(i\) specie’s mass fraction [dimensionless], \(D_i\) the diffusion coefficient for specie \(i\) [m\(^2\)/s], \(\dot{\Omega}_i\) the formation rate of specie \(i\) [mol/s], \(T\) the mixture’s temperature [K], \(C_p\) and \(C_v\), the specific heat for the mixture and for specie \(i\) respectively [J/(kg.K)], \(q\) the heat flux vector [W/m\(^2\)] and \(h_i\) the enthalpy for specie \(i\) [kJ/mol].

Since the fluid addressed can be assumed an ideal gas, density is calculated using the ideal gas equation of state (Equation 5), with \(R\) defined as the ideal gas constant taking the value of 8.31 [J/(mol.K)] and \(W_i\), the species’ molar mass in [kg/mol].

\[
p = R \rho T \sum_i Y_i/W_i \tag{5}
\]

The heat transfer interfaces use Fourier’s law of heat conduction, as depicted in Equation 6, which states that the conductive heat flux \(q_{\text{cond}} [W/m^3]\) is given as shown in 6 where \(\lambda\) is the material’s thermal conductivity [W/(m.K)].

\[
q_{\text{cond}} = -\lambda \nabla T \tag{6}
\]

Besides the heat transfer by conduction, external convection is also assumed given by Equation 7, on which \(T_0\) is the ambient temperature [K] and \(h\) the heat transfer coefficient [W/(m\(^2\).K)]. This Equation represents the effect of the exterior air cooling the channels’ walls, phenomenon often referred to as convective cooling.

\[
q_{\text{conv}} = h(T_0 - T) \tag{7}
\]

Fick’s Law of Diffusion is considered. Respectively, it is possible to define, in Equation 8, the first law of Fick and the second law of Fick. \(N_i\) represents the molar flux [mol/(m\(^2\).s)] and \(c_i\) expresses the molar concentration of specie \(i\) [mol/m\(^3\)].

\[
N_i = -D_i \nabla c_i \quad \frac{\partial c_i}{\partial t} = D_i \nabla^2 c_i \tag{8}
\]

Regarding the reaction mechanism two relevant equations are defined considering the Arrhenius law: the reaction equation and the reaction rate expression as expressed in Equation 9.

\[
R_i = k_r \prod_{i=1}^{N} c_i^{n_i} \quad k_r = A T^{\theta_r} \exp(-\frac{E_a}{RT}) \tag{9}
\]

\(R_i\) quantifies the reaction rate [mol/(m\(^3\).s)], \(k_r\) the reaction rate constant and \(v\) the concentration exponents. Regarding the second equation, \(A\) refers to the pre-exponential factor [s\(^{-1}\)], \(E_a\) [J/mol] the activation energy and \(n\) the temperature exponent.

Gas properties such as viscosity, specific heat and thermal conductivity are calculated as a mass fraction-weighted average of all species. The specific heat of each specie is calculated using a piece-wise polynomial fit of temperature.

4.1. Model Simplifications

Multiple considerations are accepted by the scientific community on the definition of these micro-combustion problems [11]: ideal gas, continuum theory, compressible flow, laminar flow, one-reaction mechanism, no radiation phenomena, symmetry and steady state solution.

4.1.1 One-step reaction mechanism

The chemical kinetic mechanism used is chosen because of its simplicity. The model chosen is an one-step reaction model proposed by Mantel et al. [12] that assumes the reaction rate expression as the one described in Equation 9, with concentration exponents coherent to the stoichiometric ones for methane combustion (as seen in Equation 10).

\[
R_i = k_r \prod_{i=1}^{N} c_i^{n_i} \quad \frac{\partial c_i}{\partial t} = D_i \nabla^2 c_i \tag{8}
\]

\[
R_i = k_r [CH_4][O_2]^{2} \tag{10}
\]

3
[CH₄] and [O₂] stand for the concentration of methane and oxygen [mol/m³] respectively and kₑ is defined as given in Equation 9. For this work the values adopted for this mechanism are E_a and A equal to 1.045 × 10⁵ J/mol and 1.53 × 10⁸ s⁻¹, respectively.

4.1.2 No radiation phenomena

Heat losses through the external walls to the surroundings were computed using Equation 7, in which natural convection is considered.

T₀ is considered the ambient temperature of approximately 300 K and the convective heat transfer coefficient hₑ was considered 17 [W/m²K]. This value is obtained by an approximation to iso-thermal walls.

4.2. Implementation Steps

The reactive flow study is implemented in two steps. First, the Reaction Engineering module is solved. This module calculates all the chemical and kinetic mechanisms associated to the reaction as a dimensionless, 0D, plug flow model. This study was run for both GRI-MECH 3.0 [13] and for the simple one-step reaction model used, as showed in the graphics portrayed in Figure 3.

The first conclusion drawn, from observing the methane concentration trends for each mechanism (Figure 3), is that methane reaction develops much faster for the simplified model, presenting an accentuate slope at the entrance of the PFR. The same is verified for all the species in the simplified system.

Regarding oxygen conversion, in the simplified model it fully reacts with methane to produce carbon dioxide and water, in an irreversible way. As a consequence it appears to have a bigger conversion percentage than for the GRI-MECH 3.0 mechanism. This phenomena is also present in the carbon dioxide and water formation, for which the values are higher than for the complex mechanism.

This 2D model is solved with the aid of two different studies. First, ignition is forced using the heat-zone method, further detailed in the section devoted to the chemistry module (Sub-Section 4.3). After, this solution is used as the initial value for a second study where the heat-zone is turned off.

When a computational error under the convergence parameter is obtained (≤10⁻³) the simulation ends and the results are exported for post-processing as 1D plots, 2D maps and data files.

4.3. Ignition Steps

Kang et al. [11] compared different ignition methods proposed in past literature. This methods can be summarised into three primary groups, all tested in this work: auto-ignition, ignition-zone and heat-zone methods. The adopted method, is defined as heat-zone method. Ignition is induced with the definition of a heat source in a small portion of the channel, then switched off computationally after reaction started. Examples of these methods are shown in Figure 4. The heat-zone method is adopted due to the numerical interest of avoiding reaction close to the entry of the channel since it creates numerical complications due to the steep gradients close to inlet boundary.

The implementation of the heat-zone is achieved by defining a two-dimensional Gaussian function at a point distant from the channel’s entry which permits a smooth temperature transition. This Gaussian function is defined in terms of an amplitude, geometric centre and radius, represented by Equation 11.

\[ f(x,y) = T_0 \exp(-\frac{(x-x_0)^2}{2\sigma_x^2} + \frac{(y-y_0)^2}{2\sigma_y^2}) \]  

The value of T₀ is set to 1500 K. Since there is symmetry the vertical centre of the blob, y₀, is defined at 0 mm and x₀ at 10 % of the total length, 1 mm. The spread is set for the heating area not to surpass the combustion chamber dimensions with the aid of a variable scaling parameter P as Equation 12 describes.

\[ \sigma_x = Px_{max} \quad \sigma_y = Py_{max} \]  

The values taken into consideration for the final simulations are P of 0.4 and x_{max} and y_{max} defined as h/4 and h respectively.
5. Solver Definition

The solver definition is separated into three main steps, associated with three different steady-state solvers. The solvers are defined as direct segregated solvers (MUMPS [14] for the first step and PARDISO [15] for the following two steps). The segregated approach treats each physic sequentially, using the results of the previously solved parameter to evaluate the parameters of the following study. The great advantage of the above approach is that an optimal iterative solver can be used in each linear sub-step.

The first solver is set to solve the initial ignition set, the following one to solve the problem keeping temperature solution contained and the last one to allow the temperature sub-step to converge. For all, a constant Newton method is used allowing the definition of a damping factor which controls the step size taken in each iteration for each segregated-step group. For this work, three main segregated step-groups are generated: one that solves pressure and velocity, one for the species’ mass fraction and a final one for temperature.

A convergence criteria has to be established regarding the maximum error criteria. The maximum allowed error is defined as \( \epsilon \leq 10^{-3} \).

5.1. Solver Implementation

On the first step, all the quantities converge for a damping factor of 0.7.

After switching off the heat zone, a first simulation is performed using the results obtained in the previous run as the initial solution for the variables for this second simulation. In a way of assuring solution stability, temperature has to be constraint defining a very low damping factor of 10\(^{-3} \) while the segregated step for velocity and pressure and segregated step for specie’s mass fractions are kept at higher damping factors, in a way of allowing solution to converge, respectively 0.7 and 0.1. After all solution’s error stabilize it is seen that the associated error for temperature is above the required criteria showing that further simulations are required. Following the same scheme, this solution is used as initial value for a new one. For this simulation, the damping factor of the temperature segregated-step is increased in order to allow the solution to “relax”. The new value for damping factor is 0.1 for the temperature segregated sub-step, guaranteeing in that way convergence of all the variables under the error criteria defined.

6. Results

Conclusions are drawn from the colour maps of: \( u \), \( T \), \( \text{YCH}_4 \) and \( \text{Ri} \). Data-sheets are also extracted, data that corresponds to the centreline results for \( T \) and \( \text{YCH}_4 \) profiles.

6.1. Baseline Case

The channel’s geometry is defined as two rectangular sections: one representing the upper wall and other the upper half of the channel. After, a symmetry condition is applied to the centre line for purposes of full evaluation of flame behaviour.

In Figure 5 the geometry values are delineated.

![Figure 5: Schematics of the model’s geometry and respective length values.](image)

Figure 6 summarises schematically all the boundary conditions applied to the system.

![Figure 6: Boundary conditions applied.](image)

At the inlet, an initial uniform velocity of 0.5 m/s is applied. The inlet temperature is set to 300 K and the molar fractions of the species considered for combustion are set to assure that the equivalence ratio is \( \phi = 0.9 \). At the outlet, a pressure condition is set, defining the pressure value as \( p = 1.01325 \times 10^5 \text{ Pa} \).

Gas diffusivity is assumed constant \( (D = 10^{-5} \text{ m}^2/\text{s}) \). Regarding the species’ transport and thermal properties, such as the molar heat capacity, entropy and standard enthalpy of formation values, the GRI-MECH 3.0 thermochemistry database is used.

The solid properties of Alumina are taken as summarized in Table 1. In this case the intermediate value of thermal conductivity is taken \( (10 \text{ W/(mK)}) \).

<table>
<thead>
<tr>
<th>Table 1: Alumina material properties [16].</th>
<th>Properties</th>
<th>Alumina</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat capacity at constant pressure</td>
<td>900 J/(kgK)</td>
<td></td>
</tr>
<tr>
<td>Density</td>
<td>3900 kg/m(^3)</td>
<td></td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>300 \times 10^9 \text{ Pa}</td>
<td></td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.22</td>
<td></td>
</tr>
</tbody>
</table>

6.2. Mesh Definition

A mapped mesh composed by 21300 quadrilateral elements, 734 edge elements and 6 vertex elements is generated. The refinement is obtained through the definition of three distributions that characterize the element growth rate in the edges highlighted in Figure 7 (1,2,3 from right to left respectively). These arithmetic distributions are outlined in Table 2.

The edge distributions are characterized by three main parameters: number of elements, element ratio and direction [16].
Figure 7: Element mesh distributions performed - distribution 1, 2 and 3.

<table>
<thead>
<tr>
<th>Distribution</th>
<th>Number of elements</th>
<th>Element ratio</th>
<th>Reverse direction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>300</td>
<td>10</td>
<td>On</td>
</tr>
<tr>
<td>2</td>
<td>240</td>
<td>1</td>
<td>Off</td>
</tr>
<tr>
<td>3</td>
<td>44</td>
<td>Fixed</td>
<td>Off</td>
</tr>
</tbody>
</table>

A stopping parameter of less than 5% alteration in the primary variable is considered. The mesh convergence study is performed increasing the elements number from 5000 to 25000.

6.3. Baseline Case Analysis

The results for the baseline simulation are presented in Figure 8. The 2D colour maps show that total methane conversion is not achieved and that the maximum reaction rate value is $1.2 \times 10^4 \text{mol/(m}^3\text{s)}$. As for temperature and velocity, the maximum values reached in the combustor are 2200 $K$ and 4 $m/s$ respectively.

Looking at the velocity profile, it is seen that near the entry, the velocity magnitude exhibits a value of 0.5 $m/s$. Near the heat zone, the flame anchors, and the velocity value rises up to 4 $m/s$ in the centre of the chamber, lowering towards the wall due to the heat loss phenomena generated by the convection of heat to the cold-walls. There is a zone where the velocity magnitude is zero close to the wall, which propagates through the whole channel.

The temperature profile obtained shows an initial inlet temperature of the premixed methane-air mixtures of 300 $K$. Then, the temperature begins to increase after 0.09 $mm$ across the axial direction, zone where the ignition process is forced. The temperature rises rapidly to 1000 $K$, contacting with the wall which preheats the reactants. There is a zone where the temperature value is close to the wall, which propagates through the whole channel.

The rate of convective heat transfer to the reactor’s wall is linearly dependent on the inverse of the gap dimension.

6.4. Influence of Gap size

The influence of the gap size is analysed for three different channel heights: 0.4 $mm$, 0.6 $mm$ and 1 $mm$.

The two-dimensional maps for the featured parameters are represented in Figures 9 and 10 for gap sizes of 0.4 and 0.6 $mm$ respectively.

For the case of smallest channel height (0.4 $mm$), the maximum velocity magnitude found in the channel is of 2.5 $m/s$, value 45 % inferior of the one estimated for the baseline case. As for temperature, the peak temperature exhibits a magnitude of 1400 $K$, 36 % lower than the one calculated for the case of a channel with 1 $mm$ height. As for the intermediate case, the values found for velocity and temperature are respectively 3 $m/s$ and 1600 $K$, corresponding to a decrease of 25 % and 27 %, respectively, regarding the reference values given in Sub-Section 6.3.

The rate of convective heat transfer to the reactor’s wall is linearly dependent on the inverse of the gap dimension.
Figure 11: Centreline axial temperature and methane fraction profiles for the three cases analysed with changing gap size.

From the data analysed (Figure 11) it is possible to observe an increase in the maximum temperature value as the channel height is incremented. Besides this, the value of axial span for which temperature values are above ambient temperature, is much higher for the largest geometry.

Figure 12: Temperature maps for gap size of = 0.4, 0.6, 1 mm from top to bottom respectively.

Figure 13: Methane mass fraction maps for gap sizes of = 0.4, 0.6, 1 mm from top to bottom respectively.

With the progressive loss of energy from the system to the exterior, is the thermal quenching in smaller channels. This phenomena is noticeable from the reducing temperature shown in Figure 12 and in the increasing area where low methane conversion occurs (graphic to the left of Figure 11).

In narrower channels, a larger portion of heat gets transferred from the gas to the solid, a part of which is lost to the surroundings. Given the low temperatures located near the wall and convected to the flame, complete combustion is never achieved. It can be seen that for the smallest channel, maximum methane conversion is only obtained in a small portion of the channel, as seen in the profiles for axial methane fraction represented in Figure 11. This area of low conversion tends to reduce with the increase of the gap size noticeable in the methane fraction maps in Figure 13.

6.5. Influence of Thermal Conductivity

This study is divided into four cases: one for adiabatic walls and three cases ranging from a low thermal conductivity of 2 $W/(mK)$ to a higher value of 50 $W/(mK)$.

Figure 14: 2D maps for the case of a thermal conductivity of the wall of theoretical 0 $W/(mK)$. From top to bottom: velocity magnitude, temperature, reaction rate and methane mass fraction.

The values obtained for adiabatic flame velocity and temperature are the highest and full methane conversion is obtained (Figure 14).

Figure 15: 2D maps for the case of a thermal conductivity of the wall of 2 $W/(mK)$. From top to bottom: velocity magnitude, temperature, reaction rate and methane mass fraction.

The results for the low thermal conductivity case (2 $W/(mK)$), depicted in Figure 15, present values of maximum velocity and temperature of respectively 4.5 m/s and 3000 K. As for the results for the highest thermal conductivity case (50 $W/(mK)$), depicted in Figure 16, the values of maximum velocity and temperature are respectively 4 m/s and 2200K.

Figure 16: 2D maps for the case of a thermal conductivity of the wall of 50 $W/(mK)$. From top to bottom: velocity magnitude, temperature, reaction rate and methane mass fraction.
Figure 17: Reaction rate maps for $\lambda = 0, 2, 10, 50$ W/(mK) from top to bottom respectively.

Looking at the reaction rate maps (Figure 17), it is possible to observe that the variation of the solid wall thermal conductivity affects the flame shape (when compared to inflow direction). It is possible to group the results obtained into three main groups: concave, flat and convex flames. The most distinctive profiles regarding flame shape (pictured in Figure 17) and temperature map (illustrated in Figure 18) are obtained for the adiabatic case. As thermal conductivity increases, the flame shape shifts to a flat shape and, in the limit case, to a convex shape until further increase of this parameter leads to extinction. This observable in Figure 17.

Figure 18: Temperature maps for $\lambda = 0, 2, 10, 50$ W/(mK) from top to bottom respectively.

Observing the colour maps (Figure 18) it is seen that, as the thermal conductivity increases, the area of high temperature reduces due to the increased heat conduction, translating into increased heat loss. This tendency is also depicted graphically in Figure 19. Besides this, higher peak temperature values are observed for the low thermal conductivity while for the intermediate and high thermal conductivity present a common maximum.

Figure 19: Centreline axial temperature and methane fraction profiles for the three cases analysed with changing thermal conductivity.

The graphic (left side of Figure 19) indicates that methane conversion also decreases with the increase of thermal conductivity. Moreover, energy loss towards the exit translates into the trend shape observed for which maximum conversion is found between 2 and 3 mm.

6.6. Influence of Heat Loss by Convection

To simulate the increase in heat loss, a forced negative power loss is imposed, by defining this power loss at the upper wall boundary as a distributed "load". This study is performed for two imposed power loss values: 5 W and 20 W.

Figure 20: 2D maps for the case of an imposed heat loss of 5 W. From top to bottom: velocity magnitude, temperature, reaction rate and methane mass fraction.

For an imposed heat loss power of 5 W (Figure 20) the maximum values obtained for velocity and temperature are of 3.5 m/s and 2000 K respectively. Regarding the 2D maps for the case of a power loss of 20 W, velocity and temperature peaks exhibit values of 2.5 m/s and 1600 K respectively (Figure 21).

Figure 21: 2D maps for the case of an imposed heat loss of 20 W. From top to bottom: velocity magnitude, temperature, reaction rate and methane mass fraction.

Figure 22: Centreline axial temperature and methane fraction profiles for the three cases analysed with changing forced heat loss parameter.
Flame extinction is characterized by the quenching distance between parallel plates. This distance is higher for superior values of heat loss and is zero if the walls are strictly adiabatic (Figure 14) as it is possible to observe in the results for methane mass fraction in Figure 22 and in the reaction rate map represented in Figure 23.

The increasing energy loss leads to an increment in the death-space, as it is possible to see by the reaction rate maps pictured in Figure 23.

Moreover, looking particularly at the methane conversion profiles for the three cases represented in the graphic to the left of Figure 22 and at Figure 25, it is possible to see that the maximum conversion occurs for the case where no heat convection is forced.

When a 5 W power loss is imposed at the wall, conversion happens efficiently at a small portion of the channel and then, close to the walls, and towards the outlet is highly incomplete due to the low velocity and temperature streamlines. Besides observable in the line graphic, this phenomena is also showed in the 2D methane mass fraction map Figure 20.

Regarding the critical case (20 W), conversion is inefficient (Figure 22). Only 52% of the initial methane mass fraction is consumed. This maximum conversion area is only found on the flame anchoring position. Looking at the temperature profiles across the axial direction of the channel (graphic to the right of Figure 22 and Figure 24), it is seen that the temperature peak reduces with the increasing heat loss value imposed. Furthermore, the cooling temperature gradients are steeper for the cases of forced convection.

In the surroundings of the flame zone, temperature reaches the ambient temperature value (300 K) for both the flames with imposed heat loss as observed by the trend lines in the graphic to the right of Figure 22 but not for the reference case where this value is higher.

Methane conversion is never fully achieved for all cases as seen in the methane mass fraction profile represented in Figure 11 and in the 2D methane mass fraction maps (Figure 25). The critical case is the one where 20 W are imposed as a power loss. For this case only a small area has significant methane conversion, specifically near the axial distance of 2 mm, where combustion occurs. Due to the low energy levels close to the wall through the whole channel, conversion towards the exit has an efficiency of only 32%.

7. Conclusions

A numerical study on a 2D laminar (inlet velocity 0.5 m/s), lean (φ=0.9), CH4–air premixed flame in a micro-channel is performed in COMSOL Multiphysics®.

The main objective of this thesis is to study how a geometric parameter (gap size), and two physical parameters (thermal conductivity of the walls and an imposed power loss to the walls) affect flame behaviour and structure at the small-scale combustion regime. A baseline simulation is defined. The peak values of temperature and velocity obtained are 2200 K and 4 m/s respectively. Regarding maximum reaction rate it assumes a value of $1.2 \times 10^4\, \text{mol/(m}^3\text{s})$.

The gap size analysis is made for channel heights of 0.4 mm, 0.6 mm and 1 mm. This study emphasizes the relevance at this scale of the ratio of surface area to volume ($S/V$). It is concluded that reducing the gap size leads to a smaller flame zone, less energy to be generated by the flame and a larger surface area for heat loss. Besides this, it is possible to conclude that the lowest thermal conductivity leads to maximum temperatures in the centreline of the channel. The same is verified for the temperatures in the walls of the chamber. A decrease in the channel’s height from the baseline case (1mm) to the critical case (0.4mm) induces a reduction of temperature and velocity of 36% and 45% respectively, which leads to lower values of methane conversion across the channel.

The effect of thermal wall conductivity on flame structure is analysed for: adiabatic walls, 2 W/(mK), 10 W/(mK) and 50 W/(mK). It is concluded that this parameter has an effect on flame shape. In this study three main flame shapes are found depending on wall thermal conductivity: concave, flat and convex. The
most distinctive results were found for the adiabatic case where no energy is lost through the wall. Flame exhibits a convex shape.

Lastly, upon forcing an energy loss gradient to the exterior (distributed negative 20 W and 5 W) a decrease on velocity and temperature are found in comparison to the baseline case: 12.5 % and 9 % for 5W and 45 % and 27 % for 20 W, regarding velocity and temperature respectively. Methane conversion for higher values of energy loss is low and only a maximum of 52% is consumed in the reaction. This leads to the conclusion that heat losses through the wall lead to a decrease in flame energy and eventually thermal quenching.

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References


