ED SMAER

Thesis subject 2014

Laboratory Institut D'Alembert

University : UPMC

Thesis supervisor : **Sergio Chibbaro**

Co supervisor : **Guillaume Legros** (UPMC)

Title of the thesis : **Theoretical analysis of microcombustion**

Collaboration within the thesis Jean-Christophe Robinet (ENSAM), Departement of mechanical engineering University of Rome « La Sapienza »,

Thesis's summary (Abstract)

The thesis will deal with the effect on the stability and dynamics of a premixed flame in a micro-channel. Significant efforts have been lately devoted to the design of microcombustor technologies, that may enable the development of micro power generation devices with low weight and long life. However, it is known that flames in microdevices show strongly unstable regimes with many different regimes. A fundamental understanding of such features is essential to control the combustion.
To characterize the stability behavior of the flame, we shall construct the stability maps delineating the regions with different flame dynamics in the inlet mass flow rate m vs. the equivalence ratio parametric space. The flame stability is analyzed for fuels with different diffusivity by changing the Lewis numbers.
A dynamical system analysis will be carried out to point out the fundamental mechanisms underlying such instabilities.
Finally, full resolved numerical simulations with detailed chemistry will be carried out with different chemical models, fuel mixtures and in diverse configurations. On one hand, these simulations will permit the assessment of scenarios put forward previousl. On the other hand, complete simulations will be used to analyse the dependence of the configuration to different parameters like diameter and Lewis number and, eventually, to develop a reliable reduced model useful for applications.

Detailed description

The improvement of the fabrication techniques has encouraged the miniaturization of mechanical and electro-mechanical devices, following the trend previously initiated by other technological areas, such as electronics or biomechanics. The primary objective of using fossil fuels to power these system is to leverage the high energy density of fuels, specifically liquid hydrocarbon fuels, relative to batteries and all other energy storage devices. As such, considering 45 MJ/kg as an average liquid fuel energy density, a miniaturized device with a power conversion efficiency of around 2–5% would compete with the energy density of around 2.5 MJ/kg found on the top Lithium/thionyl chloride primary batteries currently available in the market or the average 0.6 MJ/kg of an Alkaline battery.

According to Dunn-Rankine, to be useful as a portable power device, a system needs to achieve power densities between 10 and 1000 W/kg and working autonomies between 1 and 10 h. Among the different technologies capable of achieving such figures, we find that heat engines and, specially, rotary engines, are specially well suited for small-power generation due to its high specific power, low cost and minimum number of moving parts.

In a small-scale rotary engine, a triangular rotor revolves inside the epitrochoidal housing. The rotor admits a combustible mixture, with a given equivalence ratio, that is mechanically compressed to reach a maximum pressure when the volume of the region between the rotor and the housing is minimum near the top dead center. At that precise instant, the mixture is ignited and the flame propagates along a slender volume of width of the order of the flame thickness and length around 20 times the chamber width. The experimental feasibility of these small-scale engines has been already proven by Fu and coworkers. They built a rotary engine working with Methanol-Nitromethane mixtures with an equivalence ratio 0.4 ; 138 mm3 of average displacement, power output around 100W and thermal efficiency below 0.5%, very far from the minimum needed to make the engine an actual competitor of batteries. Larger efficiencies could have been obtained with a fuel/air ratio closer to stoichiometry, but unresolved combustion-related problems hampered the normal operation of the engine.

The reduction of the engine size brings new challenges that needs to be specifically treated to improve the engine performance, such as increasing heat losses, flame instabilities or flame quenching.

As the ratio of the reacting volume to the wall surface decreases, the proximity of the reacting volume from the colder walls can lead to higher heat losses, therefore extended flame thermal quenching. In addition, heterogeneous chemical reactions may occur at the walls, possibly contributing to radical quenching of the flame.

However, the premixed flame propagation in such ducts may exhibit different combustion modes, which can make any microcombustor's design streneous. Sustaining steady conditions, some studies reported steady mild or flameless- combustion, non-axisymmetric flames in circular ducts, asymmetric flames in planar channels, and tulip flames.

Unsteady behaviors also revealed, such as periodic flame repetitive ignition/extinction (FREI) oscillating flames and spinning flames. Therefore, the industrial development of reliable microcombustors requires fundamental understandings of premixed flame propagation at small scales.

The resemblance of the geometry of the experiments with a narrow, straight channel of great length, has motivated a great number of theoretical studies based in this simple configuration in which the particularities of the combustion in the small scale have been analyzed.

Specifically, it has been demonstrated that, for flames propagating in narrow channels, the increasing of the surface-to-volume ratio is associated with a rise in the convective heat losses to the walls of the channel proportional to the square of the ratio of flame thickness dT to the channel width h. Furthermore, for a constant mass flow rate, a reduction in the channel size is

inevitably associated with smaller residence times, what contributes to diminish further the Damkhôler number of the combustion reaction and makes the flame more prompt to quench and/or develop instabilities that make the system difficult to control.
The thermal coupling of methane and propane flames with the walls of a straight micro-channel with a step-wise wall temperature profile revealed a complex flame dynamics. These works showed that stoichiometric or near-stoichiometric mixtures give stable flames in the high and low incoming velocity regions and unstable flames in the middle velocity region, with flame extinctions and re-ignitions that are repeated periodically in time.
A similar instability has been observed by other authors for rich flames propagating in curved ducts and for lean flames propagating in a bidimensional micro-channel.
Some years ago, it has been proposed the recirculation of heat as an alternative to extend the flammability limits in small-size burners. In this type of burners, the burned gas heat is recycled to preheat the unburned mixture, reducing the effect of the heat losses through the walls. In order to understand the dynamics of a flame with heat recirculation, theoretical studies in simplified geometries showed, in particular, the extension of the flammability limits to leaner flames and the reduction of the minimum burner size that allows combustion as a function of the amount of heat recirculated.
As indicated previously, the use of liquid fuels as an alternative to batteries to power small-size devices falls on sufficiently high thermal efficiencies that have not been achieved yet. At least for rotary engines, this is, in part, due to the insufficient understanding of the effect of the fuel concentration in the incoming fresh mixture on the combustion process.
Despite of its inherent practical importance, the fundamental understanding of such behaviours and the effect of different mechanisms is far from been completed. Moreover, detailed numerical simulations of such devices with simple and complex chemistry have to be achieved.
The present thesis attempts to cover that gap by undertaking a systematic investigation about the stability of combustion in a bidimensional, micro-tube for fuels with different diffusivity.
Concretely, we aim to map the flame dynamics as a function of the mass flow rate, the equivalence ratio and the fuel Lewis number. The appropriate combination of the results obtained from the unsteady computation and from the stability analysis will be used to plot the stability maps that constitute the core of the first part of the work.
In the second part, detailed numerical simulations of Navier-Stokes equations coupled with chemical reactions will be carried out. Many of the ideas developped in the first part, will be assessed with these simulations.
More specifically, different chemical models from simplest to more complex ones will be used in order to understand which description can be retained as appropriate for microdevice. An important goal would be then to put forward a reasonable reduced model for engineering calculations. This part will benefit from the collaboration with the team headed by CM Casciola (departement of mechanical engineering of the University of Rome), where a fully parallelised code resolving Navier-Stokes with detailed chemistry is available. The agreement of the collaboration has been already discussed.
Furthermore, discussions with experimentalists at the laboratoire ICARE (Orleans) have been already started and we hope to can compare results against measurements.