Oxygen-methane combustion studies in the In Space Propulsion Programme

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Abstract
In the frame of the European framework programme 7 (FP7), the In-Space Propulsion (ISP-1) project was initiated in 2009 with the objective of improving knowledge and techniques required by future space missions relying on cryogenic propulsion. One of the work packages addresses remaining open issues for the use of oxygen and methane for in-space propulsion:: liquid-liquid injection, ignition and combustion at low pressure, film cooling and soot formation. This paper describes the work performed during the fifteen first months.
Through theoretical analyses, modelling and experimental work, this project will serve the purpose of improving the maturity of technologies which are key elements of cryogenic space propulsion systems.

1. Introduction

To improve the knowledge and the techniques which are necessary for future space missions cryogenic propulsion, the project In-Space-Propulsion (ISP-1) was initiated in 2009 within the framework of the European FP7.
ISP-1 does not focus on the early launch phase of a space flight, but on the technologies involved in the subsequent phases of a space mission, once the spacecraft or upper stage has already been placed in orbit. Hence the program name “In Space Propulsion”, which applies to launcher upper stages, orbital transfer vehicles or space exploration vehicles. The activities in ISP-1's different work packages are focussed on the concept of Low Thrust Cryogenic Propulsion, which have been presented in previous publications.
The propulsion system is using very small propellant pumps, each powered by an electric motor. The electric power can be supplied by a fuel cell.
It is considered to be more affordable than a re-startable upper stage of a launcher but as a consequence of the low thrust level, the mission lasts approximately one week instead of a few hours.
The ISP-1 program is structured into five main work packages which deal with various technological difficulties associated to the development of a Low Thrust Cryogenic Propulsion system [1] and serve the purpose of improving the maturity of technologies which are key elements of cryogenic space propulsion systems.

The second workpackage of ISP-1 deals with oxygen/methane propulsion. Indeed, this propellant combination is a possible answer to the contradictory requirements of performance and long duration in space. Up to now, only preliminary studies and lab-scale testing activities have been carried out on methane ([2],[3],[4]). These activities have been performed mainly in the frame of medium launcher main stage propulsion, for which the global advantage of methane is presently not clear, considering in particular the development effort. Basic researches are required before considering an operational engine development. In addition, in space propulsion introduces new requirements and possibly the use of new technical solutions that haven't been studied so far.
Consequently, the project will aim at extending the present knowledge on LOX/methane combustion to its use at operating conditions typical for in-space application through research on injection, ignition, combustion, soot formation and engine cooling Six main tasks have been defined to progress along the main research axes. They combine modelling activities for propellant properties and combustion with simple configuration tests to validate modelling tools and more representative tests to increase the technical knowledge in liquid-liquid injection of cryogenic propellants.

Each work package is led by a main contractor assisted by several partners who are in some case major universities, taking advantage of the know-how of large or smaller industrial organizations combined to the theoretical expertise of research laboratories. The LOX-methane combustion work package is led by ONERA (France) with main participation of University of Roma (Italy), DLR and Astrium (Germany) [1].

2. Reference engine definition

In order to focus and to bound the research domain of combustion studies, it is necessary to define some mission target.
The following propulsion systems were selected as references or “targets”

- a low thrust cryogenic (hydrogen-oxygen) space propulsion system (LTCP)
- a low thrust CH4-oxygen space propulsion system

A reference set of key parameters, or range of parameters was defined for each of these propulsion systems targets.
The foreseen missions are briefly recalled hereafter:

- the GEO mission (the payload has to be transferred from the LEO or GTO trajectory to the final GEO orbit)
- the OTV missions (the payload is transferred from an orbit to another one depending on the payload need)
- the exploration missions (Lunar or March mission) including the landing phase.

It was chosen to open as much as possible the operating conditions of the future expected propulsion systems in order to enlarge the knowledge to be made available to future designers. Furthermore, the techniques, modelling skills and tools to be improved during the project are not necessarily restricted in their application to space systems. The scope of the project should be defined but not be constrained by the chosen “reference concepts”, and is open to a wide range of operating parameters.
Detailed characteristics of reference engines can be found in [1]. For combustion studies, we will keep in mind that methane/oxygen is retained as propellant combination because hydrogen/oxygen has been extensively studied during former programs for European launch vehicles. A combustion pressure of 10 bar has been chosen as the reference, since it could be a level applicable for low thrust engines and medium thrust engines as well. Nevertheless, properties of methane, oxygen and other gases involved in the combustion as well as their mixing are studied in a wide range of pressure, i.e. up to supercritical pressure.

3. Physical and chemical characterization of Lox/methane system

The first step to calculating flows in a liquid propulsion rocket engine combustion chamber is to characterize the thermodynamic and fluid mechanic properties of the species involved in the flow and the reactive mechanism. Thus, the following activities have been planned:

- Thermodynamic and fluid mechanic properties, performed by the University of Rome
- Global reduced kinetic models for low pressure ignition and combustion , performed by DLR;
- Models for soot formation and oxidation in fuel–rich methane/oxygen combustion, also performed by University of Roma.

3.1. Thermodynamic and fluid mechanic properties

The first part of the activity deals with a extensive review of available literature models to create a database of methane properties with a selection of the most appropriate models; then, a review of mixture rules for evaluation of system equations of state and thermophysical properties has led to a database including methane properties and equations of state for multi-component (e.g. methane/oxygen/ water, hydrogen, carbon monoxide, carbon dioxide) systems.
The main goal is the selection of the most appropriate equation of state (EOS) leading to the best compromise between accuracy and computing cost. The results of the review give the Modified Benedict Webb-Rubbin EOS with the coefficients proposed by Younglove which is the most accurate EOS. Then, the implementation of subroutines able to create the database according to the degree of resolution required for the thermodynamic tables has been performed.
Beside the EOS, the specific heat capacity is modelled through the following equation:

$$c_p = c_{p0} - R - \int_0^{\rho} \left[\frac{T}{\rho^2} \left(\frac{\partial^2 p}{\partial T^2} \right)_{\rho} \right]_T d\rho + \frac{T}{\rho^2} \frac{\left(\frac{\partial p}{\partial T} \right)_{\rho}^2}{\left(\frac{\partial T}{\partial \rho} \right)_T} \quad \mathbf{(1)}$$

where c_{p0} is the rarefied gas contribution and other terms are computed integrating and differentiating EOS, except for the rarefied gas contribution c_{p0} which is given as a function of temperature only:

$$\frac{c_{p0}}{R} = \sum_{i=1}^{7} m_i T^{i-4} + m_8 \frac{m_9^2 e^{m_9/T}}{T^2 \left(e^{m_9/T} - 1\right)^2} \quad \textbf{(2)}$$

It is important to notice that the MBWR shows high accuracy to determine the correct *pvT* behaviour of a fluid and the derived thermodynamic properties (whereas simpler models fail to predict the c_p).
In the same way, transport properties (viscosity and thermal conductivity) are evaluated as the sum of two contributions: rarefied-gas term and dense-fluid term. Moreover, special attention is paid to the computation of the thermal conductivity in the vicinity of the critical point, at which it seems to reach an infinite value. Thus, a third term is added to take into account such behaviour.

The generated database includes methane properties in the following range:

- Temperature: [100; 6000.] K
- Pressure [0.1;600] bar

Validation was carried out by comparison with REFPROP [13] data from NIST (Figure 1).

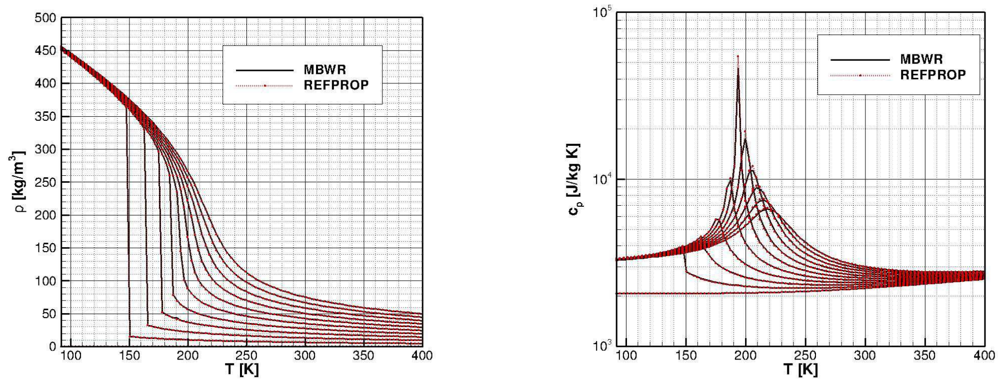


Figure 1: Validation of density and specific heat capacity at constant pressure

After having chosen the EOS for the methane, work on the mixture with oxygen was addressed. The same method was applied, and the first step was a literature review on mixture models for both perfect gases and real fluids. From the literature overview of the existing mixing rules for the real fluid, it has been found that two different groups of equations of state have been proposed:

• EOS based on the corresponding states theory. Equations of this kind allow describing also mixtures with a very low number of experimental data. Historically, this was the most widely used approach.

• EOS for the Helmholtz free energy with a departure function to take the real gas behaviour into account both for any components and for the different binary mixtures. Each binary mixture is related to another with binary parameters. The approaches are based on a very large number of experimental data.

Dealing with methane based mixtures, the most recent and reliable equations of state belong to the group based on the Helmholtz free energy in [7], which takes into account the real behaviour of fluids with some kind of departure functions from the perfect gas solution.

The mixing rules for the equation of state are commonly given in terms of Helmholtz free energy:

$$a(\delta, \tau, \overline{x}) = a^0(\rho, T, \overline{x}) + a^r(\delta, \tau, \overline{x}) \quad \textbf{(3)}$$

where δ is the reduced mixture density ($\delta = \rho / \rho_r(\overline{x})$), τ is the reduced mixture temperature ($\tau = T_r(\overline{x}) / T$), $\overline{x}$ is the species molar fraction ($\overline{x} = (x_1, \ldots x_N)$). In this equation, the first term corresponds to the perfect gas behaviour and the second term is a corrective term for real fluid, which requires experimental data and which are fitted with polynomials addressing single components and component interactions.

Finally, the model, giving the state of the mixture, is completed in a routine for the combination of the 6 species methane, oxygen, carbon dioxide, carbon monoxide, hydrogen and water.

Beside this equation of state, transport properties have been modelled with the extended corresponding states (ECS) models derived by Klein and McLinden ([8],[9]). More details on the mixture models are given in [10] where these models have been used to study LNG mixtures behaviour

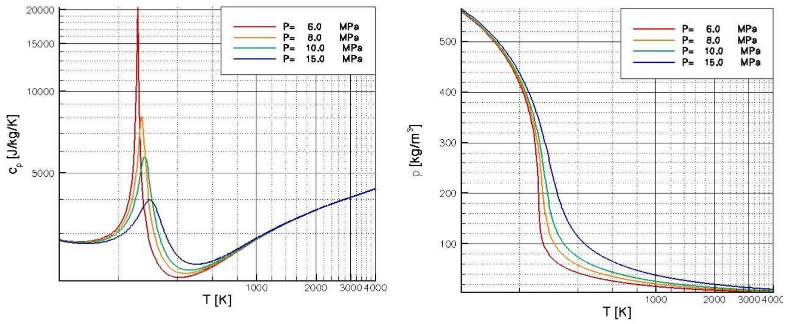


Figure 2: Isobaric specific heat (left) and density (right) for a mixture of the 6 species of the model

3.2. Global reduced kinetic models for low pressure ignition and combustion

The engine ignition study requires a global kinetic model for low pressure combustion. Such a model is today lacking. And yet, it is absolutely mandatory to increase the knowledge about the detailed chemical kinetics, which determines the ignition and combustion behaviour of this propellant combination for low pressure conditions. The final step of the development will be a reduced mechanism with sufficient predictive capabilities but still small enough to be implemented in current CFD tools.
The development logic for the construction of a reduced mechanism for low pressure CH4 combustion is composed of 3 phases :1) reaction model for CH4 low pressure oxidation; 2) mechanism validation; 3) mechanism reduction.

The first phase consists, firstly, of an extension of the Leeds Methane Oxidation Mechanism ([15],[16])and the more recent for modelling the oxidation of hydrogen, CO, methane, methanol, formaldehyde, and natural gas, leading to a mechanism, with 47 species and 311 reactions. This mechanism is presently validated for a pressure ranging from 1 bar to 60 bar, an equivalent ratio from 0.5 to 2 and an initial temperature between 300 K and 1200 K. The validation data are those of laminar flame speed, ignition delay time and soot formation. Secondly, a literature review was made to obtain thermo-chemical data and experimental data for low pressure conditions and computations with the chemkin code [2].
The last phase, corresponding to the mechanism reduction, is the biggest part of the task. It leads to a so called “skeletal mechanism” reducing the number of reaction down to 24 species and 103 reactions without any loss of predictive capabilities compared to the original scheme. Both detailed and reduced models describe experimental data under conditions: 0.2 bar $< p < 1$ bar, 900 K $< T < 1800$ K and $0.5 < \Phi < 3.0$ with satisfactory accuracy.
This is obtained by using the RedMaster [15] code which allows the selection of negligible reactions and species maintaining predictive capabilities thanks to a multitarget sensitivity analysis. These analyses are performed in several points (targets) in laminar flames or during ignition transients. For this study 60 targets were selected. Figure 3 presents the main paths of the resulting scheme.

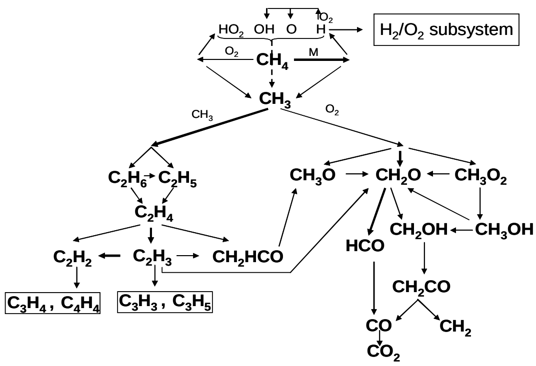


Figure 3: The main reaction paths of the methane oxidation in the reaction mechanism.

3.3. Models for soot formation and oxidation in fuel-rich operating conditions

The objective of the task is the prediction of soot yielded from methane/oxygen combustion in a chamber working under fuel-rich conditions with possible film cooling and the estimation of the ensuing radiative heat transfer.

The treatment of soot formation is based on a semi-empirical approach, solving equations for soot number density and mass fraction. The relevant source terms involve four terms, nucleation, surface growth, agglomeration and oxidation, which require both chemical and physical modelling. In particular, following Woolley et al. [19], nucleation is assumed to take place after gas-phase precursors acetylene (C_2H_2) and benzene (C_6H_6), though the latter is found to be inconsequential for the case under scrutiny (see below), and accordingly neglected. Oxidation of soot particles takes place under the action of oxygen (O_2) and hydroxyl radicals (OH).

Gas-phase chemistry is accounted for by using a thermo-chemical database (flamelet library). The laminar flamelets are generated by OPPDIF [20] (a fortran program from the CHEMKIN library for computing counterflowing diffusion flames). The flamelets are described in terms of mixture fraction (accounting for stoichiometry), scalar dissipation rate (accounting for finite-rate chemistry) and enthalpy defect (encompassing heat losses) ([21],[22]).

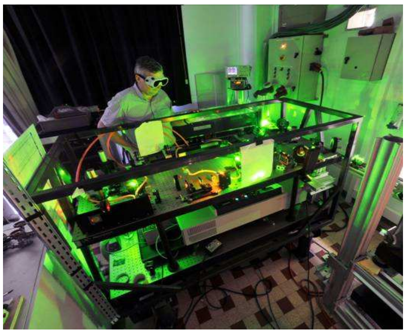
In order to identify the most suitable gas-phase chemical kinetics, three mechanisms ([23],[24],[25]) have been considered. As far as ISP-1 reference working point is concerned, results seem to indicate that acetylene is by far the main soot precursor source as compared to benzene. Model for soot formation and oxidation in turbulent methane/air flames at moderate pressures [19] has been implemented on code *XENIOS* [26], and validated against experimental results by Brookes *et al.* [27], with plausible results. However, its application to methane/oxygen combustion at relatively high pressure pointed out to some inherent limits. A modification of the model to account for the higher rates of production and oxidation in such conditions is under study.

4. Combustion

The main goal of this activity is to provide the project with detailed measurements of the hot gas temperature in a lab-scale setup at ONERA's Mascotte test bench. The first task was the choice of the operating point and the probe molecules.

According to the WP 2.1 a pressure of 10 bar was selected. But the combustion chamber used on the Mascotte test bench could not sustain mixture ratio (MR) as high as 3.4 identified as the target for the main injector [1]. Thus the combustion equilibrium temperature and species distribution was computed as a function of mixture ratio. Looking at temperature and species, the two values of 1 and 2 were selected for the mixture ratio. MR 1 has been already performed on Mascotte and results are used as reference. MR 2 exhibit molar fractions of main species which are not far from the one of MR 3.

Figure 4 shows one of the CARS measurement systems and the combustion chamber.



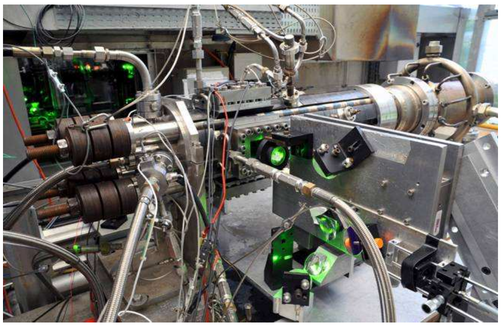


Figure 4: CARS measurement systems (left and right) and the combustion chamber (right)

First CARS measurements were performed with gaseous propellants at 3 locations downstream of the single-element injector: x = 65 mm, 105 mm and 210 mm. For each axial location, 5 points were investigate(y = 0 (on the axis), 5 mm, 9 mm, 13 mm and 16.5 mm), allowing to trace a temperature profile. To complete the results, visualisation of OH emission was performed for the beginning and the end of the flame.

Finally, 26 tests in the BHP with MR=1 and 19 tests in the BHP with MR=2 were performed. CARS measurement reduction data with H2 and H2O probe molecules gives consistent results. All the results are presented in [28].

Mean value and standard deviation of the operating point parameters have been computed, on one hand, for the 26 runs with an objective of MR1 and, on the other hand, for the 19 runs with an objective of MR2. The standard deviation for these independent runs is very small, ~1%. This leads to the definition of test cases for the CFD computation planned during the second period of the project.

5. Liquid injection

A literature survey was performed providing relevant background information on the design of injectors for LOX/CH4 for liquid-liquid as well as liquid-supercritical injection. For LOX/LCH4 injection, impingement as well as coax-shear and coax-swirl injectors have been designed and tested in the United States ([29]-[38]).
To prepare the selection of the liquid-liquid injector concept to be studied on MASCOTTE, several selection criteria were identified and weighted. For this weighting, an analytical hierarchy process methodology was applied to ensure transparency and traceability of the weighting factors [39]. The weighting of the different criteria resulted in a so-called priority vector:

Table 1: criteria and weighting factors

Criterion	Weighting Factor
Combustion Stability	0.432
Combustion Efficiency	0.280
Throttling Capability	0.132
Face Plate Heat Load	0.073
Combustor Size (L,D)	0.050
Manufacturing Issues	0.031

The weighting factors were applied to a pairwise comparison of the different concepts in a so-called Pugh-matrix [40].

The discussion about the results of this comparison leads to highlight the following points: The combustion instability criterion is of major importance and assessment of combustion stability is key for decision. Considering other technology, the pintle injector is discarded because of the fact that pintle injectors are not scalable to a multi-injector configuration; impingement is discarded because there is no heritage at any of the partners. The decision was taken to proceed to the design of two injectors: 1) coax-shear, which is of fundamental interest to broaden existing data base (gaseous propellants) and for comparison of principles with respect to spray break-up; 2) double swirl as opposite extreme with two swirling sheets and comparison with open literature on this injector type. This design promises high performance, but has never been tested before on MASCOTTE. The design of double swirl injector for Mascotte has been done and will be tested soon.

6. Ignition

6.1. Ignition experiment

During the mission in space environment, the engine will be restarted several times at low pressure and in various temperature conditions. Thus, ignition is one of the key points of a successful mission. The objective of this task is to provide the project with validated tools to describe the ignition behaviour in various conditions. Thus, the first link in the chain is the checking of the combustion scheme developed in task. To do that, ignition tests have been conducted in the micro combustor at the M3 test bench in DLR Lampoldshausen in a single-injector configuration fuel with gaseous oxygen and gaseous methane in order to acquire a ignition data base at ambient and low pressure.
The main issue in such tests is to ensure well-defined boundary conditions as close as possible to the injection plane in order to limit the computational domain. These experiments base on previous test performed with hydrogen and oxygen ([41], [42]). The lessons learned lead to some improvements in injector head design. Thus, a new injector has been designed and manufactured including a new miniaturized pressure sensor directly mounted in the injector, close to the O2-Dome, a modular design for enhanced flow path, reducing also pressure loss at LOX post inlet, and better handling and a sonic throat located directly at fuel injector part.
The instrumentation consists of pressure transducers sampled at 10 kHz, for chamber, oxygen dome, fuel dome and inlet temperature transducer sampled at1 kHz. OH-emission images and Schlieren pictures allow following the flame propagation experimentally.

Four injector geometries have been tested for varying J numbers and velocity ratios. About 60 test have been performed at ambient pressure, showing good ignition for mixture ration between 2.5 and 4. Low pressure ignition test are under way.

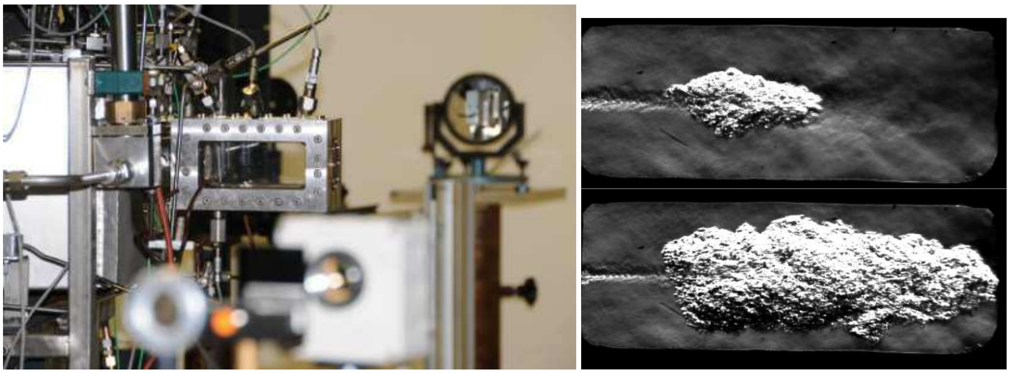


Figure 5: Chamber mounted on M3 with optical diagnostics (left) and flame propagation (right)

These tests have shown that both feed lines operate with stable parameters (pressure, flow rates) and they are decoupled from combustion chamber pressure variations during injection and ignition. This allows giving well defined boundary conditions to CFD calculations.

6.2. Ignition CFD simulation

The sequence of events possibly leading to a successful ignition can be decomposed in three main consecutive phases: 1) Energy deposition by laser pulse; 2) Primary ignition phase: spontaneous ignition, deflagration front propagation and flame kernel formation 3) Late evolution: kernel growth/propagation, flame anchoring/stabilization or blow-out.

Different strategies are envisaged in the CFD task. ONERA will apply the multi-physics CEDRE code in a LES approach. Uniroma intends to compute in more details, with more appropriate tools, the three phases mentioned above. After having computing the cold flow, with a standard procedure, a 3D compressible flow solver based on Adaptive Wavelet Multi-Level Representation with detailed kinetics will be used for the primary ignition phase modelling. Then the late evolution corresponding to the deflagration will use a 3D LES flow solver with Conditional Closure Model (CMC) for combustion sub-grid modelling

7. Methane Film Cooling

7.1. Film cooling experiments

The last open issue of the LTCP engine is the chamber cooling. Indeed, regenerative cooling requires a higher pump power due to the pressure loss in the regenerative circuit, which is contradictory to the stage requirement. Consequently, it is assumed that film cooling is the only cooling technique to be applied. After discussion during progress meetings and in order to provide a data base for code validation for all the participants of the project it was decided to operate the thruster with gaseous propellants and inject a gaseous film in order to reduce the complexity of the problem. Film cooling experiments will be performed on P6.1 test bench of DLR.

For this purpose DLR has manufactured a gas/gas injector head, which will be installed a segmented (6 segments each 50 mm long) water cooled combustor using an existing nozzle with a contraction ratio of 3.2 (Figure 6).

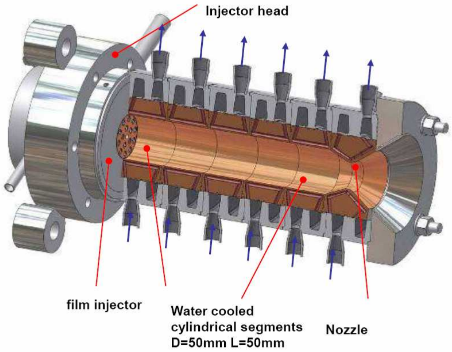


Figure 6 : Segmented combustion chamber

For the film cooling injection velocity DLR proposed an approach which keeps for one film injection slot height the film injection velocity similar to the propellant injection velocity and, by increasing the film mass flow rate increasing the injection velocity to match the average gas velocity in the combustor. Furthermore, two film injection segments with two different slot heights have been manufactured to investigate the influence of the velocity ratio between the film and main combustion chamber flow..
The heat flux to the water cooled wall and heat transfer coefficients will be calculated using a calorimetrical method. The flux is computed knowing inlet and outlet temperature, and the mass flowrate, deduced from pressure measurement as well. Combining with the measurement of wall temperature and chamber pressure leads to the evaluation of the heat transfer coefficient for each segment.
Test results will be used to evaluate CFD tools. For this purpose computations will be carried out at Astrium, DLR and University of Rome. Preliminary results are reported in [14].

8. Conclusion

Oxygen-methane combustion studies in the In-Space Propulsion Programme are aiming at providing the European Union with data and tools on open issues in order to have more knowledge for future developments of engines that will then be built with better confidence and less risks.

During the last fifteen months, experimental works have been performed leading to database for combustion of a single injector element flame fuelled with gaseous propellants and ignition at ambient and low pressure as well. At the same time, two chemical kinetic models have been developed. The first one was for low pressure methane combustion, on the base of well validated thermo-chemical data as the extension in the common hydrocarbon combustion mechanisms; the second one concern models for soot formation and oxidation in fuel-rich operating conditions on the base of semi-empirical models tailored for air/hydrocarbon combustion, and preliminary conclusion is that this soot modelling needs strong adjustment.,

In the next months, CFD activities will enter in main stage in order to continue developing and validating tools by the use of experimental results.

Acknowledgments

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