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High-fidelity LES calculation of an academic H2/air burner

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Summary

1 INTRODUCTION

1.1 Context of the project

The demands on air transport systems and electrical power generation dictates that turbines should be less polluting, less noisy and more efficient (1, 2). In addition, the scarcity of fossil fuels generates interest in the search for alternative fuels, such as bio fuels and hydrogen, which in the long term, are likely replacing traditional jet fuels (3, 4). Due to these demands, premixed combustion is a adequate choice as the preferred combustion mode since it provides lower flame temperatures when compared to diffusion flames, therefore it has lower NO_x emissions (5, 1). The high mixing quality, provided by the premixed combustion, has also shown to reduce NO_x emissions, as stated by (5, 6, 7).

To further enhance mixing quality, swirl-stabilized burners can be implemented. The swirl imposed on the flow provides sufficient mixing and creates a central recirculation zone inside the combustion chamber. The swirl-induced recirculation zone provides flame stabilization due to lowered flow velocities and by continuously feeding the flame with heat and combustion products (5). One instability present in this type of burner is the combustion induced flashback (FB), especially for highly reactive fuels (8).

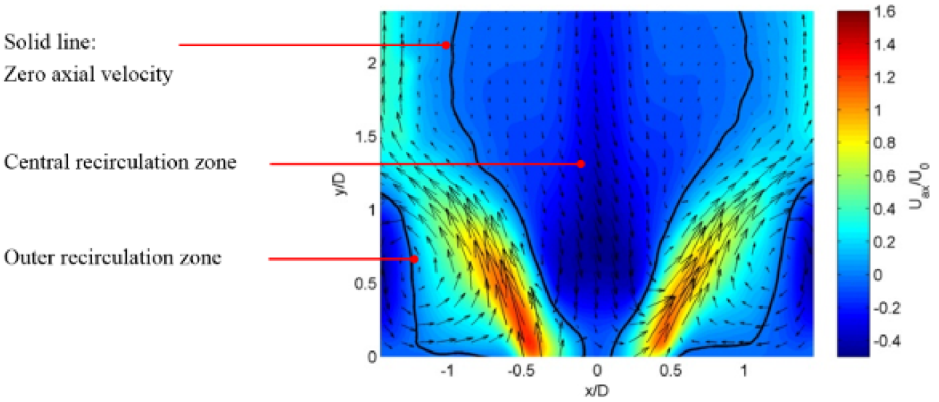

Figure 1: Swirl generated recirculation zones (2)

In recent papers the FB resistance in swirl-stabilized burners has been investigated. The position of the recirculation zone stagnation point is often used as a parameter to indicate FB resistance. This stagnation point is also referred as vortex breakdown (VB) (9). A velocity deficit along the center line makes the burner prone to FB. To avoid the flashback on the center line, (10, 11) suggested the use of a non-swirling axial jet. By doing so they were able to move the vortex breakdown position downstream and, hence, improve flashback resistance. Another effect of the addition of non-swirling axial jet is the improve in overall mixing quality (12). Reichel et al. (1) performed investigations regarding the effects of swirl number and mixing tube length on both FB resistance and mixing quality.

In the internship an academic swirl-stabilized burner was studied and simulated. The burner was developed by Reichel et al. (1). It consists of two air inlets, a radial swirler and a orifice on the central axis, both of which are fed by a shared plenum. The ratio of the the axial non-swirling flow to the overall inlet flow is defined as

$$\chi = \frac{\dot{V}_{ax}}{(\dot{V}_{ax} + \dot{V}_{sw})} \tag{1}$$

The mixing tube has a length $l = 60mm$ and diameter $D = 34mm$. Fuel is injected into the mixing tube through 16 injection holes of 1.6 mm diameter each. At the end of the mixing tube there is the combustion chamber.

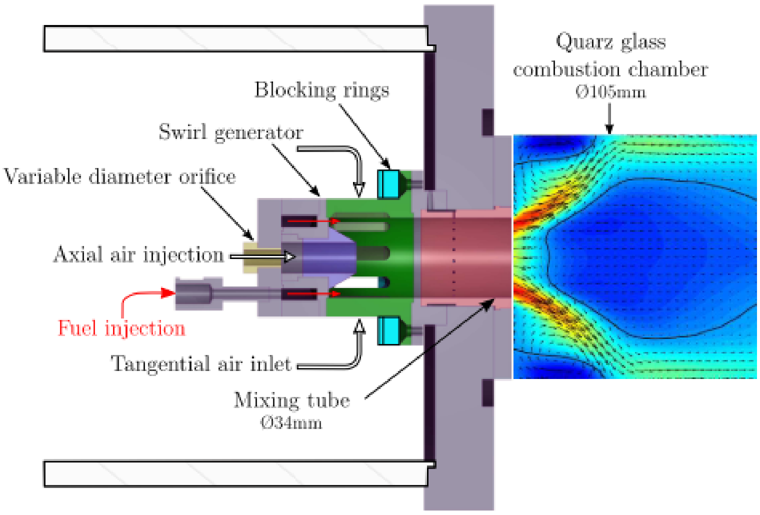

Figure 2: Swirl-stabilized burner (1)

Another parameter analyzed in the several papers was the momentum ratio. As stated by Reichel and Paschereit (9), the momentum ratio J is used to describe the impact of fuel momentum for varying combustor inlet parameters. The fuel momentum has the potential to strongly change the combustor flow field. J is defined as follows:

$$J = \frac{\rho_{fuel} u_{fuel}^2}{\rho_{air} u_{air}^2} \tag{2}$$

At a constant air mass flow rate, the momentum ratio J increases with increased equivalence ratio ϕ.

In this internship, with exception to the change in work fluid, the parameter varied in the simulated cases was the momentum ratio J. Mixing tube length l, swirl number S and the ratio χ remained constant.

1.2 Main objective

The general objective of this internship is to study and numerically simulate an academic swirl-stabilized burner (1) using the YALES2 solver developed by CORIA.

1.3 Specific objectives

The objective will be achieved through the following specific objectives:

- Familiarization with the YALES2 solver;
- Familiarization with the super computer MYRIA;
- Simulation and validation of Water test simulations;
- Simulation of CTR3, both cold and ignited simulations;

1.4 Methodological approach

The methodology of this internship consisted in first carrying out a bibliographic study in order to learn the basic aspects and functionality of the academic swirl-stabilized burner and to understand some of the instabilities related to this type of burner. After two training sessions took place in order to better understand how to use the YALES2 solver and how to perform simulations on the super computer MYRIA.

The simulations were done gradually in relation to the understanding of the subject. Firstly isothermal cold flow simulations were made using water as the work fluid following the experiments done by Reichel and Paschereit (9). Four different cases with regard to fuel mass flow rate were compared. Later a near flashback H_2/air cold flow simulation was done. The near flashback condition case was presented by (9, 13). Lastly the first attempts to ignite the flame in the simulation took place.

The internship was carried in one of INSA's classrooms, with weekly appointments with the tutor from CORIA. During these meetings, the advances and validations of the simulations, the bibliographic study and the report have been discussed. To facilitate, the presentation of weekly work was carried out in the form of slide shows. Every two weeks a meeting took place with both tutors. The internship was done with a partner. The results obtained during the internship and presented in this paper counted with the collaboration of J. Golse, student at INSA Rouen Normandie.

1.5 Document Organisation

2 Numerical simulation

In this internship all the numerical simulations were done with the YALES2 solver developed by CORIA and the calculations were done with the super computer MYRIA.

The mesh used in the calculations was provided by the tutor from SAFRAN. The mesh provided consisted of full tetrahedral elements and had close to five million cells. Using the function "MAIN GRID REFINEMENT" available in YALES2, the mesh was later refined. The refined version had close to 35 million cells.

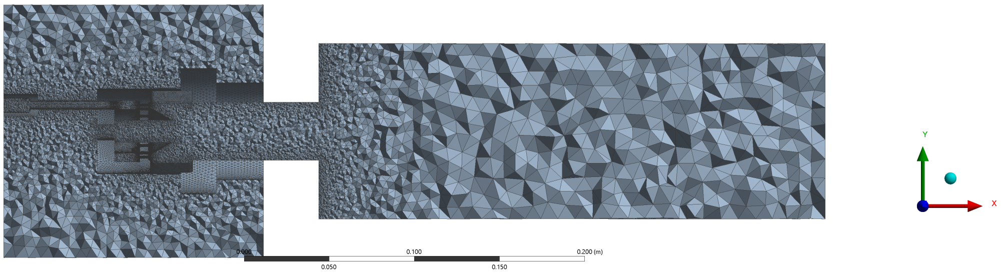

Figure 3: Mesh used in first simulations

The post processing of the results were all made using Paraview, with exception of a few graphs created with Python.

2.1 Water Test Simulation

The Water test simulations were made with the same conditions as the experiments held by Reichel and Paschereit (9). The work fluid is water, meaning both air and fuel flow were represented by water. Reynolds number was set to $Re = 40000$ with respect to the mixing tube diameter. Since the density ratio of fuel and air in the water test deviates from the density ratio of H_2 and air, the momentum ratio J was kept constant to achieve similarity between the experiments of both platforms (9, 6).

In total 4 cases were simulated. The table below summarizes the conditions used for each of the simulated cases.

Table 1: Water Test Conditions

Case	χ	J	Re	S	$\dot{V}$ [L/h]
1	7.5%	0	40000	0.9	4000
2	7.5%	2.5	40000	0.9	4000
3	7.5%	3.2	40000	0.9	4000
4	7.5%	6.3	40000	0.9	4000

where S is the Swirl number and $\dot{V}$ is the main inlet flow rate.

In order to see the influence of the momentum ratio J on the mixing quality, Reichel et al. (9) added dye to the water flow that represented the fuel and injected it through the fuel injection holes. To reproduce this experiment in the simulation, a passive scalar Z was introduced in the calculations. This scalar had a value equal to one in the fuel inlet and zero in the rest of the domain. By doing so we were able to calculate the unmixedness parameter used to analyse mixing quality.

The Unmixedness U was calculated as follows:

$$U = \frac{Z_{MEAN}^2}{(1 - Z_{RMS})Z_{RMS}} \tag{3}$$

Fig. 4 and Fig. 5 show the parameter U in the mixing chamber Y plane and in the mixing chamber outlet, respectively. Cases 2 (Upper right), 3 (Lower left) and 4 (Lower right) are shown. Case 1 is not plotted due to the absence of fuel injection ($J = 0$).

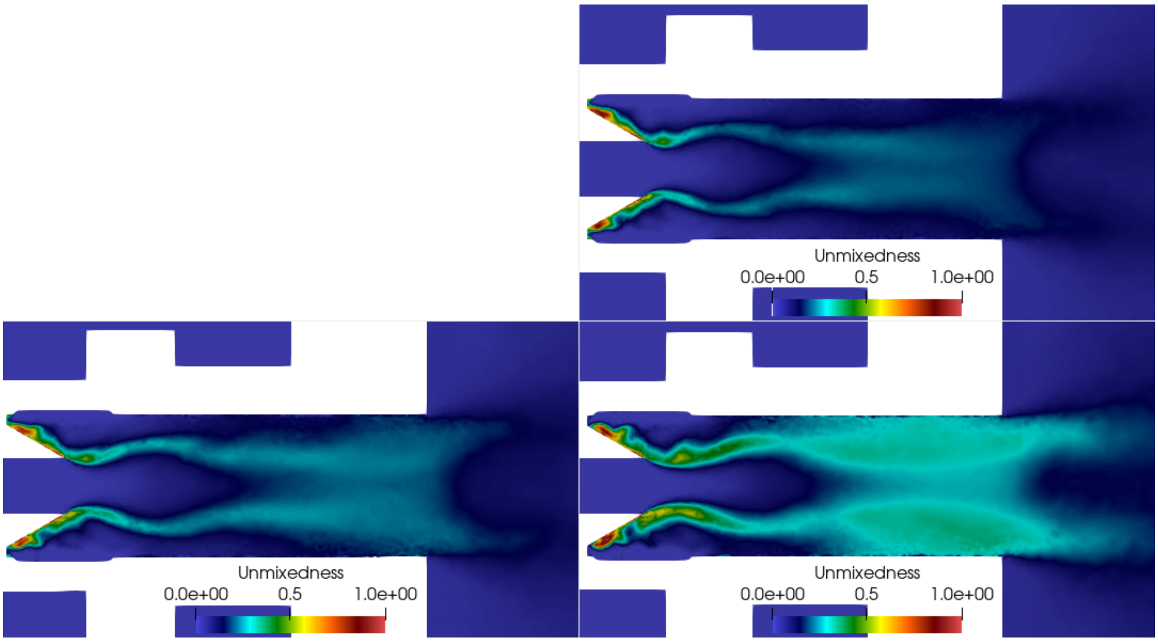

Figure 4: Unmixedness - Mixing Chamber Y Plane

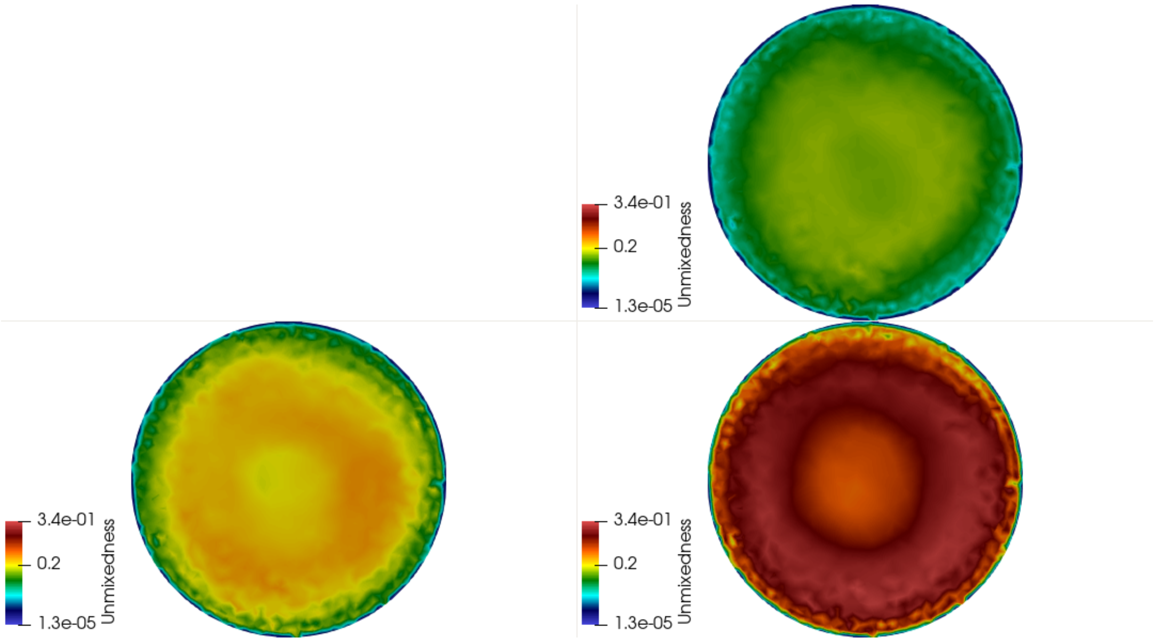

Figure 5: Unmixedness - Mixing Tube Outlet

As we can see from Fig. 4 and Fig. 5, the increase in momentum ratio J increased the unmixedness. According to Tanneberger et al. (5), a high unmixedness leads to locally higher equivalence ratios and since we increased the equivalence ratio by increasing J, this results were expected.

Another effect of momentum ratio J is on the vortex breakdown point, which indicates flashback resistance. The first set of simulations were made using the mesh with five million cells. Since the results were not in accordance with literature we used the function "MAIN GRID REFINEMENT" to refine the mesh and obtain the final mesh with around 35 million cells.

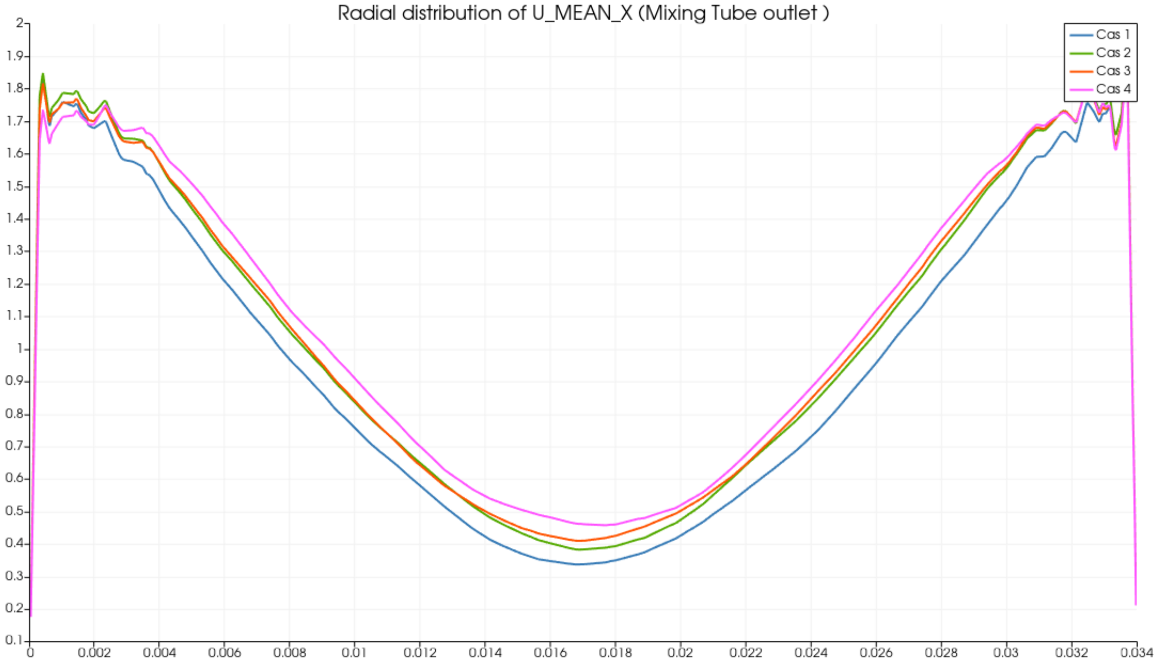

Figure 6: Radial Distribution of Mean Axial Velocity (Mixing Tube outlet)

As presented in Fig. 6, we notice the slight increase in the velocity field on the mixing tube outlet with increasing J. This phenomena is also observed in the results presented by Reichel and Paschereit (9).

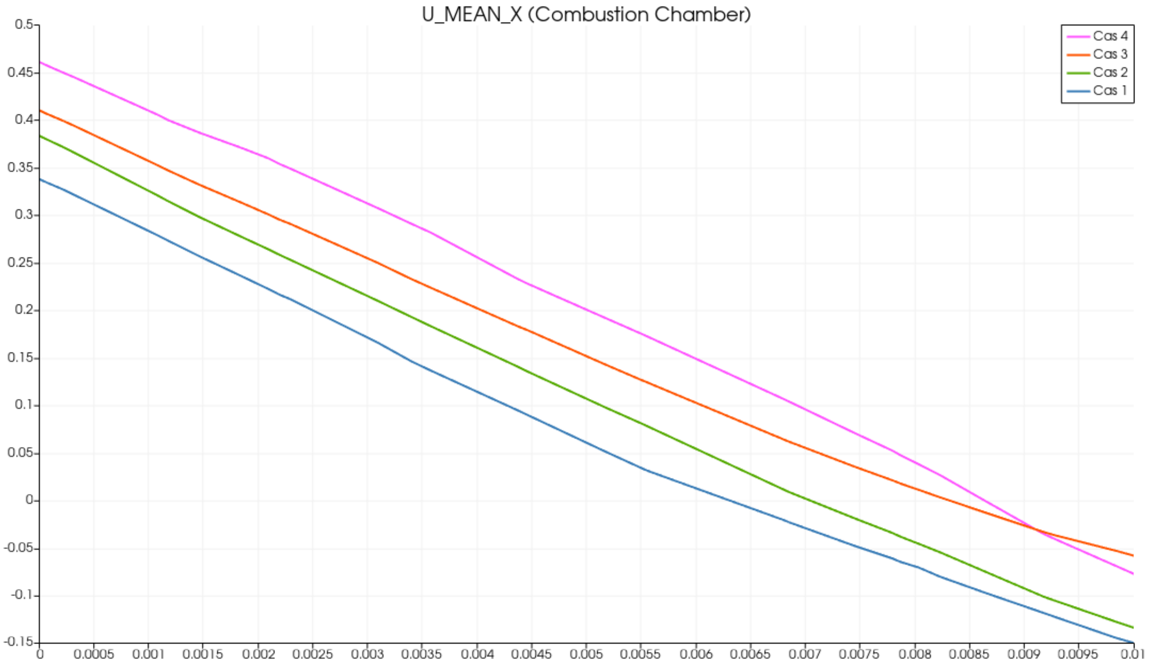

Figure 7: Mean Axial Velocity over the central axis - Combustion Chamber

Fig. 7 shows the mean axial velocity over the central axis in the combustion chamber. We can see that the vortex breakdown position was shifted downstream. This result was also reported in Reichel and Paschereit (9). This downstream shift of the vortex breakdown position leads to a increase in flashback resistance.

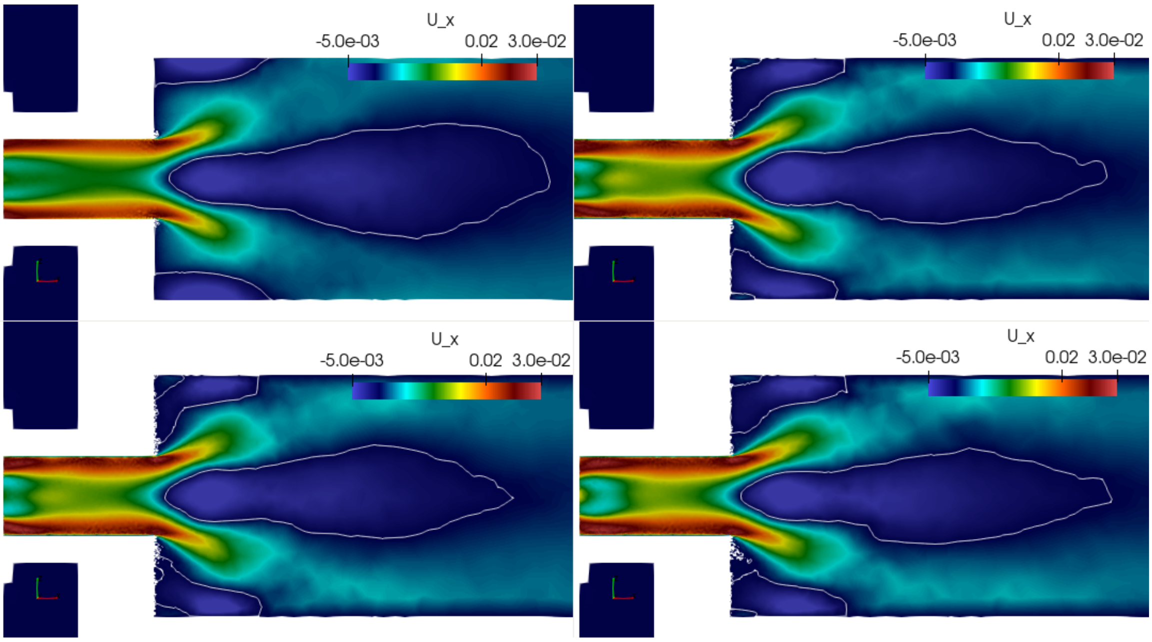

Figure 8: J impact on the velocity flow field

Fig. 8 shows the impact of the momentum ratio J on the velocity flow field for the 4 cases simulated (Case 1: Upper left, Case 2: Upper right, Case 3: Lower left, Case 4: Lower right). The solid lines in the combustion chamber represents $u_x = 0$ and, hence, the recirculation zones.

2.2 Cold Flow Hydrogen/air Simulation

Mira et al. (13) simulated 3 test cases, represented by red points on top of the experimentally measured stability map of the academic burner for a axial air injection of $\chi = 7.5\%$ (Reichel et al. (12)).

Table 2: Operating Conditions

Case	ϕ	J	Z_g	$\dot{m}_{air}$ (kg/h)	$\dot{m}_{fuel}$ (kg/h)
CTR1	0.0	0	0.0	180	2.19
CTR2	0.6	2.5	0.0171	180	3.13
CTR3	0.4	1.1	0.0115	180	0.0

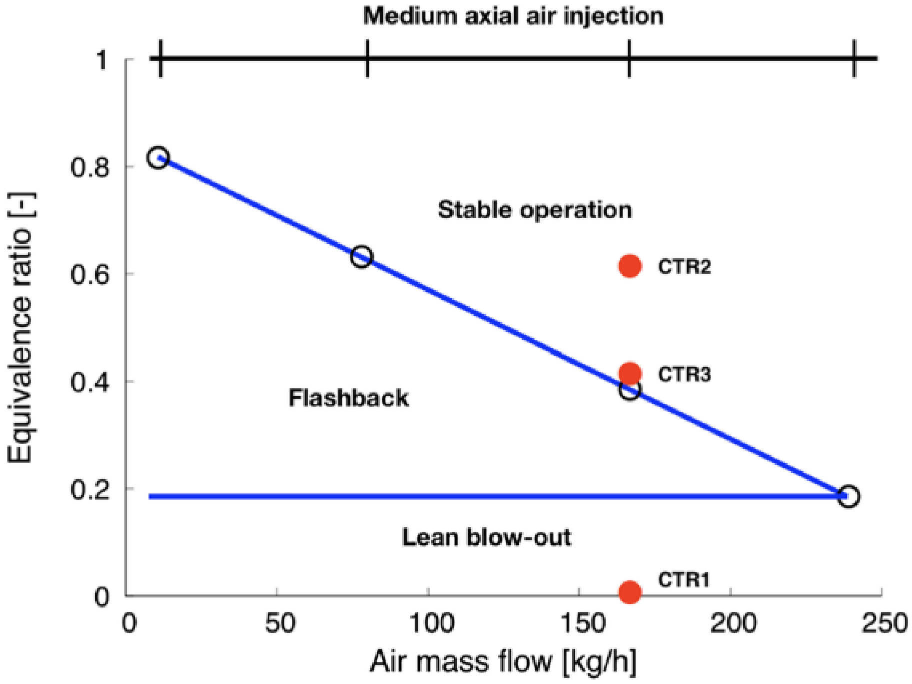

Figure 9: Stability map and selected computational cases for burner operation. Mira et al. (13)

In this paper the case called CTR3 was simulated without ignition. the operating conditions were the same as used in Mira et al. (13).

The mesh used was the refined mesh and all calculations were done in the super computer MYRIA. The total number of cores used were 840 and the simulations had to be re-launched every 24h due to limitations on the queue of the super computer. One issue faced was the size of the time step. With a time step in the order of $1e-8$ even after several days of simulation, a statistically steady state flow was not observed and the recirculation zones have not been formed completely. Increasing the CFL number was of no help since the simulation would diverge after a few iterations. The CFL used with no problems regarding divergence issues was $CFL = 0.6$.

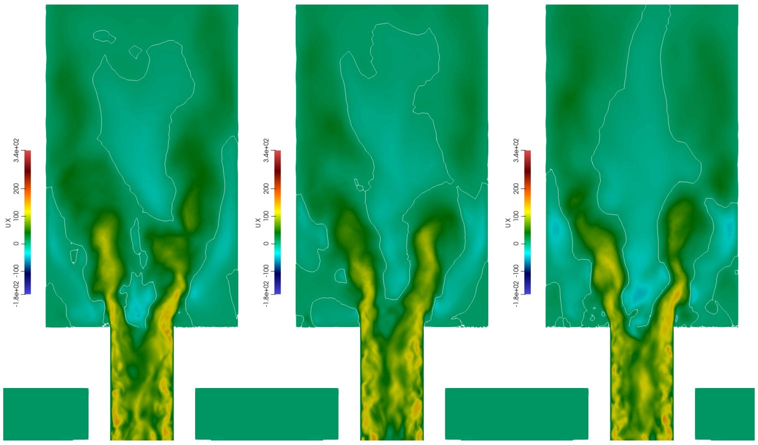

Figure 10: Velocity Flow Field a) Total time: 0.009298s b) Total time: 0.01057s c) Total time: 0.01423s

Fig. 10 shows 3 velocity flow fields for different total times. We can clearly see that the recirculation zones were still being formed. Fig. 10c) is the last simulations before the end of the internship and corresponds to the 16th day of simulation.

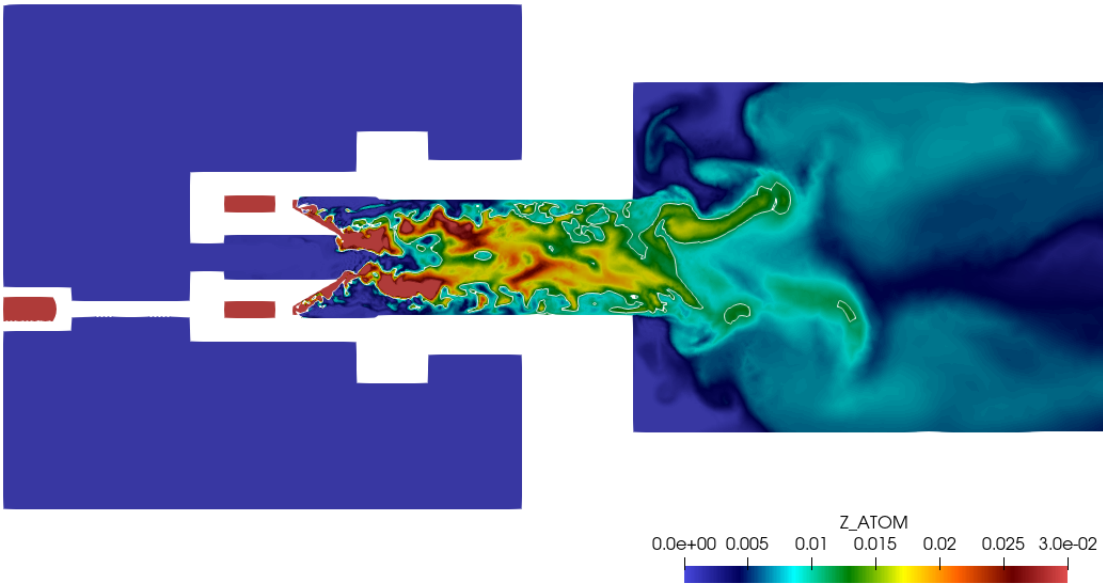

Figure 11: Z_{atom} - Bright line represents $Z_{atom} = 0.0115$ (Total time: 0.01423)

As we can see on Fig. 11, the injector is able to mix the hydrogen and air and provide a Z_{atom} field with close to $Z = 0.0115$ in the mixing tube outlet.

2.3 CTR3 Ignition

Using one of the results of the cold flow simulation for the case CTR3, we attempted to ignite the simulation. The ignition was done by increasing the temperature in a specific region. The kernel used was torus shaped and was positioned between the outer recirculation zones and the center recirculation zone. It increased the temperature to 2500 K with a a ramping time of 1e-3s and a total time of 6e-3s.

In order to set our thickening and efficiency scalars when igniting the mixture, we need to know the laminar conditions relating to our mixture. This is why we need to determine the values of the laminar flame thickness, the laminar flame velocity as well as the maximum source term of H20 in the flow. Since the case CTR3 had a equivalence ratio of $\phi = 0.4$, we conducted 1D simulations to calculate those proprieties. Table 3 summarizes the obtained results.

Table 3: 1D simulation results

δ_L	S_L	Y_{H_2O}
4.42e-4	0.794	181

where δ_L is the flame thickness, S_L is the laminar flame speed and Y_{H_2O} is the maximum H_2O source term. With this proprieties we were able to set the kernel and attempt the ignition.

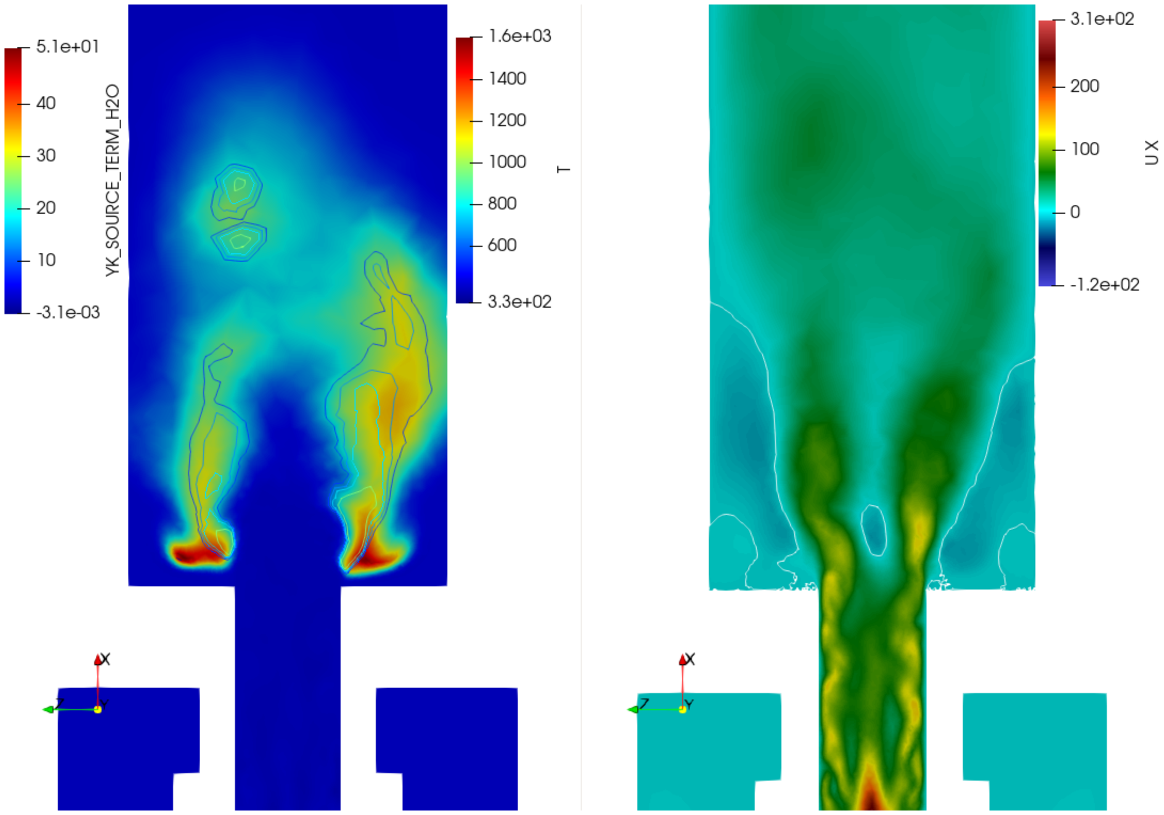

Figure 12: a) Temperature with Y_{H_2O} Source Term iso-contours b) Axial Velocity field with recirculation zones

As we can see in Fig. 12a), the positive values of the Y_{H_2O} source term shows us the existence of a combustion process. Due to the same issues faced when simulating the cold flow case, the recirculation zones are not yet formed as we can see on Fig. 12b).

In order to obtain better results for both the simulations of the case CTR3 more time would be needed.

3 Conclusion

The main objective of this work was to study and numerically simulate an academic swirl-stabilized burner. The softwares used were the YALES2 solver, Paraview and the programming language Python. For this internship, a methodology was follow-up in order to carry out the work, with 4 main steps:

- Bibliographic review on swirl-stabilized burners;

- Familiarization with the YALES2 solver and the super computer MYRIA;
- Realization of simulations;
- Post-processing and analysis of results.

The water test simulations were in accordance with the results available in the literature. We were able to observe the effects of momentum ratio J on the mixing quality and vortex breakdown position, which is a parameter used to indicate flashback resistance. Cold flow simulations of the case CTR3 were conducted on the super computer MYRIA. Further calculations need to be done in order to achieve better results. The ignition was made with a torus around the center recirculation zone, close to the flame attachment location. The Y_{H_2O} term source seems to be a good indicator of flame existence, since H_2O is a common product from combustion.

As a continuation of this work, some recommendations and indications of interesting points to study are shown below:

- The momentum ratio J effect on coherent structures;
- Implementation of a adaptive mesh;
- Further investigation on the cases CTR3 and CTR2.

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4.1 Abstract

4.1.1 English

In this paper, an academic swirl-stabilized burner was investigated. First, a brief introduction on swirl-stabilized burners is provided. The main goals of the internship as well as the specific goals are also given. Four different cases of a water test were simulated and the results were qualitatively compared with the literature. The effect of momentum ratio J on flashback resistance and mixing quality was investigated. Later the cold flow simulation of a near flashback case was done. The ignition of the cold flow case is presented afterwards. The calculations were made using the YALES2 solver and the super computer MYRIA.

Key-words: Swirl-stabilized Burner. Numerical Simulation. Hydrogen combustion. Large Eddy Simulation. Vortex Breakdown.

4.1.2 French

Dans cet article, un brûleur académique stabilisé par tourbillon a été étudié. Tout d'abord, une brève introduction sur les brûleurs stabilisés par tourbillon est fournie. Les objectifs principaux du stage ainsi que les objectifs spécifiques sont également donnés. Quatre cas différents d'un test d'eau ont été simulés et les résultats ont été comparés qualitativement avec la littérature. L'effet du rapport de quantité de mouvement J sur la résistance au retour de flamme et la qualité du mélange a été étudié. Plus tard, la simulation d'écoulement à froid d'un cas proche du flashback a été effectuée. L'allumage du cas de flux froid est présenté par la suite. Les calculs ont été effectués à l'aide du solveur YALES2 et du super ordinateur MYRIA.

Key-words: Brûleur stabilisé par tourbillon. Simulation numérique. Combustion d'hydrogène. LES. Rupture de vortex.