Stabilization of Non-premixed Turbulent Combustion by a Swirling Air Flow

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ABSTRACT

The conflict between search of combustion efficiency and fight against pollution is presented in this study as a Computational Fluid Dynamics (CFD) analysis of physical and numerical flame stability. This approach is applied in the context of influence related to the injection of a secondary air swirling flow in a non-premixed turbulent combustion chamber fed by fuel oil n°2. To achieve advantages suggested by this system, comparisons between basic, co-flow and swirl configurations are made according to the value of swirl number. Discussions about flame intensity and associated effects to the walls are established from temperature and unburned rate evolutions while considerations about pollution are given from estimations of pollutants concentrations. The final results reveal no risk of flashback or blowing phenomena, fast diminution of unburned products, significant thermal losses near walls and reduction of CO_2 production combined to a rise of NO formation.

Key words: Swirling flow, co-flow, swirl number, non-premixed turbulent combustion, reactingFOAM

INTRODUCTION

Even if Computational Fluids Dynamics (CFD) analysis has been successful in non-premixed turbulent combustion modeling and simulation, the prediction of flames stabilized by swirling jet continues to be a research area under exploration. Due to the importance of this type of fluid flow, considerable research efforts have been performed in this regard. Many projects were conducted to increase interaction between experimentalists and numerical analysts in order to reach good agreements between theory and realistic phenomena. Among these projects can be cited the International workshop on measurement and computation of Turbulent Non-premixed Flames called TNF (Albouze, 2009). To boost TNF researches, experimental simulations devices like TECFLAM (Albouze, 2009) swirl burners were developed but two limitations can be identified.

The first one concerns the nature of fuels used by TECFLAM. These are generally gas (methane, natural gas, etc.). In the present case, the fuel is a liquid (fuel oil n°2). According to CFD literature, it's less complicated to predict flames based on gaseous hydrocarbons than heavy oils

(Criner, 2008). This difficulty comes a part from strong influence of high viscosities on turbulence and combustion phenomena. And this is clearly seen during modeling and simulation of instabilities and mixtures.

Another limitation is about TECFLAM basic configurations. In most cases swirl jet is involved in primary air flows (Poireault, 1997) while this one is located in secondary air flows. In these kinds of situations the size of confinement plays an important role in the aerodynamics of flame (Criner, 2008).

In addition, the problem here is complicated by 3D assumption according to the complexity of systems and phenomena.

Despite all this, giving predictions that can satisfy industrial requirements (performance and security of systems), standards of environment protection (fight against pollution) and computational efficiency (need of precision, speed and robustness) still be a topical challenge in CFD.

DESCRIPTION OF THE PROBLEM

Geometry: In this study, the combustion chamber geometry is a typical case of those used in industrial drying furnaces (Fig. 1) (Raffak *et al.*, 2008). To obtain a non-premixed turbulent flame, the fuel oil n°2 is injected through the internal tube of the burner after being preheated and sprayed. At the same time, primary air at ambient temperature is introduced through the annular space. It is assumed that the two considered flows are coaxial. Finally, secondary air is introduced through 24 circular orifices on the edges of the front of our firebox (Fig. 1-2). To obtain a swirling flow (Fig. 3), system of axial and tangential injection of air (Criner, 2008) is used by mean of exhaust fans (Raffak *et al.*, 2008).

Boundary conditions: Experimental data obtained from measurements (Raffak *et al.*, 2008) are used in order to approach realistic situation. Entrance conditions are related to the flow rate and the temperature given from the burner exit. The inlet velocities of fuel and primary air are respectively 2.34 and 15 m sec^{-1} while their respective temperatures are 120 and 17°C. The outlet conditions are related to the pressure. The temperature of the nozzle was fixed to 980°C which is the limit of security imposed. According to the secondary air, the inlet velocity is a rotating profile field whose variation depends on the ratio of flow rates injection. About the walls, they are supposed to be adiabatic.
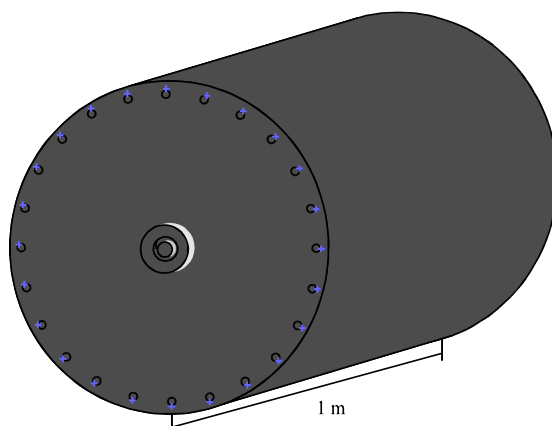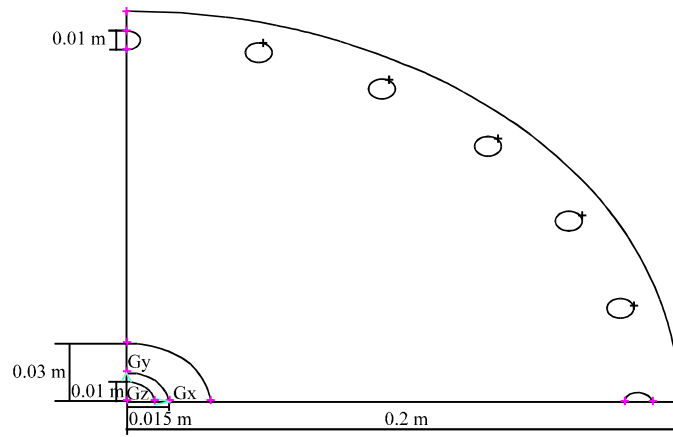

Fig. 1: Combustion chamber
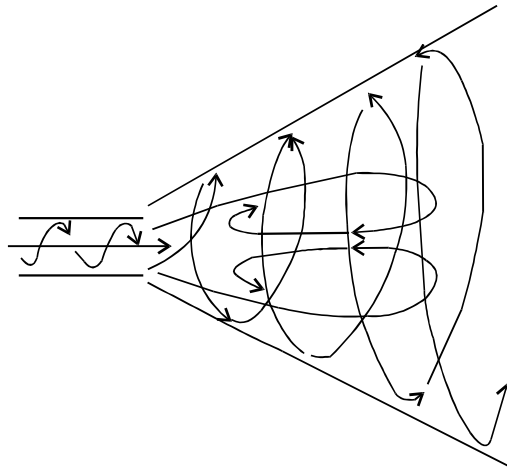
Fig. 2: Face measures

Fig. 3: Swirl flow with internal zone recirculation

MATHEMATICAL FORMULATION
Swirling flow

Swirl number (S) (Gupta *et al.*, 1984): The intensity of a swirling flow is given by a dimensionless number S called swirl number. This quantity establishes the relationship between the axial flux of kinetic momentum and the axial flux of axial momentum:

$$S = \frac{G_\theta}{RG_x} \tag{1}$$

G_θ can also be seen as the flux of tangential momentum and G_x is the flux of momentum following the direction of propagation. After developing the previous expression, S becomes:

$$S = \frac{\int_0^R \rho\left(\overline{uw} + \overline{u'w'}\right) r^2 dr}{R \int_0^R \rho\left(u^2 + \frac{\left(\overline{w}^2 - w_{max}^2\right)}{2}\right) r dr} \tag{2}$$

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where, R is the radius of the injector tube and $\vec{V}_{(u,v,w)}$ the velocity decomposed into mean and fluctuating values:

$$u = \bar{u} + u', \, v = \bar{v} + v', \, w = \bar{w} + w'$$

Equation of conservation of momentum for a swirling flow (Fluent Inc., 2000): As it has been already mentioned that the entrance of secondary air is characterized by a rotating velocity field. The absence of circumferential gradients in the swirling flow led us to consider the assumption of an axisymmetric configuration in order to establish the initial solution. We have now a 2D model with prediction of the circumferential velocity. Its equation of conservation of tangential momentum is:

$$\frac{\partial}{\partial t}(\rho w) + \frac{1}{r}\frac{\partial}{\partial x}(r\rho u w) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v w) = \frac{1}{r}\frac{\partial}{\partial x}\left[r\mu\frac{\partial w}{\partial x}\right] + \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^3\mu\frac{\partial}{\partial r}\left(\frac{\partial w}{\partial r}\right)\right] - \rho\frac{vw}{r} \tag{3}$$

Equations of the combustion: This section presents governing equations of combustion flow in the furnace. Chemical reactions that can be modeled include liquid fuel combustion in which fuel vapor is generated via evaporation of liquid droplets and a combustion reaction occurs in the gas phase.

Conservation of mass: The equation for conservation of mass, or continuity equation, can be written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla.\left(\rho.\vec{V}\right) = 0 \tag{4}$$

Conservation of momentum equation: Conservation of momentum is described by:

$$\rho\frac{\partial \vec{V}}{\partial t} + \rho\left(\vec{V}.\nabla\right)\vec{V} + \nabla\left(p\bar{\bar{\delta}} + \bar{\bar{\tau}}\right) = \rho\vec{g} \tag{5}$$

In the case of Newtonian fluids, the stress tensor $\bar{\bar{\tau}}$ is given by:

$$\bar{\bar{\tau}} = -\mu\left[\left(\nabla\vec{V}\right) + \left(\nabla\vec{V}\right)^T\right] + \left(\frac{2}{3}\mu - k\right)\left(\nabla\vec{V}\right)\bar{\bar{\delta}} \tag{6}$$

where, μ is the dynamic viscosity of the fluid, $\bar{\bar{\delta}}$ is the unit tensor, $\bar{\bar{\tau}}$ is the stress tensor associated with the fluid viscosity and k is the bulk viscosity.

Conservation of energy equation: The energy equation is solved in the following form:

$$\frac{\partial E}{\partial t} + \vec{V}.\left[\left(\rho E + p\right)\vec{V} - k\vec{\nabla}T + \left(\vec{V}.\bar{\bar{\tau}}\right)^T\right] = \rho(q + \vec{g}.\vec{V}) \tag{7}$$

where, E is the total energy, k is the thermal conductivity and q the term of internal generation of heat.

Equation of state (Albouze, 2009): The mixture formed in the furnace is supposed to be mixture of perfect gas:

$$p = \rho \frac{R}{MW(mixture)} T \tag{8}$$

The mixture molecular weight is:

$$MW(mixture) = \frac{1}{\sum_i \left(\frac{mF}{MW}\right)_i} \tag{9}$$

$R = 8.3143$ J mol^{-1} K^{-1} is the universal constant of perfect gas. MF, mF and MW are respectively the mole fraction, the mass fraction and the molecular weight of each species associated with the index i.

Conservation of chemical species equation (Elkaim *et al.*, 1989): Prediction of the local mass fraction of each species is done trough the solution of a convection-diffusion equation:

$$\frac{\partial}{\partial t}(\rho m_{i'}) + \frac{\partial}{\partial x_i}(\rho u_i m_{i'}) = -\frac{\partial}{\partial x_i} J_{i'i} + R_{i'} + S_{i'} \tag{10}$$

where, $m_{i'}$ is the local mass fraction of the ith species, $R_{i'}$ is the rate of creation or destruction, $S_{i'}$ is the creation rate in the dispersed phase:

• Mass diffusion flux for turbulent flows:

$$J_{i'i} = -(\rho D_{i'm} + \frac{\mu_t}{Sc_t}) + \frac{\partial m_{i'}}{\partial x_i} \tag{11}$$

where, Sc_t is the turbulent Schmidt number.
• Expression of the diffusive transport of species (depending on the mass enthalpy) in the energy equation:

$$\nabla.\left[\sum_{i'}^n (h_{i'}) J_{i'}\right] \tag{12}$$

IMPLEMENTATION IN OpenFOAM

The choice of implementation in OpenFOAM as CFD code compared to the commercial counterparts, e.g., Fluent and Ansys CFX etc. is justified by the fact that it offers a free advanced toolbox for solving complex physical problems involving chemical reactions, turbulence and heat transfer with the advantage to be totally open and free, both in terms of source code and in its structure and hierarchical design (Lundstrom, 2008).

Description of OpenFOAM (Open field operation and manipulation) (OCFD, 2007): Native development of OpenFOAM is done on a Linux/UNIX platform and specifically in the GCC (Gnu
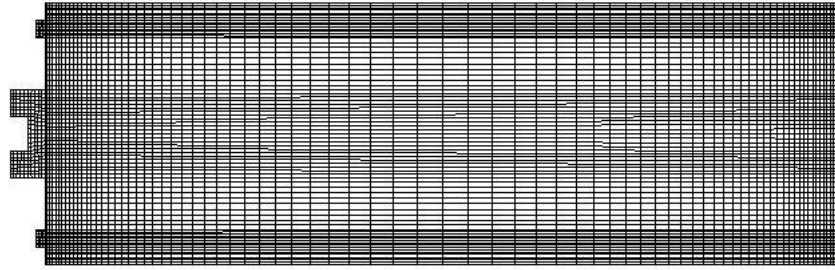
Fig. 4: 2D initial solution mesh view

Compiler Collection) C++ compiler. To pre-process and solve cases, two ways are offered: use of the graphical user interface called FoamX or the Terminal. As direct access to OpenFOAM's source code is possible (text files in C), modifications of boundary conditions or input/output control are allowed by editing the files manually. The post-processing is done by ParaView.

Mesh: Although, OpenFOAM has a mesh tool called BlockMesh exportation of other meshes is feasible. It is important to note that OpenFOAM is strictly a 3D code. To find an initial solution for a 2D axisymmetric problem (Fig. 4), the mesh must be 3D first with one cell thick and having no solution in Z-direction. We must ensure that the opening of the thickness of both sides between the Y-axis does not exceed the angle whose apex would be on the Y-axis and between 2.5 and 5° (Andersen and Niels, 2008).

TURBULENCE AND COMBUSTION MODELING

Turbulence (Fluent Inc., 2000): The Direct Numerical Simulation (DNS) is effective when simple academic problems occur otherwise it would be numerically expensive as it can be seen in our case because the phenomena and configurations are complex. The advantage of LES (Large Eddy Simulation) is to combine modeling and direct calculation but the computation of its pre-processor and solver costs a lot. Another problem related to LES is that their coupling with other models is not yet mature in OpenFOAM. Taking in account all those points RANS (Reynolds Averaged Navier-Stokes) remains the only one approach more accessible to use in our work. The model chosen is k-ε standard because of its robustness, accuracy, low cost and rich documentation. Its weakness in walls zone can be offset by the Standard Model Wall Function (SWF).

Combustion (Andersen and Niels, 2008): For combustion gas, there are three types of solvers all operating in unsteady state: reactingFOAM (Lundstrom, 2008), Xoodles and XiFoam. Only reactingFOAM models the non-premixed turbulent combustion. The concept it uses for the chemical species is the PaSR (Partially Stirred Reactor) which is a modified version of the EDC (Eddy Dissipation Concept) where the chemical time scale is handled differently:

- Expression of air-fuel reaction mechanism:

$$C_{19}H_{30} + 26.5O_2 \rightarrow 19CO_2 + 15H_2O \tag{13}$$

- Expression of the reaction rate constant according to Arrhenius kinetic model:

$$k(T) = AT^b \exp\left(-\frac{E_A}{R_u T}\right) \tag{14}$$

where, E_A is the activation energy (1.256×10^8 J kg^{-1} mol^{-1}) and A is the pre-exponential factor (2.587×10^9).

The Eq. 14 was originally made for laminar case. If we want to adapt it to turbulent case, just define the mixture rate by the ratio:

$$turb_{max} = \varepsilon/k \tag{15}$$

NB: the reaction mechanism is imported from Chemkin (software tool for solving complex chemical kinetics problems):

- ReactingFOAM Code:
- Calculate chemical reaction based on turbulent and chemical timescales
- Calculate of the density
- Calculate velocity/pressure fields
- Read species and feed them to the chemistry solver using Chemkin table
- Calculate the temperature from the chemical reactions enthalpy lookup
- Calculate the pressure field using PISO
- Correct the turbulence (pressure-corrector)
- Update the density from the temperature
- Return to step 1

NUMERICAL RESOLUTION

Discretisation method used by OpenFOAM is Finite Volume (FVM). Only transient models like reactingFOAM need temporal discretisation (Lundstrom, 2008).

Temporal discretisation: To avoid instability due to the simultaneous calculation of turbulence and combustion, the first solver to use is simpleFOAM which is a steady-state incompressible turbulence model. This is done to calculate the cold flow which will be considered as our initial solution. Knowing that reactingFOAM is an unsteady solver, the time step depends strongly on the Courant number Cr. This is possible only with the CFL (Courant Friedrichs Lewy) condition:

$$C_r = \frac{\overline{v}\Delta t}{\delta x} \tag{16}$$

If $0 < C_r = 0.5$, we have more stability and less speed. If $1 > C_r = 0.5$, we have more speed and less stability. In this case, Cr = 0.2.

Interpolation schemes:

- **Pressure:** LimitedLinear 1 (second order bounded scheme)
- **Velocity:** LimitedLinear V (TVD scheme recommended for swirl)
- **Turbulence:** Upwind (first order bounded scheme)

- **Species:** Upwind
- **Energy:** Upwind
- **Pressure-velocity coupling:** PISO (Pressure Implicit with Splitting of Operators)

RESULTS

Advantages of swirling secondary air configuration:

Tight confinement: The swirling flow affects the behavior of the flame because we are dealing with a tight confinement, in other words, the dimensions (i.e., diameter) of the injector are not negligible compared to the chamber dimensions (Fig. 1, 2) (Poireault, 1997).

Decrease of unburned rate: The Mass Fraction of Fuel (MF_f) at the outlet has almost decreased by an half as can confirm the values and graph below (Fig. 5):

- MF_f (without swirl) = ±0.1057
- MF_f (with co-flow: S = 0) = ±0.0478
- MF_f (with swirl: S = 0.3) = ±0.0478

Better protection of walls: Temperature decreases considerably near the walls (Fig. 6). This fall ΔT is inversely proportional to S. This is verified through values of transversal temperature differences observed when S = 0 or S = 0.3 (Fig. 7, 8):

- For internal transversal temperature: if S = 0.3: $\Delta T_{swirl} = T\text{-}T_{swirl} = 1150°C$ (Fig. 7)
- For outlet transversal temperature: if S = 0.3: $\Delta T_{swirl} = T\text{-}T_{swirl} = 650°C$ (Fig. 8)

Stabilization of combustion: This is done by increasing the residence time of the flame and creating recirculation in the reaction zone. The effect produced is to favor the mixture and give to the flame a more compact form (Poireault, 1997) (Fig. 9-13). The axial evolution of swirling temperature profile is almost linear (Fig. 11). It means that swirl configuration provides better and easiest control of temperature in flow direction.

Reduction of the CO_2 formation: Values and graphs of $mF(CO_2)$ below (Fig. 14, 15) reveal a decrease of the outlet CO_2 mass fraction in the case of intense swirl:
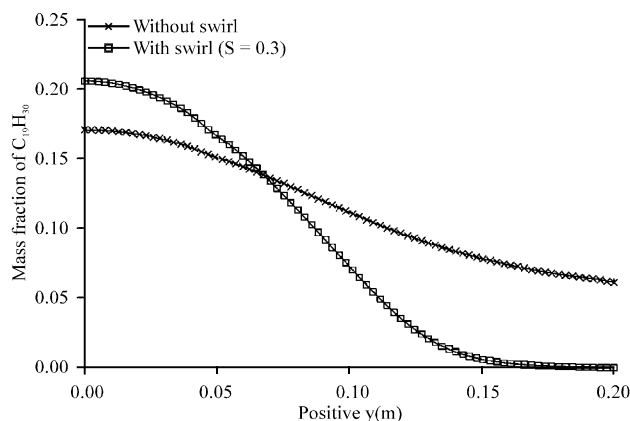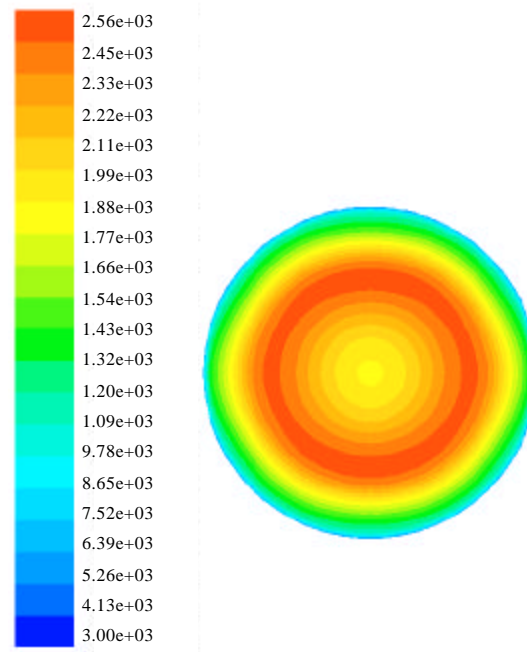

Fig. 5: Outlet mass fraction of $C_{19}H_{30}$
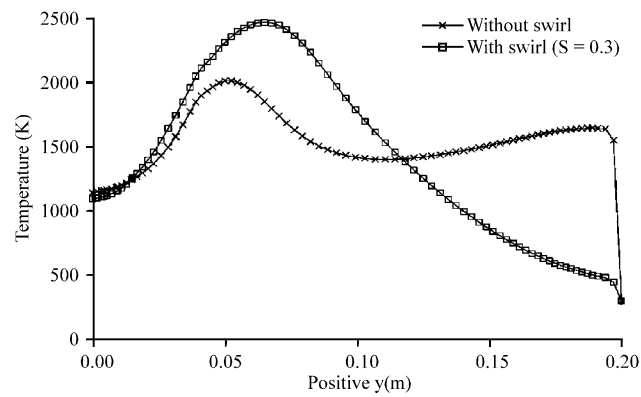
Fig. 6: Radial evolution of temperature contours

Fig. 7: Internal transversal temperature (x = 0, z = 0.52)

- Without swirl, $mF(CO_2) = \pm 0.1893$
- With co-flow (S = 0), $mF(CO_2)_{co\text{-}flow} = \pm 0.1677$
- With swirl (S = 0.6), $mF(CO_2)_{swirl} = \pm 0.1637$

Disadvantages of swirling secondary air configuration

Rise of outlet temperature: Calculation of the mass-weighted average value of temperature at outlet gives:

$$\bar{T} = \frac{\int T \rho \vec{V} d\vec{A}}{\int \rho \vec{V} d\vec{A}} \tag{17}$$

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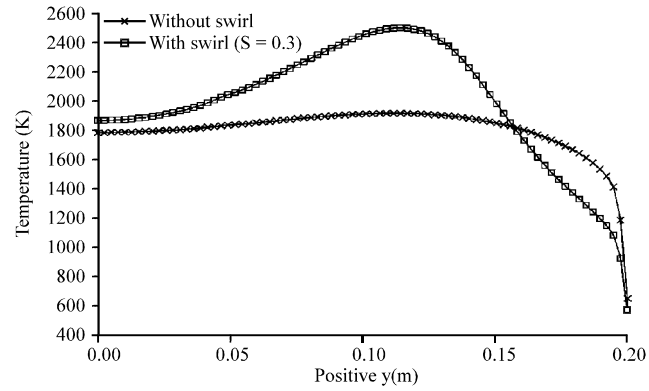
Fig. 8: Outlet transversal temperature
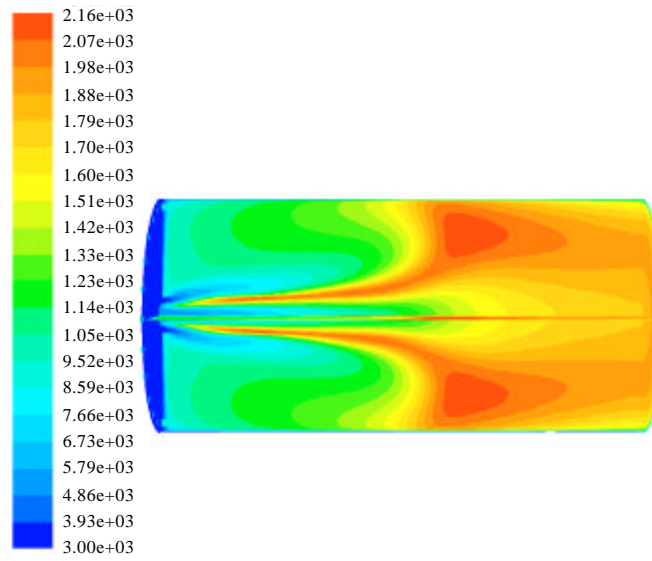
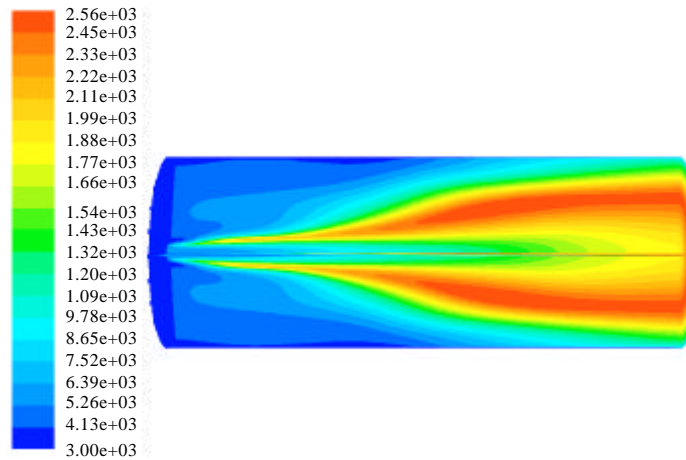Fig. 9: Temperature contours without swirl
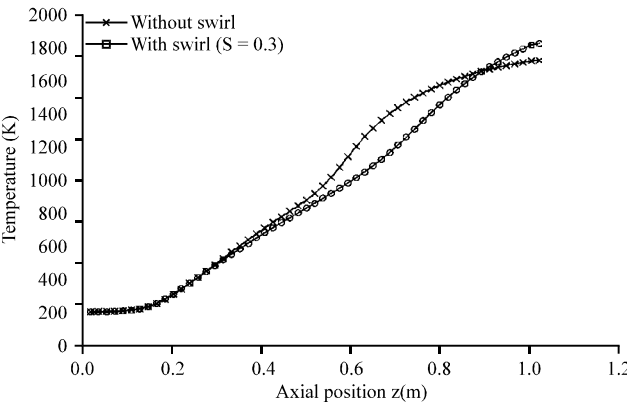

Fig. 10: Temperature contours with swirl
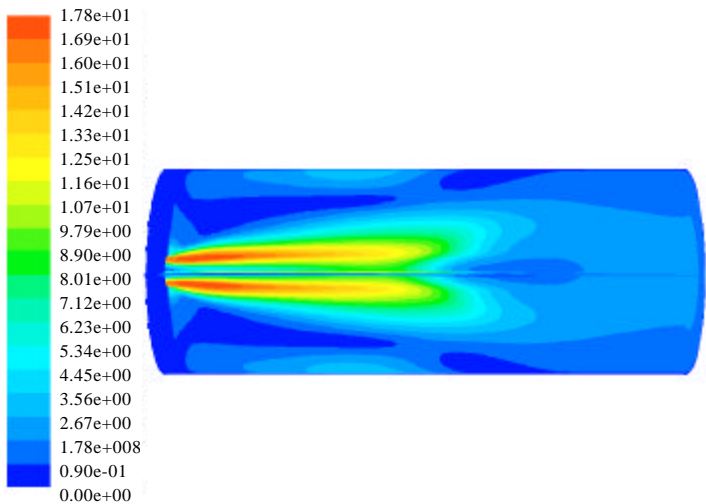
Fig. 11: Axial temperature evolution

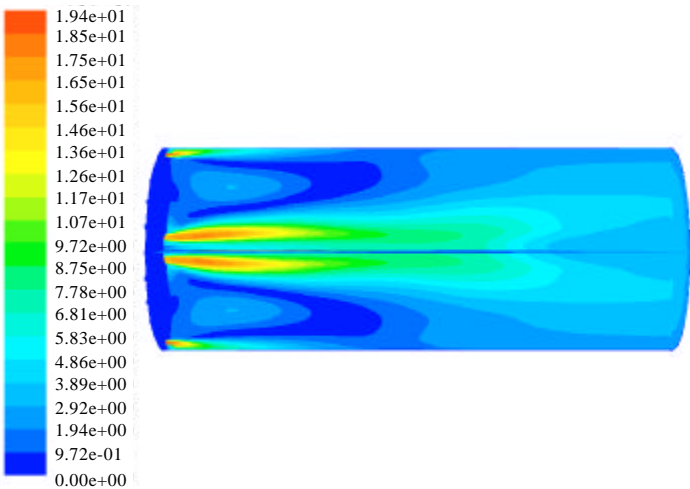Fig. 12: Velocity contours without swirl
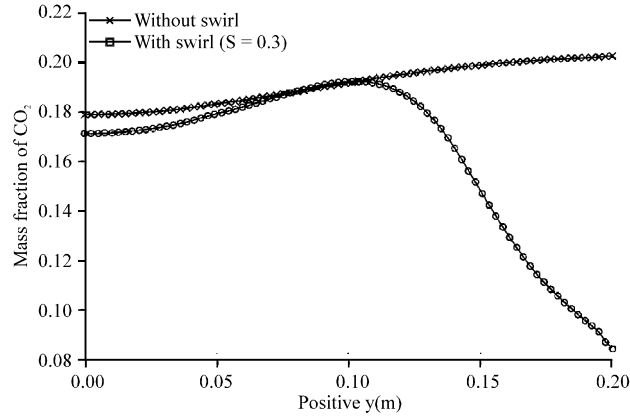
Fig. 13: Velocity contours with swirl

Fig. 14: Outlet mass fraction of CO_2

Fig. 15: Axial mass fraction of CO_2
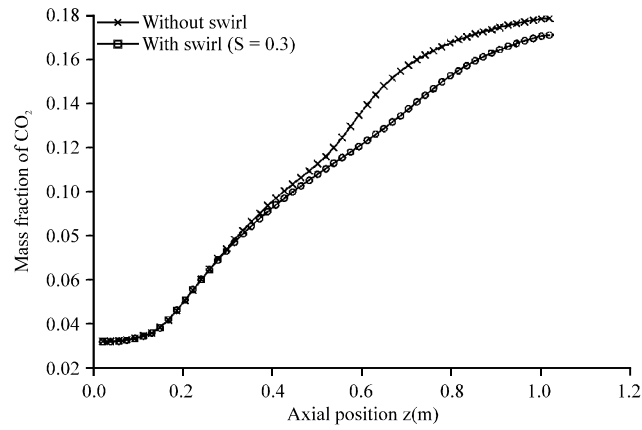
- Without swirl, $\overline{T} = \pm 1827K$
- With co-flow (S = 0), $\overline{T}_{co\text{-}flow} = \pm 1934K$
- With swirl (S=0.6), $\overline{T}_{swirl} = \pm 1879K$

Amplification of the swirl promotes NO formation: The same observation was made on a small scale by Vauchelles (2004). After 3 test cases (S = 0.3; S = 0.5; S = 0.7) of swirling secondary air injection to a combustion chamber of gas turbine engine, he asserts that the reduction of CO_2 emissions means better combustion and thus a rise of temperature controlling NO.

To reach this conclusion, the following two approaches can be used:

- Calculation of NO concentration (ppm) in the gas mixture
- NO ppm is computed from the following equation:

$$NOppm = \frac{MF(NO) \times 10^6}{1 - MF(H_2O)} \qquad (18)$$
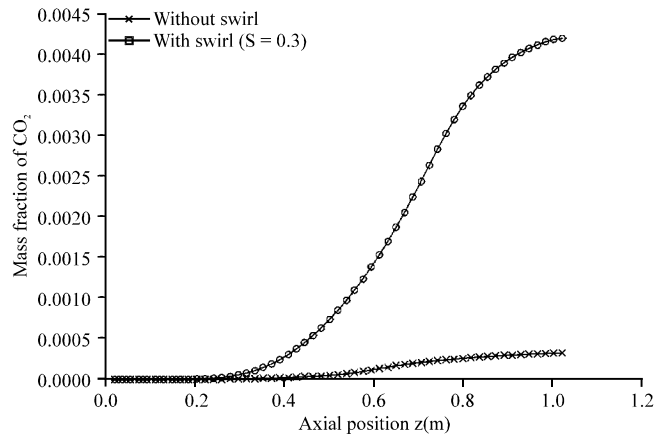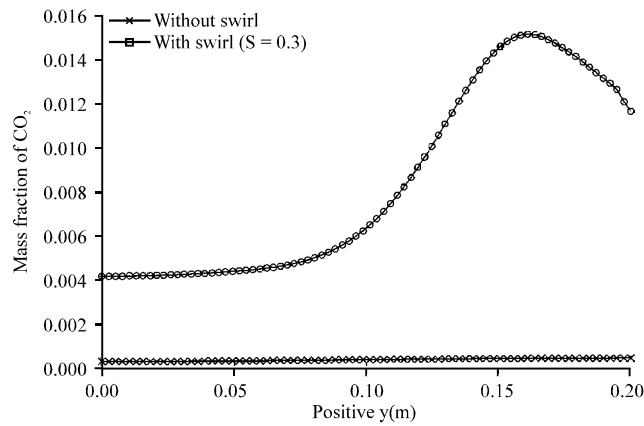
Where:

Fig. 16: Axial mass fraction of NO

Fig. 17: Outlet mass fraction of NO

$$MF(NO) = \frac{mF(NO)XMW(mixture)}{30} \qquad (19)$$

After calculation, it can be seen through the values and graphs of MW(NO) below (Fig. 16, 17) that the swirl promotes the production of NO:

- Without swirl, MW(NO) ~1019 ppm
- With co-flow (S = 0), MW(NO)co-flow ~2933 ppm
- With swirl (S = 0.6), MW(NO)swirl ~3152 ppm

Estimation of average mass fraction of outgoing NO:
The mass fraction of outgoing NO experienced a sharp increase with the intensification of the swirl:

- Without swirl, mF(NO) ~0.0011
- With co-flow (S = 0), mF(NO) ~0.0092
- With swirl (S = 0.6), mF(NO) ~0.0091

DISCUSSION

For better understanding of the potential role played by a secondary air swirling flow in a turbulent non-premixed combustion chamber, two test cases situations are considered : a pure axial jet of secondary air called "co-flow" (with S = 0) and an weak swirl jet (with S = 0.3) characterized by the presence of an IRZ (Internal Recirculation Zone). Non-premixed flames can be quenched by lowering the temperatures of the oxidizer stream, or by increasing the flow strain rate (equivalently scalar dissipation rate) (Liu *et al.*, 2012). In the first case there is a possible risk of blowing phenomenon for the secondary air flow strain rate is increased. As it is known the blow tends to get rid of the IRZ pushing the flame to hanging or extinction. In the last case (Taupin, 2003) a flashback to the injector's tube can occur and lead to a suspension of the flame. Flashback occurs when the gas velocity becomes lower than the burning velocity due to flame propagation within boundary layer, core flow or because of combustion instabilities (Sankaran *et al.*, 2006). Flashback in swirl burners (Fritz *et al.*, 2004) can be caused by a phenomena termed Combustion Induced Vortex Breakdown (CIVB) due to rapid expansion at the burner exit creating a recirculation zone which acts as a flame holder: the breakdown of this structure can occur due to flow perturbations and chemical reaction effects causing the CRZ (Central Recirculation Zone) and hence flame to propagate upstream into the premixing zone (Fritz *et al.*, 2004).

None of these two phenomena was observed because of the good tight confinement between combustion chamber and swirling air injectors. This led us to introduce confidently discussion about the flame stability based on the influence of number of Swirl (S). Studies will be extended in the next paper to deal with greater values of S.

Concerning the combustion intensity, we noticed simultaneously an increase of NO formation and a decreased of CO_2 production. We know that the two gases are the leading pollutants in combustion sites (Ferrand, 2003). This is justified by the fact that the main reaction mechanism involved for NO is that of Zeldovich (1946) which is essentially thermal as it is generated by the rise of the activation temperature in a reaction zone such as an oxidizing environment (Taupin, 2003). This observation is quite normal for in non-premixed condition, fuel is injected in shear region formed near to the zero stream line boundary and recirculation region which provides the low velocity region for flame stabilization with the evolution of high temperatures from the flame. For flames operating in diffusion mode, the reaction zone is stabilized to result in large temperature gradients and hot-spot regions in the entire combustion chamber that result in high NO levels (Gupta *et al.*, 1984) from the combustion of fuels. NO emission increased due to the accelerated chemical kinetics of the combustion process (Khalil and Gupta, 2011). Concerning CO_2 production, it is possible to reduce more by increasing the inlet air temperature but this will result in increasing the flame temperature which in its turn will increase the production of NO (Khalil and Gupta, 2011). Another solution to explore about CO_2 production can be the elevation of pressure into the combustor. As according to Khalil and Gupta (2011), this will promote the combustion kinetics to enhance the combustion reactions. At low equivalence ratios, increase in pressure diminishes CO by accelerating the rate of conversion of CO into CO_2. At high equivalence ratios, increase in combustion pressure reduces CO emissions, albeit to a lesser extent, by suppressing chemical dissociation. So in one aspect high pressures are beneficial but on the other hand, high pressure also accelerated NOx formation leading to higher NO emissions (Khalil and Gupta, 2011).

The future work will be to control temperature so as to expect a good balance between reducing pollution and improving combustion. Moreover, the protection of walls remains a priority. For complete study, it will be better to couple the influence of temperature with the humidity effects near walls by means of transversal evolution of H_2O mass fraction.

To assess the stability of reactingFOAM, the role of convection schemes in the solution was investigated. That is the reason why we used successively upwind and limitedLinear to compute the energy and species. The result was the same but instability (represented by "wiggles") occurred in the temperature profile when we tried QUICK scheme. Versteeg and Malalasekera (2007) have showed that this is due to the QUICK schemes nature which has a tendency to produce over-shoots and under-shoots in the results and thus producing the obtained "wiggles".

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