Numerical simulations of gaseous flames in combustion chamber applications

C Katona¹, C Safta², F Frunzulica³, M Goemans¹
Production Editor, Journal of Physics: Conference Series, IOP Publishing, Dirac House, Temple Back, Bristol BS1 6BE, UK

E-mail: katona.cosmin@yahoo.ro

Abstract. Recent developments and assessments of combustion models, numerical schemes and high-power computing allow simulations to be applied to real industrial thermal oxidizers and burners. In this paper, two type concepts in a complex geometry of a burner and combustion chamber is reviewed by means of measurements data from on-site during operations compared with the numerical simulation’s analysis. The combustion models as Flamelet, Flamelet Generated Manifolds (FGM) and Hybrid BML/Flamelet are performed to assess modeling and fundamental flow aspects of combustion instabilities in a swirl concept in the context of the Reynolds-averaged Navier Stokes (RANS) equations for gaseous flames. Simulations in real thermal oxidizers illustrate the prospective of the approach but the combustion modeling and chemistry sub-grid models are limited cases in terms of validations due to the lack of available advanced set of measurements. Specific issues associated to real thermal oxidizer are presented: on-site measurements during operations, multi-penetration of heat in the combustor walls and flame instabilities. The examples are assigned as mean flow predictions (velocity, temperature and species) and transient phenomena (ignition and flame instabilities). Finally, the conceptual differences of the potential perspectives are discussed in detail from a theoretical and practical point of view.

Keywords: Numerical simulations, NUMECA FINE™/Open CFD, swirl flame, gaseous combustion, combustion instabilities

1. Introduction

Industrial thermal oxidizers involve a large scale of ranges and complexities determined by the customized designs of chambers, burners and different combustion regimes developed in these devices.

Designers always were forced to develop optimized burners because of the weight and space restrictions which would be needed to assure a maximum efficiency and closeness. In the last years,
the manufactures have obtained and improved experience with the designs by adding either largely
flow recirculation with multi-fuel point injections, either multi-cooling effects with staging concepts.
To those already mentioned, adding the new pollutant regulations, the green environment community-
imposed changes to the technologies.

All these constrains and new concepts induced a high complexity of the flow and lead to specific
flow dynamics and reactive flow responses. Already in the market the manufactures are constantly
evaluating the design with Computational Fluid Dynamics (CFD), most often strategies largely rely on
Reynolds Average Navier-Stokes (RANS) approaches developed for mean stationary flows. The
benefit from these models is that the scientific community have been always with success calibrated
on fundamentals configurations. We accept as scientific community that RANS models in
unsteadiness simulations are very difficult when it comes to model unsteadiness and inhomogeneities.
In this matter, two fully unsteady computing are current available for turbulent reactive flows: Direct
Numerical Simulations (DNS) and Large Eddy Simulations (LES). Over the years the models have
grown very fast due to the network of the computing power and parallel architecture. Mainly the LES
have been replacing the RANS models because of the routinely development and bench-marked by the
turbulent combustion scientific community.

In this paper the classical flamelet, the hybrid BML and FGM method will be assessed on a series
of semi-industrial to industrial configuration cases for a non-premixed gaseous flame along with a
RANS model context. The CFD solver package and numerical modelling used are OMNIS™ for the
generation of the unstructured, hexahedral meshes and FINE™/Open with Open Labs for solving the
equations for flow, turbulence and combustion with the possibility to develop new models through the
meta-language user friendly, Open Labs. The flow solver applies a cell centered finite volume method
and time-stepping for the integration of the governing flow equations. The RANS equations are
discretized centrally by means of Jameson and Schmidt scheme, the combustion transport equation
is using a first order upwind scheme and an explicit 4-stage Runge-Kutta scheme is used for the time
among parallelization and multigrid methods.

2. Fundamentals of CFD for complex burner simulation
This paragraph describes the basics of RANS: fundamentals, models for high Reynolds number flows,
discretization of the governing model equations, turbulent combustion models with the chemical
descriptions, boundary conditions and their impact on the predictions.

2.1. Combustion models
The species and energy equations cannot be closed without a significant modelling. They are not only
governed by turbulence but also depend on mixing: different combustion cases are reliable depending
on the flow configuration, characteristics of fuel/oxidizer and injection system present in the burner.

The combustion regimes lead mostly to physical processes that influences a flame and guides to
choose the most suitable models: Flamelet, Flamelet Generated Manifold (FGM), Bray-Moss-Libby
(BML), thickened flame, rotational regimes, reaction rate etc. Laminar flames are the natural starting
point to distinguish combustion phenomena present in the real applications: diffusion flames,
premixed flames, and partially premixed flames.

Additionally, a turbulence models is introduced through the notion of combustion phenomena to
suit the use of a specific turbulent combustion model knowing the combustion regime, typically
applied in RANS models. A brief overview of major combustion/chemistry is provided below relying
on Numeca documentation.

2.1.1. Chemical description. Combustion is a multi-scale physics consisting in a large range of time
scales. Prior to their use in the CFD codes, a list of strategies can be pointed such as: constitutive
relations, chemical mechanism reduction, stiff chemistry integrators or storage chemistry approaches.
The last strategy, storage chemistry approaches, aims to accelerate the chemistry interaction while the
turbulence code integration runs. Typical models are Flamelet Generated Model (FGM or ILDM), in
situ adaptive tabulation, piece-wise reusable implementation of solution mapping (PRISM) or Artificial Neural Networks (ANN). Ultimately, the range of the applicability will create the main restriction for the all reduction methods. The final kinetic model will be strongly connected to the turbulent combustion model which is already developed with a series of assumptions. The fundamental chemical description is seriously altered from the extent of the tables and general schemes.

2.1.2. Turbulent combustion models. Like all CFD codes, the RANS turbulent combustion models rely strongly on the fundamental theories and combustion regimes: non-premixed, partially premixed and fully premixed which the main characteristics are initiated as follows:

a. For non-premixed (diffusion flames), fuel and oxidizer are different separate streams and the combustion happens in the diffusive region. The diffusive region is allowing that the molecular and the turbulent transport to mix before the reaction. Also, here the transport equations can be derived to represent the state of the mixing within the flame independently of reaction and the neglecting curvature effects, the flame will be influenced by the scalar dissipation rate.

b. For premixed flames, fuel and oxidizer are integral mixed before the reacting where the flame front represents the border between the unburned gases and the fully burnt reactants. Considering the reduced kinetic assumption and the transport, the global equations can be reduced to a single global equation usually called the progress variable having the possibility to describe a state of reaction.

c. For partially premixed, an optimization in the auto-ignition regimes are encountered and requires specific adaption to gain flame stabilization or re-ignition mechanisms.

In order to predict the governing equations, a several terms are provided due to the turbulent Reynolds number, turbulent Damkohler number and the turbulent Karlovitz number. These models are normally associated to the flamelet assumption where the reaction region is thin and only the curvature, wrinkling and stretch impacts the rate of the reaction in the iso-progress variable and iso-stoichiometry formulation.

2.1.3. Modelling methods for gaseous combustion. Balance equations for mean quantities in RANS simulations are obtained by averaging the instantaneous balance equations. This averaging procedure introduces unclosed quantities that must be modelled, using turbulent combustion models. Classical models for turbulent non-premixed flames are usually derived under the following assumptions: the thermodynamic pressure is constant and Mach number is relatively small, species heat capacity are equal and constant, molecular diffusion follows the Fick’s law and molecular diffusivities are equal for all species, Lewis numbers are equal to unity, fuel and oxidizer are separately introduced in the combustion chamber with reference state for fuel and oxidizer. Following these assumptions together with a single step chemistry in adiabatic flows (no heat losses) or multi-step chemistry in adiabatic flows (heat losses), fuel and oxidizer mass fraction and temperature are linked through the mixture fraction. In this section only two types of modelled were used, first being the classical flamelet method and secondly the flamelet generated manifolds method.

3. Thermal history root cause analysis
In order to perform an optimization to the actual combustion chamber concept, an investigation over several parameters was required. The most sensitive parameter established to be further analyzed in more detailed was the quality of the material AISI 310 as being the main material used for manufacturing. The detailed investigation revealed two main approaches: one on a macroscopic level (interoperability of the system) and one on a microscopic level (sigma phase phenomena).

The burner concept, Figure 1, was exposed to a large operation modes and different temperature range configuration. Afterwards, an examination of intergranular and interdendritic was perform over the welding to determine the effect of the loss ductility and the nature that could drove to a main
cracking mechanism along the welding. The laboratory results pointed out that the material is suitable for maximum temperature but needs to be avoid a range of 823° - 1173º K due to its vulnerability to the formation of sigma phase in the Chromium spectrum content.

![Material subject to the sigma phase phenomena:](image1)

**Figure 1** Material subject to the sigma phase phenomena: 
- a) on-site investigation on macroscopic level 
- b) on laboratory on microscopic level

4. Problem analysis and task description
The existing configuration of the support burner had its utility only for some restrictive ranges and was not covering large customized configurations. The improvement of the burner ought to be our great and immediate concern. First step was to define the support burner performance regarding:

- Assessment of combustion models for the burner application.
- Mixing of combustion air/exhaust gas with fuel support/liquid waste.
- Incineration temperature – mixt and match concept.
- Flow pattern and topology of the mixing region.
- Flame stability.
- Recirculation enhancement with a lower positioning of the internal recirculation zone (IRZ).
- Instability prediction or isolated combustion phenomena.

Secondly, was to use a continual improvement CFD code and in this matter the Numeca FINE™/Open was a new feature that expanded the scope of the new product configuration. The process of the optimization design started early by plugging in the advanced OMNIS™ CAD for the pre- and post-processing capabilities.

![The old burner configuration:](image2)

**Figure 2** The old burner configuration: 
- a) actual design in the workshop 
- b) CFD simulation with a different source code

Thirdly, was to integrate the blended air in the concept layers of the burner along with the cooling channel materials in order to achieve a high performance and sustainable configuration.
The scope of those tasks was needed to rely on a high range turn down ratio, low NOx emissions and reducing the fuel consumptions. The flame was compulsory to be non-wrinkling and non-travelling into the chamber and, to be able to exchange the heat with the combustion chamber refractory lines and to comfort the instrumentation sensors as flame eyes to a healthy control system loop.

To make sure the newly developed multifuel burner meets the new environment emissions, multi-task purpose incineration, flameless and shorten in the combustion chamber designed, all the reacting flows topology were optimized with the Numeca FINE™/Open with OpenLab.

5. Generated combustion chemistry tables

The chemical composition used in the burner application contains exotic streams as alcohols, nitriles, pyroles, pyridines, ketones, amides and piperidone. In order to achieve a chemical mechanism, we build up a rudimentary table by accounting the main available characteristics of the fuel.

Since parts of the components are not available in literature, it is recommended to create or build up a surrogate that matches other characteristics, like temperature profile, enthalpy, entropy, LHV, molecular weight etc. In this case, the enthalpy or entropy is not available. A common approach of the reaction mechanism is to use the available components by diluting or modifying the characteristics based on C/H, C/O and C/N ratios of the mixture.

The mixture of the waste was build based on the C/H, C/O, C/N ratio, adiabatic temperature, heat release and molecular weight. The treatment of the NOx (Zel’dovich mechanism) in this case was enhance.

**Table 1** Surrogates generation regarding the fuel accounting for total mass of elements, ratios between C, H, O, N, and the NASA polynomials coefficient in such matter that the surrogate matches 95% of the LHV and temperature profile of the mixture.

| Chemical composition | Total mass of element | Mixture fraction | Adiabatic Temp (K) |
|----------------------|----------------------|------------------|--------------------|
|                      | C        | H        | O        | N        | H2O     | H3      | C/H ratio | C/O ratio | C/N ratio | Flamelet | FGM** |
| Actual state         | 6.74     | 2.81     | 8.25     | 6.75     | 0.46    | 0.31    | 0.56      | 10.22     | 6.13      | 2373     |        |
| Surrogate 1          | x        | x        | -        | -        | x       | -       | -         | -         | -         | 2290     | 2290   |
| Surrogate 2          | x        | -        | -        | -        | x       | -       | -         | -         | -         | 2296     | 2298   |
| Surrogate 3          | -        | -        | -        | -        | x       | x       | -         | -         | -         | 2259     | 2282   |
| Surrogate 4          | x        | -        | -        | -        | x*      | x       | -         | -         | -         | 2312     | 2294   |

(*) the surrogate has excess heat losses added to predict accuracy in the radiation effects.

(**) Flamelet Generated Manifold Model

Table 1 is presenting the actual modifications of the mixture in such matter that the integrated chemical numerical simulation converges to a burning solution of the model by matching partially or integral the characteristics of the mixture.

**Table 2** Results of the chemistry numerical simulation for HOW waste – Surrogate 1,2,3,4 – Flamelet/FGM Model

| Position reaction layer [cm] | Flamelet | Surrogate 1 | Surrogate 2 | Surrogate 3 | Surrogate 4 |
|-------------------------------|----------|-------------|-------------|-------------|-------------|
| FGM                           | -1.6638E+00 | -1.6638E+00 | -1.6638E+00 | -1.6638E+00 |             |
| Temp. reaction layer [K]      | Flamelet | 2.2822E+03  | 2.2889E+03  | 2.2541E+03  | 2.3064E+03  |
| FGM                           | 3.2000E+02 | 3.2000E+02 | 3.2000E+02 | 3.2000E+02 |
| Flame thickness [cm]          | Flamelet | 2.8705E-01  | 2.8659E-01  | 2.9182E-01  | 2.8539E-01  |
| FGM                           | 1.3509E-01 | 1.3488E-01 | 1.3716E-01 | 1.3312E-01 |
Table 2 is presenting a summary of the results of the mixture surrogates realized with the Flamelet model and the Flamelet Generated Manifold. For a good association for the computational fluid dynamics with the combustion models, we will associate the results from the chemistry mechanism with the turbulent chemistry interaction and integrate them into the turbulent models from RANS equations (k-epsilon (steady and unsteady) and LES (WALE approach). The radiation 1 spherical order harmonics (P1) and Optical thin model was enhanced with the turbulence radiation interaction (weak and strong) and the optical properties accounted were Weighted Sum Gray Gasses.

| Stoichi. mixture fraction [non-dim] | Flamelet | 1.2862E-01 | 1.2674E-01 | 1.3928E-01 | 1.2174E-01 |
|-----------------------------------|----------|-------------|-------------|-------------|-------------|
| FGM                               | 1.2862E-01 | 1.2674E-01 | 1.39289-01  | 1.2174E-01  |
| Position stoich. mixture [cm]     | Flamelet | 2.2002E-01 | 2.2185E-01 | 2.1000E-01  | 2.2684E-01  |
| FGM                               | 1.3805E-01 | 1.3910E-01 | 1.3199E-01  | 1.4208E-01  |
| Temp. at stoich. mixture [K]      | Flamelet | 2.2643E+03 | 2.2689E+03 | 2.2379E+03  | 2.2813E+03  |
| FGM                               | 2.2902E+03 | 2.2982E+03 | 2.2821E+03  | 2.2943E+03  |
| Scalar dissipation at stoich. [1/s]| Flamelet | 1.1656E+01 | 1.1427E+01 | 1.3034E+01  | 1.0818E+01  |
| FGM                               | 0         | 0           | 0           | 0           |

Figure 3 Results of the Flamelet chemistry numerical simulation with the certain modification as per Surrogate 1,2,3,4 – mixture fraction \((f_{st} = \text{[non-dimensional]})\) over O2, H2O and CO species \((Y_{st} = \text{[non-dimensional]})\)

Figure 3 and 4 presents the regions of equilibrium with the state of the unburnerd and burned of the mixture. In figure 3 we distinguish in surrogate 1, 2 and 3 a certain gap between the contour of the species. Due to the high amount of H2O in the stream this gap might give us a lack of accuracy in the reaction rate. In figure 3 (surrogate 4) we were able to capture the interface of the all species which makes the mechanism more reliable than the others. Figure 4 uses a manifold (detailed grid) and covers the region with success in all the surrogates.
Figure 4 Results of the FGM chemistry numerical simulation with the certain modification as per Surrogate 1,2,3,4 - mixture fraction \((f_{SI} = \text{[non-dimensional]})\) over \(O_2, H_2O\) and \(CO\) species \((Y_{SI} = \text{[non-dimensional]})\)

Figure 5 and 6 shows a detailed scale over the region of interest. Figure 5, surrogate 3 shows the biggest area not covered in terms of transport equations (Fig. 5 marked with red contour) and surrogate 4 presents the smallest region not covered which makes the most accurate mechanism. In figure 6, just the surrogate 3 is not fully covered by the manifold which makes the FGM method the most robust mechanism. In the following steps, we will evaluate the coupling of combustion and radiation of the surrogate 4 from Flamelet model and surrogate 4 from FGM method being the most reliable results from the two methods.

Figure 5 Flamelet chemistry numerical simulation with the certain modification as per Surrogate 1,2,3,4 - zoomed region of stoichiometry - mixture fraction \((f_{SI} = \text{[non-dimensional]})\) over \(O_2, H_2O\) and \(CO\) species \((Y_{SI} = \text{[non-dimensional]})\)
Figure 6 FGM chemistry numerical simulation with the certain modification as per Surrogate 1,2,3,4 – zoomed region of stoichiometry - mixture fraction ($f_{SI}$ = [non-dimensional]) over O2, H2O and CO species ($Y_{SI}$ = [non-dimensional])

Figure 5 and 6 shows a detailed scale over the region of interest. Figure 5, surrogate 3 shows the biggest area not covered in terms of transport equations (Fig.5 marked with red contour) and surrogate 4 presents the smallest region not covered which makes the most accurate mechanism. In figure 6, just the surrogate 3 is not fully covered by the manifold which makes the FGM method the most robust mechanism. In the following steps, we will evaluate the coupling of combustion and radiation of the surrogate 4 from Flamelet model and surrogate 4 from FGM method being the most reliable results from the two methods.

Due to the high content of H2O in the waste stream, the combustion leads to very high radiation effects and therefore needs a strong coupling between combustion and radiation. We look at Figure 5, where the source term for the radiation model from FGM method is overpredicting compared with the Flamelet method (especially on surrogate 4). By overpredicting the source term means that the temperature at the wall will be undershoot/overshoot which makes the coupling slightly unstable.

6. Simulation strategy and set-up
Aeronautical turbulent reacting flows involve a wide range of scales and complexities caused by the specific shapes of geometries and combustion regime encountered in these devices. Most of the time the designs are being routinely evaluated by CFD, most present modeling strategies rely on Reynolds Average Navier-Stokes (RANS) approaches developed for mean stationary flows. Such models benefit from extensive research and developments from the scientific community and have been successfully calibrated on simple fundamental configurations. However, the complexity of flows in modern combustion chambers adds multiple constrains on RANS and limits their precision. Alternative numerical solutions are thus needed to further increase the share of CFD and decrease the number of real combustion chamber tests and design iterations.

In this matter, we have chosen the RANS/LES numerical method because of efficiency and time-consuming. The RANS method is a steady state method. We have considered also the LES numerical method even though is a very high time-consuming. The reduced chemical mechanism gave us the possibility to reduce the time consuming with an order of one. The sub-grid model studied for this case was the WALE method (Wall Adapted Local Eddy Viscosity). Hence, the Smagorinsky subgrid model, a simple and widely used for its simplicity, is purely dissipative and will not account for the backscatter. Also, the model does not provide the correct near-wall decay proportional to the $y$ plus.
The WALE model was considered for this study. The other numerical method, DNS, has a very high time-consuming and suppress any motion of modeling aside from the chemical model which needs to be supplied. For DNS of turbulent non-premixed reacting flows, mixing and chemical times need to be both accurately represented since the chemical time scale is controlled not only by the mixing of the adjacent streams of fuel and oxidizer but also by the consumption rate (that locates around the stoichiometric line). LES put less stringent limits for the computational size by filtering out all flow small scales which can be ideally for non-reacting flows. Evaluation of the proper scaling for turbulent reacting LES remains unclear and often depends on the turbulent combustion model used to close the corresponding sub-grid scale terms.

1. Internal of the burners
2. Combustion air inlet 2
3. Refractory line

1. Internals of the burner
2. Fuel inlet (orange contour)
3. Oxidizer inlet 1 (blue contour)
4. Inner swirler concept 1
5. Oxidizer 2 inlet (light blue contour)

1. Internals of the burner
2. Fuel inlet (red contour)
3. Oxidizer 1 inlet (green contour)
4. Inner swirler concept 2
5. Oxidizer 2 inlet (purple contour)

Figure 7 Design concept used in the simulations – general presentation

As long as, the chemical mechanism is good pre-processed, a RANS numerical method can give a sufficient clear phenomenon of the case. Indeed, it is a constrain for the RANS model to consider the unsteadiness and inhomogeneities which makes the RANS method difficult to capture. In this scope we will be using the LES to achieve the unsteadiness phenomena.

The main objective for these simulations was to simulate a combustion chamber (burners, incinerator and quenching) that provides a full-scale vision of the combustion coupled with radiation. For this reason, the RANS/LES method was implied by studying the phenomena from the non-reactive flow until combustion coupled with the radiation. The URANS method is only adding the time dependency and increases the artificial dissipation which can give discretization errors. In this matter,
we prefer the LES/DES method which is better in the sub-grid scale and shows a good agreement with physical reality of different cases.

![Figure 8 Design concept used in the simulations – general presentation](image)

The geometry model used is based on a feasibility study feedback and experience had on other similar projects. The geometry contains refinement boxes regions in order to reduce the high peaks caused by the flow penetration, combustion, transport equations and radiation effects.

![Figure 9 Design concept used in the simulation – meshing results](image)

Figure 9 shows the meshing and the results of a grid study (coarse and fine). The position of the control points (Fig. 12) was set in the middle in order to evaluate the recirculation regions and the possible interactions. The results presented are the average solution of the unsteady time steps (cycles) with 50 inner iteration per each step.

Figure 10-11 reveals the static pressure and velocity in the x direction (side motion). The coarse grid (10M cells) is less capturing of the phenomena than the fine grid (40M cells) which makes the tracked parameters to be reliable in detection and prediction of the vortices.
The figures distinguish important fluctuations in velocities due to the fine grid approach. Especially attention has been made on the x direction because this parameter is dominant in the transport of the vortices and the vortices are high carriers of energy. The coarse grid in this case is not satisfactory because the model tends to average the solution and damp useful information. Due to this reveal, the grid used in the purpose of the design will be fined and refined in the regions of interests.

7. Problem analysis and task description
RANS models’ simulations are from some time available on the literature. These simulations are more difficult to validate due to the limited set of available measurements and the extreme simplifications introduced in comparison with real operating burners.
Performing RANS in real combustion chambers imposes specific features geometrical or physical simplifications such as:

- Opposite to most experimental set-ups, fuel and oxidizer enter the combustion chamber through multiple inlets and yield a partially premixed environment.
- Local equivalence ratios are not known.
- The technology effects are present in the pre-combustion chamber as cooling devices in order to assure the burner walls sustainability and sigma phase phenomena avoidance.
- The complexity of the fuel as a kinetic model requires an exercise that could remain almost impossible to achieve even at an academic level.

One of the first steps for combustion chamber is to guarantee that the swirlers will provide the desired flow field and fuel distribution for a proper flame stabilization. Mainly the swirler design and characterization rely on RANS predictions.

Secondly, the entire combustion chamber needs to be considered because those simulations are relevant to industry for azimuthal burner thermo-acoustics stabilities, potential flame distances and flame dynamics.

The swirler presents high complexity in flow passages among with multiple obstacles in order to impose a rotation motion to the oxidizer stream. Our current technology involves an increasing number of veins, axially and radially oriented with fuel injection points located in various locations within the swirler.

The difficulty is to accurate predict the IRZ (inner recirculation zone) relative position with respect to the chamber end-wall/inner end-wall of the swirler. For a high cooling efficiency and dilution optimization were needed long and difficult design iterative loops based on RANS to be able to achieve the best primary and secondary air injection positions.

The design proposed for the numerical simulations is presented below (Fig. 12). To reduce the time-consuming, we will make the simulation over 1/3 of the geometry with a full non-matching boundary option. The difference between the two concepts we can distinguish it in Fig.31. The simulation strategy is to simulate both cases with a non-reactive flow to be able to investigate the intensity of turbulence in the mixing region, the vortices, and the fluid structure interaction. The second step is to add the combustion, radiation, and heat fluxes to the simulation, as mention further from now on as reactive flow simulation.

![Figure 12 Concept 1 and Concept 2 concept used in the following simulation](image)

Figure 13 represents the magnitude of velocity field of the concept 1 (left) and concept 2 (right). The vortices in Concept 1 are more compact then concept 2, maintaining a general dissipation into the
middle chamber but we can observe a detached vortex from the general flow heading to the wall. Concept 2 is developing higher recirculation into the upper side of the chamber but downstream we observe a smooth contact with the wall due to the high inner recirculation.

Figure 13 **Magnitude of V - Concept 1 vs Concept 2 - \( (V_{SI} = \text{m/s}) \)**

Figure 14 **Over static pressure - control points of Concept 1 vs Concept 2 - \( (P_{SI} = \text{Pa}) \)**

Figure 14 shows the over static pressure of the both concepts. Concept 2 is inducing a higher pressure drop into the burner which might become a constrain for the fans. Also, Figure 14 presents the results of pressure fluctuation in the control points and we can’t reveal high pressure fluctuation representing high carriers of energies from the vortices.
Figure 15 Velocity field – zoom over the mixing region - \( (V_{SI} = \text{[m/s]}) \)

Figure 15 shows the velocity field in a more detailed zoom. We can observe on Concept 2 a more intense region of masses around the corners suggesting a shorter recirculation region but more intense than the Concept 1 which has a longer elongation of the recirculation region.

Figure 16 Velocity field \( V_x \) - control points of Concept 1 vs Concept 2 - \( (V_{SI} = \text{[m/s]}) \)

Figure 16 presents the results of the control points tracked on both concepts in the x direction. The evaluation of control points 1 (1m into the chamber) and 2 (2m into the chamber) confirmed the high peaks of intense turbulence from the concept 2. Also, the following control points (4m and 6m into the chamber) did not predict unusually phenomena’s downstream into the chamber.

The case simulated used the Flamelet model for combustion with high heat losses and P1 model for the radiation effects. The case presented is the worst-case scenario. The maximum flow of the waste and oxidizer by matching the high content of N2 and H2O and a preheated air of 923 K. The fluid
dynamic turbulent model used is a linear eddy viscosity turbulent model with extend wall function treatment.

Figure 17 Temperature profile of Concept 1 (left) and Concept 2 (right) - Q criterion iso-surface (flame shape) contoured with temperature and wall temperature with reduced opacity ($T_{SI}=\text{[K]}$)

Figure 17 presents the simulation of both concepts. The results showed that in the upper side of the chamber we have a high radiation effect due to the high content of H2O, the flame shape is determined by the internal of the burners in which the flame is longer, less aggressive and longer recirculation with cooling purposes (Concept 1), and shorter, aggressive with the walls and short recirculation region in the upper side of the chamber (Concept 2).
Figure 18 Temperature profile - control points (same position as for the non-reactive flow) - \((T_{SI} = [K])\)

Figure 18 comes as complementary information for the temperature profiles with tracking the same control points on certain levels into the chamber. The graph in control points reveals that the injection of waste/oxidizer (preheated air) is still occurs in the first 1 m from the chamber because we observe low temperature. Control point 2 (2m into the chamber) reveals the reaction region of the waste and oxidizer by observing the temperature profile ramping up. Here, the graph reveals that the reaction position of streams is different meaning that for Concept 1 the reaction is happening after approx. 2 m and for Concept 2 is happening in less than 2m. Control point 3 (4m into the chamber) confirms the same phenomena as control point 2, meaning that Concept 1 is pulsating the flame in low frequency with high amplitude and Concept 2 in high frequency and low amplitudes.

Figure 19 Mixture fraction of the species OH - flame shape contour with temperature - \((Y_{OH} [SI] = \text{[non-dimensional]})\)
Figure 19 represents the prediction of the illuminated flame in combustion based on the OH radical. Concept 1 towards Concept 2 is developing more in the downstream of the combustion chamber.

![Figure 19](image1.png)

**Figure 20** Temperature profile of Concept 1 (left) and Concept 2 (right) - Q criterion iso-surface (flame shape) contoured with temperature and radiation gradient with reduced opacity ($T_{SI} = [K]$)

The temperature and radiation gradient are presented in Figure 20. The aspect revealed is that on the upper side of the chamber we have high radiation effects due to H2O. Concept 1 is having the wall interaction smoother, travelling along the wall in the outside part of the chamber and Concept 2 hits the middle center creating flame interactions which could suggest high release of nitrogen oxides (thermal NOx). In the further steps we will evaluate the wall effect due to the temperature profile and radiation effects.

![Figure 20](image2.png)

**Figure 21** Wall temperature defect – ($T_{SI} = [K]$)
The temperature defect is shown in the Figure 21 as a color contour. The defect is due to the high heat fluxes generated by the flame and wall interaction or by high radiation. This figure presents the outside wall of the geometry (being a 1/3 geometry, we see a section of the wall and 2 sections in center).

The upper side of the chamber (both Concepts) due to the H2O content we lose an average of 300 K. Lower, downside of the chamber we observe different patterns. Both concepts can develop possible hotspots regions on the wall.

8. Conclusions and perspectives

The objective of this study was to optimize the burner performance regarding:
- Assessment of combustion models for the burner application.
- Mixing of combustion air/exhaust gas with fuel support /liquid waste.
- Incineration temperature – mixt and match concept.
- Flow pattern and topology of the mixing region.
- Flame stability.

This study had a purpose to improve the design concept as it is on field. We started by making the validation cases from the actual data provided by the workshop and by the visit made it on site. We started as a first step by improving the design, in diameter, angles and shields regarding the inside structure. Further, after achieving a good balance regarding the mechanical design it was made the simulations for the reacting flows.

The perspective research continues by new additional cases to be investigated with more complex environment including heat transfers in the solid structure in combustors of complex geometry, inner cooling channels and two-way coupling simulations.

With the methodology and simulation tools developed by NUMECA FINE™/Open with OpenLab, we are gladly to go further in the R&D projection of transient reacting flows addressed to advanced measurements with temporarily resolved diagnostics and complement the industry on RANS predictions for design of the next generation of burners in a thermal environment.

References

[1] M. De Waele et al., “Investigation into nature and cause of the cracking of an AISI310 burner ring”, edited by BELGIAN WELDING INSTITUTE NPO, Report MDW_18-394; 2018
[2] Hinze JO. Turbulence. McGraw-Hill; 1959.
[3] Pope SB. Turbulent Flows. Cambridge University Press ; 2000.
[4] Rogallo R. et al, Numerical simulations of turbulent flows, Ann Rev Fluid Mech 1985.
[5] Poinsot T. et al Using computational fluid dynamics to study flow control, Comput. Meth COnf Appl 2002.
[6] Linan A. The asymptotic structure of the counterflow diffusion flames for large activation energies, Acta Astronautica, 1974.
[7] Cuenot B. et al, Asymptotic and numerical study of diffusion flames with variable Lewis number and finite rate chemistry, Combust Flame,1996.
[8] Givi P., Model-free simulations of turbulent reactive flows, Academic Press, 2004.
[9] Gao X., A parallel solution adaptive method for three dimensional turbulent non-premixed combusting flows, Comput Phys, 2010.
[10] Midgley K., Unsteady flow structures in radial swirler fed fuel injectors, ASME, Proceedings of ASME turbo expo, 2004.
[11] Spencer A., Vortex breakdown in swirling fuel injectors flows, J Eng Gas Turb Power 2008.
[12] Janus B., Dreizel A., Flow field and structure of swirl stabilized non-premixed natural gas flames at elevated pressure, ASME, Proceedings of ASME turbo expo, 2004.
[13] Al-Abdeli Y., Stability characteristics and flow fields of turbulent non-premixed swirling
flames, Combust Theo Model 2003.

[14] Huang Y., Dynamics and stability of lean-premixed swirl stabilized combustion, Prog Energy Comb Sci., 2009.

[15] Ranga K., Investigation of the influence of swirl on a confined coannular swirl jet., Comput Fluids 2010.

[16] TNF. Turbulent non-premixed flame series. URL: http://www.sandia.gov/TNF/abstract.html; 2006.

[17] Combustion Institute. Combustion symposium series. URL: http://www.journals.elsevier.com/proceedings-of-the-combustion-institute/; 1948.

[18] Kaufmann A., Flow forcing technique for numerical simulations of combustion instabilities, Comb Flame, 2002

[19] Sattelmayer T., Influence of the combustor aerodynamics on combustion instabilities from equivalence ratio fluctuations, J Eng Gas Turb Power, 2010.

[20] C. Katona et al., “Internal Report”, edited by NUTARA Environment NV, Report 2894-467-ENG-PRO-000-CA-0004_CFD; 2019.

[21] C. Katona et al., “Internal Report”, edited by NUTARA Environment NV, Report 2894-428-ENG-PRO-000-CA-0004_CFD; 2018.