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## CFD and Chemical Reactor Network approaches to model an inter-turbine burner

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The Flameless Combustion (FC) regime is promising to the attainment of lower emissions in gas turbine engines. The well-distributed reactions, with low peak temperatures present in the regime result in lower emissions and acoustic oscillations. However, the attainment of the FC regime on gas turbine engines has not been successful, as most of the previous design attempts failed with respect to combustion efficiency, operational range, or difficulty to integrate in an engine.

Along with a novel aircraft concept, a conceptual design of a gas turbine engine with two sequential combustion chambers was presented.<sup>1</sup> As the aircraft would allow the use of cryogenic fuels, the first (and main) combustion chamber envisages the use of hydrogen or natural gas. The inter-turbine burner (ITB) is the subsequent chamber, and would operate under the FC regime with conventional fuels.



Figure 1 – Engine concept proposed along the AHEAD project<sup>1</sup>.

Oxygen concentration would be lower and inlet temperatures would be higher in the ITB, as the oxidizer in the ITB comes from the exhaust of the first combustor. That assists the attainment of the FC regime. Furthermore, the power split between the two combustors would enhance the operational range and efficiency.<sup>2</sup>

Based on the conceptual design<sup>3</sup>, an experimental rig was designed with a scaled and simplified combustor, having three fuel ports in a 18 degree wedge, instead of the full annular combustor (Fig. 2). The fuel employed was  $CH_4$ , to simplify operation and subsequent computational simulations. Data on emissions was acquired for different values of equivalence ratio and oxidizer  $N_2$  dilution. The oxidizer was preheated to temperatures around 580 K.

Simulations aiming the replication of pollutant emissions were performed first with CFD, and then with a CRN (Chemical Reactor Network). For the CFD, the commercial code ANSYS Fluent® was employed, along with a RANS approach and the FGM (Flamelet Generate Manifolds)<sup>4</sup> as the turbulencechemistry interaction model. The *k*- $\varepsilon$  turbulence model was adopted (tests using *k*- $\omega$  SST and Reynolds Stress turbulence models did not alter the results in terms of emissions). Both adiabatic and non-adiabatic simulations were performed, with radiation and heat losses being considered in the latter.



Figure 2 – Mid-plane cut-view of the 18° combustor employed in the experiments. Quartz window in blue.

The CRN was built based on the flow field information from the CFD solutions and solved using the code Cantera. The resulting CRN was composed of 10 Perfectly Stirred Reactors (PSRs). The advantage of the CRN approach is the use of detailed chemistry with low computational costs. The detailed chemical reaction mechanisms GRI 3.0 and GRI 2.11 (an older version) were both employed, as better NOx predictions with the GRI 2.11 have been reported in the literature.<sup>5</sup>

The results of emissions show that the CRN calculations present an improvement in relation to those performed in the CFD (Fig. 3). The non-monotonic behaviour of NOx emissions with increasing global equivalence ratio were only captured by the CRN, while the values using the GRI 2.11 mechanism were closer to the experimental results, as the GRI 3.0 had a larger overprediction. Both CFD approaches showed monotonic behaviour and too high values for higher global equivalence ratios.

Additionally, the CO emissions were greatly overpredicted by the CFD approach, while the values predicted by the CRN (both for the GRI 2.11 and the GRI 3.0) were very close to the experimental data.



Figure 3 – NOx and CO emissions as functions of the global equivalence ratio.

The CRN modelling also allows the analysis of the different pathways responsible for the NOx formation. Such analysis, presented in Fig. 4, explains the unusual non-monotonic behavior across lean values of equivalence ratio. Differently from conventional systems, the prompt pathway plays the most important role (instead of the thermal pathway). The NOx increase with equivalence ratio can be accredited to the prompt pathway, with a less important contribution of the NNH pathway. Successively, NNH drops when prompt has its peak (around  $\phi = 0.24$ ). A further increase in equivalence ratio causes both NNH and prompt to lower their production, as well as increasing reburning, causing the reduction in the overall NOx production.

Further analysis pointed to the conditions in the PSRs with higher temperatures shifted their CH and HCN concentrations with equivalence ratio in a similar fashion as the NOx emissions. These intermediates are the most important drivers of the prompt pathway. Their variation was related to the C/O ratio present in these reactors and the residence time, which varied with equivalence ratio.



Figure 4 – Contributions of the different pathways to NOx formation according to the CRN modelling with the GRI 2.11 mechanism.

The CRN approach, combined with information from CFD simulations is able to provide better predictions of pollutant emissions and valuable insights into gas turbine combustors. The design of the ITB may be improved based on the conclusions taken with the aid of both modelling approaches.

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