SHORT TERM SCIENTIFIC MISSION (STSM) SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CM1404
STSM title: Large-eddy simulation of ammonia-hydrogen-air flames in a model gas turbine
STSM start and end date: 04/02/2019 to 30/04/2019
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PURPOSE OF THE STSM:

(max.200 words)
Ammonia, as a flammable carbon-free substance, is being considered as a possible alternative fuel for the mitigation of CO_2, motivating studies on its combustion. However, burning ammonia presents several drawbacks, especially low reactivity, low flame speed, as well as high NO_x and NH_3 emissions. On the other hand, kinetic models for ammonia combustion are still in development, and many studies are being done recently on the subject. In terms of turbulent flames, few experiments in this regime have been done, both fundamental studies and practical ones, while detailed CFD studies are even scarcer, being only capable of describing trends, in most cases. In this sense, the present work intends to numerically simulate the use of ammonia in gas turbines, both conceptually, using 0D reactors and 1D laminar models to explore configuration possibilities in terms of emissions mitigation for ammonia and ammonia-hydrogen blends, as well as 3D RANS and LES analysis of a real gas turbine, to which experimental data is already available, varying equivalence ratios and comparing species trends for mechanisms and turbulence model validation.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

The work conducted in the host institution was divided in two parts: a conceptual study of combustor designs for ammonia and ammonia-hydrogen blends, exploring possibilities in terms of emissions mitigation by using 0D and 1D modelling, and a 3D CFD numerical work of a real prototype combustor, on which previous ammonia combustion experiments have been done.
For the conceptual work in gas turbine combustors, three modern designs were chosen for numerical simulations: lean-burning dry-low emissions (DLE) configuration; rich-burn, quick-quench and lean burn (RQL) configuration; and moderate or intense low-oxygen dilution (MILD) configuration. The software package Cantera was used, coupled with a detailed recenty-developed kinetic mechanism. In this part, the DLE flame was modelled as a laminar premixed freely-propagating flame. The RQL configuration, on the other hand, had both combustion stages modelled that way, while the mixing part between them, for secondary air addition, was modelled as perfectly-stirred reactor, with either very low residence times or without reactions. The MILD condition was reproduced as a burner-stabilized flame with exhaust gases recirculation, generating reactants dilution and higher inlet temperatures. Initial conditions were set to those of commercial gas turbines: inlet temperature of 500K and 20 bar of pressure. Flame speeds and NO_x and NH_3 emissions were measured and compared, pointing to the best configurations. Simulations were also done at atmospheric conditions for validation, and for ammonia/hydrogen blends of 0.5 hydrogen molar fraction, for further considerations on the feasibility of ammonia in gas turbines.
For the 3D CFD part, due to the lack of experimental data for comparison, and the well known flaws in previous models – therefore jeopardizing conclusions from purely numerical studies –, the choice of the

Funded by the Horizon 2020 Framework Programme of the European Union

Tohoku University ammonia combustor, with extensive data on NO_x and NH_3 emissions available in the literature, was necessary. As reported by that group, experiments were run in the combustor for a range of conditions and configurations. The real apparatus consists of a swirler (swirl number = 0.88) mounted in a base whith 12 injection holes in the middle, all mounted in a plate and covered by a liner. The whole assembly has 13 cm in diameter and 24 cm in length. In the present work, the configuration without secondary air injection was chosen. In this case, injection angles were fixed at 45º, and a glass model liner was used. Premixed and non-premixed flames at atmospheric pressure (1 bar) and inlet temperature (298 K) were tested, with equivalence ratios varied between 0.8 up to 1.2. NO, NO_2, N_2O and NH_3 emissions were evaluated. For RANS simulations, a detailed mesh of 2 million cells was created, and the well-known EDC method was applied, modelling the fine structures as well-stirred reactors, coupled with a reduced kinetic mechanism produced by the group. For large-eddy simulations, a mesh of 6 million cells was created, and a single point has been chosen for simulations: equivalence ratio of 1.1, with premixed flame. The LES method chosen for simulations was dynamic Smagorinsky, with combustion modelled as a partially stirred reactor (PaSR).

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The work in general has allowed for a better understanding of the role of the equivalence ratio in emissions formation and mitigation paths, as well as the feasibility some solutions for ammonia in real-life combustion systems.

Both experiments and numerical simulations point to a range of equivalence ratios, between 1.1 and around 1.2, where ammonia combustion generates low NOx and NH_3 emissions without compromising flame speeds and stability, a situation enhanced by the operation at high pressures. These are conditions that can be explored in real combustion systems to make ammonia a viable smart energy carrier.

In the conceptual work, it was found that DLE combustors present very high NO_x emissions, despite presenting very low NH_3 emissions. In this configuration, only extremely lean and unstable operating points produced legally acceptable levels of these pollutants. RQL, on the other hand, presented very low NOx and relatively low NH_3 emissions in the first stage operating between equivalence ratios of 1.1 and 1.25, also producing high levels of hydrogen that were consumed in the second burner, along with residual unburned ammonia. This indicates that RQL could be a suitable solution for ammonia gas turbines. The MILD configuration also presented very low emissions values, inversely proportional to the dilution rates, which force reductive processes. This condition can be therefore considered another possible solution. Hydrogen addition, on the other hand, produces higher levels of NOx, which were kept within acceptable levels for rich combustion, also possibly enabling better stabilization due to the higher flame speeds.

Due to the mesh production time, the startup times and the computational times to take the simulations to steady state, final results have not yet been achieved for both RANS and LES simulations. Due to the known uncertainties of both the mechanism and the turbulence modelling, it is expected that simulations will produce similar trends for emissions, while producing different values. Improved turbulence/chemistry interaction models for ammonia combustion are also under development by the Lund University group, and shall be applied to the LES model in the near future.

This work has already generated a conference paper on the combustor design comparison, presented on the 9th European Combustion Meeting, and a journal paper, to be submitted to a journal of high impact. Other publications are expected from the results of the 3D RANS and LES studies.

FUTURE COLLABORATIONS (if applicable)

The present work is a continuation of a long-date partnership between the IST (Portugal) group and the Lund University (Sweden) group, which involves several works beyond ammonia combustion.

In this field, future colaborations also include a joint work on DNS of laminar flames, planned for the present year and intended to further reveal species patterns and other fundamental combustion characteristics for chemical kinetic mechanisms improvements. Other fundamental studies, both numerical and experimental ones, are also expected.

In the long term, the construction of an ammonia-fueled gas turbine is foreseen, incorporating the acquired knowledge from the STSM project into a real-life application, therefore validating designs so far only studied computationally for ammonia combustion. For instance, the results from the conceptual work shall help generate the new combustor design, while those from the RANS and LES studies shall indicate kinetics and turbulence models capable of accurately describing ammonia combustion behaviours.