COST
EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

SHORT TERM SCIENTIFIC MISSION (STSM) – SCIENTIFIC REPORT

The STSM applicant submits this report for approval to the STSM coordinator

Action number: CM 1404 SMARTCATs
STSM title: Combustion of ammonia-hydrogen mixtures in a premixed laminar burner and in a swirl burner
STSM start and end date: 17/09/2018 to 07/10/2018
Grantee name: Jakov Baleta

PURPOSE OF THE STSM/

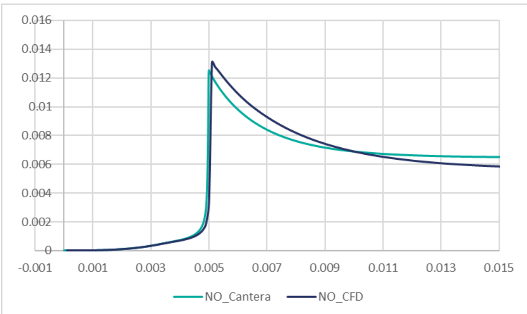
The purpose of the STSM was twofold. On one side, the goal was to increase the current understanding of ammonia/hydrogen combustion chemistry under practical industrial conditions by combining advanced numerical methods and experiments. On the other side, this STSM has initialized the cooperation between University of Zagreb Faculty of Metallurgy and IST aiming to combine the numerical expertise of the guest researcher with the experimental expertise in combustion of prof. Costa's research group. An initial plan was to focus on oxy-fuel combustion of ammonia/hydrogen mixtures in an existing premixed laminar burner operating at atmospheric pressure. In addition, focus was also placed on the numerical simulation of cases available in literature in order to evaluate the performance of reduced mechanisms of ammonia combustion and validate the numerical framework. During the course of STSM initial calculations were carried out and satisfactory agreement was achieved between 0D reactor results and CFD. Afterwards, results for a premixed swirl burner were calculated and compared with those published in literature, but no good agreement was obtained. Investigation of those discrepancies is still ongoing and will be part of future work, together with numerical simulation of other cases. It is expected that this study will contribute to enhance the current knowledge by providing new insights in ammonia burning conditions closely resembling those in industrial applications and will help to design real industrial burning systems. It is planned that the results of the joint cooperation will be published in two international conferences and in one international journal.

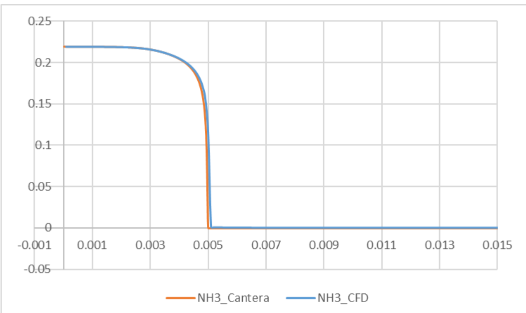
DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

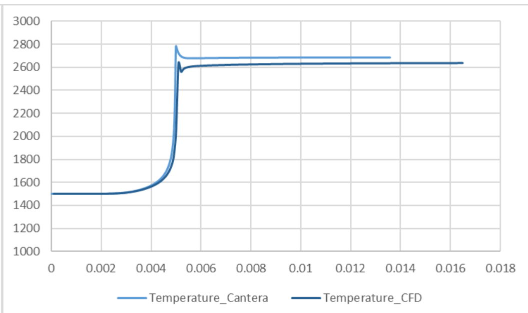
Upon arrival at IST the experimental work on the premixed burner started. At the same time, CAD models of burner geometries available in the literature were made by using suitable software for mesh generation as a part of numerical simulation. The aim of this modelling exercise was to validate reduced mechanisms of ammonia combustion developed at IST. After the literature review, few papers from the group of prof. Kobayshi were identified as a starting point, due to the fact that they have properly defined boundary conditions for simulations. Prior to simulating real industrial cases, it was decided that 0D results of reduced mechanisms obtained in Cantera should be reproduced with satisfactory agreement in CFD environment. The idea was to simulate shock tube experiments, but this approach was later neglected because the domain was very large and required much more computational resources than those available. Thus, a very simple case was established in CFD environment consisting of square shaped domain, mimicking the 0D reactor. This approach proved to be valid and results from Cantera were reproduced with satisfactory agreement. There were some discrepancies due to the fact that boundary conditions and numerical procedure were not completely identical, but the overall conclusion was that reduced mechanisms could be used for simulation of real industrial cases. As a first real case, simulation of the premixed ammonia burner described in the paper of Kobayashi and associates was performed. For this geometry there is a large body of simulation data in literature calculated using the LES approach for turbulence modelling. Unfortunately, only preliminary results were obtained until the end of the STSM, which show large discrepancies in relation with the published data. Possible sources of error could be due to turbulence modelling (RANS instead of LES) or chemical mechanism limitations. Identification of errors and their correction, as well as literature survey of new validation cases is part of ongoing work.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

Main results stem from previously described work as follows. First, the 0D results of the reduced mechanism obtained in Cantera were simulated in CFD environment. The reduced mechanism derived at IST based on the work from Mathieu et al. was employed. It consists of 66 reactions and 22 species. The reason behind this choice is justified by the fact that basic mechanism presents current state of the art NOx sub-mechanism. This mechanism possesses high importance given the fact that two main problems in ammonia combustion are emissions of unburnt ammonia and NO formation. The 0D case in CFD simulation was approximated with square shaped domain (side length of $1dm^3$) divided by 1000 equal cells. Constant pressure was imposed on the domain boundaries and simulation was initialized with suitably high temperature to ensure ignition of ammonia/air mixture with equivalence ratio of 1. The figures below compare the 0D case and the CFD simulation. As it can be seen, there are slight discrepancies, but overall the agreement is satisfactory. All trends are captured in the CFD simulation and differences can be attributed to the boundary conditions and numerical procedure not being completely identical in employed software solutions.



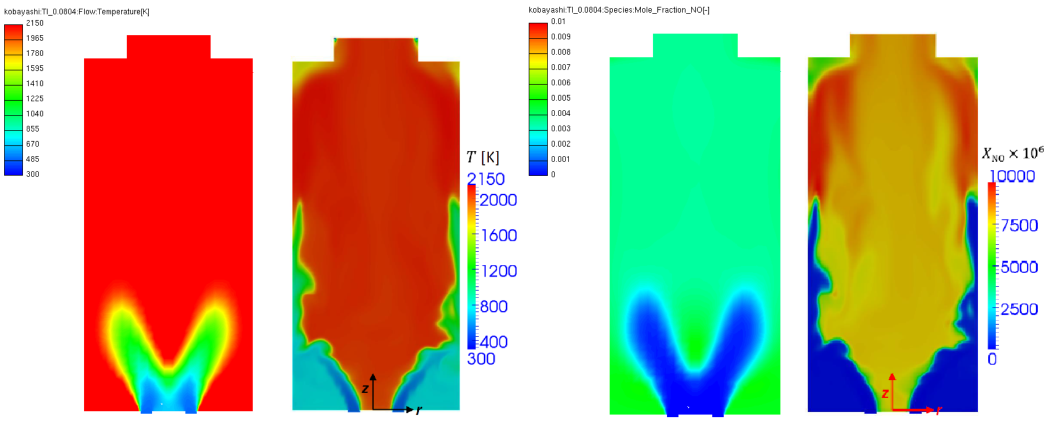




As a first real case, the simulation of the premixed ammonia burner described in the paper of Kobayashi and associates was performed. For this geometry there is a large body of simulation data obtained by using LES approach for turbulence modelling. The authors from literature used Miller's mechanism, whereas in the present simulation the reduced mechanism from Mathieu developed at IST was employed.

Preliminary results depicted in the following figures are not comparable to the published data. Temperature field and NO concentration results do not show even similar qualitative agreement with respect to the calculated gradients. The reason behind these discrepancies could be difference in turbulence modelling and consequently erroneous definition of the turbulence boundary conditions. Also, the used chemical mechanism could be responsible for different combustion of ammonia/air mixture. Identification of errors and their correction, as well as literature survey of new validation cases is part of ongoing work.

Comparison between conducted simulation (left) and published results (right) of temperature and NO concentration



FUTURE COLLABORATIONS (if applicable)

Identification of errors in the current numerical simulations is part of ongoing work. Since only a single simulation case has been established during the course of the mobility, future work will entail further literature survey in order to identify other validation cases combusting ammonia in relevant industrial environment. Once the planned experimental setup is established on IST, the measured results will be obtained by different chemical mechanisms.

There are plans to participate on several international conferences, including the First International Conference on Smart Energy Carriers in January 2019, if satisfactory results are obtained until then. Finally, it is expected that this work will result in one publication in an international journal.

In spite of the relatively short STSM duration, there is great potential for this cooperation in upcoming times. The mobility has initiated first collaboration topic and combines numerical expertise of guest researcher with experimental expertise in combustion of research group at IST in what is expected to be long term fruitful cooperation.