CONSIGLIO NAZIONALE DELLE RICERCHE

ISTITUTO DI RICERCHE SULLA COMBUSTIONE

SMARTCATs COST Action

Short Term Scientific Mission Report

Author: Magnus Fürst

Details of STSM

STSM title: Collaboration work for experimental data and uncertainty quantification for MILD combustion

Reference: COST-STSM-CM1404-37482

Period: 2017-04-20 to 2017-04-30

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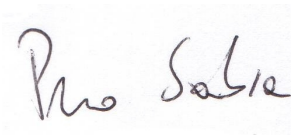
Host: Pino Sabia, Istituto di Ricerche sulla Combustione - Consiglio Nazionale delle Ricerche - Italy

I hereby confirm that Dr. Magnus Fürst, Université Libre de Bruxelles – Belgium, has spent a period (from 2017-04-20 to 2017-04-30) at the Istituto di Ricerche sulla Combustione - Consiglio Nazionale delle Ricerche – Napoli – Italy, within the framework of a Short Term Scientific Mission (STSM) under the SMARTCATs COST Action CM1404.

Thanking you,

Yours Sincerely,



Pino Sabia

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Introduction

This STSM was used for setting up a collaborative work between Istituto di Ricerche sulla Combustione - Consiglio Nazionale delle Ricerche, Naples, Italy (IRC) and Université Libre de Bruxelles, Brussels, Belgium (ULB), with the purpose of improving the performance of existing chemical kinetics with respect to Moderate or Intense Low-oxygen Dilution (MILD) combustion. The performance of existing chemical mechanisms with respect to these conditions are lacking and, based on the fact that most of them were developed and validated with respect to conventional combustion, there are room for improvements.

The experimental data from IRC was therefore used in the framework of Uncertainty Quantification (UQ) which is a statistical method used for quantifying and minimizing uncertainties in the chemical kinetics, with respect to specified experimental data. The overall performance of the new kinetics is highly related to the amount of experimental data considered in the UQ process, which is why this data exchange between CNR and ULB is very important and the future collaboration between these two groups is very beneficial for the community.

Activities

The mission started with a tour of all the lab facilities and discussions focused on the experimental facilities, especially the Plug Flow Reactor (PFR) which data is the focus of this work. This facility is used to analyze the auto-ignition delay time for different fuels during MILD conditions. Based on the fact that MILD combustion is a spontaneously auto-igniting process, this property is very important for accurately predicting the conditions in MILD combustion numerically. The facility consists of a 1.4m long tube which is equipped with thermocouples every 5cm which are used to capture the temperature trend in the reactor. The whole reactor is encapsulated in an oven which keeps the surrounding temperature the same as the inlet temperature of the mixture, which decreases the heat losses to the surrounding. The auto-ignition delay time is then defined as the time elapsed before the temperature is 10 degrees higher than the inlet temperature. The data considered in this work is from an experimental campaign where biogas was evaluated. In order to reach MILD conditions, the injected mixture was diluted in nitrogen at different percentages. The mixture was then preheated to different inlet temperatures and the auto-ignition delay time was measured. The large set of experimental data was thereafter simulated using the OpenSMOKE++ open source software. One case can be plotted in a so called Arrhenius plot in Figure 1 below, where the simulations were run with three different detailed chemical mechanisms, namely POLIMI C1C3 [1], Zhukov [2] and AramcoMech2.0 [3].

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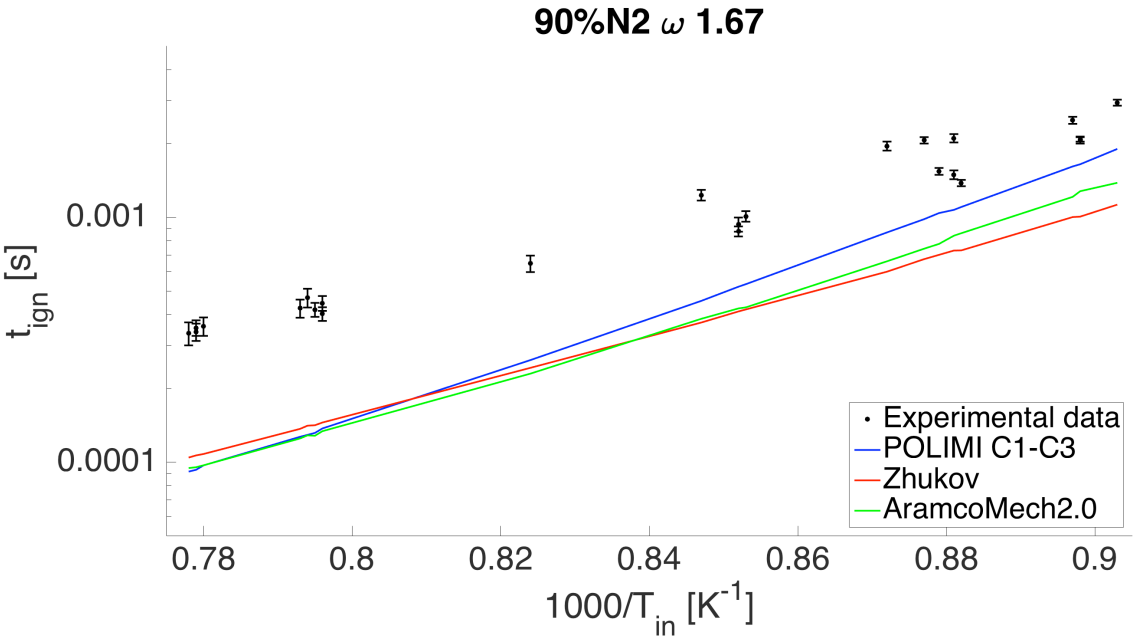

Figure 1: Auto-ignition delay times at different inlet temperatures at 90% N2 dilution and ω of 1.67. The experimental data is presented in black with corresponding error bars, while the simulation results are presented with the lines.

Based on these curves, it can be seen that none of the mechanisms are accurately predicting the experimental data. This confirms the conclusions already published in [4] and gives room for improvement.

Further, a very fruitful discussion was conducted with respect to how the experimental uncertainties were evaluated for this process. Considering that the UQ process is trying to fit the chemical kinetics within the experimental uncertainty, this range is very important. For this case, the experimental uncertainty is evaluated considering the displacements of the thermocouples and the velocity of the mixture, which then represents the possibility that ignition will occur in-between two thermocouples. The experimental error ranges between 2.4 and 10.8% for this specific case presented.

Conclusions

Based on the work and discussions carried out during this mission, the collaboration between IRC and ULB was initiated. The experimental data from IRC will be used in the framework of UQ, which will improve the proficiency of existing chemical kinetics with respect to MILD combustion. The results from this collaboration will thereafter be published in a relevant journal or format to be discussed later.

References

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[3] Metcalfe WK, Burke SM, Ahmed SS, Curran HJ. A hierarchical and comparative kinetic modeling study of C1 - C2 hydrocarbon and oxygenated fuels. Int J Chem Kinet 2013;45:638–75. doi:10.1002/kin.20802.

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