SHORT TERM SCIENTIFIC MISSION (STSM) – SCIENTIFIC REPORT

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

Action number: CM1404
STSM title: Development of an Optimization toolbox for chemical kinetics
STSM start and end date: 16/04/2018 to 26/04/2018
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PURPOSE OF THE STSM/

The use of detailed chemical kinetics for large scale simulations is becoming more realizable as computational power increases. However, due to inherent uncertainties in chemical kinetics, the performance of existing kinetics can vary depending on the fuel and system in question. The use of efficient optimization tools is therefore very prominent in order to improve the performance of existing kinetic mechanisms. The purpose of this STSM is therefore to work on the coupling of two existing software that together can be used to perform such optimizations. The software in question are OpenSMOKE++ (Cuoci et al., 2015) and Dakota (Adams et al., 2017). OpenSMOKE++ is a framework developed at Politecnico di Milano for solving reacting systems using detailed kinetics. Dakota is a broad toolkit developed by Sandia National Laboratories for studies such as Sensitivity Analysis, Unceratinty Quantification, Optimization and Calibration. This work will therefore allow the user to perform any of these studies for detailed kinetics using this coupling.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

Through the use of an interface created, the two software OpenSMOKE++ and Dakota was used to perform a series of optimization studies. The main focus has been on experimental data from a Plug Flow Reactor (PFR) from (Sabia et al., 2015) where Biogas was used as a fuel. The coupling enabled us to perform and test different optimization capabilities available in the Dakota toolkit and the most efficient methodology was used for the case mentioned above.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

By using the tool developed in this STSM, 3 reactions were optimized, including 7 kinetic parameters. By using a non-linear least squared optimization approach, the performance of the optimized kinetics was drastically improved. A plot of this can be seen in Figure 1 below where the green line represents the nominal POLIMI C1-C3 mechanism (Ranzi et al., 2012) and the blue line is the optimized mechanism.

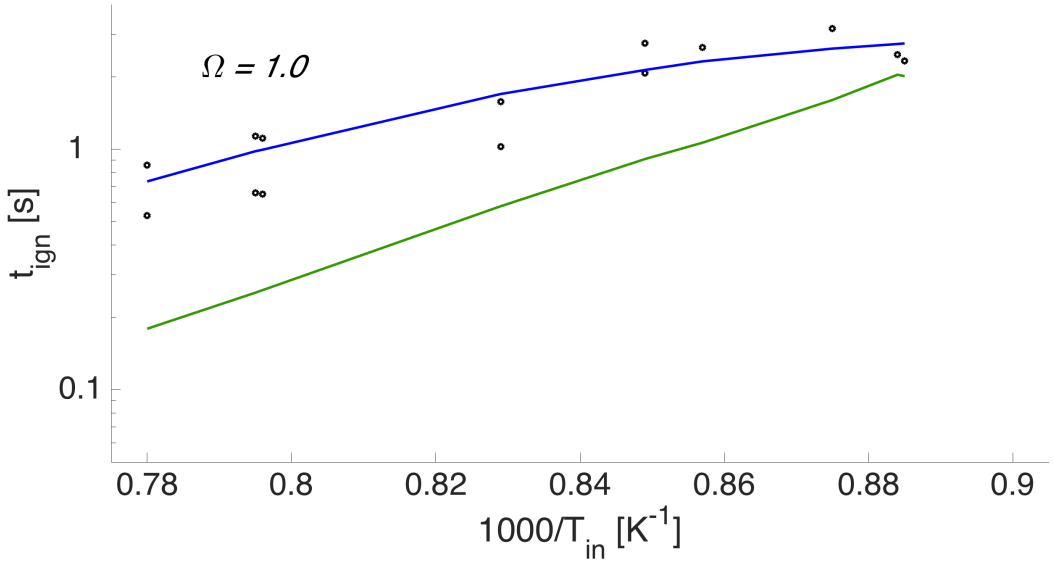

Figure 1 - Ignition delay time for Biogas in MILD conditions at stoichiometric conditions at different inlet temperatures. The green line represents the original POILIMI C1-C3 mechanism (Ranzi et al., 2012) and the blue line is the optimized mechanism from this work.

It can clearly be seen that the blue line is performing much better with respect to the experimental data. The optimizer needed about 90 min on a single core in order to arrive with these results, however considering that 222 different parameter combinations were evaluated, this is still very efficient.

FUTURE COLLABORATIONS (if applicable)

The work started in the STSM will be continued, including more functionality to the toolbox. The next steps would be to include restrictions on the proposed kinetic parameters to ensure that the reaction rate will always stay within its specific uncertainty limits. Thereafter more experimental targets will be added in order to improve the performance of the proposed kinetics for more conditions. As more data is added to the optimization procedure, parallelization options of the Dakota software will be explored in order to speed up the optimization procedure.

This work is also planned to be presented at the 37th International Symposium on Combustion in Dublin 29 July – 3 August 2018 in the form of a Work in Progress Poster.