COST STSM Report

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The aim of my visit to the Prof. Turanyi's group at the Eotvos Budapest University has been to identify an efficient and general format to exchange and store the large amount of experimental data nowadays produced in combustion research. In fact, Professor Turanyi's group is undoubtedly the world reference in this key topic.
Starting from the large amount of experimental information stored in the ReSpecTh database [1] the main goal of my activity has been to connect such database to the code I've been developing during my Master Thesis activity under the supervision of Prof. Tiziano Faravelli in Milan. In turns, the final goal is to automatically link the experimental database to the usual ideal reactors kinetic simulations performed with OpenSMOKE++ developed by Cuoci et al. [2] In fact, as the size and complexity of kinetic mechanisms for combustion application increases, together with theoretical and experimental capabilities, it is of outstanding importance to automatically check and re-validate a kinetic mechanism (e.g. CRECK modeling kinetic mechanism [3]) after every new implementation, extension or update. The final goal of the code we have been working on is to read the experimental database, together with its conditions (Reactor type, temperature, pressure and composition, observed variables), set the input files for OpenSMOKE++ simulations according to the operating conditions, compare model results and experimental data and evaluate the new performances through the Curve Matching framework [4] and decide whether the reliability of the new mechanism is satisfactory. For the first step (read and select the experimental data of interest) it is convenient to adopt the formatting method well established in Prof. Turanyi's group.

Every experimental dataset in the ReSpecTh database is stored as a .xml file and categorized based on the paper reference (year, volume, pages, journal and authors), on the type of experiment (ignition delay time, laminar flame speed, speciation…), on the type of reactor (shock tube, laminar flame, jet stirred reactor…). This .xml file is generated starting from a .txt file, more easy to write and read.

The main issue was to translate the information stored in such files into something matching keywords and formatting of OpenSMOKE++ kinetic simulations.

Two significance differences were identified between their standards and our needs:

1. They used to define the type of experiment in a way OpenSMOKE++ cannot use
2. We need to specify the type of reactor starting from the type of experiments and the ReSpecTh database did not allow this (the type of reactor was not defined)

Therefore we agreed to specifically define also the type of reactor in the existing files updating the formatting standards and making them useful for both the groups. Now we are able to use their database effectively, and to exchange data in a more efficient way.
We also discussed about possible future developments such as creating an FTP repository where all the universities and research center in the combustion community can upload and download information, according to the new standards. The critical point in this would be to supervise the uploading process, making sure the format is coherent.

Prof. Turanyi's group already has a management system where every file's name is defined based on some rules such as: direct or indirect measurement (e.g. rate constants measurements), type of experiments, type of the project and number of Project.

We agreed also to rename the .xml file in a more useful way, allowing a better connection with the input file to be written for the kinetic simulation.

In the last days we talked about another very critical aspect: the nomenclature of the chemical species in the kinetic mechanism. In fact, while for small species more or less every kinetic mechanism adopt the same name (ethylene=C2H4, methane=CH4, methyl radical=CH3 etc.) for larger species (e.g. fatty acid methyl esters, alcohols etc.) the names adopted by different research groups can differ quite a lot (butanol= N1C4H9OH in CRECK mechanism, and C4H9OH-1 in LLNL mechanism). A solution might be to construct a database where every different name is stored with their standard nomenclature (e.g. IUPAC).

References

[1] http://garfield.chem.elte.hu

[2] Cuoci, Alberto, et al. "OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms." *Computer Physics Communications* 192 (2015): 237-264.

[3] http://creckmodeling.chem.polimi.it
[4] Bernardi, M. S., et al. "Curve matching, a generalized framework for models/experiments comparison: An application to n-heptane combustion kinetic mechanisms." *Combustion and Flame* 168 (2016): 186-203.