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: Integrating the OpenSMOKE++ framework into Optima++ for the extensive validation of optimization of detailed kinetic mechanisms
STSM start and end date: 07/02/2019 to 21/02/2019
Grantee name: Máté Papp

PURPOSE OF THE STSM:

–

The participants of Working Group 4 have elaborated a series of principles on data collection and storage, and the participants at ELTE, Budapest are working on the implementation of these principles.

The group of the ELTE Eötvös Loránd University, Budapest has created the ReSpecTh Kinetics Data format ("RKD format") standard.

Optima++ is a general framework program for creating the RKD format files from text files containing the experimental data. Also, Optima++ may test of a reaction mechanism by carrying out simulations, reproducing the experimental data defined in a series of RKD files. These calculations are carried by an external simulation code.

Before the STSM, Chemkin-II and FlameMaster were the two simulation codes implemented in Optima++.

OpenSMOKE++ is an object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms, developed by the CRECK Modeling Group of Politecnico di Milano. According to the experience of the Budapest group, the best approach is the simultaneous usage of these simulation codes for PSR and flame simulations, because unexpected numerical instabilities or too large computational requirements may occur. Integrating OpenSMOKE++ into Optima++ will significantly extend the mechanism testing capabilities of the Optima++ code.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

–

Máté Papp has started the integration of OpenSMOKE++ to Optima++ in December

2018. Since the framework program Optima++ directly controls the simulation code and the return of the simulation results have to be very efficient, a deep level integration of the two codes is needed. Most of this work has been done by February, but there were some points, when modifications in the OpenSMOKE++ code were also necessary.

In the ReSpecTh Kinetics Data format, the ignition delay can be defined in six different ways. During the STSM, the OpenSMOKE++ code was extended to be able to handle all ignition delay definition types. The Optima++ code was also modified to write OpenSMOKE++ inputs with the new options and to read the results from the OpenSMOKE++ output files.

Optima++ can be used for effective flame calculations using a solution database. During a flame simulation, Optima++ takes the most similar solution from the database and forward it to the simulation software as an initial guess. This feature was extended to work effectively with OpenSMOKE++.

Some calculations performed by Optima++ (optimization of kinetic parameters or sensitivity analysis) require a large number of simulations which differ only in a few kinetic parameters. In order to do these calculations efficiently, an interface may be necessary in the simulation package. Professor Alberto Cuoci added a possibility in OpenSMOKE++ to change the kinetic parameters of a mechanism without repreproccesing it.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The main results obtained during the STSM can be summarized in the following points:

- The OpenSMOKE++ framework is able to calculate all of the ignition delay times defined in the ReSpecTh Kinetics Data format.
- A new interface was added to OpenSMOKE++ to change the kinetic parameters of a mechanism without repreproccesing it.
- Optima++ can carry out simulations with OpenSMOKE++ in a much more effective way.
- Efficient flame calculations are possible using a solution database.
- Automatic OpenSMOKE++ input file generation from the RKD format files is fully supported by Optima++.
- After the STSM, a new version of Optima++ has been released and it is now available on the respecth.hu web site.

FUTURE COLLABORATIONS (if applicable)

Some further collaborations may be needed to improve the interconnection between the two software. For example, the modification of the low pressure limit parameters is not possible in the current implementation, but it can be easily extended in the future.