COST Action CM1404 – Chemistry of Smart Energy Carriers and Technologies

Final Report on the Short Term Scientific Mission (STSM)

Tabulated Chemistry in 3D CFD Simulations

From Adina Werner

Grand period: September 2nd, 2018 – September 21st, 2018

Host institution: Lund Combustion Engineering LOGE AB

Home institution: Technical University of Technology Cottbus-Senftenberg

Purpose of the STSM

The purpose of the STSM from Adina Werner was the knowledge transfer regarding tabulated chemistry implementation strategies in CFD software. Furthermore, an aim was to finalize a joint publication on validation of tabulated chemistry in CFD.

Description of the work carried out during the STSM and major results

During the first two weeks, there was a daily two-hour seminar, where we discussed different theoretical fundamentals of the combustion progress variable (CPV) model and compared the LOGE model to other approaches from other research teams.

The base of the combustion progress variable (CPV) model from LOGE AB is to use the chemical enthalpy h_{298} as a progress variable. Therefore, they use the constant pressure homogeneous reactor approach. Other research teams working with similar or different approaches. Other approaches based for example on the flamelet model. We had a look at different publications, for example:

- Knop et al.: Modelling and Speciation of Nitrogen Oxides in Engines, 2013
- Michel et al.: On the Formulation of Species Reaction Rates in the Context of Multi-species CFD Codes using Complex Chemistry Tabulation Techniques, 2010
- Pera et al.: Development of a FPI Detailed Chemistry Tabulation Methodology for Internal Combustion Engines

One more is the paper from O. Colin and A. Benkenida (The 3-Zones Extended Coherent Flame Model (ECFM3Z) for Computing Premixed/Diffusion Combustion) from 2004. This model based also on a homogeneous reactor. The progress variable based on temperature, our model on thermodynamics. We also had a look at the different source terms.

In further seminars, we had a look at the code behind the CPV model. We picked up some equations and discussed the theory behind, for example the soot model.

In the first week I create my first own CPV table. There was already an existing table for a n-dodecane mechanism that I used for the Spray A cases for the publication. I create a new table with a newer table generator and try out the new CPV table at an old Spray A case.

Another aim of the stay was to finalize a publication called “Further Application of the Fast Tabulated CPV Approach”. In this work, the CPV model is validated against the SAGE detailed chemistry

combustion model and the some experiments. Therefor it was very useful that we discussed the theories of the CPV model.

The main application in this publication is the Spray A from the ECN. The first results looked very good. Based on the created post processing plots we could see that there is a difference between the ignition behaviour of SAGE and CPV and that both cases ignite at places where we it not expected. We run some simulations with some little changes and can so improve the ignition behaviour (Figure 2).

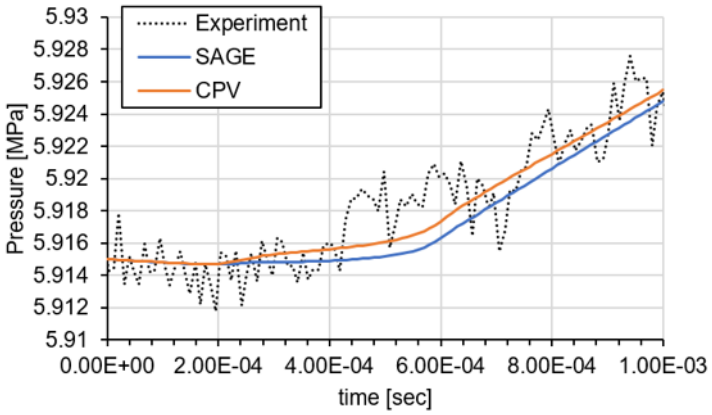

Figure 1: Pressure comparison between experiment, SAGE and CPV.

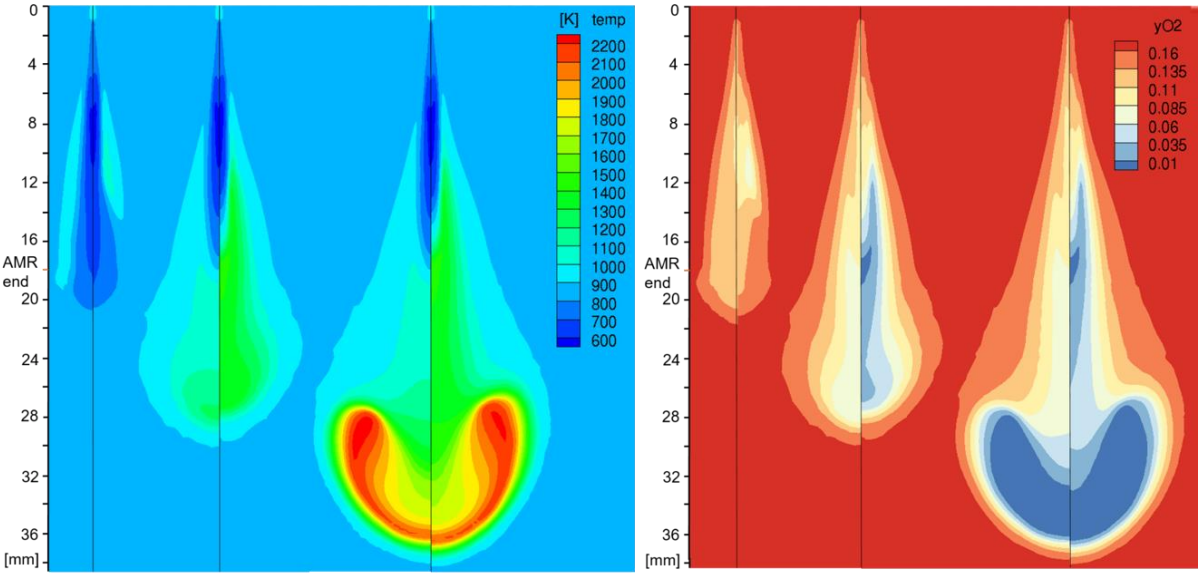

Figure 2: Temperature- and O_2-mass fraction profile compared SAGE (left) and CPV (right) at 0.2 ms, 0.425 ms and 0.725 ms.

During the discussions, we decided to compare also the combustions durations and the lift-off length for the Spray A at different temperatures. Therefor I set up new simulations based on the experiments from the ECN site done by Sandia National Laboratories. The results show a difference in the ignition delay (Figure 3), but the trend is the same. We expected this difference because we used only the RANS approach for our simulations.

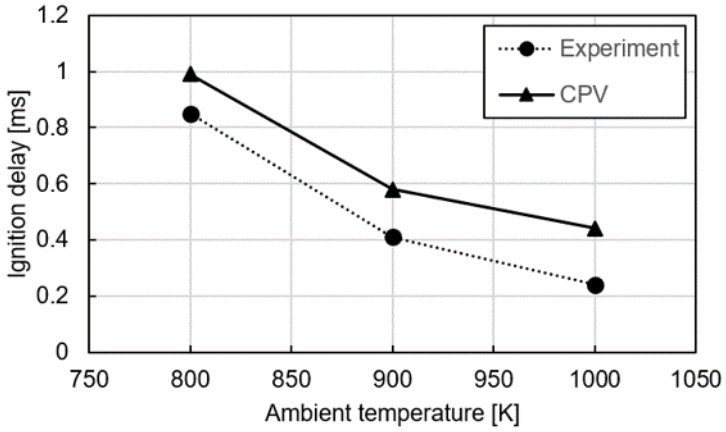

Figure 3: Ignition delay time comparison between experiment and CPV at three different temperatures.

The results show that there is a very good agreement between SAGE and CPV. The biggest advantage of the CPV model is the very short CPU time. For example, the Spray A case with SAGE needs 108 h, with CPV only 8 h. In addition, the agreements with the experiment are also good. At the end of the stay, we had every important plot that we are decided to show in the publication. A future step will be to have a look at the soot and compare the simulation results to the Spray A experiments.

How the STAM has contributed to the Action's aim

The STSM was very helpful for me. It was great to work together with the people that I only know from skype meetings. It was much easier to have together a first look at the code and to speak together about the fundamental theory. I am sure that we will work together to in the future. The first next thing is to finalize the publication.