COST STSM CM1404-30762 SCIENTIFIC REPORT

STSM Topic: Chemistry of Smart Energy Carriers and Technologies (SMARTCATS)

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Period of STSM: 24 January - 3 February 2016

Background/ Purpose of the STSM

The use of Computer modelling in the development of clean and efficient engines and fuels has in recent time become a valuable tool for the achievement of lower carbon emissions in the transportation and energy sector. However, to simulate practical combustion systems such as the spark ignition engine and HCCI engines, accurate and reliable chemical kinetic model of fuel oxidation are needed as input into engine simulation. The overall aim of my research work is to bridge the gap between our current chemical kinetic understanding of alternative fuels combustion in fundamental systems and their performance (behaviour) in real engines under blending conditions. My current focus is on n-butanol when blended with gasoline. So far, as part of my research work, I have carried out ignition delay time experiments with the Leeds University Rapid Compression Machine (RCM) for a range of fuels including gasoline, TRF, gasoline-butanol blends and TRF-butanol blends and have also been working with researchers at KAUST to develop suitable chemical kinetic mechanisms for simulating ignition of gasoline-butanol fuel blend within the RCM. In the course of my work, I have performed evaluation of the chemical kinetic modelling of a range of oxygenated fuels like DME, butanol, gasoline and gasoline-butanol blends within a zero-dimensional modelling framework via comparison of predicted data with rapid compression machine data and the application of local sensitivity and global uncertainty/sensitivity methods. In addition, I have carried out engine test studies using the Leeds University Ported Optical engine (LUPOE) for a range of fuels including gasoline, TRF, gasoline-butanol blends and TRF-butanol blends. We would like to link these studies with computer simulations of the combustion chemistry which occurs within the engine under as close as possible conditions for the range of fuels mentioned above in order to explore auto-ignition and knock behaviours of these fuels blends under real engine conditions. LOGEengine, software developed by LOGE Company is being adopted for our computer simulations. The LOGEengine software is based on a stochastic reactor model (SRM) with inbuilt initial condition calibration tool and mixing time optimisation tool. One of the advantage of LOGEengine is that detailed and skeletal reaction mechanism could be employed in full engine simulations and inhomogenieties and chemistry-flow interaction in the engine are well accounted for. However there have been several challenges with the use of LOGEengine software. The purpose of the STSM visit was therefore to allow me to learn the functionality of the code and to test its application against the TRF and TRF-butanol fuel data from our research engine. The visit is expected to lead to ongoing collaborations and submitted journal publications on the role of alternative fuel blending in engines.

Description of the work carried out during the STSM

Day 1 -3 (25th- 27th January) Heat release analysis and compression phase matching

The first three days of the STSM was dedicated to gaining experience on how to set up a case for tuning and calibration of initial conditions to match compression phase of experimentally obtained pressure data. During this period, I was introduced to the basics of the Graphical user interface (GUI) in LOGEengine software and how to use the set up wizard for setting up and running a heat release analysis case for compression matching. I was also introduced to the help column on the set up wizard which is needed for acquiring information regarding any parameter.

Some of the specific work carried out with the software during the above period include:

- Loading of experimental pressure data and checking of units for consistency
- Selection of optimisation limits for pressure offset, cylinder head temperature, compression ratio, temperature and start CAD etc.
- Use of advanced option which requires the mass flow of fuel before compression in kg/s/cylinder and atomic fractions of fuel components for optimum compression phase matching
- Running of several heat release/compression phase matching set up with varying input parameters in order to gain experience on how the various input parameters like pressure offset, pressure multiplier, cylinder head temperature, cylinder wall temperature, compression ratio, temperature and start CAD etc, can be controlled to get better matching of compression phase. Figure 1 below shows a sample of the set up wizard while Figure 2 shows the result of the heat release analysis for LOGE sample data.

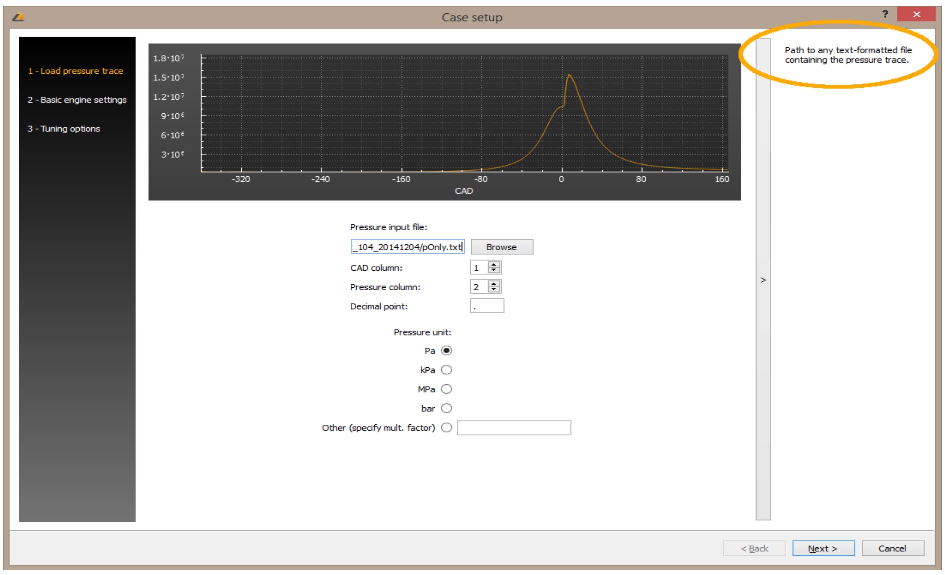

Figure 1: set up wizard for heat release analysis and compression phase matching

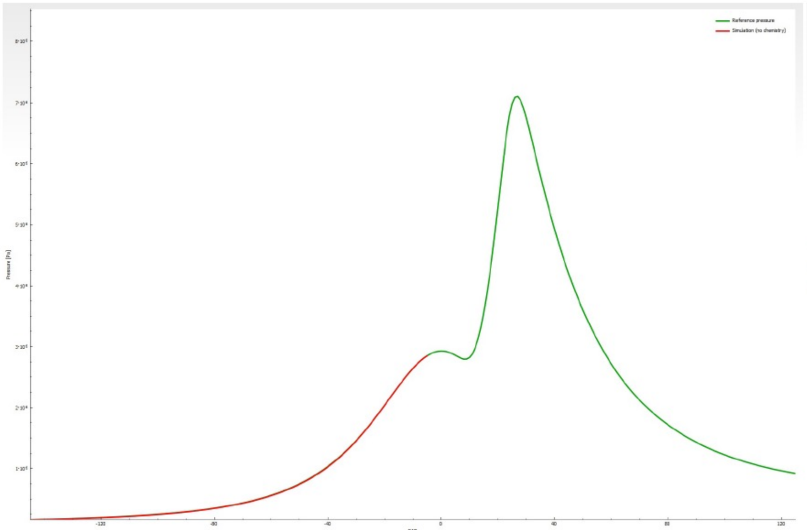

Figure 2: Heat release analysis and compression phase matching obtained for LOGEengine sample case

<u>Day 4-5 (28th -29th January) Generation and testing of cylinder profile for combustion phase matching</u>

For accurate matching of the combustion phase using the optimisation algorithm in LOGEengine, it is required to provide an accurate profile of the experimental cylinder clearance volume and the provided profile must be consistent with the right format recognised by LOGEengine. During the above period, I was given a tutorial on the procedure for developing an appropriate cylinder profile for any shape of engine cylinder clearance volume. Based on the methodology, I was able to generate an appropriate cylinder profile in excel program for the cylinder clearance volume of the Leeds University Ported Optical engine (LUPOE) while using the relevant dimensions of the engine cylinder. I also carried out testing of the generated cylinder profile in LOGEengine using the default chemistry files. Figure 3 below shows the cylinder profile developed for LUPOE.

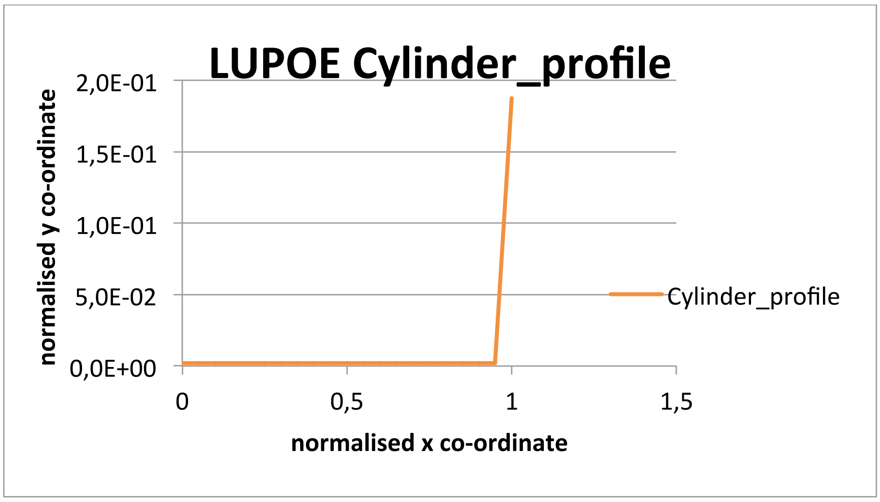

Figure 3: Cylinder geometry input profile for LUPOE, visualisation of the first intersection

Day 6-7 (1st- 2nd February) Combustion phase matching through SRM calculation and mixing time/spark timing optimisation.

Matching of the combustion phase is the most difficult part of LOGEengine application and this require some experience with tuning of the turbulence theta (spark timing) and mixing time. Day 6 of my STSM was dedicated to learning how to match the combustion phase using LOGEengine sample pressure data, cylinder profile and default chemistry file while day 7 was dedicated to learning how to match the combustion phase using Leed University gasoline pressure data, engine cylinder profile and Lawrence Livermoore National Laboratory (LLNL) gasoline chemistry file. The following specific work was carried during day 6 and 7 of my STSM.

- Selection of appropriate tuning limits for turbulence theta and mixing time and running of SRM calculations for optimal matching of combustion phase
- Tracking of optimization parameter development and target parameter development for improvement of simulation results.
- Trouble shooting of failed calculations via the use of YAGA optimiser output window and output file (ESSA file) generated by genetic algorithm for the failed combination in the particular generation.

Figure 4 and Figure 6 shows the result of parameter tuning in SRM calculations for combustion phase matching using LOGE sample pressure data and Leeds pressure data respectively.

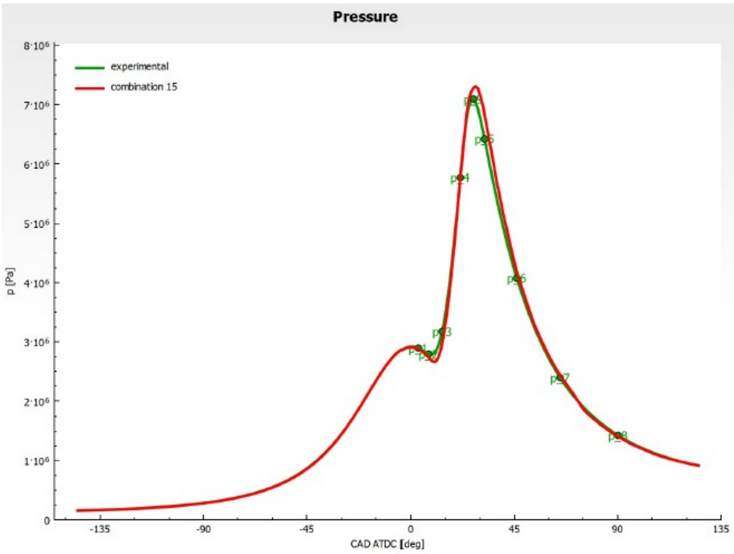

Figure 4: SI-SRM-based Simulation of combustion process with mixing time Optimisation (LOGE sample case).

Best combination: 15

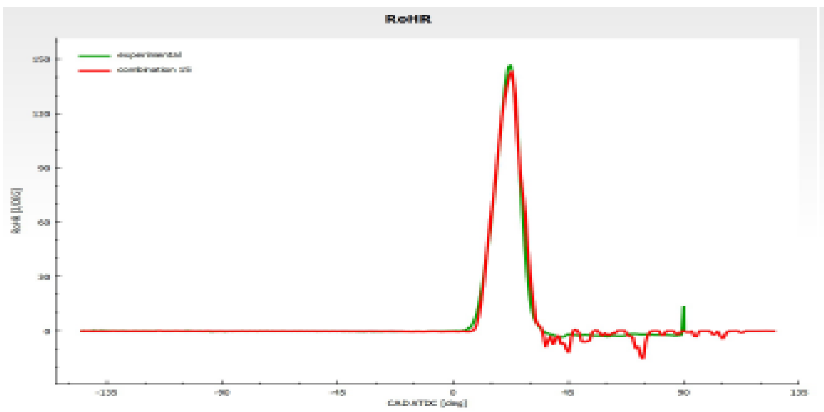

Figure 5: Rate of Heat Release obtained for sample case in LOGEengine

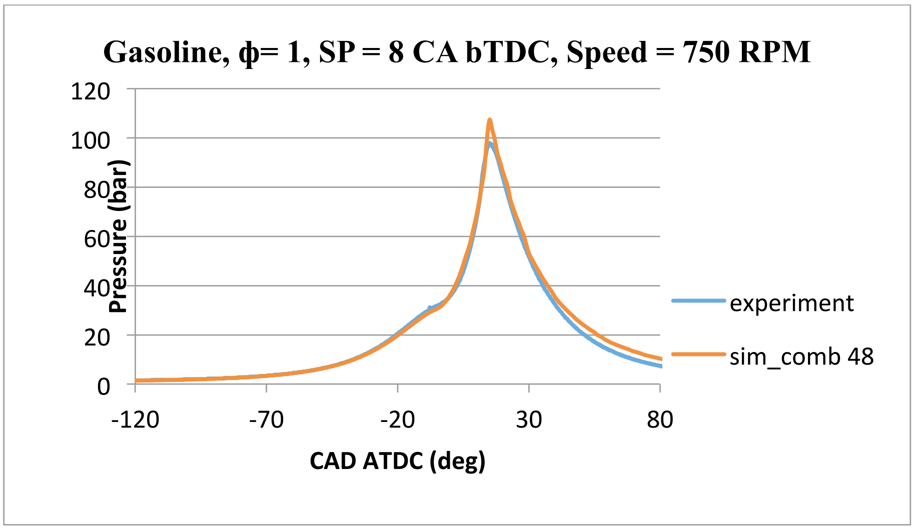

Figure 6: SI-SRM-based Simulation of combustion process with mixing time Optimisation obtained for Leeds condition.

Day 8 (3rd February) Tutorial on post processing of result for knock analysis and performance of chemistry.

During day 8 of the STSM I was introduced to how to access and identify each parameter in the output results of the SRM optimisation calculations. I addition, we also explored how the results of LOGEengine optimisation calculations in the unburned zone could be used for auto-ignition/knock prediction via the heat release and species concentration history. Figure 7 and Figure 8 shows the heat release rate in the unburned zone obtained for under knocking conditions for LOGE sample case and Leeds data. The position of second peak in the heat release rate graph indicates the onset of knock.

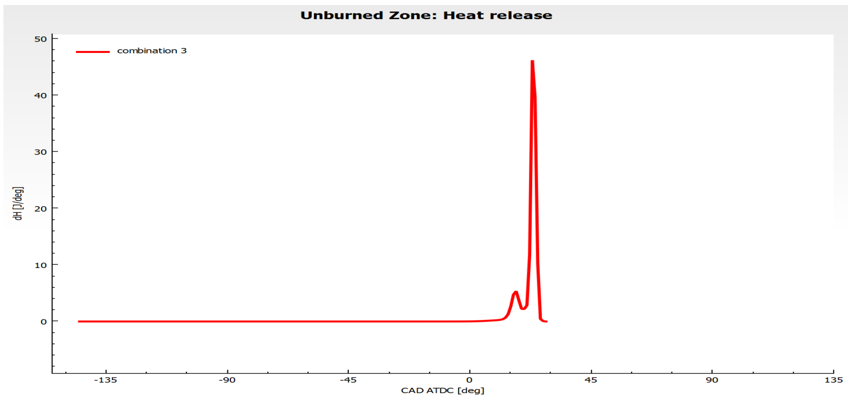

Figure 7: Rate of Heat Release of the unburned zone obtained for sample case in LOGEengine

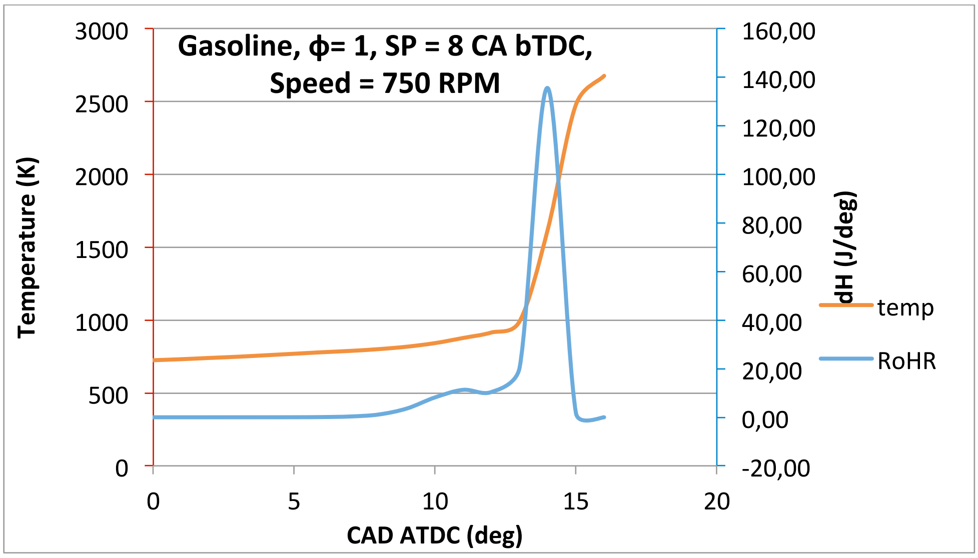

Figure 8: Predicted Rate of Heat Release and Temperature history in the unburned zone obtained for Leeds condition

Description of the main results obtained

Heat release analysis and compression phase matching: One of the main results of the STSM is the skill I acquired regarding heat release analysis and tuning and calibration of initial conditions to match compression phase of any experimental pressure data. The methodology was tested on Leeds data with good success. Figure 2 above shows the result of the heat release analysis/compression phase matching obtained for LOGE sample data.

SRM calculation and mixing time optimisation: Another major result of the STSM is the ability for me to setup and do SRM engine calculations in LOGEengine with spark timing and mixing time calibration for combustion phase matching using a specific cylinder profile and detailed reaction mechanism. The methodology was tested on LOGEengine sample data and Leeds data with reasonable success. Figure 4 and Figure 6 below shows the result of the mixing time calibration in SRM calculation obtained for LOGEengine sample case and Leeds condition.

Future collaboration with host institution

We have an offer of collaboration with LOGE group and Professor Fabian Mauss with regards to modelling of Leeds engine data using LOGEengine software and a recent gasoline-butanol chemical kinetic model developed in collaboration with KAUST group. The host institution has granted University of Leeds a free academic licence to use LOGEengine and the LOGE group has also offered to continue to provide support for the use of LOGEengine. Both institutions plans to maintain the ongoing collaboration that would lead to a joint paper publication on the role of alternative fuel blending in spark ignition engines.

Confirmation of the Host Institution of the successful execution of the STSM

See attached letter

Other Comments

I sincerely appreciate the COST office for giving me this valuable opportunity to visit LOGE Lund Combustion Engineering Company, Cottbus, Germany. My thanks also go to my host supervisors, Prof Fabian Mauss and Dr Michal Pasternak and the entire team at LOGE Company for their support. I am also grateful to my home supervisor, Prof Alison Tomlin for her support.