SHORT TERM SCIENTIFIC MISSION (STSM) – SCIENTIFIC REPORT

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

Action number: CM1404
STSM title: Modelling of photo chemically ignition controlled fuels in HCCI mode
STSM start and end date: 15/04/2018 to 28/04/2018
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PURPOSE OF THE STSM/

The ignition event in engines operated in Homogeneous Charge Compression Ignition (HCCI) mode are often unstable, show large cyclic variations and are therefore difficult to control. In this study a novel “Smart fuel” is analyse to control the ignition event, so called Reaction Controlled Compression Ignition (RCCI).

To the regular gasoline, in the experimental study represented by a primary reference fuel (PRF surrogate), 1,3-cyclohexadiene (CHD) is added 5% by mass. This mixture is then subjected to UV exposure in a photo reactor. This compound undergoes electro-cyclic ring-opening, resulting in the formation of 1,3,5-hexatriene (HT). The experiments carried out using a novel optically accessible compression ignition chamber (OACIC) show a significant delay in the ignition event by adding the CHD and an additional delay by injection the UV treated fuel containing HT.

In the STSM, the LOGEsoft software suite [1] is used to model the ignition behaviour of those fuels in a zero-dimensional Stochastic Reactor Model (SRM). The main features of this model are the discretization of the cylinder volume in non-dimensional particles, which allow for inhomogeneities as in a real engine. Due to the zero-dimensional model type, detailed reaction schemes can be used for the combustion prediction within minutes, which is a significant gain in computational costs compared to often applied three-dimensional Computational Fluid Dynamics (CFD) simulations.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

For further investigations on the chemistry, the experiments are modelled using the HCCI SRM model available in the LOGEsoft software suite [1]. For this purpose, three steps have been carried out:

1) Analysis of available reaction mechanisms and their application to the problem,

2) Analysis of the initial conditions for the simulations and

3) Simulation of the combustion processes.

The analysed mechanism are the JetSurf mechanism v1.1 [2], a mechanism for the auto-ignition of cyclo-pentane and cyclo-hexane from Sirjean et al. [3] and an ETRF (ethanol containing toluene Reference Fuel) mechanism from Seidel [4]. In this step, it is analysed if the additive 1,3-cyclohexadiene (CHD) and the photo

product 1,3,5-hexatriene (HT) are available in the mechanism and if the mechanism can be used to reproduce the PRF mixture used in the experiments. Further, ignition delay times τ are calculated since the prediction of the auto-ignition is essential for the simulations of HCCI.

In engine simulations, the choice of the initial conditions is a key to reproduce the compression and combustion. From the experiment, the temperature of the inflow is known, whereas the temperature at Inlet Valve Closure (IVC), which is the starting point for the engine simulation, is unknown. Further, it is know that some of the trapped mass is lost due to leakage. The inlet conditions for two cases (T_{inlet} = 95°CA and T_{inlet}=115°C) performed with OACIC are optimized using LOGEengine [1]. Found properties are pressure and temperature at IVC, the compression ratio and trapped mass.

In the LOGEsoft toolbox there is no module available that accounts for an optical chamber additional mounted at the cylinder head. To account for this additional volume, the regular HCCI module is applied using a correction of the cylinder bore to correct the volume at top dead centre. Drawbacks of this approach are first, that both chambers (optical chamber and main cylinder) are treated as one volume, which might affect the auto-ignition behaviour and second, due to the correction of the bore, the volume during the whole engine cycle is increased, which leads to a higher need trapped air mass in the simulation compared to the experiment. The advantage is that the model can be used and calibrated easily, so that the focus of the study can be set on the investigation of the detailed chemistry. Two cases (T_{inlet} = 95°CA and T_{inlet}=115°C) are predicted and compared to the experiment.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

The analysis of the reaction schemes showed that none of the anylased mechanisms is applicaple to repdruce the experiment. The Jetsurf meachanism [2] is not further considered because *n*-octane is a fuel species, not *iso*-octane and the reactions for C6H8-135 (HT) are comment out. The mechanism from Sirjean [3] has the species C6H8#6 which is supposed to be CHD and C6H8Z3-135 to be HT. Figure 1 shows the predicted ignition delay times for the pure species and their mixture accoring to the conversion in the experiments. The simulations are perfomrmed for differenrt equivalence ratios ϕ and at 40 bar, which corresponds approximately to the pressure in the egine case at auto-ignition. In Figure 1 D) the pure components are compared to the the mixture for ϕ = 0.3. The pure HT has the shortes ignition delay times, the mixture of CHD and HT, that can be genrated by the UV light treatment has the longest ignition delay times. This trend is also found in the experiment. However, using the same mixture in the HCCI SRM leads to a promoted auto-ignition (Figure 2). To understand this beahvior a flow analysis has been performed (Figure 3). In both cases, stoichometric and lean, the HT forms the cyclic molecule CHD, which is then decomposed. From theory, the UV light is expected to break a bond of CHD, which reranges as consequence its electrones and forms the more stable HT. So this found transformation back to CHD is considered as unreasonable. Considering the reactions that envolved HT, no decompostion pathways are available. The dominating reaction seams to be “C6H8Z3-135=C6H8#6” which is the reformation or ringopening reaction. In the project proposal n-pentane has been used as fuel species. Using this meachanism, there was no ignition using pure n-pentane and differenet ϕ predicted.

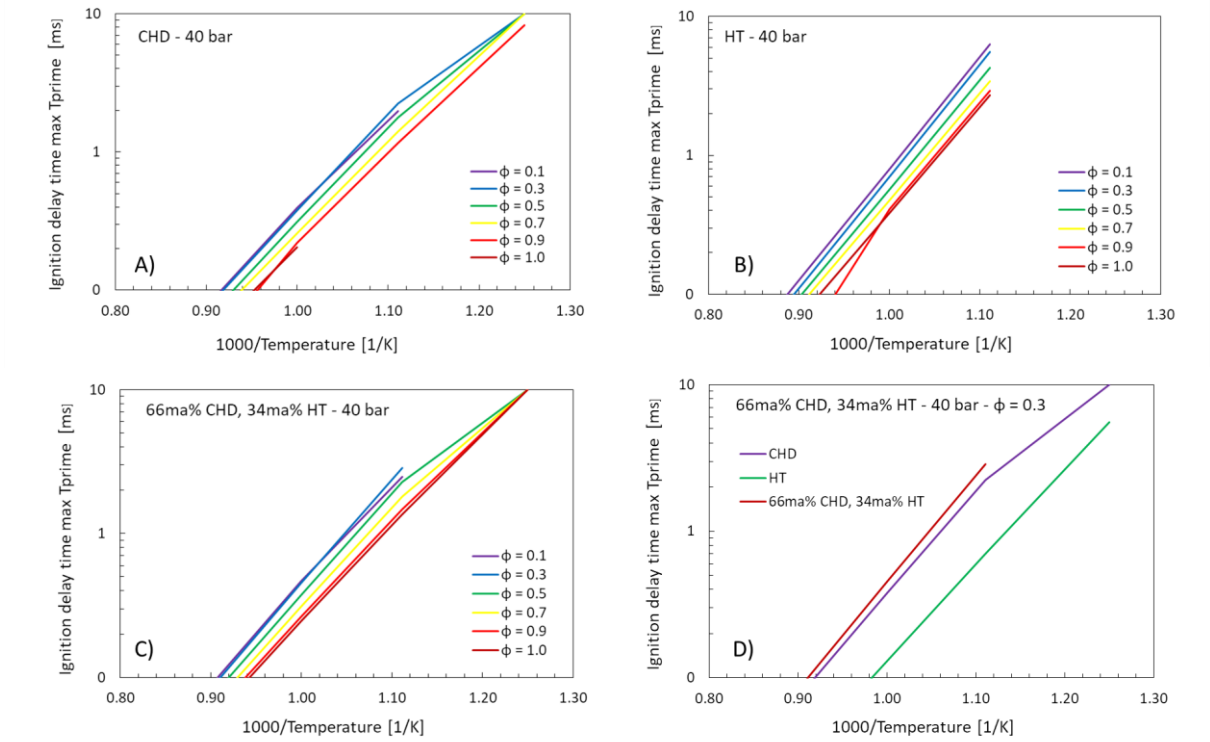

Figure 1: Ignition delay time prediction using constant volume reactors and the mechanism from Sirjean et al. [3]. A) 1,3-cyclohexadiene (CHD) and B) 1,3,5-hexatriene (HT) C) 66 mass% CHD and 34 mass% HT at 40 bar and different equivalence ratios and D) CHD, HT and their mixture at 40 bar and ϕ = 0.3.

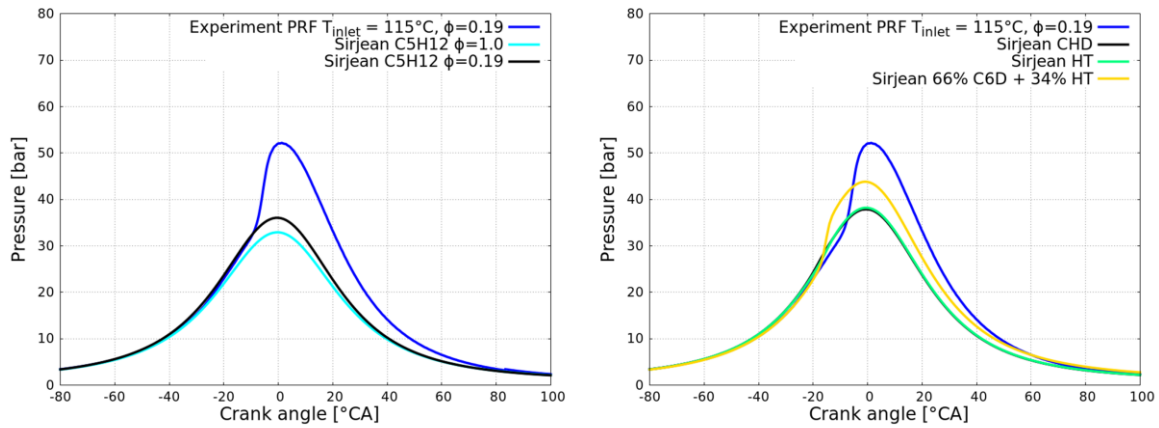

Figure 2: Measured pressure for ϕ=0.19 using PRF RON 90, Simulations using the mechanism from Sirjean [3].Left figure: pure pentane for ϕ=1.0 and ϕ=0.19. Right figure: applying CHD and HT as pure fuel species and their mixture (66 mass% CHD and 34 mass% HT).

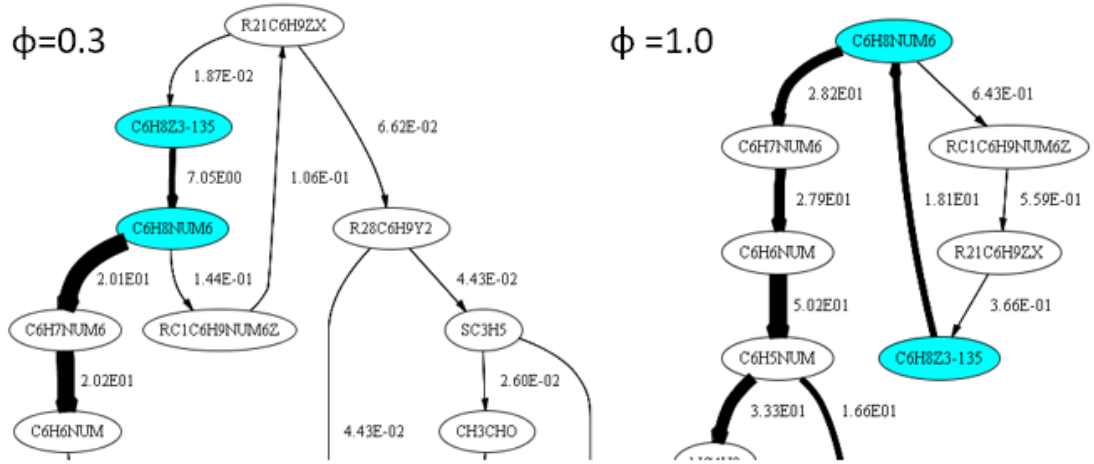

Figure 3: Flow analysis using HT (C6H8Z3-135) as fuel species for ϕ=0.3 and ϕ=1.0 predicted using the mechanism from Sirjean et al [3].

To repduce the PRF auto-ignition, the mechanism from Seidel [4] is applied. In this meachnism the photo reaction is not present, but it is validated for PRF mixtures. To find a good aggreemnet to the experiment, the air mass was corrected. The found equivalence ratios are tehrefore ϕ =0.16 (instead of ϕ =0.18) for T_{inlet}=95°C) and ϕ =0.165 (instead of ϕ =0.19) for T_{inlet}=115°C. The predicted pressure traces agree well with the ones form the experiment, eventhough the volume has beed corrected (Figure 4). The deviation at the end of the expansion of experiment and simulation is due to mass conservation in the simulation, but leakage in the experiment and therefore expected to be seen.

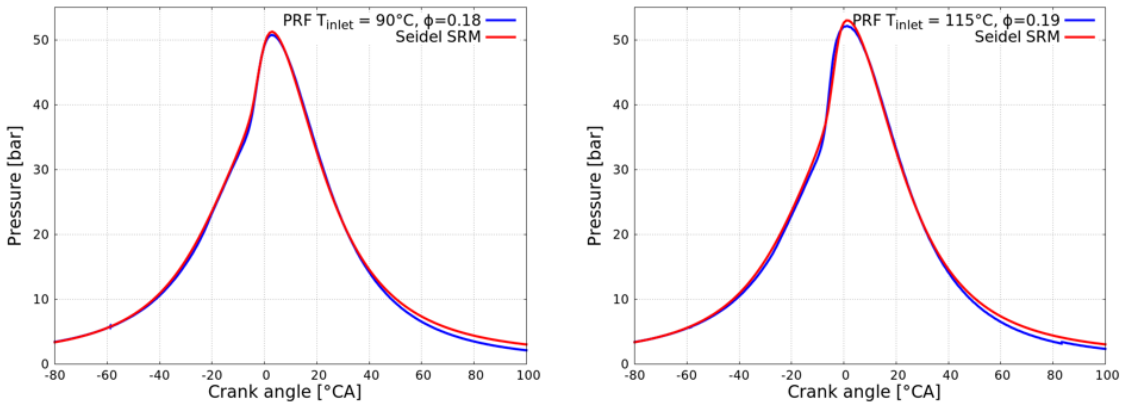

Figure 4: Measured and predicted pressure for ϕ=0.18 and ϕ=0.19 using PRF RON 90. Simulations are performed using the mechanism from Seidel [4].

FUTURE COLLABORATIONS (if applicable)

During the STSM a coopertaion between the “engine modelling groups” of both institutions has been started and will be continued, not only for the SmartFuel project, but also for the investigations of Diesel combustion.

The analysis of the reaction mechanisms showed that there is no reaction scheme available that can be used to describe both the main fuel species (*iso*-ocatane and *n*-heptane) and the photo chemical ignition. A new reaction scheme needs to be composed and validated, which can be a fruitful cooperation for both institutes.

Both groups plan to deepen their cooperation in the combustion modelling field after this STSM.

References

[1] *LOGEsoft v1.08,* LOGE AB, www.logesoft.com, 2018.

[2] Sirjean, B., Dames, E., Sheen, D.A., Egolfopoulos, F.N., Wang, H., Davidson, D.F., Hanson, R.K., Pitsch, H., Bowman, C.T., Law, C.K., Tsang, W., Cernansky, N.P., Miller, D.L., Violi, A., Lindstedt, R.P., "A high-temperature chemical kinetic model of n-alkane, cyclohexane, and methyl-ethyl-, n-propyl and n-butyl-cyclohexane oxidation at high temperatures, JetSurF version 1.1," 15 September 2009. [Online]. Available: http://melchior.usc.edu/JetSurF/JetSurF1.1.

[3] Sirjean, B., Buda, F., Hakka, H., Glaude, P.A., Fournet, R. , "The autoignition of cyclopentane and cyclohexane in a shock tube," *Proceedings of the Combustion Institute ,* vol. 31, p. 277–284, 2007.

[4] Seidel, L., Development and Reduction of a Multicomponent Reference Fuel for Gasoline, Brandenburg University of Technology Cottbus-Senftenberg: PhD thesis, 2017.