SHORT TERM SCIENTIFIC MISSION (STSM)
SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CM 1404
STSM title: Experimental study and detailed evaluation on the laminar flame speed of alcohol-water-air mixtures
STSM start and end date: 03/09/2018 to 31/10/2018
Grantee name: Lisa van Treek

PURPOSE OF THE STSM

The purpose of the Short Term Scientific Missions (STSM) was focused to performing experiments to determine the laminar flame velocities of alcohol-water-air mixtures. These newly acquired experimental results will contribute to broadening the understanding of the combustion chemistry of alcohol-based fuel blends.

Next to the use of fossil fuels, other fuels are increasingly becoming the focus of public discussion. Reasons for the search for alternatives are the limited crude oil reserves, but also the environmental pollution and emissions that occur during the combustion of mineral oil products and their additives.
An alternative to diesel or gasoline offer bio-alcohols such as ethanol. The laminar flame velocity of alcohols is an important parameter in combustion. The experimental results can provide a thorough knowledge of the combustion chemistry of alcohol-based fuel mixtures.

To understand the impact of water content in ethanol, either due to long term storage or due to water injection strategies during combustion, an extensive measurement campaign was carried out.

For this purpose, the STSM was carried out in the Department of Combustion Physics at Lund University in Sweden. With the STSM experimental and scientific experiences in the established methods of the University of Lund should be gained. The focus was on acquiring skills and handling in determining the laminar flame velocities of a liquid fuel with the heat flux burner.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSM

During this STSM experiments were carried out to determine the laminar flame velocities of ethanol-water-air mixtures. The determination of the laminar burning velocity was performed with the heat flux method. The mixture containing 0 to 40 % water by mole. The flames were investigated with the initial temperature of 358 K and the equivalence ratio (ϕ) range was varied from 0.7 to 1.4 at atmospheric pressure.

The experimental burner consists of a perforated plate burner, where the flame stabilizes above a 2 mm thick brass burner plate. The plate has a diameter of 30 mm and is perforated with small holes of 0.5 mm diameter at 0.7 mm pitch. The burner head and plenum chamber has heating and cooling jackets respectively to keep the temperature constant. To keep the temperature at 358 K constant two water bath were used. Mass flow controllers have been used to regulate the flow rates of the oxidizer and the fuel. The liquid fuel mixture (ethanol and water) was gasified using an evaporator. The laminar burning velocity was determined by varying the velocity of the unburned gas for a given gas mixture until a constant temperature distribution is reached.

At the beginning experiments were carried out with gaseous fuels (methane-air mixture) to get acquainted with the setup (devices and instrumentation) and the process at division of Combustion Physics at Lund University. By gaining familiarity with the combustion setup we started with the main part of measurements and evaluations of laminar burning velocities of liquid fuels.
Numerical calculations were conducted with CHEMKIN-PRO software package and LOGEresearch [1] to compare the experimental data. Three detailed kinetic mechanism, derived from Konnov et al. [2], Moshammer et al. [3] and Shrestha et al. [4], have been used.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

To determine laminar flame velocities of ethanol-water-air flames for different equivalence ratios the following mixing ratios were selected and performed. In Table 1 the experimentally investigated conditions in this study are presented.

Table 1: Experimental conditions of ethanol-air-flames

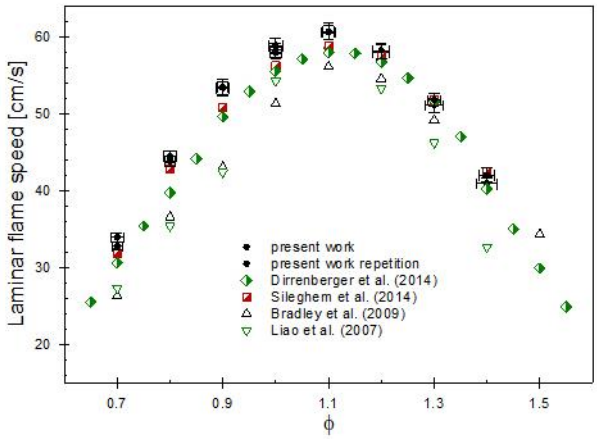
Ethanol [%]	H2O [%]	ϕ
100	0	0.7 - 1.4
90	10	0.7 - 1.4
80	20	0.7 - 1.4
70	30	0.7 - 1.3
60	40	0.7 - 1.2

The experimental laminar flame speed (S_L) of ethanol-air at T = 358 K and at atmospheric pressure was performed. The S_L are measured for different equivalence ratios form ϕ = 0.7 to 1.4, as present in Figure 1. Figure 1 compares the present data including error bars with published data and shows good agreement.

At lean and near stoichiometric conditions the obtained S_L is slightly faster slightly in comparison to other experiments. The S_L measured by Sileghem et al. [5] agrees very good for lean and rich mixtures. At stoichiometric mixtures it is observed that the present S_L are (systematically) higher.

For rich conditions the results of Dirrenberger et al. [6], Bradley et al. [7] and Sileghem et al. [5] are within the present measurements. At equivalence ratio of 1.2 the present data found to be close to the data of Dirrenberger et al. [6] and Sileghem et al. [5].

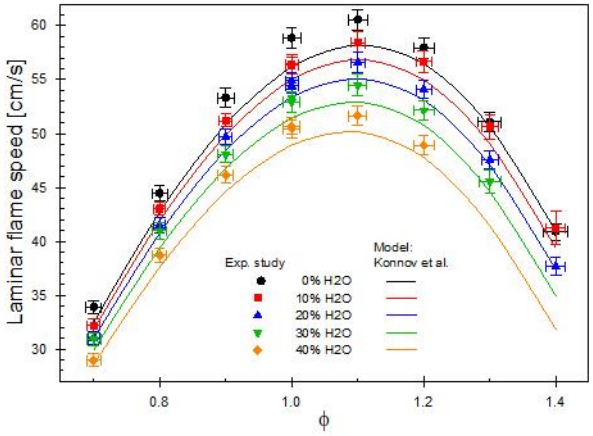
Data from Bradley et al. [7] are in good agreement with the data of Dirrenberger et al. [6] for rich conditions. The S_L of Liao et al. [8] are generally slower at all conditions than the presented results. It should be noted that Liao et al. [8] used a different method (combustion bomb) to determined the S_L. The Figure 1 shows also that the repetition of the S_L of ethanol-air flames are in the range of error bars.



In Figure 1: Laminar flame speed of ethanol-air at T = 358 K and atmospheric pressure with error bars in comparison with references [5]–[8].

The experimental and simulated laminar burning velocities of ethanol-water-air mixtures are shown in Figure 2 to Figure 4. The laminar burning velocities obtained in this study, along with there uncertainties, are compared against with the predictions of three models: the mechanism developed by Konnov et al. [2], the model of Moshammer et al. [3] and Shrestha et al. [4].

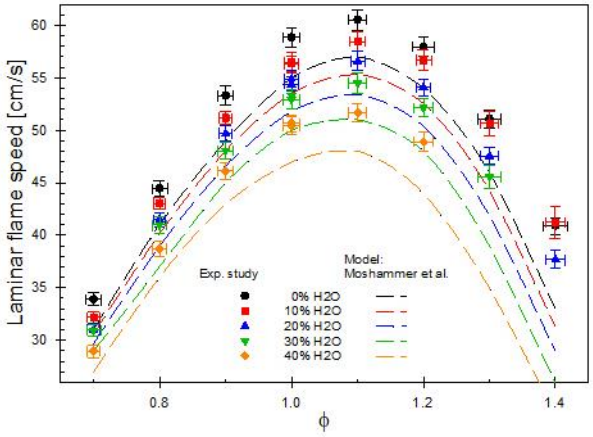
In all Figures (Figure 2 and Figure 4) it is seen that the experimental laminar flame speed (S_L) for ethanol-water-air mixtures decrease with increasing the water content 10 - 40%. General the experimental data for S_L show a better agreement with the model of Konnov et al. [2].



In Figure 2: S_L of ethanol-water-air at T = 358 K at different water contents. The solid lines represent the numerical results predicted to the model [2].

The model of Konnov et al. [2] leads to a slight underestimation of the S_L in particular at rich conditions. A very close agreement is observed for lean mixtures. The largest deviation is seen close to the stochiometric mixtures and the maximum S_L for the equivalence ratio of 1.1.

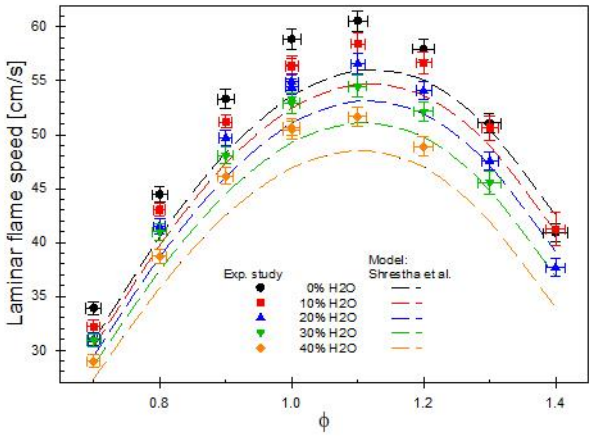
Figure 3 displays the experimental results for ethanol-water-air flames, which are good agreement with the model at lean conditions.



In Figure 3: S_L of ethanol-water-air at T = 358 K at different water contents. The dash lines represent the numerical results predicted to the model [3].

For equivalence ratio above 0.9 the deviation increase between the model of Moshammer et al. [3] and experimental data.

Finally, Figure 4 compares the present data with the model of Shrestha et al. [4]. The model of Shrestha et al. [4] predicts the experimental results very well at rich mixtures. At lean- and stochiometric conditions this model shows larger deviations than the model of Konnov et al. [2].



In Figure 4: S_L of ethanol-water-air at T = 358 K at different water contents. The dash lines represent the numerical results predicted to the model [4].

HOW THE STSM HAS CONTRIBUTED TO THE ACTIONS´S AIM

Regarding the SMARTCATs COST action (CM1404), this STSM represents a collaboration between two partners of a workgroup (WG 1: Smart Energy Carriers gas phase chemistry: from experiments to kinetic models).

FUTURE COLLABORATION WITH THE HOST INSTITUTION

At last year's conference, organized in the COST Framework of Action, there were opportunities to discuss experimental results and error estimation of laminar flame velocities.

The collaboration group of Lund University during the STSM was an excellent opportunity to broaden the knowledge about experimental design. In addition, the collaboration with the Department of Combustion Physics at Lund University provided a good opportunity to strengthen the link between the two universities and, where appropriate, to conduct future joint activities in the SMARTCATS COST Action.

FORESEEN PUBLICATIONS / ARTICLES RESULTING FROM THE STSM

Regarding the work during the STSM there is a plan to present the results at the next upcoming COST Meeting (First International Conference on Smart Energy Carriers) in January 2019. Furthermore, a joint publication of a paper in a international scientific journal is planned.

REFERENCES

[1] http://logesoft.com/de/loge-software/.

[2] A. Fomin, T. Zavlev, V. A. Alekseev, I. Rahinov, S. Cheskis, and A. A. Konnov, “Experimental and modelling study of $^{1}CH2$ in premixed very rich methane flames,” Combust. Flame, vol. 171, pp. 198–210, 2016.

[3] K. Moshammer, L. Seidel, Y. Wang, H. Selim, S. M. Sarathy, F. Mauss and N. Hansen, “Aromatic ring formation in opposed-flow diffusive 1,3-butadiene flames,” Proc. Combust. Inst., vol. 36, pp. 947–955, 2017.

[4] K. P. Shrestha, L. Seidel, T. Zeuch and F. Mauss, “Kinetic modelling of NOx formation and consumption during Methanol and Ethanol oxidation,” Submitt. to Rev. Combust. Sci. Technol.

[5] L. Sileghem, V. A. Alekseev, J. Vancoillie, E. J. K. Nilsson, S. Verhelst, and A. A. Konnov, “Laminar burning velocities of primary reference fuels and simple alcohols,” Fuel, vol. 115, pp. 32–40, 2014.

[6] P. Dirrenberger, P. A. Glaude, R. Bounaceur, H. Le Gall, A. P. Da Cruz and A. A. Konnov, F. Battin-Leclerc, “Laminar burning velocity of gasolines with addition of ethanol,” Fuel, vol. 115, pp. 162–169, 2014.

[7] D. Bradley, M. Lawes, and M. S. Mansour, “Explosion bomb measurements of ethanol-air laminar gaseous flame characteristics at pressures up to 1.4 MPa,” Combust. Flame, vol. 156, no. 7, pp. 1462–1470, 2009.

[8] S. Y. Liao, D. M. Jiang, Z. H. Huang, W. D. Shen, C. Yuan, and Q. Cheng, “Laminar burning velocities for mixtures of methanol and air at elevated temperatures,” Energy Convers. Manag., vol. 48, no. 3, pp. 857–863, 2007.