

# The Laminar Burning Velocity of Iso-Octane, Ethanol and Iso-Butanol using the Heat Flux Burner and the Closed Combustion Vessel

F. Rau<sup>1,\*</sup>, B. Schoen<sup>1</sup>, S. Hartl<sup>2</sup>, S. Voss<sup>1</sup>, C. Hasse<sup>2</sup>, D. Trimis<sup>3</sup>

<sup>1</sup>TU Bergakademie Freiberg, Institute of Thermal Engineering, Freiberg, Germany

<sup>2</sup>TU Bergakademie Freiberg, Chair of Numerical Thermo-Fluid Dynamics, Freiberg, Germany

<sup>3</sup>Karlsruhe Institute of Technology, Engler-Bunte-Institute, Division of Combustion Technology, Karlsruhe, Germany

## Abstract

Two methods to measure the laminar burning velocity, the Heat Flux burner and the closed combustion vessel, are compared against each other. The investigated fuels are commonly used to measure the influence of the biofuel blending with ethanol as the state-of-the-art surrogate and iso-butanol as a possible alternative. The comparison of measured and published laminar burning velocities show deviations between the methods on average of about 2 cm/s and on maximum of about 3 cm/s. Also numerical mechanisms are investigated, showing prediction performances in range of deviation on average between 1 cm/s and 4 cm/s.

## Introduction

The laminar burning velocity is an important fuel property, which is commonly used for the validation of chemical reaction mechanisms. It is defined as the velocity of a laminar adiabatic premixed propagation of an unstretched one-dimensional flame into a fuel/air mixture. Based mainly on different measurement techniques, a wide distribution of the measured laminar burning velocities appears. To quantify this proposition for chosen fuels, the results of two techniques are compared against each other in this article: the Heat Flux method (HF) and the closed combustion vessel method (CV).

The investigated fuels are orientated on the well discussed displacement of gasoline with biogenic fuel. These biofuels need to be produced with renewable primary resources to contribute to the emission reduction within the traffic sector [1]. Since the most common production path is the fermentation of sugar cane and crops, the surrogates belong to the group of alkanol. The best-known representatives of this substance group are, in order of size, methanol, ethanol and butanol. Ethanol is actually well established in several countries as a surrogate (e.g. Brazil, USA and the countries of the European Union). Additionally, butanol is considered, because of its higher energy content. Further the travel range, which is reduced by the use of ethanol blending, shows an improvement. Butanol consists of four carbon atoms, therefore the chemical composition allows four isomers, namely 1(n)-butanol, 2-butanol, 3-butanol and iso-butanol. Actually the use of 1-butanol is promoted due to the fact, that it can be easily produced with a retrofitting of existing ethanol production facilities. However, recent efforts are made towards iso-butanol, since its properties allow the highest increase of the octane number of the blended gasoline.

In this article the laminar burning velocity of these three fuels, which are required for a mixture of a reference fuel for state-of-the-art biofuels (iso-octane/ethanol) as well as for prospective biofuels (iso-octane/iso-butanol), is investigated. The results of two

measurement methods, the Heat Flux and the closed combustion method, are compared against each other. The conditions for the experiments are an unburned gas temperature of 373 K and absolute pressures up to 10 bar. The investigated equivalence ratio is in the range of 0.8 to 1.3. The measurement results are furthermore compared to existing chemical reaction mechanisms calculated with the Cantera software package.

## Experimental Method

The laminar burning velocity is measured at atmospheric conditions with the Heat Flux burner and the closed combustion vessel, while only the closed combustion vessel is used for the high-pressure investigations.

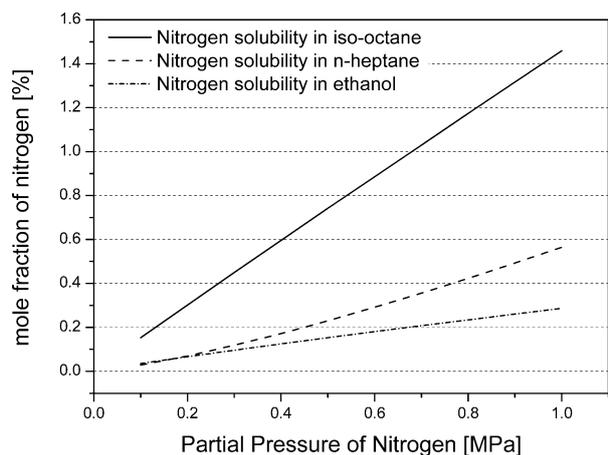
The method of the Heat Flux burner has been proposed by de Goey et al. in 1993 [2] based on the earlier work of Botha and Spalding [3]. Additionally information about the method can be found in [4].

The used test rig is explained in detail in [5]. Since then, the liquid fuel handling has been modified. In the previous version, the liquid fuel was stored in a stainless steel tank and pressurized with nitrogen to 5 bar(g) to operate a coriolis mass flow controller (mini-CORIFlow™, Bronkhorst B.V.). With this dosing system, the dissolved nitrogen had to be removed with a gas separator before the evaporation. The pressure-dependant solubility of nitrogen in iso-octane, ethanol and n-heptane is shown in Figure 1. In the actual version, the stainless steel tank is replaced by a hydraulic accumulator, which separates the liquid and the gas phase. Since the solubility is excluded, the gas separator could be removed and a source of disturbance in the measurement of the laminar burning velocity is eliminated.

The method of the closed combustion vessel is well known due to the work of the groups around Beeckmann and Pitsch [6], Varea and Renou [7], Broustail and Mounaim-Rousselle [8] as well as Kelly and Law [11]. The technical construction of the test rig is consistent with [6]. The principle of the optical setup is shown in Figure 2.

---

\* Corresponding Author: Florian.Rau@iwtt.tu-freiberg.de  
Proceedings of the European Combustion Meeting 2015



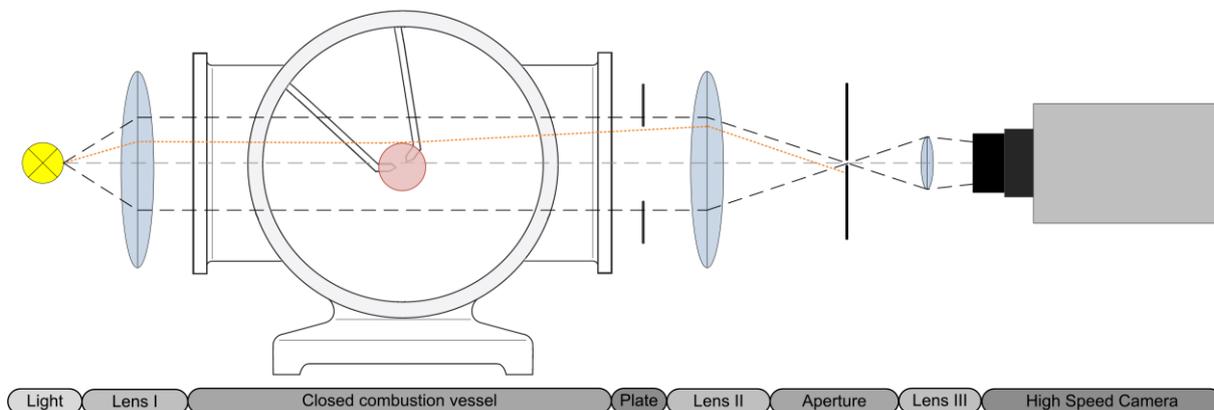
**Figure 1** –Pressure-dependant solubility of nitrogen in iso-octane, ethanol and n-heptane at 298 K [10]

The used visualization technique is the Schlieren method. The source for the parallel light is a standard white LED with a biconvex lens afterwards. The beams of light pass the optical windows of the combustion vessel and some are diffracted by the density gradient at the flame front (red line, Figure 2). The beams of light are focused with a second biconvex lens on an iris aperture and the diffracted beams are blocked. The third lens focuses the image for the high speed camera. The images are recorded with a resolution of 768 x 768 pixel at a frame rate of 10 000 fps. To convert the pixel into a length scale a calibration plate is placed inside the visible range of the camera.

The radius of the flame front is extracted from the images of the high-speed camera with the method of Kasa [9], while the laminar burning velocity is derived with the non-linear approach of Kelly and Law [11].

### Numerical Method

The Cantera software package is used to model one-dimensional adiabatic steady laminar premixed flames. The transport properties are evaluated by using the mixture average diffusion model. Furthermore, an adaptive grid refinement is used with an average of over 500 grid points on a domain up to 0.3 meter to ensure a chemical equilibrium state in the burned gas and grid independent results. An overview of the used mechanisms for the specific fuels is given in Table 1.



**Figure 2** - Principle of the optical setup of the closed combustion vessel test rig

**Table 1** - Overview of the used mechanisms

Name	Fuel	# of Species	# of Reactions
Zhong&Zheng	Iso-octane	51	204
Golovitchev	Iso-octane	120	677
Saxena&Williams	Ethanol	57	383
CRECK	Butanol	317	12251

During this work, the iso-octane/air flames are modelled using the Zhong&Zheng mechanism [12] and the Golovitchev mechanism [13]. The mechanism of Zhong&Zheng is developed for ignition and oxidation processes of the three-component fuel mixture iso-octane, n-heptane, and ethanol. It is based on the detailed ethanol mechanism created by Marinov [14], whose major species and reactions were incorporated into the kinetic PRF model. Based on this mechanism a previous model is developed for ignition delay times. This did not accurately describe reactions related to the H-atom radical, which results in a not accurate laminar burning velocity. Hence, some significant reactions that affect the laminar burning velocity are extracted. The mechanism is validated against ignition delay data of shock tube measurements, laminar burning velocities of iso-octane, n-heptane, ethanol, and the ternary mixtures and a rich iso-octane/air premixed flame.

The Golovitchev mechanism is developed for the combustion of gasoline-ethanol blends in respect to the modelling of engines in CFD calculations. It is based on chosen sub-mechanisms of gasoline surrogates and ethanol. The mechanism is validated against experimental data on laminar burning velocities and ignition delay times, obtained for various iso-octane, toluene, ethanol and n-heptane air mixtures under various conditions for the equivalence ratios, initial temperatures, and pressures.

The ethanol/air flames are modelled using the mechanism by Saxena&Williams [15]. The foundation of this chemical-kinetic mechanism is an assembly of mechanisms developed for the combustion of hydrogen, carbon monoxide, methane, ethane, ethylene, acetylene, propane, propene, propyne, allene and methanol.

Due to simplifications ( $p \leq 100$  bar,  $T > 1000$  K,  $\phi < 3$ ,  $a > 50$  s) it is relatively small for a detailed mechanism. This mechanism is extended to ethanol by adding 33 reactions that involve ethanol and 22 reactions that involve acetaldehyde. It describes the formation of oxides of nitrogen as well as compounds involving three carbon atoms. The mechanism is tested against data for shock-tube auto-ignition delay times, laminar burning velocities of ethanol at atmospheric pressure and initial temperatures of 298 K to 453 K, counterflow diffusion flame extinction and the structure of counterflow partially premixed and diffusion ethanol flames.

The butanol/air flames are modelled using the PRF mechanism by the CRECK Modelling Group [16]. Within this mechanism optimisation, different isomers of butanol are treated, since it is known that the structure of fuel molecules is important with respect to the intermediate species. The updated mechanism is compared to major and intermediate species profiles for the combustion of the four butanol isomers under low-pressure premixed flame conditions. Further the formation of acetone in 2- and tert-butanol flames, acetaldehyde in the 1-butanol flame and formaldehyde and propene in 1- and iso-butanol flames is analysed.

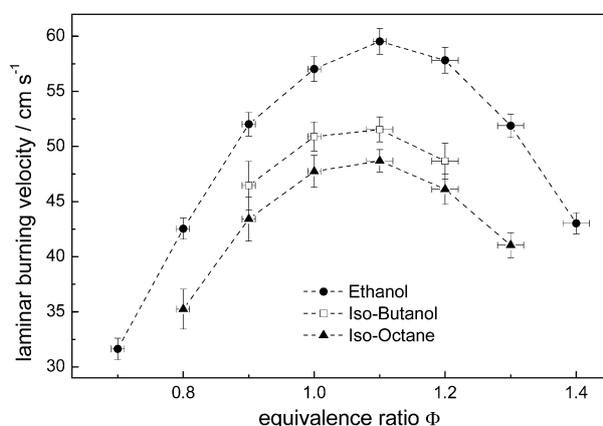
The modelling is mainly used to evaluate the mechanisms with respect to the present set of experimental data for the pure iso-octane, ethanol and iso-butanol investigations. Furthermore, it is possible to provide a pressure dependent comparison of the experimental data using all three pure fuels.

## Results and Discussion

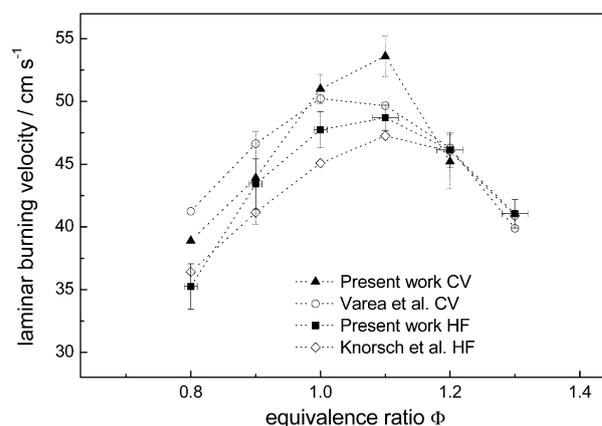
All results of the laminar burning velocities for iso-octane, ethanol and iso-butanol were measured and calculated at an unburned gas temperature of 373 K. The equivalence ratio is considered from 0.8 to 1.3.

### 1. Atmospheric Investigation

An overview of the relation between the investigated liquid fuels iso-octane, ethanol and iso-butanol at 373 K is given in Figure 3.



**Figure 3** - Laminar burning velocity of iso-octane, ethanol and iso-butanol measured with the Heat Flux method at 373 K and atmospheric pressure



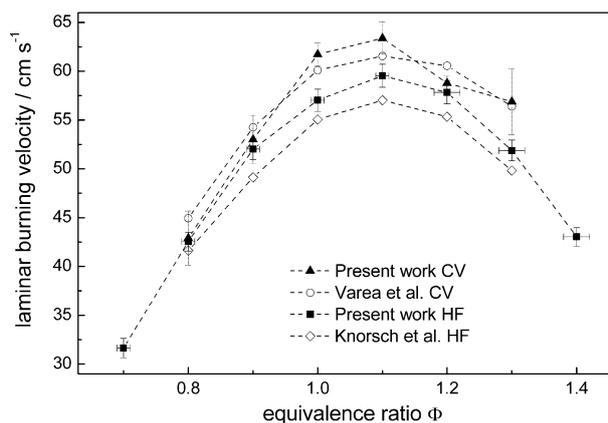
**Figure 4** - Laminar burning velocity of iso-octane measured with the Heat Flux and the closed combustion vessel method at 373 K and atmospheric pressure

The laminar burning velocity of the primary reference fuel iso-octane shows the lowest laminar burning velocity values for the atmospheric investigations. It is followed by iso-butanol. With a maximum velocity of 59.5 cm/s ethanol has an about 11 cm/s higher laminar burning velocity than iso-butanol.

The comparison of the measurements of iso-octane with the closed combustion vessel and the Heat Flux burner is shown in Figure 4. The published data of Varea et al. [17] and Knorsch et al. [18], executed for the same conditions, are also included. The literature data and the HF results are in a good agreement for an equivalence ratio range from 1.0 to 1.3. However, the decrease of the laminar burning velocity at lower equivalence ratios shows higher discrepancies. On the other side, the laminar burning velocities for equivalence ratios above 1.2 are closely distributed at about 46 cm/s and 40 cm/s with a standard deviation of 0.4 cm/s and 0.5 cm/s, respectively. The maximum deviation is 2.4 cm/s at an equivalence ratio of 1.1.

The comparison for ethanol is presented in Figure 5. The overall behaviour of the laminar burning velocity measurements over the equivalence ratio is comparable for the four data sets. The lowest laminar burning velocities are measured by Knorsch et al. [18] while the own measurements using the closed combustion vessel are the highest. The spread of the measurements is, contrary to iso-octane, lower for low equivalence ratios. The maximum deviation has the same value and shows differences at the same position as the iso-octane measurements. Figure 5 is giving the misleading impression of a lower deviation between the data sets compared to the iso-octane measurements. This is disproved by the minimum deviation of 1.2 cm/s and a maximum with 3.0 cm/s.

Since 1-butanol is actually the scope of the investigations of other groups, the available data for the comparison of iso-butanol at 373 K and atmospheric pressure is reduced to the measurements of Knorsch et al. [18], Figure 6.



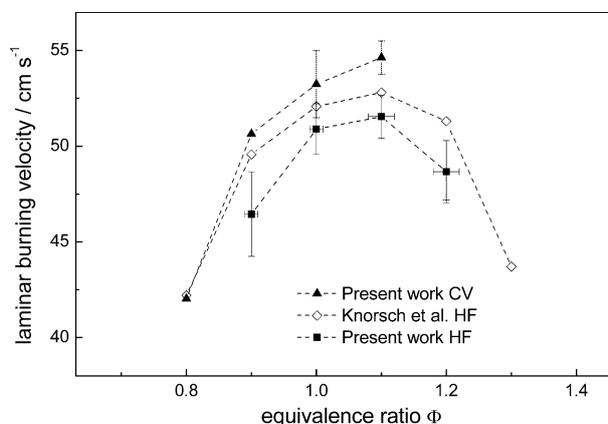
**Figure 5** - Laminar burning velocity of ethanol measured with the Heat Flux and the closed combustion vessel method at 373 K and atmospheric pressure

The trend of the burning velocity is consistent for the three sets of data. So far the maximum deviation is the lowest with a value of 1.8 cm/s. Since the own measurements with the closed combustion vessel as well as with the Heat Flux burner are not finished yet, a detailed analysis is omitted.

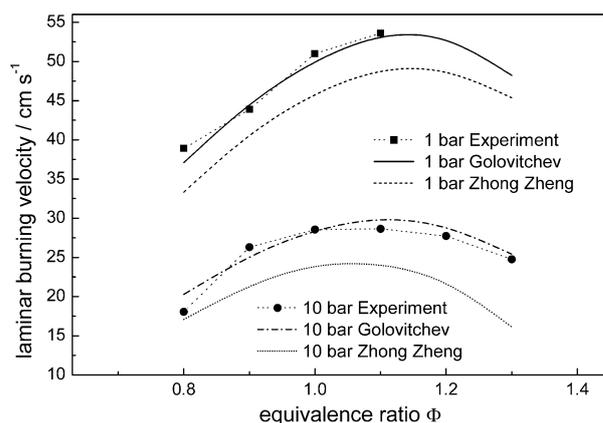
## II. Pressure Investigation

The dependence of the laminar burning velocity on the pressure is studied within a closed combustion vessel at 373 K for atmospheric and elevated pressure cases.

Figure 7 shows the results for iso-octane for an absolute pressure of atmospheric and 10 bar in comparison with the chemical mechanism of Golovitchev [13] and Zhong&Zheng [12]. The increase of the pressure from atmospheric to 10 bar leads to a decrease of about 50% of the laminar burning velocity. At the atmospheric case, the prediction of the Golovitchev shows very good agreement with the results of the closed combustion vessel, which is indicated by a maximum discrepancy of 1.8 cm/s at an equivalence ratio of 0.8 and a mean discrepancy of 1.0 cm/s.



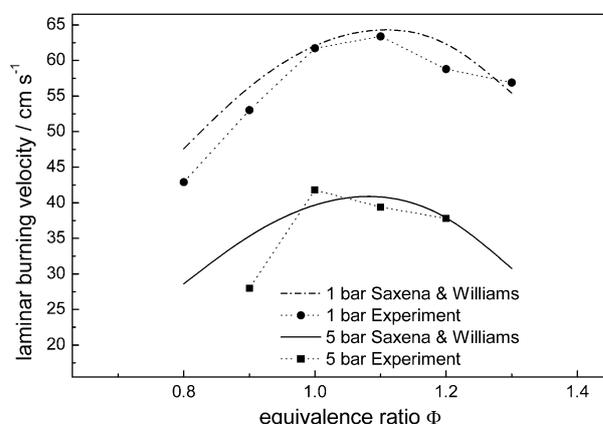
**Figure 6** - Laminar burning velocity of iso-butanol measured with the Heat Flux and the closed combustion vessel method at 373 K and atmospheric pressure



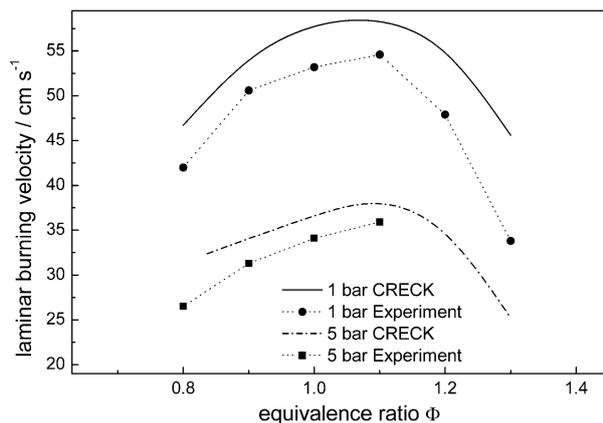
**Figure 7** - Laminar burning velocity of iso-octane measured with the closed combustion vessel at 373 K and absolute pressure of atmospheric and 10 bar in comparison with numerical predictions

At the higher pressure case, the predictions of Golovitchev stay at a high level of consistency resulting in a maximum discrepancy of 2.2 cm/s and a mean discrepancy of 1.1 cm/s. The mechanism of Zhong&Zheng is still predicting a lower laminar burning velocity than measured and the maximum discrepancy remains above 5.0 cm/s.

Figure 8 shows the ability of the mechanism of Saxena&Williams [15] to predict the laminar burning velocity of ethanol at atmospheric and 5 bar. The maximum velocity of the atmospheric case of 63.4 cm/s at an equivalence ratio of 1.1 is calculated with a deviation of 0.9 cm/s. So the overall agreement between experiment and numerical mechanism is very good. At equivalence ratios below stoichiometry the Saxena&Williams mechanism tends to underpredict the laminar burning velocity, which leads to a discrepancy of 4.7 cm/s at an equivalence ratio of 0.8. With the actual set of measurements at an absolute pressure of 5 bar, the evaluation of the calculation show good results.



**Figure 8** - Laminar burning velocity of ethanol measured with the closed combustion vessel at 373 K and absolute pressures of atmospheric and 5 bar in comparison with numerical predictions



**Figure 9** - Laminar burning velocity of iso-butanol measured with the closed combustion vessel at 373 K and absolute pressures of atmospheric and 5 bar in comparison with numerical predictions

The comparison between measurements and numerical predictions for iso-butanol is shown in Figure 9. At atmospheric conditions the CRECK mechanism [16] tends to overpredict the laminar burning velocity at a mean deviation over the entire investigated equivalence ratio of 5.8 cm/s. This mean deviation is reduced at 5 bar to 3.5 cm/s.

### Conclusions

Within this paper the comparison of the laminar burning velocities measured with different measurement techniques, data from the literature and numerical predictions for the three liquid fuels iso-octane, ethanol and iso-butanol are shown. Based on the lack of data at 373 K and atmospheric pressure only data from Varea et al. and Knorsch et al. are available for the comparison. The own and the published measurements for iso-octane have a mean deviation of 1.6 cm/s and a maximum discrepancy of 2.4 cm/s at an equivalence ratio of 1.1, the highest laminar burning velocity. For ethanol the mean and maximum deviations are higher with values of 2.2 cm/s and 2.6 cm/s, respectively. The peak of the deviation is at an equivalence ratio at 1.3. For iso-butanol only Knorsch et al. measured the laminar burning velocity. At this point of progress the set of data gives reliable results.

The comparison of the laminar burning velocity measured with the closed combustion vessel and calculated with numerical mechanisms should prove the reliability of dedicated numerical predictions. For iso-octane the mechanism of Golovitchev shows very good agreement. At atmospheric conditions the mean deviation is 1.0 cm/s and the maximum is 1.8 cm/s. The mean deviation for an absolute pressure of 10 bar stays nearly constant at 1.1 cm/s as well as the maximum with 2.2 cm/s. The mechanism of Zhong&Zheng underpredict the laminar burning velocity over the entire investigated equivalence ratio. The laminar burning velocity of ethanol is calculated with the mechanism of Saxena&Williams and shows a good agreement for atmospheric pressure with a mean deviation of 2.3 cm/s. The increasing discrepancy at

lower equivalence ratios leads to a maximum deviation of 4.7 cm/s. The third investigated fuel is iso-butanol, which is predicted with the CRECK mechanism. At atmospheric pressure the discrepancy is at a high level with 4.1 cm/s in mean and 11.8 cm/s at maximum. With rising pressure, the performance is intensively improved to a mean deviation of 3.5 cm/s and a maximum of 4.9 cm/s.

### Acknowledgements

The authors would like to gratefully acknowledge the financial support of the European Commission through the European Social Fund (ESF) and the Saxon State Ministry of Science and the Arts for the project BioRedKat (no. SAB 100097882).

### References

- [1] International Energy Agency, Technology roadmap. Biofuels for Transport, 2011.
- [2] L.P.H. de Goey, A. van Maaren, R.M. Quax, *Combust. Sci. And Tech.* 92 (1993) 201-207.
- [3] J.P. Botha, D.B. Spalding, *Proc. R. Soc. Lon. Ser. A* 225, Issue 1160 (1954), 71-95.
- [4] Heat Flux Method, Web January 2015, <http://heatfluxburner.org>.
- [5] F. Rau, S. Hartl, S. Voss, M. Still, C. Hasse, D. Trimis, *Fuel* 140 (2015), 10-16.
- [6] J. Beeckmann, L. Cai, H. Pitsch, *Fuel* 117 (2014), 340-350.
- [7] E. Varea, J. Beeckmann, H. Pitsch, Z. Chen, B. Renou, *Proceedings of the Combustion Institute* 35 (2014), 711-719.
- [8] G. Broustail, F. Halter, P. Seers, G. Moréac, C. Mounaïm-Rousselle, *Fuel* 106 (2013), 310-317.
- [9] I. Kasa, *IEEE Transactions on Instrumentation and Measurement* IM-25 no.1 (1976), 8-14.
- [10] R. Battino, T.R. Rettich, T. Tominaga, *J. Phys. Chem. Ref. Data* 13 (2) (1984), 563- 600.
- [11] A.P. Kelley, C.K. Law, *Combust. Flame* 156 (2009) 1844-1851.
- [12] B.-J. Zhong, D. Zheng, *Combust. Sci. And Tech.* 185 (2013), 627 – 644.
- [13] C. Huang, V. Golovichev, A. Lipatnikov, *SAE Technical Paper* 2010-01-0543 (2010).
- [14] N.M. Marinov, *Int. Journal of Chem. Kin.* 31 (1999), 183–220.
- [15] P. Saxena, F.A. Williams, *Proceedings of the Combustion Institute* 31 (2007), 1149-1156.
- [16] A. Frassoldati, R. Grana, T. Faravelli, E. Ranzi, P. Obwald, K. Kohse-Höinghaus, *Combust. Flame* 159 (2012) 2295-2311.
- [17] E. Varea, V. Modica, B. Renou, A. M. Boukhalfa, *Proceedings of the Combustion Institute* 34 (2013) 735-744.
- [18] T. Knorsch, A. Zackel, D. Mamaikin, L. Zigan, M. Wensing, *Energy and Fuels* 28 (2) (2014), 1446-1452.