Validation of a SI Auto-Ignition Onset Model for Hydrogen and Methanol against Measurement Data

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Abstract: With the increasing focus on carbon neutrality, synthetic fuels are gaining popularity. This work investigates the prediction of the auto-ignition of hydrogen and methanol. With a wide range of potential applications, such as land and marine transportation, construction vehicles, and automotive applications, they could replace fossil fuels in sectors with high carbon dioxide emissions and high requirements to power density. Obviously, this future use of synthetic fuels will require experimental testing. Simulations are an important tool to minimize costly and time-consuming tests. Compared to other simulation classes, 0D/1D simulations offers high predictive capability with low computational time requirements and are therefore well suited for more extensive investigations such as concept studies. Due to the energy-intensive production of synthetic fuels and the limited availability of renewable energy, an efficient use in internal combustion engines is essential. Knocking is an important limiting factor for peak efficiency in spark ignition engines. It is caused by an unwanted auto-ignition in the unburned mixture. This indicates, that an accurate auto-ignition model is essential for knock modeling.

The 0D auto-ignition simulation method used in this work is originally developed by Fandakov for gasoline fuels and validated for these. It has been adapted for the use of hydrogen and methanol, and in this work validated against a measurement database of these synthetic fuels. To predict their auto-ignition onset, an integral which considers the state of the chemical pre-reactions in the unburned mixture is calculated. For this purpose, the ignition delay times, which are strongly dependent on the boundary conditions, are required for each calculation step. Since their acquisition with detailed reaction kinetics requires a lot of computational time, an approach is used for the auto-ignition model, which benefits the typical low computational effort of 0D/1D simulations. The calculations are performed in advance and the results are stored in correlation equation. From there, they are provided at simulation runtime. To validate the modeled auto-ignition onset, an extensive database of test bench measurements has been collected. Single knocking working cycles are used to validate the modeled results against measured data. The knock onset is determined from the filtered indicated pressure curve and set equal to the auto-ignition onset. To accurately determine the knock onset from the extensive measurement data, an automated method based on a bandpass filter is used.

1 Introduction

Due to climate change, our atmosphere continues to warm every year, with devastating consequences for humanity and the environment [1]. With the “Green Deal”, the European Union aims to make Europe the first climate-neutral continent. To achieve this, net greenhouse gas emissions from all sectors are to be reduced to zero by 2050 [2]. As shown in [3], a mix of powertrains with carbon-neutral energy carriers is needed, which includes finding alternative fuels for internal combustion engines (ICE). Due to their surpassing properties, hydrogen and methanol are promising fuel candidates for a wide range of. applications in the future, such as land and marine transportation, construction vehicles, and automotive applications.

Since the production of green hydrogen and green methanol is very energy-intensive and there is a lack of renewable energies [4], an efficient use in ICE is essential. The resulting costs also incentivises the minimization of test bench measurements. Instead, simulation tools can help develop engine designs and operation strategies that are optimized to their respective fuels. Especially the 0D/1D simulation, with its high prediction quality and low computational time requirements, is well suited for extensive studies.

To achieve peak efficiency in ICEs, the limiting factors must be well predictable in simulations. Knocking is one of the most important limiting factors in spark ignition (SI) engines. It is caused by an unwanted auto-ignition in the unburned mixture. In this work, a method for simulating auto-ignition developed by Fandakov [5] and extensively validated for gasoline data by Hess [6] is used. The method is adapted for auto-ignition onset prediction of hydrogen and methanol. To validate the results, measurement data from knocking single working cycles are used.

2 Measurement Data

The measurement data has been obtained from a single-cylinder SI test bench engine from RWTH Aachen University. It is measured at the Institute for thermodynamics of mobile energy conversion systems and center for mobile propulsion. Different engine configurations were used for the measurements of hydrogen and methanol. Table 1 shows the most important geometrical parameters of these two engine configurations.

Table 1: Test bench engine configurations

	Unit	**Hydrogen**	**Methanol**
Bore	mm	75	84
Stroke	mm	113.2	113.2
Stroke-to-bore ratio	-	1.51	1.35
Connecting rod length	mm	220	220
Displacement volume	cm^3	500	627
Compression ratio	-	12.2	19.5
Peak pressure capability (mean)	bar	180	190

For the validation of hydrogen auto-ignition, this work uses 3621 knocking indicated single working cycles of 69 different operating points. All operating points share the same engine speed of 2000 rpm but include variations of:

- Indicated mean effective pressure (IMEP): 6, 9, 12, 15 and 18 bar.
- Air-to fuel equivalence ratio: 1.0, 1.1 and 1.2.
- Injection: Central, lateral and shared.
- Variation of the injector retraction: 0, 3, 4 and 6 mm

To validate the modelled methanol auto-ignition, 62 knocking indicated single working cycles of 6 different operating points are used. The operating points are located at the same engine speed of 2500 rpm and the same air-to fuel ratio λ of 1. They include a variation of the valve timing and two different loads with 15 and 18 bar IMEP.

3 Applied Methods

Not every auto-ignition result in a knocking phenomenon, but every knocking phenomenon is caused by an auto-ignition. For validating the modeled auto-ignition against measurement data of a real SI-ICE, the knock onset is thus set equal to the auto-ignition onset. The following two sections will describe on the method of auto-ignition modeling and the detection of the knock onset from the measurement data.

3.1 Auto-Ignition Onset Modeling

To predict the auto-ignition onset, this work uses a so called Livengood-Wu integral as shown in equation (1). It was originally defined by Livengood and Wu [7] and estimates the state of the chemical pre-reactions in the unburned mixture. The auto-ignition onset is defined as the time step where the integral reaches a value of 1.

$$\int_{t}^{t_e} \frac{1}{\tau} \mathrm{d}t = 1 \tag{1}$$

Following Fandakov's procedure for gasoline data, the calculation of the integral starts at inlet valve closes (IVC) and ends at the auto-ignition onset (AI), as can be seen in equation (2). To ensure sufficient accuracy, integration steps of 0.1 °CA are chosen.

$$I_k = \frac{1}{n}\int_{\alpha_{IVC}}^{\alpha_{AI}} \frac{1}{\tau}\,\mathrm{d}\alpha \tag{2}$$

The equations show that the ignition delay time of the unburned mixture is required for each calculation step. To obtain the ignition delay times, time- and computationally-intensive reaction kinetic calculations are necessary. Fandakov [5] developed a procedure for gasoline data in which these calculations are performed a priori and provided to the simulation via correlation fit. In this way, the advantages of the low computing time of 0D/1D simulations can be conserve. Crönert [8] adapted this procedure for the use of different fuels and automated it. His approach involves three successive modules and is shown in figure 1. Each module is using the results of its predecessor.

Figure 1: Schematic structure of the automated approach to handle ignition delay times from different fuels in simulation. [8]

To use the automated approach, a wide range of boundary conditions for the reaction kinetic calculations must be defined to ensure an extensive area of validity. The chosen boundary conditions for hydrogen and methanol calculations are shown in Table 2.

Table 2: Boundary conditions for the reaction kinetic calculations for hydrogen and methanol performed for the use in this work

	Unit	Hydrogen	Methanol
Temperature	K	300 - 1400	300 - 1400
Pressure	bar	1 - 200	1 - 200
Air-to fuel equivalence ratio	-	1 - 5	0.9 – 2.2
Exhaust gas recirculation rate	%	0-50	0 - 10

The correlation fits in the second module of the automated approach are generated using an Arrhenius-type correlation, shown in equation (3).

$$\tau_\alpha = A_\alpha \cdot e^{\left(\frac{B_\alpha}{T}\right)} \quad with\ A_\alpha, B_\alpha = f(BC) \tag{3}$$

Figure 2 shows an example of the reaction kinetic calculations with the corresponding correlation fits for selected boundary conditions of hydrogen and methanol.

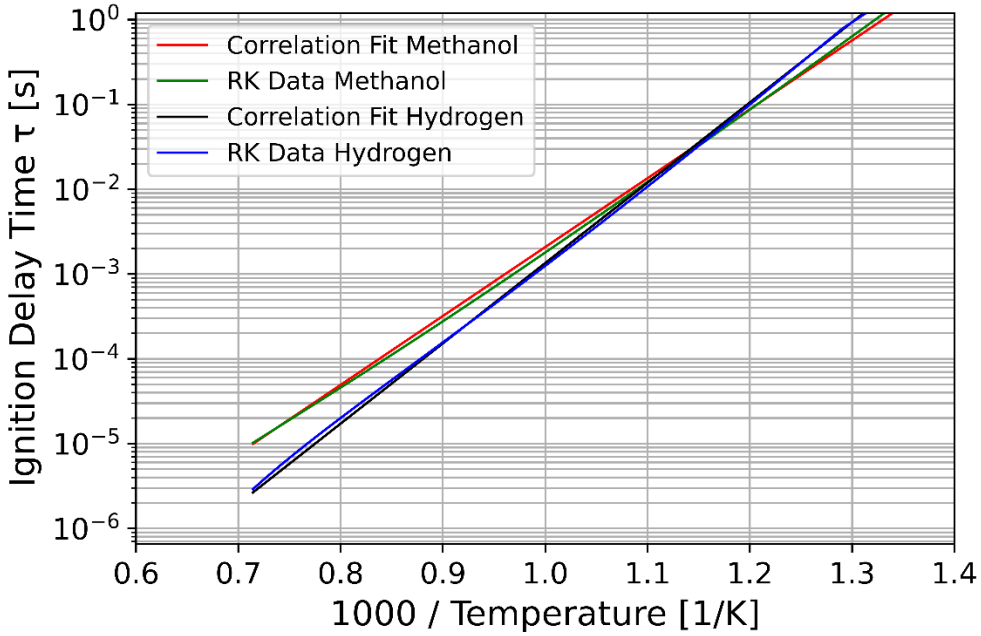

Figure 2: Exemplary reaction kinetic calculations and corresponding correlation fits for hydrogen and methanol. Stoichiometric conditions without any EGR influences and a pressure of 100 bar are shown.

The described auto-ignition model is integrated into a quasi-dimensional simulation tool. It models the auto-ignition onset as a post-processing tool by calculating the Livengood-Wu integral fed by the stored correlation fits. As a post-processing tool, the results are influenced by all previous models, e.g. the wall heat model. Furthermore, the reaction kinetic calculations and the corresponding fits may have errors and with the quasi-dimensional simulation, temperature inhomogeneities cannot be considered. In order to minimize the resulting deviations, it is possible to calibrate the auto ignition model. Ignition delay times are highly temperature dependent. Therefore, as shown in equation (4), the temperature of the unburned mixture can be adjusted using two calibration factors a and b. This temperature of the unburned mixture T_{ub*} is only used for the auto-ignition model and has no influence on the other results of the simulation.

Calibration factor b is used as a correction of a temperature offset, while calibration factor a affects the temperature influence depending on the cylinder pressure p_{cy}. This way, pressure-dependent deviations can also be minimized.

$$T_{ub*} = T_{ub} \cdot (1 + a \cdot p_{cy} + b) \tag{4}$$

For this work, pressure trace analyses (PTA) were carried out with each knocking single working cycle of the available measurement data. The results of this PTA are used as input for the auto-ignition model.

3.2 Knock Onset Detection

To determine the knock onset in the measurement data, an automated method developed by Hess [6] is used. As input the indicated cylinder pressure and the value of the knock-peak-to-peak (KPP) threshold are needed. The KPP is used to identify a working cycle as a knocking one. Its value is the distance between the highest and lowest value of the pressure oscillation caused by the knocking phenomenon, schematically shown in figure 3. The KPP threshold at which a working cycle is defined as knocking one depends on the engine speed n in rpm. It is calculated as shown in equation (5). Thus, for example, a value of 2.5 bar results as the $KPP_{threshold}$ for an engine speed of 2500 rpm.

$$KPP_{threshold} = \frac{n}{1000} \tag{5}$$

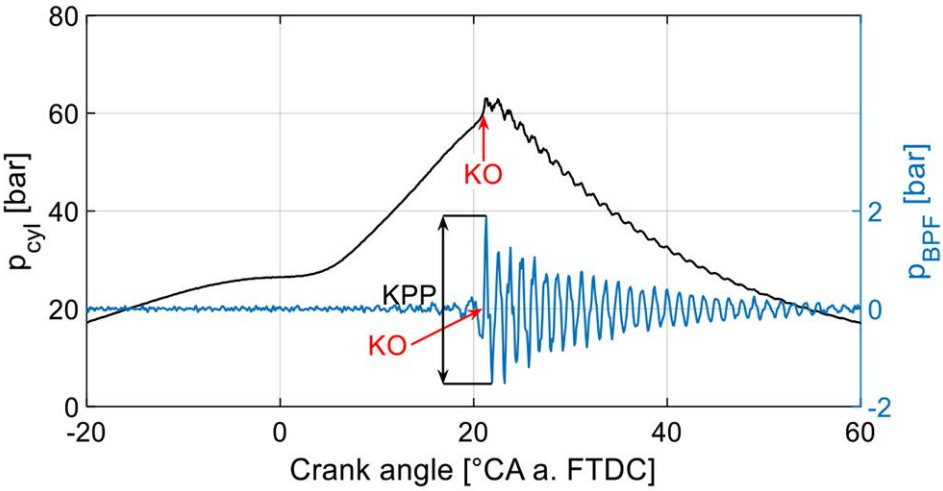

Figure 3: Indicated cylinder pressure p_{cy} and filtered cylinder pressure p_{BPF} with KPP and specified knock onset (KO). [6]

The method is based on the bandpass filtered indicated cylinder pressure, where the lower cut-off frequency needs to be smaller than the second circumferential resonance frequency of the combustion chamber. This means that this frequency depends on the engine geometry. The schematic workflow of the method to detect the knock onset is shown in figure 4 with cut-off frequencies for the hydrogen test bench engine configuration. In this case, the second circumferential resonance frequency is calculated as 12.11 kHz. The upper cut-off frequency is set to 30 kHz to avoid high-frequency disturbances and measurement noise.

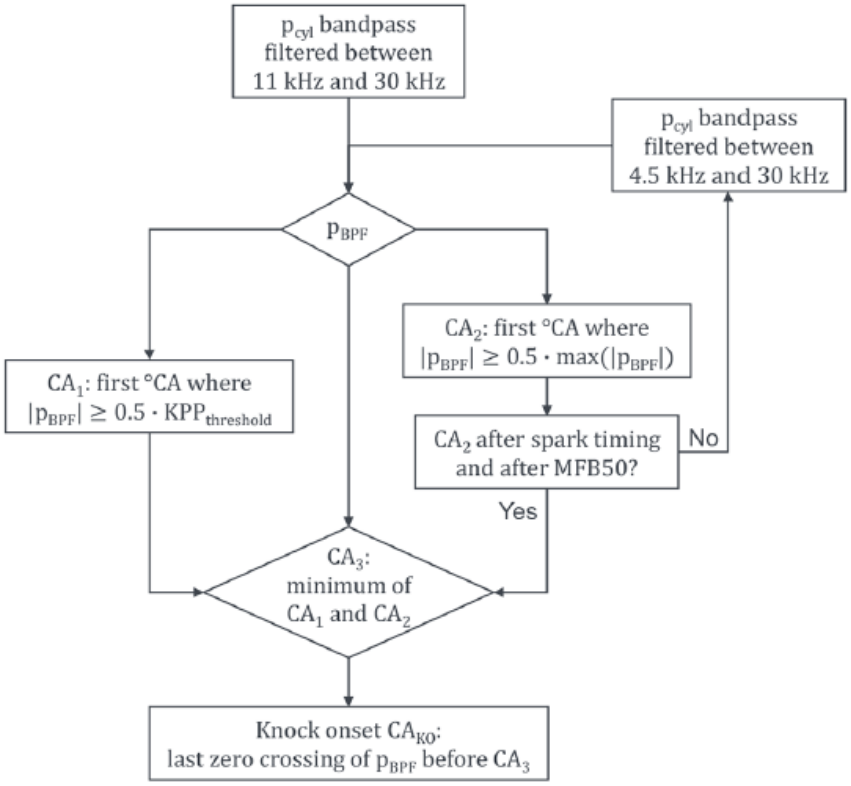

Figure 4: Schematic workflow to detect the knock onset with the automated method from Hess with exemplary cut-off frequencies for the hydrogen test bench configuration of this work. [6]

4 Validation of modeled Auto-Ignition Onset against Measurement Data

In this chapter, the modeled and measured auto-ignition onsets are compared. For this purpose, the auto-ignition model is calibrated according to equation (4), whereby only calibration factor b is used in this work.

In order to simulate a practical use of the model, it is calibrated only once per fuel, where calibration factor b is utilized. A random operating point is selected for this purpose. It can thus be assumed that better values will be achieved with a more complex calibration.

Figure 5 shows the results for the hydrogen data, where the modeled auto-ignition onset is compared to the detected knock onset of the single work cycles. The red line shows the angle bisector on which perfect results would lie in this illustration. To obtain good modeling results, a root-mean-square error (RMSE) of less than 2 °CA is desired. For the 3621 working cycles shown in figure 5, the RMSE is 1.51 °CA. The majority of the points are distributed around the bisector. There are only a few outliers with larger deviations. These are probably due to phenomena that cannot be captured by the quasi-dimensional simulation. But it can be seen that even with a single calibration and with only one calibration factor used, good results can be obtained over a wide range of operating conditions.

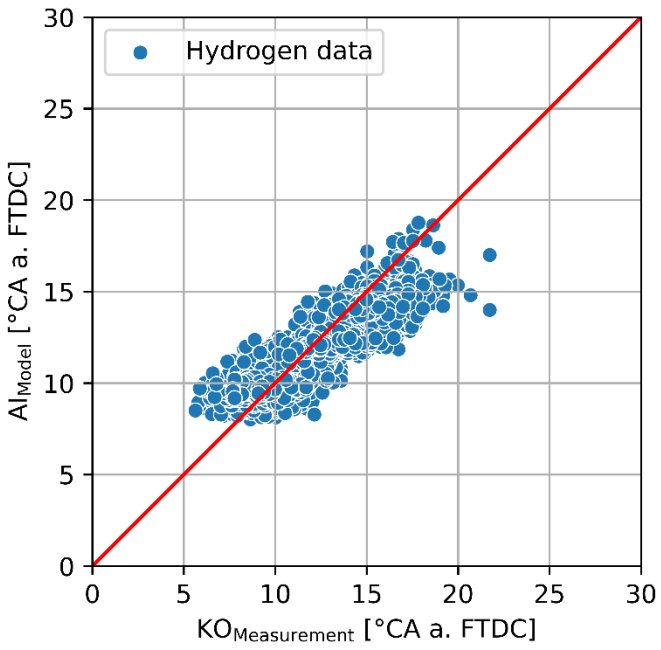

Figure 5: Comparison of the modeled auto-ignition onset with the detected knock onset from the hydrogen measurement data.

The results of the methanol data are in the same way shown in figure 6. For a better overview, the scaling of the axes is adjusted, which must be considered when viewing the results. For the results of the 62 working cycles shown, the RMSE is 1.36 °CA, which means that good results can also be obtained for the methanol data. However, the number of working cycles used and the range of the operating conditions is significantly smaller than for the hydrogen data.

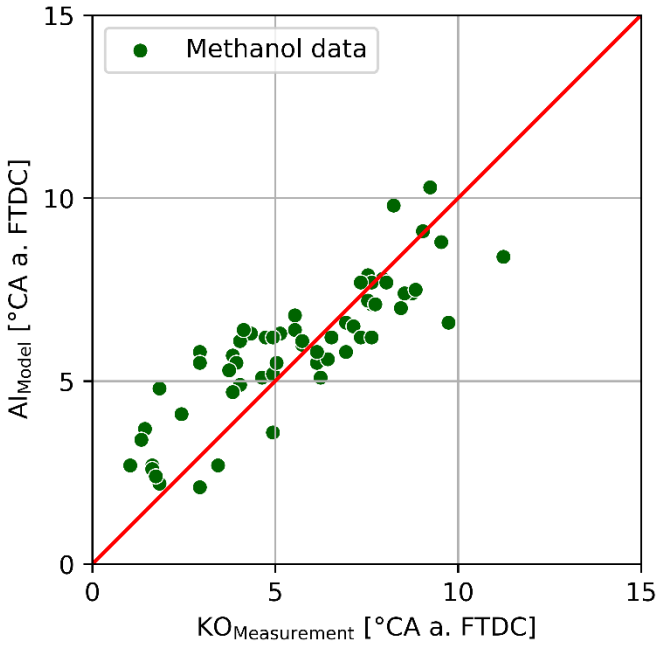

Figure 6: Comparison of the modeled auto-ignition onset with the detected knock onset from the methanol measurement data.

5 Conclusion and Outlook

It has been shown that the method to predict the auto-ignition onset is successfully adapted for the use with hydrogen and methanol. By using indicated knocking single working cycles the results could be validated. For hydrogen, good results were shown for 3621 single working cycles and over a wide range of operating conditions with a RMSE of 1.51 °CA. The results of methanol are also good with a RMSE of 1.36 °CA for 62 working cycles and thus a smaller range of operating conditions.

Further knocking measurement data from hydrogen and methanol are currently available, which will enable even more extensive investigations and validations in the future. In addition, it is planned to adapt the shown method for the use with ammonia (ammonia-hydrogen blends). Once the studies on auto-ignition has been completed, they should serve as basis for the development of a knock model for synthetic fuels.

Acknowledgments

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