Control of Auto-ignitive Wave Propagation Modes from Hot Spots by Mixture Tailoring in Shockless Explosion Combustion

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Abstract. Shockless Explosion Combustion is a novel combustion concept that achieves pressure gain combustion by quasi-homogeneous auto-ignition of the fuel/air mixture. Shockless Explosion Combustion is, like other combustion concepts based on auto-ignition, prone to premature ignition and detonation formation in the presence of reactivity gradients, so called hot spots. Two measures to inhibit detonation formation and to achieve quasi-homogeneous auto-ignition, dilution and fuel blending, are investigated by means of zero-dimensional simulations of generic hot spots. Experimental ignition delay times measured in a high pressure shock tube are used to select suitable chemical-kinetic models for the numerical investigation and the calculation of temperature sensitivities of ignition delay times. The main focus of this investigation are the two non-dimensional regime parameters ξ and ε, as they enable characterization of the mode of auto-ignitive wave propagation from hot spots. ξ is the ratio between the speed of sound and the auto-ignitive wave propagation velocity and ε describes the ratio between the time a pressure wave travels through the hot spot and the excitation time. Dilution of the combustion mixture with steam and CO_2 aims at extending excitation times and therefore decreasing the parameter ε. Fuel blending of Dimethyl ether with hydrogen or methane aims at reducing the temperature sensitivity of ignition delay time and low values of ξ. It is demonstrated that both measures are effective at mitigating detonation development while maintaining quasi-homogeneous auto-ignition in presence of hot spots.

Keywords: Ignition delay time · Excitation time · Knock · Auto-ignition · Detonation peninsula · Dilution · Fuel blending

1 Introduction

The novel combustion concept Shockless Explosion Combustion (SEC) is a way to implement pressure gain combustion in a gas turbine [1]. It promises a substantial increase in efficiency over a conventional gas turbine cycle [2,3], while it

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circumvents the disadvantages associated with using detonation waves to achieve pressure gain combustion like high pressure peaks or deflagration-to-detonation and exergy losses [1].

In SEC the pressure rise is achieved by quasi-homogeneous auto-ignition of the fuel-air mixture. The ensuing pressure wave generated by the volumetric heat release is reflected at the end of the combustion chamber as a suction wave. It is used to refill the combustion tube with a fresh fuel-air mixture to initiate the next combustion cycle. The quasi-homogeneous auto-ignition that is required for the process is achieved by matching the residence time of the fuel-air mixture in the combustion chamber with its ignition delay time through fuel stratification. Realizing quasi-homogeneous auto-ignition in a real combustion environment demands on-the-fly control of fuel stratification and is still a topic of on-going research [4]. Nevertheless, it is experimentally proven that the homogeneity of ignition correlates with the pressure increase in SEC [5,6].

Combustion concepts that are based on auto-ignition are prone to detonation formation and inhomogenoues ignition. Premature ignition in a local spot with increased reactivity can lead to the development of undesired detonation waves. These local spots with increased reactivity are here referred to as hot spots and can be caused by a temperature or concentration gradient. This is not only a challenge for SEC, but also for different auto-ignition based combustion concepts such as HCCI (homogeneous charge compression ignition) [7]. Detonation development from hot spots can be explained with the SWACER (Shock Wave Amplification by Coherent Energy Release) mechanism [8]. Premature ignition leads to localized heat release. This local heat release causes a pressure rise, which propagates as an acoustic pressure wave. If this pressure wave is in phase with heat release resulting from the auto-ignition of subsequent discrete mixture volumes along the reactivity gradient, the heat release can reinforce the pressure wave and a detonation wave may form.

Zeldovich et al. [9] demonstrated the importance of the temperature gradient of the hot spot for detonation formation. Different modes of auto-ignitive wave propagation can be initiated depending on the value of the temperature gradient [10]. Premature ignition along the reactivity gradient of the hot spot generates an auto-ignitive wave. In the following a hot spot with a temperature gradient is considered as in the analysis in [11]. The velocity of the ensuing auto-ignitive wave u_{ai} that results from the gradient in ignition delay time $\partial\tau_i/\partial r$ can be expressed by the temperature gradient of the hot spot $\frac{\partial T}{\partial r}$ and the temperature sensitivity of ignition delay time $\frac{\partial\tau_i}{\partial T}$ [11],

$$u_{ai} = \left(\frac{\partial\tau_i}{\partial r}\right)^{-1} = \left(\frac{\partial\tau_i}{\partial T}\frac{\partial T}{\partial r}\right)^{-1}. \tag{1}$$

When the auto-ignitive wave velocity is close to the speed of sound, the pressure wave is reinforced by the heat release and a detonation wave may form. However, when the auto-ignitive wave velocity exceeds the speed of sound characterizing the pressure wave propagation, reinforcement of the pressure wave by the heat release is not possible and the auto-ignitive wave will propagate without being

affected by pressure waves as a supersonic auto-ignitive wave. In the limiting case of infinite auto-ignitive wave velocity the gas auto-ignites homogeneously as a thermal explosion. When the auto-ignitive wave velocity is below the speed of sound, wave propagation occurs with two different propagation mechanisms depending on the velocity: subsonic auto-ignitive propagation, which is driven by the reactivity gradient in the hot spot and flame propagation, which is driven by diffusive processes.

The aim to classify the wave propagation led to the development of non-dimensional parameters ξ and ε [11]. The non-dimensional parameter ξ normalizes the speed of sound of the gas a to the velocity of auto-ignitive wave,

$$\xi = \frac{a}{u_{ai}}, \tag{2}$$

and expresses the influence of the auto-ignitive wave velocity on the propagation mode based on the work of Zeldovich [10] which is discussed above. In theory, the heat release of the auto-ignition can reinforce the pressure wave when ξ equals one, i.e. the auto-ignitive wave propagates with a velocity at the speed of sound, and detonations may occur. In practice, lower and upper bounds in ξ are defined for detonation formation depending on the conditions and fuel/oxidizer mixture, as the initial temperature gradient of the hot spot may change during the induction period [11]. This is attributed to heat conduction, mass diffusion and gas expansion [11]. For small values of ξ the regime of supersonic auto-ignitive wave propagation is observed, while subsonic auto-ignitive wave propagation appears at large values of ξ. A second non-dimensional parameter ε is proposed, to account for the rapidness of heat release rate, which is expressed by the excitation time [11]. It describes the ratio of the transit time of an acoustic wave though the hot spot relative to the excitation time of the gas τ_e, which is the characteristic time scale of the heat release,

$$\varepsilon = \frac{r_{hs}/a}{\tau_e}, \tag{3}$$

where r_{hs} describes the radius of the hot spot. Small values of ε indicate that heat release is much slower than acoustic waves traveling through the hot spot. Therefore, reinforcement of the pressure wave becomes less likely.

To classify modes of wave propagation from a hot spot a regime diagram as $\xi - \varepsilon$ diagram has been proposed [11]. The area in regime diagram where detonation formation is observed is usually referred to as detonation peninsula.

Furthermore, a criterion is proposed to discern whether detonation formation is possible [12–14]. If the excitation time τ_e is much longer than the difference in ignition delay time between the hot spot and the surrounding gas $\Delta\tau_i$, the surrounding gas ignites before the formation a of detonation wave is possible. Only for negative $\Delta\tau_i$ premature ignition appears in the hot spot that can possibly lead to the formation of a detonation wave. Hence, in the case of premature ignition the following condition

$$\left| \frac{\Delta\tau_i}{\tau_e} \right| < 1 \tag{4}$$

is fulfilled when the surrounding gas ignites before a detonation wave can form. The criterion in Eq. (4) has also been used to classify experimentally observed detonation transition [15].

In the following it is demonstrated, that the condition in Eq. (4) can be reformulated in terms of the non-dimensional parameters ξ and ε. $\Delta\tau_i$ can be expressed by the mean ignition delay time gradient $\overline{\frac{\partial\tau_i}{\partial r}}$ and the radius r_{hs} of the hot spot,

$$\Delta\tau_i = -r_{hs}\overline{\frac{\partial\tau_i}{\partial r}} = -r_{hs}\bar{u}_{ai}^{-1} \tag{5}$$

and can thus be related to the mean auto-ignitive wave velocity $\bar{u}_{ai}$. In other words, the difference in ignition delay time $\Delta\tau_i$ equals the time that the auto-ignitive wave that originates at the maximum reactivity in the hot spot needs to reach the surrounding gas. As the temperature sensitivity of ignition delay time may vary with temperature, also the ignition delay time gradient and auto-ignition velocity may vary within the hot spot. Therefore, the mean values $\overline{\frac{\partial\tau_i}{\partial r}}, \bar{u}_{ai}$ are chosen such that relation (5) holds. The ratio in criterion (4) can be rearranged using Eq. (5) for the case of premature ignition in the hot spot to

$$\left|\frac{\Delta\tau_i}{\tau_e}\right| = \frac{r_{hs}\bar{u}_{ai}^{-1}}{\tau_e}\frac{a}{a} = \frac{a}{\bar{u}_{ai}}\frac{r_{hs}/a}{\tau_e} = \xi\varepsilon, \text{ for } \overline{\frac{\partial\tau_i}{\partial r}} > 0. \tag{6}$$

Thus, when premature ignition appears in the hot spot the formation of a detonation wave is suppressed due to the auto-ignition of the surrounding when the following condition holds,

$$\xi\varepsilon < 1. \tag{7}$$

While it is shown above that the product of ξ and ε can be used interchangeably to the ratio $\frac{\Delta\tau_i}{\tau_e}$ to discern suppression of detonation development for the case of auto-ignition of the surrounding gas, it has also been used in the literature to distinguish between auto-ignitive wave propagation and deflagration [16,17]. It is proposed that values of $\xi\varepsilon$ over 1500 are associated with deflagration [16]. However, the border between both propagation modes is not very sharp [16].

Temperature or concentration inhomogeneities that may cause premature ignition are always present in technical systems, which also pose a challenge for SEC. Both detonations, as well as subsonic auto-ignitive wave propagation are to be avoided in SEC, as it is not designed for the former and the latter results in burned gas expansion with insufficient pressure gain. SEC requires supersonic auto-ignitive wave propagation or thermal explosion to a achieve (quasi-)homogenous ignition even in the presence of hot spots, i.e. low values of ξ and/or ε.

The parameters that influence the wave propagation mode are highly dependent on the physicochemical properties of the fuel-air mixtures and the thermodynamic conditions. Especially, the ignition and heat release characteristics of a mixture, namely the temperature sensitivity of ignition delay time and the

excitation time, play an important role for the mode of auto-ignitive wave propagation. This enables tailoring of the mixture with focus on these properties. In this work two approaches are investigated: the extension of excitation time by dilution with CO_2 and steam [14,18], which is targeted at decreasing ε; and decreasing temperature sensitivity of ignition delay time by fuel blending [19,20], which is targeted at decreasing ξ.

Dimethyl ether (DME) is used as a fuel, respectively fuel component, in both investigations. The reason is that it is suited for auto-ignition based concepts due to its relatively high reactivity [21]. DME's negative temperature coefficient (NTC) behavior, i.e. an increase in ignition delay time with increasing temperature within a certain temperature range, makes it suitable as a fuel blend component. Due to the application of SEC in gas turbines, usually similar conditions as in conventional gas turbines are of interest [19]. Rähse et al. [2] demonstrated, that a gas turbine with SEC achieves a significantly increased efficiency for pressures between 24 and 50 bar and temperatures between 823 to 1039 K. For the investigations in this study a thermodynamic condition of 35 atm and 887 K, is chosen which resembles the condition at the inlet of a gas turbine combustor. It is determined by compression from ambient conditions with a pressure ratio of 35 and a compression efficiency of 90%.

The overall goal of this study is to assess the impact of dilution and fuel blending on the non-dimensional detonation parameters in the presence of hot spots.

2 Experimental and Numerical Methods

In order to determine the temperature sensitivity of ignition delay time and choose suited chemical kinetic models to investigate the effects of the proposed mixture tailoring, ignition delay times are measured behind reflected shock waves in a high-pressure shock tube. Detailed information about the facility and the measurement procedure can be found in [20,22,23].

Zero-dimensional homogeneous reactor simulations are performed for both, the choice of the chemical-kinetic model and the determination of the relevant gas properties for the calculation of ξ and ε as explained below. The reactor models are implemented in *Python* with the software package *Cantera* [24]. Excitation time is defined as the time that elapses between 5% of the maximum heat release rate and the maximum heat release rate. This definition is very common and used in e.g. [11,18,25]. Furthermore, it is chosen because it is also used in the simulations in [25–27], which the obtained results will be compared to.

Generic hot spots of a defined radius and fixed temperature gradient are used to investigate the effect for the two investigated measures, i.e. dilution and fuel blending. Equations (2) and (3) are then used to calculate the respective ξ and ε parameters, utilizing excitation times and temperature sensitivity of ignition delay time determined by reactor simulations.

Firstly, the influence of temperature on the non-dimensional parameters is studied for a fixed hot spot. A single generic hot spot with a radius of 5 mm and a temperature gradient of ±1 K/mm is chosen, as these are commonly used radii [16,18,25] and temperature gradients [20,28]. In the NTC region a hot spot with a temperature decrease is needed to excite an auto-ignitive wave. Therefore the sign of the temperature gradient is adjusted depending on whether a hot spot with a temperature increase or decrease is present. For this investigation, the non-dimensional parameters are evaluated at the surrounding gas temperature to enable comparison with figures that depict the temperature sensitivity of ignition delay time and excitation time over the temperature.

Secondly, the influence of the two investigated measures is studied for the thermodynamic condition that resembles a gas turbine combustor. By varying the hot spot radius and temperature gradient multiple points in the $\xi - \varepsilon$ diagram are created. The radius of the generic hot spots is varied between ±1 and ±10 mm and the temperature gradient is varied between 1 and 10 K/mm. These are common orders of magnitudes for similar kinds of investigation [16,25,28]. The effect of the two proposed measures is investigated on the points in the regime diagram by using the same hot spot properties, however the mixture is altered either by diluting or fuel blending. Note, that the values of ξ and ε depend on where in the hot spot they are defined, as they are temperature dependent. For the construction of regime diagrams they are evaluated in the middle of the hot spot at $0.5r_{hs}$ and a temperature of

$$T_{hs} = T_0 - 0.5r_{hs} \left(\partial T/\partial r\right)_{hs},$$

where T_0 defines the surrounding gas temperature, as this is a common definition [11,18].

3 Extension of Excitation Time by Dilution

The effect of dilution on the non-dimensional parameters is studied for a stoichiometric DME/air mixture and by adding steam or CO_2. The chemical-kinetic model AramcoMech 2.0 [29–35] is chosen for the investigation because it reproduces experimental ignition delay times of both undiluted DME/air mixtures [23] and CO_2-diluted DME/air mixtures [22] well. For comparison to simulation data from [25] the same chemical-kinetic model from Zhao et al. [36] is chosen, which also shows acceptable agreement with the experimental data [22,23].

3.1 Influence of Dilution on Excitation Time and Temperature Sensitivity of Ignition Delay Time

The modeling results indicate that dilution can significantly increase the excitation time (Fig. 1). The effect of CO_2-dilution is slightly stronger, which may be attributed to a physical effect (i.e. increased heat capacity) and/or a chemical

effect. An increase in the duration of the heat release can mitigate the reinforcement of the pressure wave by the heat release and may prevent detonation formation.

Adding dilution also affects the temperature sensitivity of ignition delay time (Fig. 1). The temperature sensitivity of all investigated mixtures exhibits large negative values for low temperatures (Fig. 1), i.e. an increase in temperature will strongly decrease the ignition delay time. Positive values are attained in the NTC region. The absolute temperature sensitivity increases with dilution for most of the considered temperatures (Fig. 1). Due to the shift of the NTC region that is caused by dilution the absolute temperature sensitivity is reduced on the borders of the NTC region at around 800 and 930 K when dilution is added to the DME/air mixture (Fig. 1).

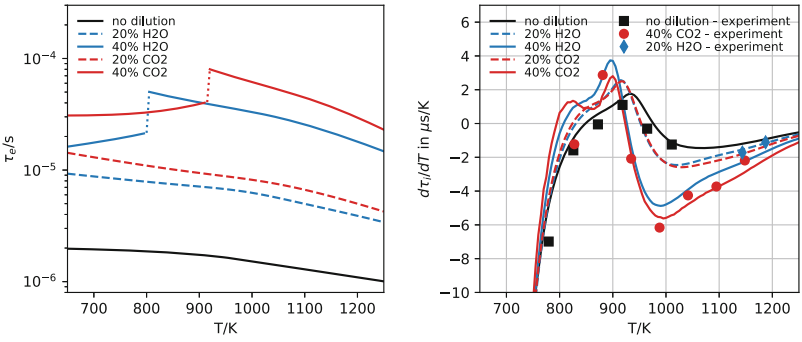

Fig. 1. Excitation time (left) and temperature sensitivity of ignition delay time (right) for undiluted and diluted stoichiometric DME/air mixture. Curves - prediction with AramcoMech 2.0, symbols - extraction from experimental ignition delay time.

3.2 Influence of Dilution on the Non-dimensional Regime Parameters

In the following the effect of dilution on the non-dimensional detonation parameters ξ and ε is studied over a range of temperatures by utilizing a generic hot spot with fixed properties as explained in Sect. 2 (Fig. 2). The non-dimensional parameter ε is strongly decreased by dilution over the whole investigated temperature range (Fig. 2). The effect on ε is slightly stronger for CO_2 dilution due to its longer excitation time (Fig. 1).

The temperature-dependent effect of dilution on the non-dimensional parameter ξ is illustrated in Fig. 2. The auto-ignitive wave velocity decreases strongly with temperature at low temperatures, which results in very high values of ξ (Fig. 2). The large values in ξ indicate that an auto-ignitive wave with subsonic propagation speed is expected at low temperatures. In the NTC region and at high temperatures, dilution decreases the auto-ignitive wave velocity below

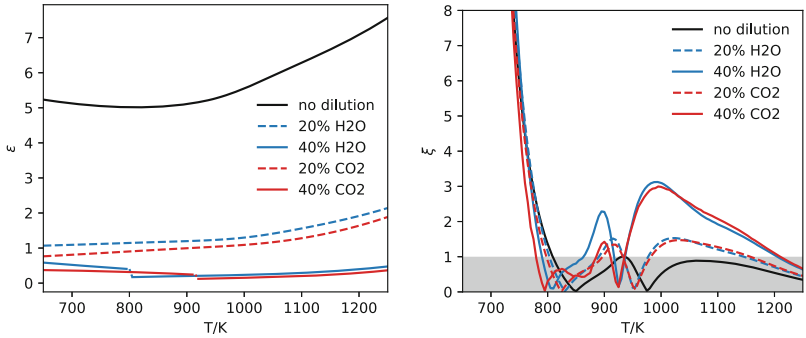

Fig. 2. Non-dimensional parameter ε for hot spot with radius of 5 mm (left), and non-dimensional parameter ξ for temperature gradient of ± 1 K/mm for undiluted and diluted DME/air mixture (calculated with AramcoMech 2.0).

the speed of sound, which also results in an increase in ξ above one (Fig. 2). Nonetheless, ξ is close to one in the intermediate and high temperature range and therefore in a range that is possibly prone to detonation formation. Therefore, the effect of dilution on the location in the $\xi - \varepsilon$ diagram will be studied in the following at 35 atm and 887 K.

The ξ and ε parameters of different hot spots with radii of 2, 5 and 8 mm and temperature gradients of 1, 4, 7 and 10 K/mm are used to create multiple points in the $\xi - \varepsilon$ diagram. Keeping the hot spot properties constant, the DME air mixture is further diluted and the effect on the location of the points is studied (Fig. 3). The arrows in Fig. 3 link the undiluted mixture to the diluted mixtures for hot spots with the same properties and hence demonstrate the effect of dilution. The excitation time, temperature sensitivity of ignition delay time and speed of sound are evaluated in the middle of the hot spot as explained in Sect. 2. The temperature at the location of evaluation lies within the NTC region for all considered mixtures and ensures that a hot spot with a decrease in temperature can be used for all considered points in the $\xi - \varepsilon$ plane. In order to link each hot spot in Fig. 3 to its temperature of evaluation, the arrows in Fig. 3 are color coded with respect to the evaluation temperature.

For all considered hot spots diluting the DME/air mixture significantly shifts towards smaller ε values. The non-dimensional parameter ξ is increased when adding dilution compared to the undiluted mixture (Fig. 3). When adding 20% dilution the effect on ξ is similar between steam and CO_2 dilution, due to their similar temperature sensitivity of ignition delay time (Fig. 1). However, dilution with 40% steam increases ξ stronger compared to CO_2 dilution. This is due to the fact that the applied chemical-kinetic model predicts the temperature sensitivity of mixtures with 40% steam to be significantly larger compared to the same amount of CO_2 dilution (Fig. 1). There is a small temperature range, where the temperature sensitivity of the mixture with 40% CO_2 is lower than that of the mixture with 20% CO_2 (Fig. 1). This results in ξ values of the mixture

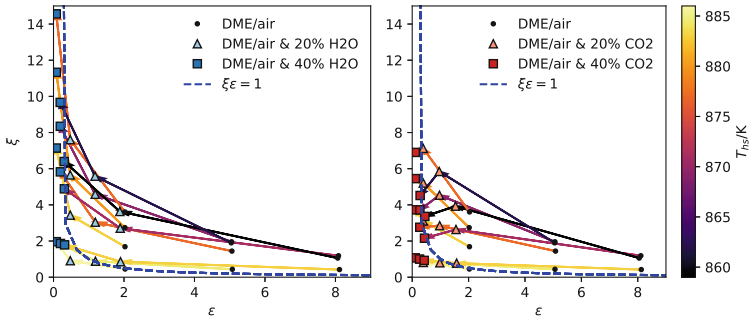

Fig. 3. Regime diagram at of stoichiometric DME/air mixture with and without dilution. Surrounding gas is at 35 atm and 887 K (calculated with AramcoMech 2.0).

with 40% CO_2 being lower compared to the mixture with 20% CO_2 dilution for hot spots with a larger temperature diminishment. For all points below the curve $\xi\varepsilon = 1$ detonation formation is prohibited according to the criterion in Eq. (7). When diluting the DME/air mixture with 40% steam or CO_2 the location in the $\xi - \varepsilon$ diagram is below or very close to the curve $\xi\varepsilon = 1$ for all considered hot spots in Fig. 3, which indicates that dilution decreases the propensity to detonation development.

To relate the effect of dilution on the location in the $\xi - \varepsilon$ diagram to the actual wave propagation mode, a second set of zero-dimensional simulations is conducted at 40 atm and 982 K and compared to results obtained at the same conditions of a spherical one-dimensional hot spot from [25] (Fig. 4). The pressure is comparable to the condition considered in this study and the temperature is also within the NTC region. Note, that the depicted detonation peninsula from [25] is only determined for the undiluted DME/air mixture and that it may differ for the diluted mixtures. Therefore, additionally the curve $\xi\varepsilon = 1$ is shown in Fig. 4, as it demarcates the region where detonation formation can be excluded, according to the criterion in Eq. (7). Compared to the detonation peninsula by Dai et al. [25] the criterion is rather conservative. This is because it considers the strictest case where detonation formation is not possible due to the ignition of the gas surrounding the hot spot. Other cases, where e.g. insufficient reinforcement of the pressure wave by the heat release leads to the prevention of detonation formation are not considered by criterion (7). However, these cases are considered in the regime diagram in Fig. 4 that is obtained through one-dimensional simulations [25]. The results demonstrate again, that dilution significantly reduces the ε parameter (Fig. 4). With the simulation results from [25] it is possible to evaluate the effect of the change in ε on the propagation mode and possible mitigation of detonation formation. For the undiluted mixture there are four hot spots that are within or on the borders of the detonation peninsula. Dilution with 20% steam or CO_2 shifts the points out of the detonation peninsula. Dilution with 40% steam or CO_2 shifts the points even into the region below the curve $\xi\varepsilon = 1$, indicating that detonation formation is mitigated according

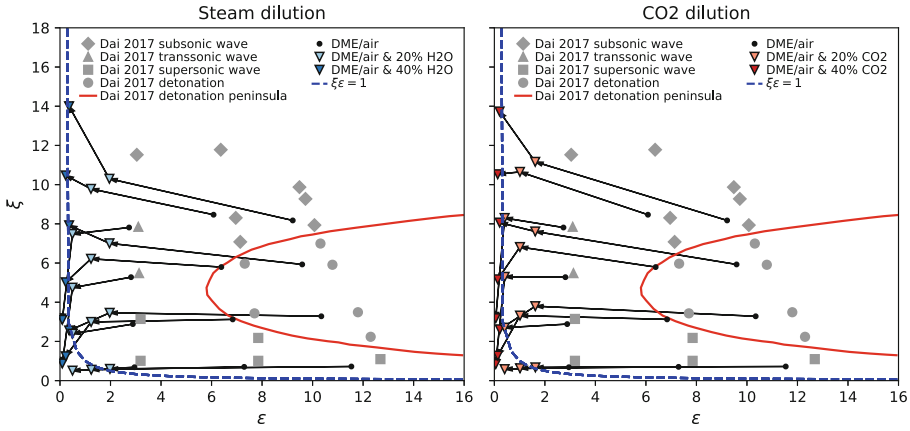

Fig. 4. Regime diagram of stoichiometric DME/air mixture with and without dilution compared to data from Dai et al. [25]. Surrounding gas is at 40 atm and 982 K (calculated with the model from [36].)

to the stricter criterion in Eq. (7). Hence, hot spots that would result in the formation of a detonation wave will not result in a detonation when dilution with CO_2 or steam is added. Instead, the ξ and ε values are shifted into the region where Dai et al. [25] observe transonic or supersonic auto-ignitive waves. The shift from the detonation regime to supersonic auto-ignitive deflagration is desired for stable SEC operation. The resulting very rapid ignition of the fuel-air mixture can achieve the aerodynamic confinement that is necessary for pressure gain in SEC without the formation of a detonation wave. In the case of transonic auto-ignitive wave propagation no mutual reinforcement appears between the pressure and reaction wave even though the speed of the auto-ignitive wave is close to the speed of sound [25]. Transonic auto-ignitive wave propagation is therefore closely related to small ε values. The appearance of transonic wave propagation is attributed to the small hot spot radius in [25], while it is achieved by an increase in excitation time in this study. Note, that the boundaries of the detonation peninsula and the region of transonic wave propagation are observed at ξ values larger than one in the one-dimensional simulations [25]. This can be attributed to the transient evolution of the temperature gradient and mass diffusion [11,37], which alter the ignition delay time gradient in the hot spot. For hot spots with a higher temperature difference to the surrounding gas the location in the regime diagram is within the subsonic propagation regime for the undiluted mixture. For these points, the ξ value increases with dilution compared to the undiluted mixture, while the ε value is strongly reduced.

The regime diagram in Fig. 4 shows cases, where an auto-ignitive wave with transonic or subsonic auto-ignitive propagation will ensue from a hot spot for diluted mixtures. This raises the question whether ignition in these cases is still homogeneous enough to achieve the necessary aerodynamic confinement in SEC. With the applied methods this cannot be finally assessed in this study. However, even if the ξ value is large, it does not necessarily mean that the whole gas in the SEC combustor will be burned ineffectively through a deflagration. The gas surrounding the hot spot is very close to auto-ignition. It may be possible that a subsonic reaction wave is created within the hot spot. However, it may not propagate very long before the surrounding gas auto-ignites and quasi-homogeneous auto-ignition can still be achieved, considering that subsonic processes are relatively slow.

To conclude, it is demonstrated that dilution is a very effective measure to prevent detonation formation in SEC and facilitate quasi-homogeneous auto-ignition in presence of reactivity gradients.

4 Decreasing the Temperature Sensitivity of Ignition Delay Time by Fuel Blending

Fuel candidates like hydrogen and methane can be produced from renewable resources and are therefore interesting for SEC application, but both fuels have generally long ignition delay times and very high temperature sensitivities of ignition delay times at the relevant conditions.

To decrease the non-dimensional parameter ξ by reducing the temperature sensitivity of ignition delay time, fuel blends with a fuel component with NTC behavior can be used. A ternary fuel blend of DME, methane and hydrogen, which was proposed by Cai and Pitsch [19] and experimentally investigated in [20], is further studied here. The intention in this case is to show that DME is capable to reduce the high temperature sensitivity of ignition delay time of H_2 and CH_4, while at the same time reducing the relatively large ignition delay time characteristic for those fuels to a level relevant for SEC.

Suited mechanisms and a validation for the ternary fuel blend containing DME, H_2 and CH_4 can be found in our previous study [20]. It was shown, that the chemical-kinetic model AramcoMech 3.0 [38] and the mechanism from Cai and Pitsch [19] are in good agreement with the conducted ignition delay time measurements. For the further analysis the AramcoMech 3.0 is used, based on the findings in the mentioned study.

4.1 Effect of Fuel Blending on Temperature Sensitivities of Ignition Delay Times

The temperature sensitivities of ignition delay times of the pure components are compared to those of fuel blends to show the effectiveness of the fuel blending. Using an Arrhenius-fitting and derivation approach the available experimental

data is used to extract temperature sensitivities of ignition delay times for comparison with mechanism predictions, as shown in Fig. 5. Predicted temperature sensitivities of ignition delay times show good agreement to the temperature sensitivities derived from the experimental ignition delay time data.

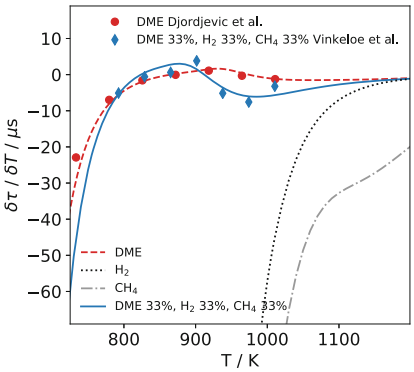

Fig. 5. Temperature sensitivities of ignition delay times derived from experimental data (data for DME from Djordjevic et al. [22] and data for ternary equimolar fuel blend from Vinkeloe et al. [20]) and numerical simulations (AramcoMech 3.0 [38]) at stoichiometric conditions and a nominal pressure of 35 bar.

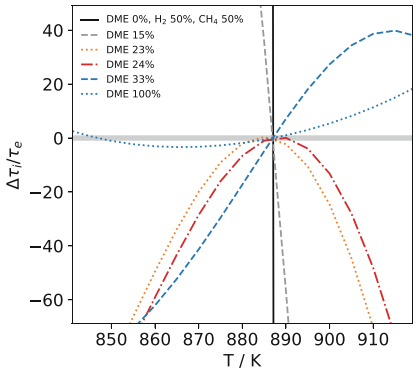

Fig. 6. Ratio of difference in ignition delay time between hot spot and surrounding gas to excitation time over varying hot spot peak temperature; 35 atm, 887 K and stoichiometric conditions and the ternary fuel blend DME/H_2/CH_4 with constant ratio between H_2 and CH_4

Compared to pure hydrogen and methane, DME and the equimolar fuel blend exhibit significantly reduced temperature sensitivity of ignition delay time in a temperature range between 700 and 1100 K. In between 800 and 900 K temperature sensitivities of ignition delay times of DME and the ternary fuel blend exhibit the same order of magnitude (Fig. 5).

Due to the low temperature sensitivity of ignition delay time the ternary fuel blend is interesting for the SEC application. Nevertheless, the probability of developing detonations in hot spots depends also on the hot spot's temperature gradient, size, fuel/oxidizer mixture properties and transient coupling of the pressure wave and the auto-ignitive wave. The criterion in Eq. 4 is applied to investigate the impact of the fuel blends. For absolute values of this criterion lower than unity, detonation formation is improbable. In that case, the gas surrounding the hot spot has enough time to ignite, before the pressure is rising due to premature ignition in a hot spot. Hence, the formation of a detonation is inhibited.

Figure 6 shows this criterion for the ternary fuel blend and varying hot spot temperatures. The considered fuel blends contain an equimolar hydrogen/methane fuel blend, blended with varying percentages of DME. Different blends lead to varying temperature ranges where the criterion is lower than 1, which is associated with conditions, where no detonation wave can form. The fuel blend of H_2 and CH_4 has a very small temperature range, where the criterion is valid, whereas adding 23% and 24% DME has a strong positive effect. A higher DME content leads to a reduction and a DME content near 100% leads to a wider temperature range, where the criterion is valid. Due to the varying DME content the shape and temperature range of the NTC range of ignition delay time change, hence, this criterion has a non-linear behavior, which depends on the conditions.

Nevertheless, the criterion shown in Fig. 6 is very conservative. To further investigate the impact of fuel blending on auto-ignitive wave propagation mode in presence of a hot spot the non-dimensional parameters ξ and ε are analyzed.

4.2 Influence of Fuel Tailoring on Non-dimensional Regime Parameters

The introduced detonation regime parameters ξ and ε give more information about the possible mode of auto-ignitive wave propagation in hot spots. As shown above fuel blends have a significant impact on the temperature sensitivities of ignition delay times, and therefore also on ξ (compare Eq. (2)). Due to the different fuel components, properties of the combustion mixtures like the speed of sound and the transient process of heat release vary. Hence, in addition to ξ also ε is affected by fuel blends.

Figure 7 shows values of ξ over the temperature of the surrounding gas for various blending ratios, assuming a temperature gradient of $-1\,\mathrm{K/mm}$ (or $1\,\mathrm{K/mm}$ in case of a positive temperature sensitivity) inside a generic hot spot. DME is the component in the considered ternary blend, that has the greatest impact on the overall ignition delay time and its temperature sensitivity. Hence, the percentage of DME has an impact on the overall magnitude of ξ as well as the temperature range of low values of ξ. Without DME it is not possible to get near the target of $\xi < 1$. For high percentages of DME in the fuel blend the temperature range where $\xi < 1$ increases. The relative hydrogen to methane ratio in the ternary fuel blend has only minor impact on ξ [20] and is thus not further studied here.

Due to the varying fuel composition the excitation time differs, which has an impact on ε. Figure 8 shows the impact of different fuels and fuel blend ratios on the non-dimensional parameter ε. For small percentages of DME in the ternary fuel blend ε remains at the same level. Higher percentages of DME decrease ε significantly.

When fuel blends are used to reduce ξ for SEC application, the impact on ε should also be taken into account. Compared to dilution the impact of the fuel on ε is lower for low percentages of DME.

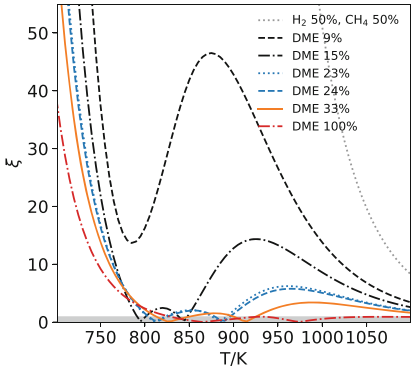

Fig. 7. Impact of fuel blends with varying blending ratios on the non-dimensional parameter ξ over temperature (AramcoMech 3.0, temperature gradient $\pm 1\,\mathrm{K/mm}$, 35 atm, 887 K and stoichiometric conditions)

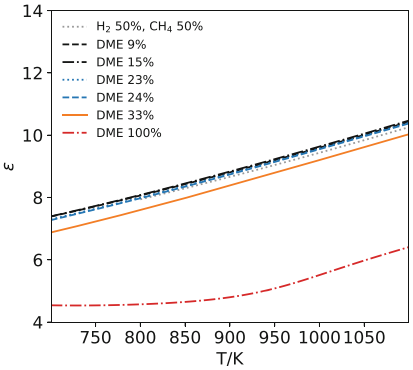

Fig. 8. Impact of fuel blends with varying blending ratios on the non-dimensional parameter ε over temperature (AramcoMech 3.0, hot spot radius 5 mm, 35 atm, 887 K and stoichiometric conditions)

At the condition of 35 atm and 887 K Fig. 9 shows the $\xi - \varepsilon$ diagram for the considered ternary fuel blends. For the numerical simulations, hot spot temperature gradients range from $\pm 1\,\mathrm{K/mm}$ to $\pm 10\,\mathrm{K/mm}$ and hot spot radii range from 1 mm to 10 mm. The conditions of the surrounding gas are kept constant, while varying fuel blend ratios. Simulations with the same hot spot parameters are connected with grey lines to illustrate the effect of DME addition.

Reference points (black asterisks) are hot spots with negative temperature gradients, because the fuel blend of CH_4/H_2 exhibits negative temperature sensitivities of ignition delay times. It can be shown that small percentages of DME in the ternary fuel blend with H_2 and CH_4 reduce the very high values of ξ for the H_2/CH_4 blend very effectively, whereas the impact on ε is rather weak (Fig. 9). DME contents higher than 33% have only a reduced impact on ξ, but an increasing impact on ε. Depending on the hot spot temperature gradient and radius, DME addition reduces ξ values in some cases to the necessary order of magnitude to fulfill the conservative criterion $\xi\varepsilon = 1$. But for most of the considered cases this criterion is not fulfilled, even for high DME contents.

Nevertheless, to reach values for ξ and ε under the $\xi\varepsilon = 1$ curve is a very strict requirement for detonation prevention. Usually a detonation peninsula is used to identify points where detonation formation occurs. In contrast to the $\xi\varepsilon = 1$ curve, which has a fixed position in the $\xi\varepsilon$ diagram, a peninsula is dependent on many parameters like temperature, pressure and fuel. Hence, fuel blending has an impact on the shape and position of the detonation peninsula.

Detonation peninsulas from literature are used here to compare the auto-ignitive wave propagation modes of pure fuels to the effect of fuel blending on ξ and ε. For this purpose numerical simulations at the same conditions and varying hot spot parameter (temperature gradients range from $-1\,\mathrm{K/mm}$ to $-10\,\mathrm{K/mm}$

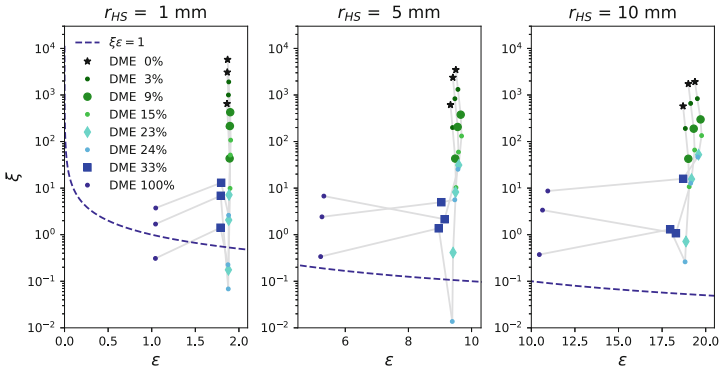

Fig. 9. $\xi - \varepsilon$ diagram at 35 atm, 887 K and stoichiometric conditions using AramcoMech 3.0

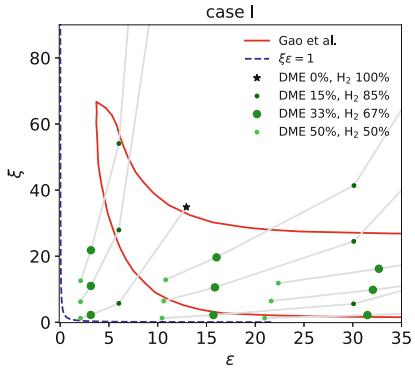

Fig. 10. Impact of blending DME and hydrogen on ξ and ε compared to regime diagram from Gao et al. [27] at 40 atm, 1000 K and stoichiometric conditions simulated with AramcoMech 3.0

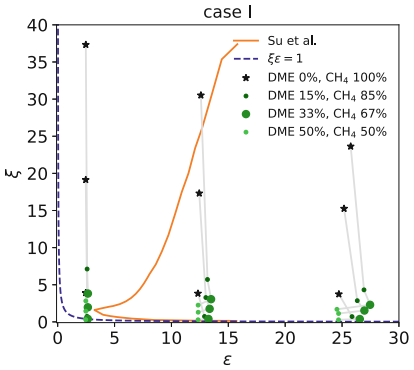

Fig. 11. Impact of blending DME and methane on ξ and ε compared to regime diagram from Su et al. [26] at 40 atm, 1300 K and stoichiometric conditions simulated with AramcoMech 3.0

and hot spot radii range from 1 mm to 8 mm) are conducted. Two dual fuel blend cases are investigated, because there are no detonation peninsulas available for fuel blends of hydrogen and methane. A detonation peninsula for hydrogen/air mixtures was investigated by Gao et al. [27] at 40 atm and 1000 K. Su et al. [26] conducted simulations to create a detonation peninsula for methane/air mixtures at 40 atm and 1300 K. Figure 10 shows the impact of blending DME and hydrogen, simulated with the AramcoMech 3.0. Values of both, ξ and ε decrease with DME addition. Depending on the hot spot parameters, DME addition can move the points out of the detonation peninsula for pure hydrogen/air mixtures and into the targeted area of supersonic auto-ignitive wave propagation. Figure 11 depicts the corresponding comparison for blends containing DME and

methane. Similarly, a reducing effect on ξ can be observed, while the impact on ε is much lower than for hydrogen DME blends. Not all hot spot trajectories can be moved out of the detonation peninsula because the blending ratio in both dual fuel cases are not optimized and DME addition over 50% is not considered, because the detonation peninsula is only valid for pure H_2 or CH_4. Nevertheless a clear trend of the reducing effect of DME addition on ξ can be observed.

To conclude, it is demonstrated that adding a fuel exhibiting NTC behavior, such as DME, can be an effective measure to prevent detonation formation in SEC in presence of hot spots, when fuels with a strong temperature dependency of ignition delay time, such as H_2 and CH_4, are used. Additionally, the high reactivity of the blended DME reduces ignition delay times of those fuels at the relevant conditions to a level to make their utilization in SEC feasible.

5 Conclusions

The novel combustion concept SEC requires a quasi-homogeneous auto-ignition to achieve pressure gain combustion, which is associated with an advantage in efficiency. At the same time, processes based on auto-ignition are prone to the formation of undesired detonation waves, which needs to be avoided to evade damage to the machinery. To achieve that goal, the ignition and heat release characteristics of the fuel air mixture are modified by dilution aiming at extending the excitation time; and by fuel blending aiming at reducing the temperature sensitivity of ignition delay time. The effect on the non-dimensional regime parameters is investigated for a range of generic hot spots by means of 0-dimensional constant volume reactor simulations.

Increasing the excitation time by dilution with steam or CO_2 leads to a strong reduction in the non-dimensional parameter ε over the whole considered range of temperatures, indicating that the rapidness of heat release is decreased such that the reinforcement of the pressure wave through the heat release is mitigated. In comparison to findings from Dai et al. [25], dilution moves points in the regime diagram in the desired direction (low ε), out of the detonation peninsula into the area of super sonic auto-ignitive wave propagation leading to quasi-homogeneous auto-ignition.

It is shown that criterion $\xi\varepsilon < 1$ for regions where detonation formation is improbable is more conservative compared to detonation peninsula from [25]. Depending on the temperature and utilized diluent, dilution can lead to an increase in temperature sensitivity of ignition delay time and therefore also the ξ value. This unwanted effect can be eliminated by tailoring the fuel blend. Nevertheless, it was shown that tailored dilution of the combustion mixture with CO_2 or steam is a promising measure to mitigate detonation development and thus engine knock in auto-ignition based combustion concepts.

Reduction of the temperature sensitivity of ignition delay time and hence reduction of ξ is the main target of fuel blend tailoring in this study. In a ternary fuel blend with DME, H_2 and CH_4, DME is capable of increasing the overall reactivity and simultaneously reducing the high temperature sensitivities of ignition

delay times of methane and hydrogen, which could not be used for SEC application as pure fuels. Numerical results show a strong impact of fuel blend ratio on ξ and a wider temperature range, where $\xi < 1$ or even $\xi\varepsilon < 1$, which is associated with inhibited detonation formation.

To achieve the goal of quasi-homogenous auto-ignition and inhibited detonation formation (low values for ξ and ε), fuel blending and dilution can be applied at the same time. Another advantage when using both methods at the same time is, that a larger parameter space is possible to adjust the ignition delay time, its temperature sensitivity and the excitation time simultaneously. Beside the SEC the presented findings are also interesting for other technical applications based on auto-ignition like the HCCI-engine, which are also prone to engine-knock or detonation formation.

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