Knock Control in Shockless Explosion Combustion by Extension of Excitation Time



Lisa Zander, Giordana Tornow, Rupert Klein and Neda Djordjevic

Abstract Shockless Explosion Combustion is a novel constant volume combustion concept with an expected efficiency increase compared to conventional gas turbines. However, Shockless Explosion Combustion is prone to knocking because it is based on autoignition. This study investigates the potential of prolonging the excitation time of the combustible mixture by dilution with exhaust gas and steam to suppress detonation formation and mitigate knocking. Analyses of the characteristic chemical time scales by zero-dimensional reactor simulations show that the excitation time can be prolonged by dilution such that it exceeds the ignition delay time perturbation caused by a difference in initial temperature. This may suppress the formation of a detonation because less energy is fed into the pressure wave running ahead of the reaction front. One-dimensional simulations are performed to investigate reaction front propagation from a hot spot with various amounts of dilution. They demonstrate that dilution with exhaust gas or steam suppresses the formation of a detonation compared to the undiluted case, where a detonation ensues from the hot spot.

Keywords Shockless explosion combustion • Dilution • Detonation formation

L. Zander (⋈) · N. Djordjevic

Institute of Fluid Dynamics and Technical Acoustics, Combustion Kinetics, Technische Universität Berlin, Müller-Breslau-Str. 8, D-10623 Berlin, Germany e-mail: lisa.zander@tu-berlin.de

N. Djordjevic

e-mail: neda.djordjevic@tu-berlin.de

G. Tornow · R. Klein

Department of Mathematics, Geophysical Fluid Dynamics, Freie Universität Berlin, Arnimallee 6, D-14195 Berlin, Germany e-mail: gtornow@math.fu-berlin.de

R. Klein

e-mail: rupert.klein@math.fu-berlin.de

© Springer Nature Switzerland AG 2019
R. King (ed.), *Active Flow and Combustion Control 2018*,
Notes on Numerical Fluid Mechanics and Multidisciplinary Design 141,
https://doi.org/10.1007/978-3-319-98177-2_10

1 Introduction

A substantial efficiency increase is expected for constant volume combustion systems compared to conventional gas turbines utilizing constant pressure combustion. A novel system utilizing constant volume combustion is Shockless Explosion Combustion (SEC). It was first described by Bobusch et al. [1]. A qualitative analysis indicates an efficiency gain of the SEC process compared to the Joule cycle [2].

SEC is based on quasi-homogeneous autoignition of the gas in the combustion tube and utilizes pressure waves for filling and purging. To achieve quasi-homogeneous autoignition the fresh gas mixture's equivalence ratio is stratified such that the ignition delay time of each discrete gas volume is correlated to its residence time in the combustion tube. As a result, the total volume of the combustion mixture auto-ignites simultaneously after filling is completed.

Because SEC relies on homogeneous autoignition it has several advantages compared to constant volume combustion systems that use detonation waves. Sharp pressure rises which can be harmful to the machine are avoided. Smaller exergy losses are expected for SEC because the kinetic energy in detonation waves cannot be used entirely. Furthermore, losses due to the deflagration to detonation transition which appear in detonative combustion processes are not present in SEC.

Nonetheless, a process that relies on autoignition is strongly dependent on the chemical-kinetic properties of the combustible mixture. Under certain circumstances, a detonation wave can ensue from a more reactive spot caused by premature ignition and lead to knocking. Consequently, the SEC process is very sensitive to deviations in temperature or mixture composition from the ideal distributions that guarantee nearly homogeneous autoignition after completion of the charging process. The formation of detonations in SEC can be explained with the SWACER (Shock Wave Amplification by Coherent Energy Release) mechanisms proposed by Lee et al. [3]. Premature ignition in a more reactive spot, e.g. a hot spot, generates a pressure wave which moves into the not yet ignited gas. Additionally, the gradient in ignition delay time around this reactive spot leads to an autoignition wave. If the autoignition wave propagates at a speed, such that the heat release is in phase with the pressure wave running ahead of the autoignition wave, the pressure wave is amplified and a detonation may be formed.

Multiple researchers investigated the conditions for the occurrence of detonation waves in general. Zeldovic et al. [4] identified that the slope of the temperature gradient influences whether a detonation is formed for a combustible mixture with an inhomogeneous initial temperature distribution. Later, Zeldovich [5] distinguished four modes of reaction front propagation for mixtures with inhomogeneous initial temperature distributions theoretically: weak detonation (also referred to as supersonic deflagration), with propagation governed by autoignition at a velocity higher than Chapman–Jouget (C–J) velocity and without the formation of a shock wave; developing detonation and detonation; subsonic flame propagation controlled by autoignition and flame propagation which is governed by heat conduction and diffusion. Zeldovich regards adiabatic explosion at constant volume (also referred to as

thermal explosion) as a limiting case of weak detonation, because chemical conversion happens simultaneously in the complete combustion volume and the propagation speed reaches infinity. Gu et al. [6] identified all of the modes described in [5] in simulations with hot spots of different radii and temperature gradients. They underlined the importance of the rapidness of the heat release into the shock for the successful formation of a detonation. Based on this idea, they proposed a regime diagram for the occurrence of detonations defined by two non-dimensional quantities, the normalized temperature gradient of the hot spot and the acoustic time normalized by the excitation time. The range of values for which detonations can occur in this regime diagram is commonly referred to as detonation peninsula.

Sources of perturbations in SEC can be heat convection or radiation from the combustion tube's walls, equivalence ratio perturbations caused by the filling process or residual gas that remains in the combustion tube from the previous cycle. These fluctuations are difficult to predict and control and the process has to be robust against them. Sources of perturbations in SEC that may be predicted up to a certain level are temperature changes due to the filling process. Their order of magnitude amounts to $\mathcal{O}(10)$ K [7]. When using fuels with two-stage ignition the heat release of the first stage can cause inhomogeneous ignition and possibly the formation of a detonation wave [7].

Different strategies were investigated to alleviate the sensitivity of the SEC process to inhomogeneities. The effects of equivalence ratio perturbations on homogeneous ignition can be mitigated by reducing the range of equivalence ratios used for the fuel stratification [8]. The negative temperature coefficient (NTC) behavior of most hydrocarbons, which leads to an increase in ignition delay time with increased initial temperature over a certain range of temperatures, can be utilized to tailor the combustible mixture for SEC. Mixing fuels with and without NTC behavior yields a fuel blend with temperature independent ignition delay time over a range of initial temperatures, which ideally eliminates the effect of temperature perturbations in the SEC process [9].

Berndt et al. investigated the SEC process by means of simulations with a simplified reaction mechanism [10]. They showed that even when the temperature dependency was reduced for a range of initial temperatures, the heat release of the first ignition stage still led to inhomogeneous ignition and concluded that the temperature dependency of the ignition delay time needs to be reduced further. Additionally, Berndt et al. determined the detonation peninsula in the regime diagram qualitatively [7]. They proved that the lower bound for detonation development in SEC is linked to the C–J speed and found that long excitation times can prevent detonation formation, even when there are fair perturbations in the ignition delay time.

To avoid the formation of a detonation caused by inhomogeneous ignition not only the temperature dependency of the mixture has to be decreased but an increase in excitation time would substantially reduce the demands on the accuracy of mixture stratification and temperature homogeneity. However, it was not possible to increase the excitation time by blending different fuels [9] because relevant fuels have similar excitation times.

In order to prolong the excitation time and mitigate knocking we consider the possibility of diluting the fresh gas mixture with exhaust gas and steam in the present study. To evaluate the proposed methods we conduct simulations of a combustible mixture subjected to a temperature inhomogeneity in form of a hot spot with various amounts of dilution.

2 Numerical Setup and Methods

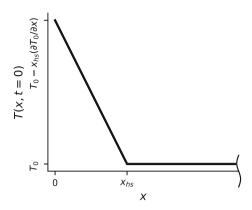
One-dimensional numerical simulations are conducted to assess the effect of dilution on ignition and wave propagation in a setup with an initial temperature perturbation. A section of a cylindrical tube with a hot spot is considered. The gas mixture is at rest initially. The hot spot is modeled as a linear temperature increase at the left part of the domain. The initial temperature distribution T(x, t = 0) containing a hot spot is described by the following equation:

$$T(x,t=0) = \begin{cases} (x - x_{hs}) \left(\frac{\partial T_0}{\partial x}\right) + T_0, & x \le x_{hs} \\ T_0, & x > x_{hs} \end{cases},$$

where T_0 is the temperature of the gas outside of the hot spot, x_{hs} is the hot spot's spacial extension and $\frac{\partial T_0}{\partial x}$ is the temperature gradient in the hot spot (it is negative to obtain a temperature elevation within the hot spot). Figure 1 sketches the initial temperature profile defined by the equation above. The hot spot's extension is chosen to be 0.5 mm and the maximum temperature elevation (at T(x = 0, t = 0)) amounts to 10 K. The gas in the tube is assumed to be radially homogeneous. Thus, the problem reduces to one dimension along the tube axis. The section that is modeled has a length of 5 cm. Because the domain represents merely a section of a tube there are no reflections at the boundaries. Hence, continuous boundaries are used which force the gradients to be zero. The gas mixture in the tube section is a homogeneous dimethyl ether (DME)/air mixture with stoichiometric composition. Various amounts of steam and exhaust gas are added to the reactants. The exhaust gas is assumed to be composed according to the global products composition of stoichiometric DME/air combustion. The initial thermodynamic state in the tube is calculated assuming the gas is compressed with a pressure ratio of 20 from ambient conditions before entering the tube with an isentropic efficiency of 90%. The pressure ratio is chosen such that the ignition delay time is of the order of 1 ms to ensure feasible tube lengths (compare e.g. [11] for the relation between tube length and ignition delay time). From this reasoning, the conditions inside the tube result to 20 bar and 755 K.

The processes inside the tube are simulated using a code developed for simulating the SEC process [12]. The reactive Euler equations with chemical source terms in the energy equation and species mass fraction conservation equations are solved using the finite volume method with a HLL (Harten, Lax, van Leer) solver with Einfeldt correction. It was demonstrated in [13] that the choice of the solver is appropriate for the problem to be modeled. A second order integration scheme is used. Chemical

Fig. 1 Sketch of initial temperature distribution with a hot spot



kinetics is integrated into the scheme by Strang splitting. The chemical kinetics of DME is modeled using a detailed mechanism developed by Zhao et al. [14] which was validated for a range of temperatures and pressures relevant to the present study. However, none of the available mechanisms for DME was validated for dilution with exhaust gas and steam and experimental data of ignition delay times in such mixtures are necessary to quantitatively prove the effects of dilution on the chemistry. Nevertheless, the physical influence of dilution on ignition and the characteristic time scales is reproduced.

All simulation results provided in this work were obtained with a spacial resolution of 5×10^{-5} m and a CFL (Courant, Friedrichs, Lewy) number of 0.5.

3 Results

As described in the introduction, the two time scales of interest are the ignition delay time τ_i and the excitation time τ_e . To investigate how these time scales change with dilution, zero-dimensional isochoric reactor simulations are performed with the software package Cantera [15]. The ignition delay time is determined through the time it takes the gas mixture to reach the maximum temporal change in temperature. The excitation time is defined as in [12] as the time needed for the temperature to rise from

$$0.85T(t=0) + 0.15T(t=t_{\infty})$$

to

$$0.15T(t=0) + 0.85T(t=t_{\infty}).$$

In the equation above $T(t=t_{\infty})$ denotes the temperature the gas mixture attains in equilibrium after ignition. Other researchers define the excitation time from the instant when a given fraction of the maximum heat release rate (e.g. 5% in [6] and 1%

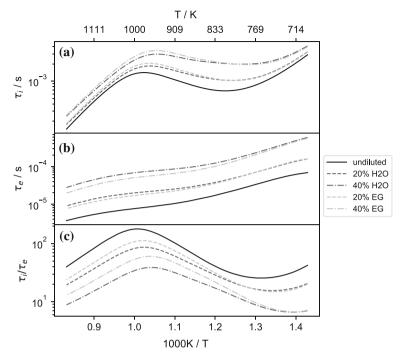


Fig. 2 Ignition delay time a, excitation time b and their ratio c over initial mixture temperature for 0%, 20 vol% and 40 vol% dilution with steam (H2O) and exhaust gas (EG) for a pressure of 20 bar

in [9]) is achieved until the instant of maximum heat release. For the considered mixtures these definitions are ambiguous due to the presence of multiple ignition stages for certain conditions. The definition from [12] was chosen because the monotonous increase of the temperature yields an unambiguous definition of the excitation time. The predominant trends in the following results are similar regardless of the chosen excitation time definition.

The variation of excitation times and ignition delay times with initial temperature is depicted in Fig. 2a, b for a pressure of 20 bar as in the one-dimensional simulations. The excitation time increases with increasing amount of dilution (Fig. 2b), and can thus be used to mitigate knocking as proposed. The prolongation of excitation times is higher for steam dilution, except for lower temperatures and lower dilutions rates, where excitation times are similar for both diluents.

However, dilution with steam or exhaust gas also increases the ignition delay time (Fig. 2a), which influences the combustion process of SEC including filling and purging. For intermediate to high temperatures the ignition delay time is prolonged more with exhaust gas dilution compared to the same amount of steam dilution, while ignition delay times are similar for both diluents at low temperatures. Furthermore, the ignition delay times in Fig. 2a show that DME exhibits a pronounced NTC behavior

in the temperature range between 820 and 980 K for the undiluted case. The range of temperatures where NTC behavior is prevailing shifts to lower temperatures with increasing amount of dilution.

In order to evaluate the effect of initial temperature on both chemical time scales the ratio of ignition delay time to excitation time is depicted in Fig. 2c. Dilution enables the desired prolongation of the excitation time (Fig. 2b), but it also increases the ignition delay time (Fig. 2a), thus influencing the combustion process and operation of SEC. It is desired that the effect of dilution on the excitation time is stronger than on the ignition delay time. Hence, a low ratio of ignition delay time to excitation time τ_i/τ_e is desired. With increasing dilution this ratio is decreased (Fig. 2c). For intermediate to high temperatures the ratio of ignition delay to excitation time is smaller with steam dilution, while it is similar at low temperatures for both diluents.

When the temperature in a combustion volume is perturbed at a specific spot, ignition can appear there earlier compared to the surrounding mixture. Generally, this is the case for hot spots, or for cool spots within the NTC region. In the following analysis we refer to the temperature of the perturbation as T_p and define the ignition delay time deviation $\Delta \tau_i$ from the surrounding mixture's ignition delay time caused by a temperature perturbation as

$$\Delta \tau_i = \tau_i(T_p) - \tau_i(755 K).$$

In the equation above, the reference temperature which represents the surrounding mixture's temperature is chosen to be 755 K as in the one-dimensional simulations.

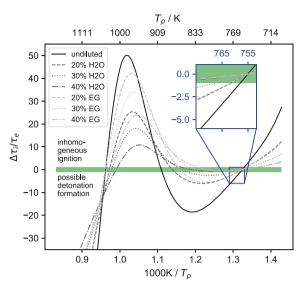
Depending on the temperature gradient of the perturbation, the perturbation size and mixture properties, a detonation can ensue from an ignition spot. In the following, the influence of the rapidness of heat release on detonation formation is investigated. If the temperature perturbation in a hot spot leads to premature ignition, the local heat release results in a local increase in pressure. The pressure then propagates into the gas surrounding the hot spot, which is already close to autoignition. The compression due to the pressure propagation from the hot spot may accelerate the autoignition of the surrounding gas and trigger a detonation. However, if the time scale of the pressure rise in the hot spot is longer than the difference in ignition delay time between the hot spot and the surrounding gas, the surrounding gas will have enough time to autoignite when its actual ignition delay time expired without being affected by the hot spot. Thus, the hot spot would pose no risk with respect to detonation formation [12]. Since the time scale of the pressure rise is determined by the excitation time τ_e , this is qualitatively fulfilled if

$$|\Delta \tau_i| < \tau_e. \tag{1}$$

In order to examine the fulfillment of condition (1), Fig. 3 shows the ratio of the ignition delay time deviation $\Delta \tau_i$ to the excitation time of the temperature perturbation $\tau_e(T_p)$ over the perturbation's temperature T_p .

When the ratio $\Delta \tau_i/\tau_e$ depicted in Fig. 3 is negative, the ignition delay time of the perturbation is smaller than the surrounding mixture's ignition delay time. In

Fig. 3 Ratio of ignition delay time deviation $\Delta \tau_i$ caused by a temperature perturbation to the excitation time of the mixture with perturbed temperature τ_e over the perturbation temperature T_p with various amounts of steam (H2O) and exhaust gas (EG) dilution. The green shaded area denotes condition (1)



the opposite case, where the ratio $\Delta \tau_i/\tau_e$ is positive, the ignition delay time of the surrounding mixture has expired before the hot spot ignites. In Fig. 3 the ignition delay time of the hot spot is higher than the ignition delay time of the surrounding mixture in the range of perturbation temperatures between 900 and 1040 K for the undiluted mixture because of the NTC behavior of DME.

As explained above, only negative ignition delay time deviations which describe a decrease in ignition delay of a hot spot compared to the surrounding mixture's ignition delay time can lead to premature ignition and the formation of a detonation wave. Nonetheless, positive ignition delay time deviations can lead to inhomogeneous ignition. In order to investigate the possibility of knock control by dilution, only negative ignition delay time deviations $\Delta \tau_i$ (respectively negative ratios $\Delta \tau_i/\tau_e$) will be considered because they can possibly result in a detonation.

The condition in Eq. (1) can be transformed to

$$\left| \frac{\Delta \tau_i}{\tau_e} \right| < 1. \tag{2}$$

Condition (2) is represented by the green shaded area in Fig. 3.

The magnitude of the ratio of ignition delay deviation to excitation time $|\Delta\tau_i/\tau_e|$ is decreased by dilution (Fig. 3). Exhaust gas dilution is decreasing it more for intermediate temperatures, while steam dilution does for high temperatures. For dilution with 40 vol% steam the ratio of ignition delay time deviations to the excitation time remains within the green shaded area for temperature perturbations of up to 860 K, indicating that condition (1) is fulfilled and knocking may effectively be mitigated for these temperatures. For perturbation temperatures above 1040 K dilution is less effective, because the magnitude of the ignition delay time deviation increases much

more with increasing perturbation temperature than the excitation time. The insert in Fig. 3 shows the diagram magnified to a perturbation temperature of 765 K, which is the amplitude of the hot spot present in the one-dimensional simulations. Dilution with more than 30 vol% exhaust gas or steam decreases the ratio $|\Delta \tau_i/\tau_e|$ such that it fulfills condition (1), which indicates that the prolongation of excitation times may become effective for reducing knocking in the one-dimensional simulations at about this amount of dilution.

To conclude, dilution alters the characteristic time scales of the mixture in such a way that condition (1) is met for a wider range of perturbation temperatures compared to the undiluted case. This indicates that the increase in excitation time caused by dilution may in fact prevent detonation formation. However, the aforementioned zero-dimensional analysis does not consider the influence of the properties of the temperature perturbation, such as its radius and temperature gradient.

While the previous analysis shows the influence of dilution on the magnitude of the relevant time scales, the following considers the effect of dilution on the gradient in ignition delay time which influences the autoignition wave propagation mode. The propagation speed u of an autoignition wave equals the inverse of the ignition delay time gradient [5, 6] and is related to the temperature gradient in a mixture as follows:

$$u = \left(\frac{\partial \tau_i}{\partial x}\right)^{-1} = \left(\frac{\partial \tau_i}{\partial T_0} \frac{\partial T_0}{\partial x}\right)^{-1} \tag{3}$$

When the temperature gradient in a mixture close to autoignition reaches a certain critical value, such that the autoignition wave generated by this temperature gradient propagates at approximately the speed of sound a into the unburned gas a detonation can be initiated through coupling of the pressure wave with the reaction front [5]. This critical temperature gradient can be expressed as [6]

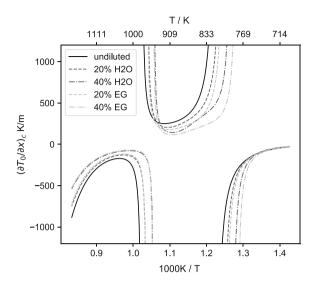
$$\left(\frac{\partial T_0}{\partial x}\right)_C = a^{-1} \left(\frac{\partial \tau_i}{\partial T_0}\right)^{-1}.$$
 (4)

It is usually defined from the initial temperature distribution in a combustion volume. However, the ignition delay time gradient in a hot spot will be altered by species diffusion and heat conduction. Therefore, a detonation develops not exclusively for the critical temperature gradient, but for a range of temperature gradients [6].

Equation (4) is evaluated to determine the critical temperature gradient over a range of temperatures (Fig. 4). Due to NTC behavior cold spots (with a positive temperature gradient) can initiate detonations in the intermediate temperature range. At the transition temperatures from NTC to the non-NTC region there are two singular points, because a change in temperature results solely in a small change in ignition delay time. In general, dilution of the fresh gas alters the critical temperature gradient.

After identifying the main parameters influencing the occurrence of knocking qualitatively with zero-dimensional calculations, the effect of dilution is studied for the case of a hot spot in a tube by means of one-dimensional simulations. Figure 5b, c

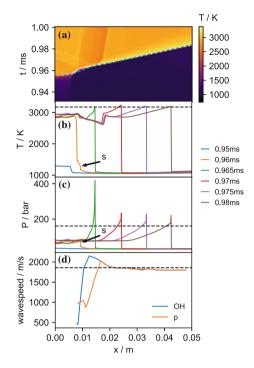
Fig. 4 Critical temperature gradient over initial temperature for 0%, 20 vol% and 40 vol% dilution with steam (H2O) and exhaust gas (EG)



shows temperature and pressure distributions at different times inside the combustion tube for the undiluted case of a stoichiometric DME/air mixture. The reaction front and shock wave are traced by the maximum change in OH mass fraction and pressure respectively. Their trajectories are represented by a white and dashed blue curve in the space-time diagram of the temperature in Fig. 5a and their propagation speeds are plotted over the axial coordinate in Fig. 5d. In all of the performed one-dimensional simulations temperature, pressure and OH mass fraction are sampled every us. At t = 0.95 ms the temperature has risen to a value of approximately 1000 K throughout the domain, which indicates that some heat was already released (Fig. 5b). Later, at $t = 0.96 \,\mathrm{ms}$, a shock forms, which is indicated by the sharp pressure rise in Fig. 5c and the letter s. It is propagating ahead of the reaction front (Fig. 5a). The shock and reaction front couple at $x \approx 0.015$ m where the propagation speeds of both waves coalesce in Fig. 5d and the detonation wave is fully developed. Eventually the propagation speed of the detonation wave approaches the speed of a C-J detonation (Fig. 5d) and the C–J temperature and pressure are distinguishable in the profiles in Fig. 5b, c (C–J conditions are computed according to [16, 17]). This wave propagation mode corresponds to the shock-detonation mode observed by Dai et al. [18].

In the following, dilution is added to the reactants mixture aiming at mitigation of knock behavior. Figures 6, 7 and 8 show the ignition processes inside the tube when adding different amounts of exhaust gas and steam dilution. Compared to the undiluted case the shock propagates a longer distance in front of the reaction front before they form a detonation wave in the 20 vol% steam or exhaust gas diluted mixture. This can again be observed by the trace of the reaction front and pressure wave in Fig. 6a, e or by the distance it takes until their propagation velocities are equal in Fig. 6d, h. At an axial location of $x \approx 0.03 \text{ m}$ for exhaust gas dilution, respectively $x \approx 0.035 \text{ m}$ for steam dilution, the reaction front reaches a propagation speed close

Fig. 5 a Space-time diagram of the temperature, white curve—reaction front, dashed blue curve—pressure wave. b, c Temperature and pressure distributions at different times. d Velocities of reaction front (OH) and leading pressure wave (p). Dashed lines in b-d C-J values of temperature, pressure and C-J detonation velocity



to a C–J detonation. The distributions in Fig. 6b, c, f, and g exhibit pressures and temperatures close to the C–J state. Dilution with 30 vol% exhaust gas delays the formation of a fully developed detonation even more (Fig. 7a, d).

When diluting with 30 vol% steam the formation of a detonation fails, as indicated by the temperature distributions in Fig. 7f and the pressure distributions in Fig. 7g, which reach values below their respective C–J values and do not exhibit steep profiles as in the undiluted case in Fig. 5. Ignition and wave propagation for dilution with 40 vol% exhaust gas or steam show a similar behavior (Fig. 8). The heat release of the reaction front creates a pressure wave which runs ahead of it. It compresses the gas and raises the temperature. However, the pressure wave does not steepen into a shock wave (Fig. 7g). Eventually the reaction front propagates at a speed greater than C–J detonation velocity, which indicates that the wave is driven by autoignition (Fig. 7h). This propagation mode is described in [5, 6] as supersonic autoignitive deflagration. It is an approximation to constant volume combustion [12] and indicates that successful SEC can be achieved without knocking even with the presence of a hot spot.

The simulation results show that dilution decreases the detonation propensity of the mixture in fact and indicates that knocking can effectively be reduced by diluting the reactants mixture with steam or exhaust gas. Although the Euler equations do not completely represent all processes relevant to combustion, they do cover the mechanism of detonation formation. Diffusion processes are generally unimportant in detonation formation except in the course of the initial formation of a detonation.

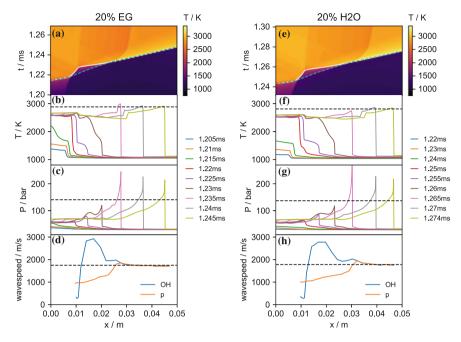


Fig. 6 a/e Space-time diagram of the temperature, white curve—reaction front, dashed blue curve—pressure wave. b/f, c/g Temperature and pressure distributions at different times. d/h Velocities of reaction front (OH) and leading pressure wave (p). Dashed lines in b-d/f-h C-J values of temperature, pressure and C-J detonation velocity. For 20% exhaust gas (EG) and steam (H2O) dilution

Once autoignition is taking place in a regime prone to detonation formation, the gas dynamic and reactive time scales are far shorter than those of diffusive processes. As a consequence, molecular transport does not have enough time to sizeably interfere with the ignition event. Of course, Euler simulations are limited in that they cannot accurately capture the course of events when temperature gradients are rather steep and diffusion controlled deflagrations develop, but this regime is not of interest here.

In general, dilution alters multiple gas properties that support avoiding detonation formation and knocking:

1. When diluting the reactants mixture, the volumetric energy density decreases. Less amount of energy is transferred from the reaction front into the pressure wave. For a sufficient amount of dilution only a pressure wave is produced, that does not develop into a shock. A similar observation was made in [19] by changing the initial temperature of the gas. Rudloff et al. [20] pointed out that the energy in the gas determines how severe knocking can get. This indicates that even when knocking appears in SEC, it might be less harmful for diluted fresh gas mixtures.

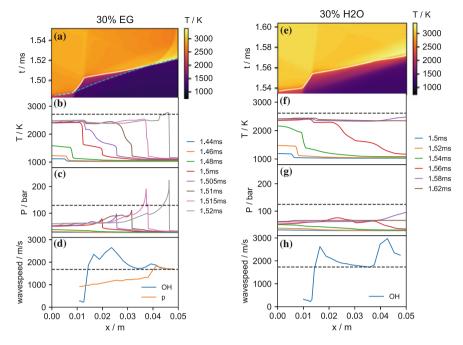


Fig. 7 a/e Space-time diagram of the temperature, white curve—reaction front, dashed blue curve—pressure wave. **b/f**, **c/g** Temperature and pressure distributions at different times. **d/h** Velocities of reaction front (OH) and leading pressure wave (p). Dashed lines in **b-d/f-h** C–J values of temperature, pressure and C–J detonation velocity. For 30% exhaust gas (EG) and steam (H2O) dilution

- 2. Dilution alters both the speed of sound in the unburned gas as well as the gradient in ignition delay $\partial \tau_i / \partial x$ (by changing $\partial \tau_i / \partial T$). Hence, the propagation speed of the autoignition and pressure wave emanating from the hot spot are different such that they may not couple. This is expressed in the critical temperature gradient (Fig. 4).
- 3. Dilution increases the excitation time (Fig. 2b), which decreases the rapidness of heat release into the shock. Figure 3 shows that the heat release caused by premature ignition is slow compared to the perturbation in ignition delay time when the combustible mixture is diluted. This can mitigate detonation formation.

The performed one-dimensional simulations show, that dilution of the combustible mixture with exhaust gas or steam alters the aforementioned gas properties such that detonation formation is suppressed.

Dilution changes both non-dimensional parameters in the regime diagram proposed by Gu et al. [6]. Dai et al. [19] underlined that a decrease in volumetric energy density narrows the detonation peninsula. This indicates that dilution shifts the location of the detonation peninsula and narrows it, which can benefit engine operation because operation points that are prone to detonation formation may be decimated.

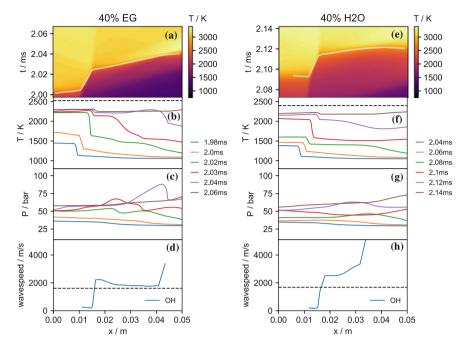


Fig. 8 a/e Space-time diagram of the temperature, white curve—reaction front. b/f, c/g Temperature and pressure distributions at different times. d/h Velocities of reaction front (OH) and leading pressure wave (p). Dashed lines in b-d/f-h C-J values of temperature, pressure and C-J detonation velocity. For 40% exhaust gas (EG) and steam (H2O) dilution

4 Conclusions

We investigated the influence of dilution of the combustible mixture with exhaust gas and steam on knocking in SEC. The main influences were identified by analysis of the change of mixture properties with dilution. It showed that the excitation time is increased while the volumetric energy density is decreased and the critical temperature gradient is altered, which are beneficial for the prevention of detonations in a combustion system. Simulations with the Euler equations with different amounts of dilution proved that the propensity of the mixture to detonate is decreased with increasing amount of dilution. For a hot spot with a temperature elevation of $10 \, \mathrm{K}$ diluting with 30% steam or 40% exhaust gas is sufficient to prevent the formation of a detonation.

The results show that the approach is promising to prevent knocking. In order to support the development and implementation of SEC further, the location of the detonation peninsula in the regime diagram needs to be determined for relevant mixtures with and without dilution.

Furthermore, the influence of dilution onto the whole SEC process needs to be assessed. The SEC design has to consider that dilution increases the ignition delay

time and therefore the combustion tube's length. Moreover, the impact of dilution on the efficiency needs to be determined.

A challenge for further research is that most kinetic models are not validated for dilution with exhaust gas or steam. In order to increase the confidence in the determination of the detonation peninsula as well as for the process design and control of SEC with diluted gas mixtures the experimental database needs to be extended for ignition delay times of mixtures with steam and exhaust gas dilution. If necessary, kinetic models need to be adjusted.

Nevertheless, the study shows that by influencing the excitation time through dilution it is possible to prevent knocking. Exhaust gas or steam are well suited as potential diluents because their integration into a conventional, respectively wet, gas turbine cycle is feasible.

Acknowledgements The authors gratefully acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) as part of collaborative research center SFB 1029 "Substantial efficiency increase in gas turbines through direct use of coupled unsteady combustion and flow dynamics" on project A08.

References

- Bobusch, B.C., Berndt, P., Paschereit, C.O., Klein, R.: Shockless explosion combustion: an innovative way of efficient constant volume combustion in gas turbines. Combust. Sci. Technol. 186(10–11), 1680–1689 (2014)
- Rähse, T.S., Paschereit, C.O., Stathopoulos, P., Berndt, P., Klein, R.: Gas dynamic simulation
 of shockless explosion combustion for gas turbine power cycles. In: ASME Turbo Expo 2017:
 Turbomachinery Technical Conference and Exposition, pp. V003T06A005–V003T06A005.
 American Society of Mechanical Engineers (2017)
- 3. Lee, J.H., Knystautas, R., Yoshikawa, N.: Photochemical initiation of gaseous detonations. Acta Astronaut. **5**(11–12), 971–982 (1978)
- 4. Zeldovich, Y.B., Librovich, V.B., Makhviladze, G.M., Sivashinsky, G.I.: On the development of detonation in a non-uniformly preheated gas 15, 313–321 (1970)
- Zeldovich, Y.B.: Regime classification of an exothermic reaction with nonuniform initial conditions. Combust. Flame 39(2), 211–214 (1980)
- Gu, X.J., Emerson, D.R., Bradley, D.: Modes of reaction front propagation from hot spots. Combust. Flame 133(1), 63–74 (2003)
- 7. Berndt, P., Klein, R.: Modeling the kinetics of the shockless explosion combustion. Combust. Flame 175, 16–26 (2017)
- 8. Bobusch, B.C., Berndt, P., Paschereit, C.O., Klein, R.: Investigation of fluidic devices for mixing enhancement for the shockless explosion combustion process. In: Active Flow and Combustion Control 2014. Springer (2015)
- 9. Cai, L., Pitsch, H.: Tailoring fuels for a shockless explosion combustor. In: Active Flow and Combustion Control 2014. Springer (2015)
- Berndt, P., Klein, R., Oliver Paschereit, C.: A kinetics model for the shockless explosion combustion. In: Proceedings of the ASME Turbo Expo (2016)
- 11. Bobusch, B.C.: Fluidic devices for realizing the shockless explosion combustion process. Ph.D. thesis, Technische Universitt Berlin (2015)
- 12. Berndt, P.: Mathematical modeling of the shockless explosion combustion. Ph.D. thesis, Freie Universität Berlin (2016)

- Berndt, P.: On the use of the hll-scheme for the simulation of the multi-species euler equations.
 In: Finite Volumes for Complex Applications VII-Elliptic, Parabolic and Hyperbolic Problems,
 pp. 809–816. Springer (2014)
- Zhao, Z., Chaos, M., Kazakov, A., Dryer, F.L.: Thermal decomposition reaction and a comprehensive kinetic model of dimethyl ether. Int. J. Chem. Kinet. 40(1), 1–18 (2008)
- Goodwin, D.G., Moffat, H.K., Speth, R.L.: Cantera: an object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes (2017). http://www.cantera.org, Version 2.3.0
- Gordon, S., McBride, B.J.: Computer program for calculation of complex chemical equilibrium compositions and applications. I: analysis. Technical report, NASA (1994). NASA Reference Publication 1311
- 17. Lee, J.H.S.: The Detonation Phenomenon. Cambridge University Press, The Detonation Phenomenon (2008)
- 18. Dai, P., Chen, Z., Chen, S., Ju, Y.: Numerical experiments on reaction front propagation in n-heptane/air mixture with temperature gradient, vol. 35, pp. 3045–3052. Elsevier (2015)
- Dai, P., Qi, C., Chen, Z.: Effects of initial temperature on autoignition and detonation development in dimethyl ether/air mixtures with temperature gradient, vol. 36, pp. 3643–3650. Elsevier (2017)
- Rudloff, J., Zaccardi, J.-M., Richard, S., Anderlohr, J.M.: Analysis of pre-ignition in highly charged SI engines: emphasis on the auto-ignition mode, vol. 34, pp. 2959–2967. Elsevier (2013)