COMBUSTION REGIMES IN SEQUENTIAL COMBUSTORS

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ABSTRACT
This numerical study compares the combustion process of a gas turbine sequential combustor at atmospheric and high pressure (10bar) conditions. Flame propagation is found to be the driving combustion regime at 1bar, whereas at high pressure autoignition dominates. The transition from propagation to autoignition is mapped over a range of unburned gas temperature and pressure based on 1-D flame simulations. A new Analytically Reduced Chemistry (ARC) mechanism for methane/air combustion at high pressure with 16 transported species is obtained to perform compressible 3-D Large Eddy Simulation (LES) with the Dynamic Thickened Flame model (DTF).

INTRODUCTION
Thermoacoustic instabilities are one of the major challenges in gas turbine engineering, especially at high pressure and lean conditions [1, 2]. They can appear in almost every combustion system resulting from a constructive interaction between acoustic pressure and unsteady heat release rates transmitted from the flame. Most of the laboratory research is done with setups operating at atmospheric pressure, such as e.g. [3–12]. This numerical study compares combustion processes in a second stage sequential combustion system, or also referred to as axial staging concept [13–15], at atmospheric and high pressure (10bar).

Fuel is injected into vitiated hot gas coming from a first stage swirled flame [16] and mixing temperatures range from about 1200K to 1400K. In these operating conditions experimental data such as flame speeds are lacking. As reviewed by Ranzi et al. [17] experimental data for laminar flame speeds $s_L$ for methane/air combustion is available only up to an unburned gas temperature of 400K [18]. Turbulent flame speeds were measured up to 770K and 14bar [19]. To the authors knowledge no data is available for vitiated flow conditions. Nevertheless there are several studies with conditions closer to the ones found in engines, such as [10, 20, 21]. In the well documented lifted flame experiment of Cabra et al. [20] an extensive number of numerical studies, e.g. [20, 22–27] identified flame propagation and autoignition burning regimes. In regions dominated by propagation one can detect unburned mixing temperatures ranging from approximately 1150K to 1300K. These studies show good agreements with experimental data, which indicates that the used methane/air chemistry schemes can be applied up to these temperatures. The atmospheric Cabra experiment features a cold methane/air jet injected into a hot vitiated coflow where turbulence chemistry interactions are expected to be similar to the sequential burner. Propagation and autoignition burning regimes coexist and the dominant flame stabilisation mechanism has been characterised as autoignition (e.g. [22–24]).

The aim of this study is to identify the dominant combustion mechanisms of a sequential burner at 1 and 10bar. It investigates if the coexistence of propagation and autoignition applies for this configuration. Based on 1-D flame simulations it also examines how the combustion process changes with increasing pressure closer to engine conditions.

CONFIGURATION AND NUMERICAL SETUP

The Sequential Burner
A sketch of the configuration is shown in Fig. 1a. Only the second stage of the sequential combustion system is simulated. Perfectly premixed first stage combustion products diluted with additional fresh air at a velocity of 65 m/s are imposed at the domain inlet. The hot gas temperature is set to 1450K at 1bar and is decreased to 1300K at 10bar with the aim of having comparable flame lengths. One might argue that inlet temperatures should be equal to investigate the influence of pressure. It is not possible to find such a condition for this...
configuration: for example, decreasing the inlet temperature at 1 bar increases the flame length, while increasing the inlet temperature at 10 bar shortens it. Later in the paper it will be shown that at 10 bar autoignition is the dominant combustion regime. Assuming an inlet temperature of 1400 K instead of 1300 K at 10 bar autoignition times decrease by factor one third and the flame is expected to be located in the mixing zone, which is not acceptable. The effect of temperature difference is further discussed in the context of Fig. 6. Fuel (methane/air at 320 K) is injected via jet in cross flow further discussed in the context of Fig. 6.

Figure 1 shows iso-contours of the Q-criterion [28] (5 × 10^7), CH₄ mass fraction (0.04) and heat release rate (1 × 10^7 W/m^3). Atmospheric Pressure.

Numerical Methods

Compressible Large Eddy Simulation (LES) are performed with the explicit cell-vertex code AVBP [30] using the numerical scheme TTGC [31] with third order accuracy in space and time. The Smagorinsky approach was used to model subgrid Reynolds stress. Non-reflecting Navier-Stokes Characteristic Boundary Conditions [32] are imposed at the inlets and outlet. The heat loss formulation $q = (T_{wall} - T_w)/R_w$ is applied to the domain walls. At atmospheric pressure the thermal resistance $R_w$ is set to 0.02 K m^2/W in the mixing zone and 0.04 K m^2/W in the combustion chamber. At 10 bar $R_w$ is decreased to 0.005 K m^2/W and 0.01 K m^2/W respectively. 2-D wall resolved simulations with characteristic velocities, pressure and temperatures show that these $R_w$ result in wall temperatures of 700 K in the mixing zone and 1000 K in the combustion chamber. Heat losses decrease mixing temperatures, nevertheless wall temperatures are similar at 1 and 10 bar allowing a comparison of both cases.

Simulations were performed on an unstructured mesh with 1.9 million nodes (11.1 million cells) and a characteristic cell size of 0.7 mm in the reaction zone. The wall boundary layer is not resolved, which is compensated by a coupled velocity/temperature wall-model [33]. The Dynamic Thickened Flame (DTF) Model [34] was used for turbulent combustion modelling. The flame front is thickened to have a minimum of 4.5 cells inside the flame front allowing to resolve it on the LES grid and maintaining the correct laminar flame speed. At atmospheric pressure this results in thickening factors of approximately 9. The DTF model has not yet been applied to pure autoignition flame fronts as they appear at 10 bar. As shown in the upper part of Fig. 2 the flame position only depends on the autoignition time $\tau_{AI}$ and the inlet velocity $u$. The inlet velocity $u$ also affects the flame thickness: A decreased $u$ decreases the flame thickness and vice versa. One can imagine a homogeneous mixture transported in physical space: for the same mixture chemistry time scales stay constant, whereas the transport time scales change with $u$. With a minimum velocity of 10 m/s and therefore a flame thickness $\delta$ of 0.3 mm (compare with Fig. 2) a maximum thickening factor of 13 is obtained at 10 bar. Here the reader should note that a velocity of 10 m/s is chosen conservatively and represents the worst case. As shown later in the paper velocities close to the centre line reach easily 60 m/s and therefore thickening factors smaller than 13 are obtained. One can also refer to [22] for an application of the DTF to the Cabra flame configuration.
FIGURE 2. Profiles of temperature and mass fractions of a stoichiometric 1-D autoignition flame at 10 bar. Width of blue region highlights flame thickness $\delta x$. Top: Temperature profile with autoignition length $\tau_{AI} \cdot u$. Bottom: Zoom into flame region with profiles of temperature and mass fractions derived from detailed (lines) and reduced chemistry scheme ARC_16_10BAR_GRI30 (symbols).

Analytically Reduced Chemistry

In the 1 bar simulations the analytically reduced chemistry (ARC) scheme ARC_22_GRI211 with 22 transported species is used. For a detailed validation of the scheme the reader is referred to [22, 35]. The ARC scheme for 10 bar is obtained from the detailed GRI-MECH 3.0 mechanism [36]. For this study NO$_x$ prediction is not of interest and therefore 17 species involved in the NO$_x$ pathways, namely: N, NO, N$_2$O, NO$_2$, NH, HNO, NH$_2$, NNH, CN, NCO, HCN, HCNO, H$_2$CN, HCN, HCNO and NH$_3$ were removed in a first reduction step. At this stage the error for autoignition times obtained by Perfectly Stirred Reactor (PSR) simulations is less than 1%. In a second reduction step the following 12 species were removed using the directed relation graph with error propagation (DRGEP) method [37]: C, CH, C$_2$H$_2$, C$_2$H, HCCO, CH$_2$CO, CH$_2$OH, HCCOH, CH$_2$CHO, C$_3$H$_7$, CH$_3$CHO, C$_3$H$_8$ and AR. In the last reduction step the species HCN, CH$_2$GSG-CH$_2$, CH$_3$O, HCO, CH$_2$, C$_3$H$_5$, H$_2$O$_2$ and C$_2$H$_3$ were identified suitable for quasi-steady state (QSS) assumption with analytical expressions of their concentrations [37]. Hence only the following 16 transported species remain in the scheme, named ARC_16_10BAR_GRI30: N$_2$, H, H$_2$, O, OH, O$_2$, H$_2$O, HO$_2$, CH$_3$, CH$_2$O, CO$_2$, CO, CH$_2$OH, CH$_4$, C$_2$H$_6$ and C$_2$H$_4$.

Profiles of temperature and species mass fractions for a 1-D autoignition flame derived using AVBP with ARC_16_10BAR_GRI30, as well as CANTERA with detailed chemistry are shown in Fig. 2. For the AVBP simulation (symbols) the inlet velocity $u$ is set to 10 m/s. With $\tau_{AI} = 4.4$ ms this results in an autoignition length of $\tau_{AI} \cdot u = 44$ mm. For the CANTERA simulation $u$ is increased to 10.8 m/s compensating an error in autoignition time of 8%. Profiles for temperature and species mass fractions are in excellent agreement.

Autoignition times $\tau_{AI}$ from PSR simulations at 10 bar for the two reduced schemes in comparison with GRI-MECH 3.0 are presented in Figure 3. In this study $\tau_{AI}$ is taken at maximum temperature gradient. ARC_22_GRI211 is not able to predict autoignition times correctly whereas the maximum error using ARC_16_10BAR_GRI30 is less than 10% which was considered acceptable for this study.

As shown in [35] including NO$_x$ chemistry will result into 9 additional QSS species and 4 additional transported species, the latter one increasing computational cost by approximately factor 1.2.
THE ROLE OF AUTOIGNITION AND PROPAGATION FROM 1 TO 10 BAR

Figure 4 shows the autoignition time $\tau_{AI}$ over mixture fraction $Z$ for 1 bar and 10 bar computed with PSR simulations. Throughout the paper the mixture fraction definition by Bilger et al. [38] is used. Note that at 10 bar the hot gas cross flow temperature was decreased to 1300 K compensating the decrease of $\tau_{AI}$ with increased pressure, whereas the species composition is kept constant. The most reactive mixture fraction $Z_{mr}$ defined at minimum $\tau_{AI}$ is found on the very lean side: $Z_{mr,1bar} \approx 0.002$ corresponding to an equivalence ratio of $\phi_{mr,1bar} \approx 0.053$ and $Z_{mr,10bar} \approx 0.001$ corresponding to $\phi_{mr,10bar} \approx 0.027$.

The laminar flame speed $s_L$ over mixture fraction $Z$ derived from 1-D propagating premixed flame simulations at 1 bar is shown in Fig. 5 (highlighted in orange). Below $Z_{trans} \approx 0.01$ (subscript trans denotes transitional) corresponding to $\phi_{trans} \approx 0.27$ freely propagating flames cannot be observed anymore and autoignition of the mixture starts to dominate (in blue). Similar observations were shown for the Cabra configuration in [22, 25]. At 10 bar (inset plot) mixture fractions are governed only by autoignition. Note that $Z_{trans}$ is shifted to higher mixture fractions ($\approx 0.2$) larger than the maximum mixture fraction in the sequential burner just upstream of the flame ($Z_{max} \approx 0.04$) and is therefore not of interest for this study.

In Fig. 6 the transition from propagation to autoignition at stoichiometry ($\phi = 1$) is presented over a wide range of unburned gas temperature $T_u$ and pressure. The composition was kept constant and corresponds to stoichiometry or $Z_{\phi=1} = 0.0365$. Note that in the sequential burner going from 1 to 10 bar the inlet hot gas temperature is decreased resulting in stoichiometric mixing temperatures of 1409 K and 1264 K respectively (both are marked in Fig. 6). Open circles represent 1-D propagating flame (in orange area), as well as 1-D autoignition flame (in blue area) simulations with CANTERA. The reader should note, that these data are not obtained using the autoignition index $AI$ [22], which is introduced later in the paper. For a constant pressure the temperature is increased until a freely propagating flame is not observed anymore. This temperature marks the transition between propagation and autoignition, which is similar to the approach in Fig. 5, where the same phenomenon is investigated in mixture fraction space.

With increasing pressure one can observe the transition from propagation to autoignition at lower $T_u$. As shown for example in [17] laminar flame speeds $s_L$ decrease with increasing pressure. For example, at $T_u = 1100$ K and 1 bar a 1-D propagation flame simulation with detailed chemistry gives $s_L = 1.96$ m/s. Increasing the pressure to 10 bar and keeping the same temperature (going in horizontal direction in Fig. 6) a propagating flame is still observed and $s_L$ decreases to 0.64 m/s, which is agreement with $s_L \propto p^{1/2}$ [39]. A further increase of pressure (moving further in horizontal direction in Fig. 6) results in decreased autoignition times $\tau_{AI}$ and even lower $s_L$, hence a dynamic balance between flow velocity and flame propagation speed cannot be achieved anymore and autoignition starts to dominate. An increase in $T_u$ (moving in upper vertical direction) increases laminar flame speeds [18], nevertheless $\tau_{AI}$ decreases and autoignition starts to dominate.

In the following the effect of different inlet temperatures $T_{in}$ is discussed on the basis of Fig. 6. One can imagine a decrease of $T_{in}$ at 1 bar and an increase of $T_{in}$ at 10 bar to equal values. As a consequence the 1 bar case is shifted further down into the propagation region and the 10 bar case (both marked in Fig. 6) is shifted further up into the autoignition region. Indeed, when keeping the same mixture composition, higher temperatures promote autoignition and one can argue that the temperature difference does not change the conclusions drawn in the present study, but rather supports them.
COMPARISON OF FLAME ANCHORING MECHANISMS

Figure 7 compares instantaneous (top) and time averaged (bottom) temperature flow fields at 1 bar (right) and 10 bar (left). The horizontal y-cut is taken at half the height of the mixing zone and combustion chamber. At 10 bar the flame is more compact and one can observe an autoignition type flame shape being less conical compared to 1 bar. Here the reader is referred to compare with high pressure flame fields in [40–43]. With the aim of quantifying autoignition and propagating type flames time averaged velocities $\bar{u}$ and autoignition times $\tau_{AI}$ based on mixture compositions are extracted along an axial line for both simulations (brown lines, offset from centerline 12 mm). Along these lines compositions do not change significantly and a mixed state is assumed. The equivalence ratio $\phi$ and $u$, as well as $\bar{\phi}$ and $\bar{u}$ are plotted along the lines.

At 10 bar the time and spatially averaged equivalence ratio $\bar{\phi}$ is determined as 0.66, which corresponds to a mixture fraction $Z$ of 0.0245 and an autoignition time $\tau_{AI}$ of 2.9 ms computed with a PSR simulation (compare with Fig. 4). With an averaged velocity $\bar{u}$ of 67.1 m/s the autoignition length is determined as $\tau_{AI} \cdot \bar{u} = 195$ mm and is marked with a brown cross, which matches well with the average flame position at 10 bar. Although this is a complex 3-D configuration with strong turbulence chemistry interactions time scales from 0-D PSR simulations do not become meaningless and can be used to have a first guess on the autoignition length under the assumption that conditions along the path do not change significantly.

At atmospheric pressure (right part of Fig. 7) the same procedure is repeated. With $\bar{\phi} = 0.87$ ($Z = 0.032$) and a corresponding $\tau_{AI} = 5.8$ ms, as well as $\bar{\pi} = 64.3$ m/s the theoretical autoignition length (373 mm) is located far downstream of the flame stabilisation position visualised by the cross outside the bottom averaged $T$ field. The flame position cannot be determined using an autoignition length which indicates that it is mainly driven by propagation. At this height the flame changes from an autoignition flame to a mainly propagating driven type flame when decreasing pressure from 10 to 1 bar, which is in agreement with findings in Fig. 5.

The above statement is made from an “autoignition point of view”. It shows that the 10 bar case is autoignition driven and the 1 bar case is not. In the following it will be shown that a “propagation point of view” gives the same results. The stoichiometric laminar flame speed at 1 bar is computed as $s_L = 5.1$ m/s. With $s_T/s_L \approx 1 + u' / s_L$ [44] the turbulent flame speed has an estimated value of 11 m/s. The rms velocity $u'$ = 6 m/s is extracted in the central heat release zone. With a decrease in temperature of 150 K (as it is done at 10 bar) $s_L$ decreases to 3.3 m/s and therefore the turbulent flame speed drops to 9.3 m/s using the same $u'$. In the following we could imagine a propagating type flame at 10 bar. It is assumed that the turbulent flame speed is pressure independent [19]. Hence at 10 bar a turbulent flame speed of 9.3 m/s would result in a stretched flame with a flame tip located further downstream compared to 1 bar or even in flame blow off. However the opposite trend is observed: the flame is more compact, which suggests that the driving mechanism is autoignition.

Figure 8 shows scatter plots of scalar dissipation rate $\chi$ against
FIGURE 8. Scatter plots showing scalar dissipation rate $\chi$ against mixture fraction $Z$ [38] coloured by heat release rate $Q$ at 10 bar (left) and 1 bar (right). Data extracted at horizontal $y$-line at half the height of the combustion chamber (red line in sketch). Scatter conditioned on $Y_{CH_4} > 1 \times 10^{-5}$ to disregard post-flame chemistry. Dashed square in left plot marks region favourable for autoignition (low $Z$ and low $\chi$) where no point with low $Q$ (black) are observed. Scatter size as function of heat release rate $Q$: large for $Q > 1 \times 10^7$, medium for $1 \times 10^7 > Q > 1 \times 10^6$ and small for $Q < 1 \times 10^6$.

mixture fraction $Z$ coloured by heat release rate $Q$ at 10 bar (left) and 1 bar (right). $\chi$ is defined as

$$\chi = \frac{1}{Sc} \left[ \left( \frac{\partial Z}{\partial x} \right)^2 + \left( \frac{\partial Z}{\partial y} \right)^2 + \left( \frac{\partial Z}{\partial z} \right)^2 \right]$$  \hspace{1cm} (1)

with Schmidt number $Sc$. As shown in the sketch data are extracted along a horizontal $y$-line at half the height of the combustion chamber. Only points with $Y_{CH_4} > 1 \times 10^{-5}$ are considered, which allows to focus on reaction regions in the bulk flow and the flame without post-flame chemistry. As shown in [45] turbulent autoignition is observed when mixture fractions are close to the most reactive one and when the conditional scalar dissipation rates $\chi|_{Z_{mr}}$ (mr stands for most reactive) are low. In Fig. 8 it is shown that mixture fractions at this axial position range between approximately $0.008 < Z < 0.065$ for both pressures, which is due to mixing effects. Therefore $Z$ are larger than the most reactive ones ranging between $0.0008 < Z_{mr} < 0.003$ for 10 bar and $0.001 < Z_{mr} < 0.004$ for 1 bar (compare with Fig. 4). Nevertheless autoignition is expected to be favourable at low autoignition times and therefore low mixture fractions, here denoted as $Z_{low}$, as well as low conditional scalar dissipation rates $\chi|_{Z_{low}}$. Indeed, as shown in the left part of Fig. 8, at 10 bar most of the points with large $Q$ are located at low $Z$ and low $\chi$. One can also see that once favourable conditions for autoignition are reached, heat is
always released and there are even regions where no scatter with low \( Q \) (black dots) are observed anymore (marked by the dashed square). In contrary, at 1 bar (right plot and inset with zoom) points with low \( Q \) are observed over the whole \( Z \) range, even at conditions favourable for autoignition. This is a strong indication that here autoignition is not the driving combustion regime, which is in agreement with the above observations.

Previous results indicate propagation as the dominant combustion regime at 1 bar. Nevertheless as seen in Fig. 5 autoignition type flames can occur at lower mixture fractions, which is visualised in Fig. 9 showing instantaneous heat release rate \( Q \) in logarithmic scale (top) and the autoignition index \( AI \) [22] (bottom). \( AI \) allows to distinguish between autoignition and propagation based on the relative contribution of two reactions for hydroperoxyl (HO$_2$) consumption:

\[
AI = \left| \frac{\omega_{\text{HO}_2}^{(R8)}}{\omega_{\text{HO}_2}^{(R8)} + \omega_{\text{HO}_2}^{(R6)}} \right|,
\]

with HO$_2$ reaction rates \( \omega_{\text{HO}_2} \) for the following two reactions (same numbering as in [22] and [27]):

\[
\text{HO}_2 + \text{H} \leftrightarrow \text{OH} + \text{OH}, \quad \text{R6}
\]

\[
\text{HO}_2 + \text{OH} \leftrightarrow \text{H}_2\text{O} + \text{O}_2, \quad \text{R8}
\]

For \( AI > 0.5 \), HO$_2$ reaction rates of R8 locally dominate over the ones of R6 and an autoignition burning regime is identified; propagation is detected for \( AI < 0.5 \). A 1-D propagating flame simulation (not shown here) at 1 bar and \( Z = 0.01 \) was performed to validate the autoignition index. \( AI \) is extracted at maximum heat release rate \( Q \) and a value of 0.5 is obtained. Hence, the index predicts properly the transition between autoignition and propagation, which, as shown in Fig. 5, is located at \( Z = 0.01 \).

In the present turbulent configuration \( AI \) is conditioned on \( Q \) and CH$_2$O (as done in [22]) allowing to include the autoignition kernel, but not the post flame chemistry. CH$_2$O is present during initialisation of autoignition and drops with high temperature chemistry [27]. In Fig. 9 an autoignition kernel with relatively low \( Q \) is located inside the mixing zone close to the wall and gets convected downstream. One can also see a thin autoignition region close to the lower rim. However the stabilised flame is mainly driven by propagation especially in regions with high \( Q \) coloured in yellow, which is in agreement with results in Fig. 7. Note that \( AI \) is not valid at high pressure and therefore cannot be used in the 10bar case. As shown for example in [46] dominant reactions change compared to atmospheric pressure and \( AI \) needs to be redefined for high pressure.

**CONCLUSIONS AND OUTLOOK**

In the present paper the combustion regimes of a sequential combustor are investigated at atmospheric and high pressure. Flame propagation is identified as the dominant mechanism at 1 bar. An analysis of the average flow field mixing zone shows that autoignition times from PSR simulations cannot be used to determine the flame front position. Nevertheless a study in mixture fraction space \( Z \) indicates that at low \( Z \) autoignition exists, which was shown in an instantaneous field using the autoignition index \( AI \).

A mapping of temperature and pressure dependent transition between propagation and autoignition highlights that with increasing pressure autoignition starts to dominate at lower temperatures. At 10 bar autoignition is the dominant burning regime and flame anchoring mechanism. In the relevant mixture fraction space of the sequential configuration only autoignition regions are present. The mixing zone analysis illustrates that autoignition times from PSR can be used to have a first guess on the flame front position.

This work highlights the difference of the combustion regimes at low and high pressure conditions. Although both flames look qualitatively similar they are subject to very different combustion processes. In the scope of thermoacoustic instabilities future work should address the differences in flame response to flow perturbations. One could assume that propagating flames and autoignition flames show a different behaviour, especially for temperature fluctuations due to the non-linear dependence of the reaction rate on the temperature in the Arrhenius expression.

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**REFERENCES**


