A COMPUTATIONAL ASSESSMENT OF COMBUSTION SUBMODELS FOR PREDICTIVE SIMULATIONS OF PRE-CHAMBER COMBUSTION ENGINES

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ABSTRACT

Pre-chamber combustion (PCC) modeling has been progressing in recent years, while there are lingering questions on fundamental modeling aspects, whether a flame-based or an ignition-based model predicts the combustion with higher fidelity. This mode of ignition concept is known to enable a stable engine operation at ultralean conditions with a short combustion duration, thus enhancing engine efficiency. The current work utilizes computational fluid dynamics to assess well-known combustion models: multi-zone well-stirred reactor (MZ-WSR) and G-Equation. The former models combustion as an ignition-based phenomenon while the latter as a flame propagation type of combustion. A pre-chamber containing twelve nozzles divided into two layers on a narrow throat was chosen. The jets from the two layers of nozzles and the local thermodynamic conditions differ substantially, which makes it a suitable configuration for assessing the predictive capabilities of distinct combustion models. The fuel utilized was methane and the global air-fuel ratio ($\lambda$) was varied, ranging from global-$\lambda$ of 1.6, 1.8, and 2.0, and the total fuel injected through the pre-chamber was varied for one of the cases (3%, 7%, and 13%). The results suggest that both combustion models can potentially match experimental engine performance data upon appropriate calibration; however, fundamental differences in jet topology arise since the G-Equation formulation accounts for turbulence-chemistry interaction, while MZ-WSR does not.

Keywords: Pre-chamber, G-Equation, MZ-WSR

1. INTRODUCTION

Stringent policies on emissions from the transportation sector drive the industry towards carbon-neutral mobility. To comply with the targets, multiple technologies are being investigated and deployed. Among those, pre-chamber combustion (PCC) is attracting substantial attention in favor of its potential to decrease emissions, while delivering diesel-like thermal efficiencies through the burning of ultra-lean mixtures. Lean burn is characterized by an excess air-fuel ratio (AFR) compared to a stoichiometric operation. The former comes with attractive advantages relative to the latter: lower nitric oxide (NOx) emissions (due to lower combustion temperature), decreased fuel consumption, lower carbon dioxide ($CO_2$) emissions, lower pumping losses by averting throttling, and higher efficiency. In addition, a lean charge can withstand larger compression ratios before knock onset, while its specific heat ratio is higher [1]; these combined can be quickly observed to increase the thermodynamic efficiency if an Otto cycle is considered.

The major challenges in operating engines in ultra-lean conditions come from the high ignition energy needed to initiate the flame, the considerable decrease in the flame propagation speed, and poor combustion stability, which can detriment the engine performance. The utilization of an active pre-chamber (PC) can circumvent these drawbacks simultaneously. The flame is initiated within the pre-chamber where the local composition can be controlled to facilitate flame initiation. As the flame grows within the PC and propagates towards the main chamber (MC), it is forced to pass through small nozzles, which generate considerable turbulence, thus compensating for the lower burning velocity of the main lean
In summary, the mechanism for the main charge consumption relies on highly reactive and spatially distributed jets/ flames instead of a conventional spark plug as in common spark-ignited (SI) engines. This effectively extends the lean limit of operation [2] and promotes faster burn rates [3] to values hardly achievable with SI engines [4, 5].

The small pre-chamber concept proposed by Gussak [6] is one of the most investigated concepts in recent years. It is a small component (volume is usually less than 5% of the engine clearance volume) placed on the engine cylinder head with a tip that protrudes into the main chamber [7, 8]; nozzles are drilled in this tip to allow for the charge exchange between PC and MC. The pre-chamber can be directly fueled, called active, or scavenged. Otherwise, it is called passive or unscavenged, and its air-fuel ratio is bounded to be the same as in the main chamber. The main goal is to tailor the pre-chamber geometry and operating conditions to control the jet properties and maximize the main chamber response to the jets. The objective is to command the thermal, chemical, and turbulence aspects of the jet [9].

It is widely documented that the PC engines have a multi-variable dependence: PC design [10-12], the fuel of choice [13], and operation mode [14] are some to mention. Active PC is known to extend the limit more than the passive due to the straightforward flame initiation within the PC using a common spark plug. After the flame is established, propagating through an ultra-lean charge is manageable [15]. Nonetheless, faster charge consumption in the MC is possible when the PC is operated actively and close to stoichiometry [14] which expectedly yields higher PC pressure build-up, thus higher jets temperature and momentum. Previous works by Toulsen et al. [2, 16] showed the potential of using different fuels (H2, C3H8, LPG, CH4) with a proven extension of lean limit and substantial emission reduction. Recently Inna et al. [13] developed a merit function toward optimum PC fuel properties, suggesting that high research octane number (RON) and mid-low octane sensitivity (OS) fuels are preferable.

Towards tailoring the PC behavior, multiple geometrical aspects are documented. Korb et al. [17] found that the nozzle offset can influence the PC scavenging. Similarly, Bolla et al. [18] observed that it is crucial for the PC charge mixing. Shah et al. [19] showed that larger PC volumes can prolong the lean limit. Gentz et al. [20] showed that λ ≈ 1 favors uniform volumetric distribution of jet within the chamber, thus enhancing combustion progression. However, in leaner conditions, smaller nozzles are needed to trigger combustion. Similarly, Shah et al. found that smaller nozzles facilitate the early flame development in the MC. Hlaing et al. [21] demonstrated experimentally that larger PC volumes yield faster combustion while enhancing combustion stability relative to small-sized PCs. 

Alongside experiments, computational modeling provides incremental knowledge to pre-chamber combustion. In the Reynolds-averaged Navier-Stokes (RANS) based approach, the assessment of various combustion models is documented. The multizone well-stirred reactor (MZ-WSR) model was utilized by Silva et al. [11, 14] with a satisfactory prediction of pre- and main chamber combustion on multiple pre-chamber compositions and geometries. The G-equation model was utilized in numerous works. Silva et al [21] utilized it and successfully reproduced the pressure evolutions behavior of a narrow throat PC engine operated with methane. Kim et al. [22] proposed that the turbulence-chemistry constants in Peters’s relation could be tuned to achieve correct pressure prediction, while the current work preserves the originally proposed turbulent constant values. Alkhamsi et al. [23] utilized the G-equation approach and demonstrated the significance of the laminar flame speed at ultralean conditions. That work verifies that once the turbulence generated by the pre-chamber is mostly dissipated and the role of convective transport is comparable to the turbulent enhancement, the correct prediction of the laminar flame speed becomes crucial to the correct prediction of the pressure build-up in a pre-chamber engine. Kammel et al. [24] utilized the extended coherent flame model (ECFM) and showed that adjustable injection timing can optimize the jet’s momentum utilization for combustion of the main charge.

Albeit extensive investigation, the comprehensive understanding of PC fundamentals at engine conditions remains incomplete. For example, whether the combustion is mainly driven by flame propagation or auto-ignition phenomena remains inconclusive [25-27]. Furthermore, the additional feature of a narrow throat and double layer of nozzles pre-chamber utilized in the current work promotes distinguishable nozzle behavior, thus is suitable for additional assessment. In addition, it is documented that both pre- and main chambers combustion occur with a large variation of turbulence-chemistry interaction (TCI) - time scales and length scales [21, 28] therefore, an adequate combustion model for predictive pre-chamber combustion modeling must account for these ample scales. A recent work by Tang et al. [27] performed in an optical engine suggested that, under stable engine operating conditions, a flame-based phenomenon is likely to represent the PC combustion. Among the previously discussed models, the G-equation has the advantage of explicitly accounting for the effect of TCI at various scales on its formulation, thus being attractive, provided that the pre-chamber combustion can be modeled by flame propagation.

Whatever the underlying physical mechanisms governing PC combustion might be, it is highly needed to assess and develop predictive models capable of representing the real physical processes involved in it. Multiple turbulence and combustion models were used in computational fluid dynamics (CFD) frameworks to replicate the pre-chamber combustion processes; it is crucial to comprehend these models and their simplifying assumptions before linking the computational results to measured data. To this end, the current work aims to utilize CFD to assess two combustion submodels: an MZ-WSR, and the G-equation model. While the former describes combustion as ignition of a locally homogenous mixture, the latter represents the bulk combustion phenomena as flame propagation. For broader applicability, five different operating conditions are chosen. The results suggest that both combustion models can potentially match experimental engine performance data upon appropriate calibration. Finally, all the turbulence-chemistry parameters ahead of the flame were obtained from the simulation data and were analyzed to understand the role of the TCI, depending on the corresponding combustion regime classification according to the Borghi-Peters diagram.
2. MATERIALS AND METHODS

2.1 Experimental data acquisition

Detailed explanations of experimental and numerical setups are discussed in previous works [21] and will be briefly quoted in the current work. The experiments were conducted at KAUST; the schematic of the testbed is found in [7, 8, 10]. The research engine is a Volvo D13C500 heavy-duty diesel engine modified to operate as a single-cylinder research engine and further equipped with a PC. The geometric compression ratio of 11.5 and a bowl-in re-entrant piston design were used. The air intake is fitted with port fuel injectors. The fuel supply to the pre-chamber is controlled with a mass flow controller. Both chambers were equipped with pressure sensors. Fuel was injected at -360 CAD for both chambers. The recorded data have a coefficient of variation of gross indicated mean effective pressure (CoV of IMEPg < 5%). Specifics of the engine are found in TABLE 1.

<table>
<thead>
<tr>
<th>TABLE 1: ENGINE SPECIFICATIONS [21]</th>
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<tbody>
<tr>
<td>Engine model</td>
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<tr>
<td>Piston shape</td>
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<td>Valve mechanism</td>
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<tr>
<td>Number of valves</td>
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<tr>
<td>Bore</td>
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<tr>
<td>Stroke</td>
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<tr>
<td>Connecting rod length</td>
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<tr>
<td>Compression ratio</td>
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<tr>
<td>Displacement volume</td>
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</table>

Table 2 displays the experimental conditions; methane with 99.5% purity by volume was utilized. The global $\lambda$ was adjusted while the total amount of fuel is split for active pre-chamber operation; for the current cases, the fraction of fuel energy delivered to the pre-chamber directly (pre-chamber fueling ratio - PCFR) was varied between 3-13%.

<table>
<thead>
<tr>
<th>TABLE 2: ENGINE OPERATING CONDITIONS</th>
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<tbody>
<tr>
<td>Engine Speed</td>
</tr>
<tr>
<td>Coolant temperature</td>
</tr>
<tr>
<td>Lubricant oil temperature</td>
</tr>
<tr>
<td>Intake temperature</td>
</tr>
<tr>
<td>Intake pressure</td>
</tr>
<tr>
<td>PC and MC fuel injection</td>
</tr>
<tr>
<td>PCFR</td>
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<tr>
<td>Excess air-fuel ratio ($\lambda_{global}$)</td>
</tr>
</tbody>
</table>

The KAUST pre-chamber dimensions are shown in Table 3. The benefit of the narrow-throat PC is to retrofit a diesel injector thus requiring minimal engine modification [8, 29]. Twelve nozzles are distributed in two layers, each containing six nozzles shifted by 30°.

<table>
<thead>
<tr>
<th>TABLE 3: PRE-CHAMBER DIMENSIONS (ADAPTED [21])</th>
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</thead>
<tbody>
<tr>
<td>Feature</td>
</tr>
<tr>
<td>Throat diameter</td>
</tr>
<tr>
<td>Nozzle diameter</td>
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<tr>
<td>Nozzle length</td>
</tr>
<tr>
<td>Number of nozzles</td>
</tr>
<tr>
<td>Volume</td>
</tr>
</tbody>
</table>

2.2 Modeling setup

CONVERGE™ was chosen as the CFD solver. Figure 1 shows the fluid domain. A fixed grid of 0.250 mm was used for the PC; the nozzles were kept at 0.125 mm; further information can be found in previous works [12]. To capture the early transients of the jet, a fixed embedding was utilized within the main chamber (after the nozzles) in an umbrella-like manner. A base grid size of 4 mm was initially adopted with AMR, with 3 levels of refinement (the finest mesh is 0.5 mm) in the main chamber far from the PC nozzles.

Unsteady Reynolds-averaged Navier-Stokes (RANS) with RNG k-ε turbulence model [30] was utilized to model turbulence. The coupling between pressure and velocity was done by the pressure-implicit with the splitting of operator (PISO) algorithm. The wall heat transfer model by O’Rourke and Amsden [31] was utilized. The Redlich-Kwong equation of state was used with real gas properties as a function of temperature, mixture-averaged diffusion coefficients, turbulent Prandtl number of 0.9, and turbulent Schmidt number of 0.78. A variable time step algorithm was used, with time steps ranging from $1 \times 10^{-8}$ to $1 \times 10^{-6}$ seconds, while limited by the Courant Friedrich Lew (CFL) number for convection of 1.0.

To further calibrate initial and boundary conditions, a full-system 1D GT-Power simulation was performed a priori. For that, the simplified PC object along with the SI turbulence flame combustion model was considered; the MC combustion was modeled using the built-in jet ignition combustion model. To ensure agreement, the heat release-based calibration (HRBC) was employed, where the apparent heat release rates are computed from the measured pressure traces. Additional boundary calibration ensured that the pumping loop of the pressure versus volume diagram was matched between the
model and the experiment. Details and illustrations on the calibration are found in [7, 10].

The models are initialized quiescently at exhaust valve opening (EVO) of the previous cycle; the major species (CO₂, CO, O₂, N₂, H₂O), pressure (from the experiment), and temperature (from 1D GT-power) are initially considered. The in-cylinder trapped mass and trapped fuel amounts are kept as the matching parameter between CFD and 1D models to ensure concordant energy content between the two. Initializing at EVO of the previous cycle allows for a complete exhaust stroke proceeded by a complete intake stroke, thus decreasing eventual effects from field initialization on the combustion stroke. The effective compression ratio was found to be 11.1, against 11.5 of the geometrical value, by matching the experimental motoring pressure curve [8]. The PC fueling was performed during the intake stroke; a detailed explanation of the injection strategy can be found in [7].

For combustion modeling, the multi-zone well-stirred reactor (MZ-WSR) and the G-Equation were considered. The detailed chemistry was obtained from the skeletal mechanism derived from GRI Mech 3.0 by Lu and Law [32]. The MZ-WSR is a detailed chemistry solver [33] which uses a set of CHEMKIN-formatted files to model chemical kinetics and uses the CVODE solver to compute the system of ordinary differential equations. MZ-WSR calculates the reaction rates for each elementary reaction present in the mechanism, while the CFD solver is responsible for handling the transport of species. Detailed derivation can be found in [15].

The reaction rate progress parameter \( q_i \), with \( i \) representing each individual reaction, is given by:

\[
q_i = k_{ri} \prod_{m=1}^{M} [X_m]^n_{m,i} - k_{fi} \prod_{m=1}^{M} [X_m]^{n'}_{m,i} \tag{1}
\]

where \( n' \) and \( n'' \) represent the stoichiometric of reactants and products, respectively, for a given reaction \( i \) and species \( m \); \( M \) is the total number of species. \( [X_m] \) is the molar fraction of the specie \( m \) and \( k \) is the reaction rate for each elementary reaction, with \( f \) and \( r \) representing forward and reverse reactions respectively, calculated from the Arrhenius law.

The G-Equation (2) is a non-reacting scalar level-set equation that describes the flame front in space and time. In combustion, it is a model for turbulent premixed combustion regimes, where \( G \) represents the flame location; the iso-scalar field \( G(x, t) = G_o \) marks the boundary between the unburned and burned mixture under the assumption of an asymptotically thin reaction zone with a defined local burning velocity. In CONVERGE, \( G_o = 0 \) is chosen as the flame location, while \( G < G_o \) represents the unburned premixed field and \( G > G_o \) represents the burned region, following the original formulation [34]. The specific derivations and scaling arguments are found in [35].

\[
\langle \rho \rangle \frac{\partial \tilde{G}}{\partial t} + \langle \rho \rangle \tilde{V} \cdot \nabla \tilde{G} = \langle (\rho S_T) - (\rho)k \tilde{D}' \rangle \nabla \tilde{G} \tag{2}
\]

where \( \rho \) is the density, \( \tilde{u} \) the field velocity, \( S_T \) the turbulent flame speed, \( \tilde{k} \) is the flame curvature, and \( D' \), the turbulent diffusivity. \( S_T \) is modeled using the well-known Peters’ correlation (3) [35]. It accounts for small and large-scale turbulence and is described as:

\[
S_T = S_L + u' \left\{ -\frac{a_1 b_1^2}{2b_1} Da + \left( \frac{a_1 b_1^2}{2b_1} Da + a_1 b_1 Da \right)^{\frac{1}{2}} \right\} \tag{3}
\]

where \( u' \) is the fluctuating turbulent component, \( l_T \) the turbulent length scale, \( \delta_T \) the flame thickness, \( b_1 \) and \( b_1 \) are model constants corresponding to large and small-scale turbulence enhancement, respectively, and \( S_L \) the laminar flame speed. The constants \( a_1 \) and \( b_1 \) were set to 0.78, 2.0, and 1.0, respectively, following the original formulation [35]. The Damkohler number \( (Da) \) is a ratio between the flow time scale \( (l_T/u') \) over the chemical time scale \( (\delta_T/S_L) \). \( u' \), was obtained from the transport equation for the turbulent kinetic energy \( (k) \) under the assumption of homogeneous and isotropic turbulence. Additional discussion can be found in previous works [21].

\( S_L \) was tabulated using the 1D utility tool in CONVERGE using the 30-specie skeletal mechanism by Lu and Law [32]. For the table generation, the initial temperature range was 600-1200 K, with a step size of 50 K, pressure ranging from 10-90 bar, equivalence ratio between 0.4 to 2, with step size was 0.05, and 0-15% of residuals with 5% step size. For the MZ-WSR model, the spark was modeled as a spherical source mimicking the arching and glowing phases. For the G-Equation, the G-field is sourced and the flame is initiated; in either case, the spark is located between the spark plug electrodes. When G-equation is used, the MZ-WSR is coupled on, behind, and ahead of the flame to compute the intermediate and post-reaction species.

3. RESULTS AND DISCUSSION

For a thorough validation, five cases at three different load conditions were considered and are shown in Table 4. Cases 1, 3, and 5 have the same PC fuelMEP (fuel mean effective pressure) with distinct global-\( \lambda \); cases 2, 3, and 4 have distinct PC fuelMEP and the same global-\( \lambda \). The spark timing was distinct since the considered experimental cases were the ones with maximum break torque.

### TABLE 4: SPECIFICS OF OPERATING CONDITIONS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>C-1</th>
<th>C-2</th>
<th>C-3</th>
<th>C-4</th>
<th>C-5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spark timing [CAD aTDC]</td>
<td>-11</td>
<td>-13</td>
<td>-13</td>
<td>-13</td>
<td>-15</td>
</tr>
<tr>
<td>Global – ( \lambda ) [-]</td>
<td>1.6</td>
<td>1.8</td>
<td>1.8</td>
<td>1.8</td>
<td>2.0</td>
</tr>
<tr>
<td>PCFR [%]</td>
<td>7.0</td>
<td>7.0</td>
<td>7.0</td>
<td>7.0</td>
<td>7.0</td>
</tr>
<tr>
<td>IMEP, [bar]</td>
<td>9.7</td>
<td>8.5</td>
<td>8.5</td>
<td>8.5</td>
<td>8.5</td>
</tr>
</tbody>
</table>

Figure 2 shows the comparison for the pressure build-up accompanied by the flame at the imminence of reaching the piston for the considered combustion models. The 500 experimental individual pressure cycles are overlaid in gray. In general, a satisfactory agreement was observed with both combustion models with an inherent minor mismatch in peak pressures and PC peak phasing. There are two major sources of
mismatches in the results: the early transients of pre-chamber pressure build-up result in distinct MC combustion initiation; in addition, the jet topologies are distinct among the combustion models, which inherently influences the early MC combustion process.

The 3D contours reveal that, although the PCs have 12 nozzles, it mostly relies on the major activity of 6 bottom nozzles. Silva et al. [21] discussed this unusual behavior, which is a combination of high-speed flow along the throat, followed by transonic flow at the top nozzle location, which prevents the comparable behavior to the bottom nozzles. Moreover, a major distinction in the jet topologies is observed; while G-Equation shows small jet exiting the top nozzles, the MZ-WSR only manifests the six bottom nozzle jets. Marquez et al. [36] utilized the same pre-chamber of the current study in an optically accessible engine configuration. His work with chemiluminescence imaging with active PC conditions revealed qualitatively agreement with the modeling results predicted by G-Equation, as shown in Figure 3 (small top jets and well-developed bottom jets).

Scanning through cases C1-C3-C5, it is possible to see the effect of main chamber enleanment, while in cases C2-C3-C4 the effect of pre-chamber enrichment is observed. Overall, when the MC enleanment is considered, a remarkable decrease in jet area is qualitatively observed, despite the PC pressure build-up being comparable. This suggests that the MC composition and its corresponding slower laminar flame speed play a crucial role in jet development. Damkohler’s first hypothesis [37] suggests that in high turbulence scenarios, the turbulent flame propagation scales with the turbulence enhancement; recent direct numerical simulation (DNS) [38] data confirmed that, while Kerstein [39] demonstrated the significance of the laminar component.

In addition, the differences in jet topology predicted by MZ-WSR become pronounced as the PC is enriched (C-4 having the richer PC). MZ-WSR models combustion as a mere ignition event, thus relying on the chemical kinetics of a well-stirred reactor model, therefore, the jet development is compromised provided the fast time scales imposed by the

FIGURE 2: COMPARISON OF DISTINCT COMBUSTION MODELS AGAINST EXPERIMENTS (PRESSURE CURVES OF C1 THROUGH C5 FROM LEFT TO RIGHT ON TOP) AND THE CORRESPONDING JET TOPOLOGY FOR DISTINCT COMBUSTION MODELS AT THE IMMINENCE OF REACHING THE PISTON (BOTTOM)

FIGURE 3: CHEMILUMINESCENCE IMAGING: ACTIVE PRE-CHAMBER OPERATION FOR THREE DISTINCT FUELMEP CONDITIONS (ADAPTED FROM MARQUEZ ET AL. [36]): (a) $\lambda_{GLOBAL} = 1.47$ AND PCFR 9%, (b) $\lambda_{GLOBAL} = 1.43$ AND PCFR 13%, (c) $\lambda_{GLOBAL} = 1.2$ AND PCFR 7%
high-speed jet. Whereas, G-Equation considers the established flame as an asymptotically thin layer embedded into the turbulent flow and explicitly accounts for the turbulence-driven wrinkling of the flame front. It is reasonable to affirm that the jet issuing event into the MC is a process with strong turbulence, therefore, having a model which explicitly accounts for the TCI effect is crucial for capturing the early transients of jet development.

The summary of the engine performance metrics is shown in Figure 4. The cases C1-C3-C5 are taken for analysis provided that the PCFR sweep had a minor influence on engine parameters, which was also reported in previous studies [40]. The indicated specific fuel consumption (ISFC) was, in general, kept similar as the MC was leaner. Note that among distinct combustion models the difference observed was small relative to the order of magnitude of the predictions. The maximum pressure ($P_{\text{max}}$) was at most different by 5%; minor differences are expected since no case-by-case tuning was performed.

It is worth noting that the maximum pressure rise rate (MPRR), although shows negligible differences among the combustion models, the trends were consistent regardless of the model utilized. Moreover, the higher MPRR for each individual case corroborates with the PC peak pressure phasing and inherent MC combustion initiation; for C1 and C5, G-Equation has a slightly higher MPRR provided its PC pressure peak is slightly advanced compared to MZ-WSR; by similar analysis, the C-3 trend is justified. Therefore, the results suggest that small deviations in the PC pressure phasing should be carefully considered. In general and consistently, G-Equation predicted longer combustion durations; Kim et al [38] observed the same and found it to be linked to the late combustion stages and associated near-wall combustion.

Prior to the near-wall combustion, the $CA_{50}$ was reasonably comparable among the distinct combustion models. As shown by Silva et al. [21], nearly 50% of the mass fraction of fuel burned is mainly driven by the convective field brought by the jets. The observed sweep in the trend from C3 to C5 is mainly associated with the inherited late phasing of the PC combustion, which was delayed for the G-Equation in the C3 case. More critically, the general trends were captured without any major model modifications.

Overall, as the main chamber is made leaner, the peak pressure tends to be lower provided that most of the fuel is consumed after the jet issuing event ceases and relies on flame propagation/ignition of a leaner charge. Inherently, the thermal sNOx formation follows the main chamber composition and the predicted pressure build-up between the two models; as the MC is leaner, thus with lower temperature, less sNOx is expected; similarly, the slightly lower peak pressure predicted by G-Equation corroborates the slightly lower sNOx values compared to MZ-WSR. Note that the accuracy of NOx prediction at such lean levels is still an open problem. Using the standalone extended Zel’dovich model may miss part of NO produced through $N_2O$ path; therefore, the development of NOx models validated at ultralean conditions is needed for improving the PC modeling predictions.

Ultimately, the energy distribution (Figure 5), reveals that the critical engineering metrics remain comparable among the distinct combustion submodels. Although the qualitative results on jet development suggest that the correct capturing of the TCI is crucial to describe the jet development, the hot jets are short-lived and the main bulk mixture combustion could be described by both combustion models with minor differences; this resulted in minor differences on the main engineering metrics among both combustion models. Therefore, as long as engineering metrics are considered, both combustion models can potentially match experimental data upon careful calibration for the considered condition.
The combustion regime for the PC/MC is shown in Figure 6 employing the Borghi-Peters (B-P) diagrams; the local $u'/S_L$ and $l_T/\delta_L$ trajectories are values computed from the simulation data at computational cells near (ahead) the flame as a mass-averaged quantity, as described by Silva et al [21]; the resolution of points was 0.1 CAD from spark timing until top dead center (TDC), and 1 CAD from TDC to end of combustion. For the considered cases, the initial flame, while in the PC, is located in the thin reaction zone regime, where $u'$ nearly one order of magnitude higher than $S_L$.

Detailed analysis of jet developments and turbulence-chemistry interaction can be found in previous work [21, 23]. As the jets are issued into the MC, $u'/S_L$ substantially aggrandizes with concomitant decrease in $l_T/\delta_L$ provided that the region around the jet has significant shear thus smaller turbulent structures. As the jet issuing finishes, the trend monotonically decays as the small-scale turbulent structures are quickly dissipated and subsequently enter the corrugated flamelet regime. Note that as the MC composition becomes leaner (C5), a critical modeling implication arises, provided that the original G-Equation formulation has arguable validity beyond Karlovitz

$$= 100 (K_{aS} = 1) [35, 41, 42].$$

Therefore, the predictive modeling of ultra-lean engine operation at high turbulent conditions should consider additional investigation on the validity of the original formulation and scaling arguments to predict combustion accurately at ultralean turbulent conditions.

Note, however, that the flamelet assumption being overshadowed by the existence of the broken reaction zone, until today, remains debatable as widely reported in the literature [41, 42]. The so-called distributed regime has not been observed either experimentally [42] or from DNS data [38, 41]. Recent works on active optical PC engines, despite the high turbulence levels, suggest it to be a flame dominant phenomenon [27, 36, 43-46], provided the consistent attachment of the flame to the nozzle exit.

### 3.1 Detailed analysis of jet development

Figure 7 shows the flame development in both pre-chamber (a) and main chamber (b). The case with $\lambda_{\text{global}} = 1.8$ and PCFR 3% (C2) is taken for further analysis of detailed jet development; this case is considered since its pressure curves have a minor mismatch, thus being a good candidate to isolate the combustion model effects on the jet development.

In general, minor deviations between model and experiments arise from locally stratified mixtures within the PC which are inherently carried over to the MC prediction. It is vital to ensure that the PC pressure is nearly the same as in the experiments and the following behavior must be a consequence of the combustion progression. The pre-chamber flame development (Fig. 7 (a)) shows the early transients to be different. Kim et al. [47] observed similar differences when comparing the two models. Despite the flame initiation mechanism being distinct, all the cases show faster pressure rise rate when utilizing G-Equation compared to MZ-WSR, with exception of one case (C-3). Mainly, G-Equation, considers an established flame that will further propagate, while MZ-WSR relies on energy deposition and subsequent ignition, thus justifying the delayed response.

Analyzing the jets for the bottom nozzles, as they leave the PC and develop into the MC, considering engine times for similar jet tip locations, the transients of their topology are...
significantly distinct. The initial jet (Figure 7 (b)-I) is much thinner (arrows 1 and 2) for the MZ-WSR case; while the transport of $\dot{G}$ depends on physical variables, MZ-WSR relies on the autoignition at a cell level to capture the jet formation. Provided that the jets are significantly fast, the associated small flow time scales compete with the ignition time-scale, and the jet development is radially deficient, while the axial jet development is comparable. More critical, as the jets enter the main chamber, it is expected that the strong turbulence around the jet will enhance its radial propagation, therefore, the results suggest that having TCI on the model formulation is crucial for capturing the early jet transients.

The faulty bottom nozzle behavior in the early transients can be understood by investigating Figure 8. While the bottom nozzles have a larger flow rate, the top nozzles have compromised flow and temperature; note, however, that still there flow through them. Provided that G-Equation models combustion as a flame propagation, even though the top nozzle flow is compromised, the flame propagates outwards. On contrary, the MZ-WSR model took longer until autoignition happened at the nozzle vicinity (Figure 7 (b)-IV); from that point onwards, the subsequent combustion is qualitatively comparable, thus justifying the similarities in global engine metrics.

3.2 A priori note on major modeling uncertainties

The major sources of uncertainties need to be identified and understood prior to fine-tuning physical models utilized in predictive PCC modeling. One major uncertainty is the correct prediction of the lambda inside the pre-chamber. Haling et al. [7] demonstrated the calibration methodology while Silva et al. [14] demonstrated the major mismatches that may arise if the pre-chamber is artificially enriched. More recently, Alkhamis et al. [23] demonstrated that a dominant effect on PC modeling resides in the correct prediction of the laminar flame component. Figure 9 shows the G-Equation results for pressure prediction comparison when utilizing distinct laminar flame speeds and the Peters’ relation for the turbulent flame speed following the original formulation.
Note that the discrepancy among the three cases arises only after the strong jet issuing event ceases and the convective transport of the $G\tilde{c}$ field by the jet is minimized so that the effects of turbulent transport and turbulent flame propagation become crucial in determining the overall burning rate. Alkhamsi et al. [23] demonstrated (not shown here) that by tailoring Gulder’s model a perfect match was possible, thus proving the significance of correct laminar flame speed for ultralean PC engine modeling. While ultralean $S_l$ measurements with conventional methods are challenging, the ultralean engine data serves as a practical benchmark for the validation of newly developed mechanisms for ultralean engine operation. Ultimately, towards high fidelity modeling of pre-chamber engines, the major sources of uncertainties need to be identified and corrected prior to proposing fine-tuning of turbulence-related constants and combustion models.

4. CONCLUSION

The comparison between G-Equation and MZ-WSR models revealed that the turbulence-chemistry interaction (TCI) at the early jet development is crucial and should be captured by the combustion model formulation to predict the jet topology with high fidelity. G-Equation, which explicitly accounts for TCI, revealed significant differences in early jet topology compared to the ignition-based MZ-WSR model.

Despite major differences in the early jet development between the two combustion models, the overall engine performance metrics remained comparable. Therefore, both combustion models can potentially match experimental engine performance data upon appropriate calibration. The combustion regime according to the Borghi-Peters diagram revealed that further fundamental studies are needed to evaluate the validity of the G-Equation beyond the combustion regimes it was derived for. Finally, the combustion submodels showed relatively minor effects on global engine metrics, while the basic model calibration and the choice of chemical mechanism with an accurate prediction of the laminar flame speed are among the dominant components toward high fidelity pre-chamber combustion modeling.

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