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A large-eddy simulation study on the influence of diesel pilot spray quantity on methane-air flame initiation



H. Kahila*, O. Kaario, Z. Ahmad, M. Ghaderi Masouleh, B. Tekgül, M. Larmi, V. Vuorinen

Department of Mechanical Engineering, Aalto University School of Engineering, Puumiehenkuja, 502150 Espoo, Finland

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ABSTRACT

The present study is a continuation of the previous work by Kahila et al. (2019), in which a dual-fuel (DF) ignition process was numerically investigated by modeling liquid diesel-surrogate injection into a lean methane-air mixture in engine relevant conditions. Earlier, the injection duration (t_{ini}) of diesel-surrogate exceeded substantially the characteristic autoignition time scale. Here, such a pilot spray ignition problem is studied at a fixed mass flow rate but with a varying t_{inj} . The focus is on understanding the influence of pilot quantity on spray dilution process and low- and high-temperature chemistry. In total, ten cases are computed with multiple diesel pilot quantities by utilizing a newly developed large-eddy simulation/finite-rate chemistry solver. The baseline spray setup corresponds to the Engine Combustion Network (ECN) Spray A configuration, enabling an extensive validation of the present numerical models and providing a reference case for the DF computations. Additionally, experimental results from a singlecylinder laboratory engine are provided to discuss the ignition characteristics in the context of a real application. The main results of the present study are: (1) reducing t_{inj} introduces excessive dilution of the DF mixture, (2) dilution lowers the reactivity of the DF mixture, leading to delayed high-temperature ignition and slow overall methane consumption, (3) low enough pilot quantity ($t_{ini} < 0.3$ ms) may lead to very long ignition delay times, (4) cumulative heat release is dominated by low/high-temperature chemistry at low/high t_{inj} values, (5) analysis of the underlying chemistry manifold implies that the sensitivity of ignition chemistry on mixing is time-dependent and connected to the end of injection time, and 6) long ignition delay times at very low t_{ini} values can be decreased by decreasing injection pressure.

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1. Introduction

Utilization of natural gas as a primary fuel in stationary gas engines is gaining more attention as stringent emission and thermal efficiency requirements rise, and liquefied gas distribution networks become more common [1,2]. As natural gas consists mainly of methane, it produces low CO_2 emissions per unit of energy and when operated in lean conditions, low NO_x emissions can be obtained due to low combustion temperatures [2]. Since methane is a potent greenhouse gas and a relatively low reactivity fuel [3], an engine ignition system must provide a locally sufficient energy source to ensure ignition at a right timing and to avoid incomplete combustion of the charge (i.e. methane slip). To ensure a successful premixed flame initiation in engines, manufacturers seek

* Corresponding author, E-mail address: heikki.kahila@aalto.fi (H. Kahila). for a better understanding and control over the ignition and the early premixed flame initiation to develop a more reliable ignition system.

Besides conventional electrode-based spark and pre-chamber [4] ignition systems, a dual-fuel (DF) pilot ignition concept is utilized in some commercial gas engines. Here, by DF pilot ignition we refer to a concept where a relatively small quantity of highreactivity fuel, e.g. liquid diesel fuel, is injected into an engine cylinder filled with a gaseous premixed primary fuel-air charge. The high-reactivity fuel autoignites and releases an energy deposit, high enough to initiate a premixed flame. Typically, the contribution of the pilot-fuel to the total energy is held below 10% [5] but in demand, a completely conventional diesel combustion mode (100%) can be retained in many commercial implementations [3].

Even though there are already various commercial implementations of DF pilot ignition systems, only recently, details of the flame initiation process have been investigated in experiments and simulations. In particular, Schlatter et al. [6], Srna et al. [7] and

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Fig. 1. An artistic illustration of the comparison between a conventional diesel spray and a dual-fuel pilot ignition process. The art work is based on the authors' numerical work on diesel sprays [9] (left) and data used to compile the present publication (right).

Kahila et al. [8] have investigated the topic in detail. While Schlatter et al. and Srna et al. conducted optical imaging in a rapid compression machine (RCM), Kahila et al. [8] utilized a large-eddy simulation (LES) to investigate 3d ignition chemistry. We summarize the main findings of these recent DF studies by a visual illustration in Fig. 1, where a comparison between a conventional single-fuel (SF) diesel spray flame and a DF pilot fuel ignition concept is presented. Besides a different oxidizer composition (presence of methane in DF), the key difference between the two configurations in Fig. 1 is the quantity of injected diesel surrogate, which is considerably lower for the DF pilot case. Typically in DF pilot ignition system, a relatively short injection duration (t_{ini}) is applied, which leads to a more diluted diesel mixture within the spray envelope after the end of injection. According to the aforementioned studies [6-8], there are three common stages during the SF and DF autoignition processes: (I) turbulent mixing, (II) volumetric activation of low-temperature chemistry (LTC), i.e. first-stage ignition, and (III) volumetric activation of hightemperature chemistry (HTC), i.e. second-stage ignition, at the spray tip. For a SF spray, high-temperature ignition is followed by a highly luminous lifted quasi-steady diffusion flame, whereas for a DF pilot spray, ignition is followed by a premixed methane-air flame initiation and its subsequent propagation in space (IV). Each of these stages is illustrated in Fig. 1 for a conventional diesel spray flame and for a DF pilot spray ignition. In the following, these stages are further explained from the literature point of view.

Within the LTC regime, diesel fuel is decomposed into various intermediate/radical species with a considerable heat release [7,8,10]. In particular, LTC (stage II) is experimentally observed by laser diagnostics on formaldehyde in both SF [7,10] and DF [7] configurations. Following LTC, chemical progress leads to local high-temperature ignition pockets (i.e. kernels) around the spray tip (III), which has been observed experimentally [6,7,10,11] and numerically [8] in both SF and DF configurations.

Srna et al. [7] observed in RCM experiments that both the low- and high-temperature ignition stages of diesel fuel are delayed with an increase in ambient methane concentration [7]. For reference, a factor of ~ 1.3 delay in high-temperature ignition between a no-methane and a lean equivalence ratio $\phi_{CH_4} = 0.5$ cases was found (ambient temperature and pressure at start of injection corresponded to \sim 850K and \sim 25 bar, respectively). The experimental observations indicated that a significant part of the overall delay was attributed to the inhibited low-temperature ignition chemistry. This observation was further strengthened by numerical investigations by Kahila et al. [8] in terms of 1d and 3d simulations, and reaction sensitivity analysis. In particular, the inhibiting influence of methane was observed throughout the oxidation process with the strongest impact on LTC. Furthermore, Kahila et al. [8] report that ignition favors mixture fraction values close to the most reactive mixture fraction, consistent with earlier findings by Demosthenous et al. [12] who carried out a direct numerical simulation (DNS) study on ignition of inhomogeneous n-heptane-CH₄-air mixtures with presence of decaying homogeneous isotropic turbulence. Both works by Demosthenous et al. [12] and Kahila et al. [8] report that methane consumption is initiated due to heat release and interaction with intermediate species originating from the diesel surrogate oxidation.

Aside from the above studies on diesel-methane DF pilot spray ignition, there is a body of literature in the context of homogeneous charge compression ignition (HCCI) [13,14] and reactivity controlled compression-ignition (RCCI) [15,16] concepts, where the oxidation of mixed low- and high-reactivity fuels is an important aspect to explore. Burke et al. [17] observed an influence of methane on early decomposition reactions of DME in homogeneous mixtures (0d problem). Ghaderi Masouleh et al. [18] concluded that the molar ratio of diesel surrogate and methane is a key variable when considering ignition characteristics of homogeneous mixtures. The DNS studies by Bhagatwala et al. and Luong et al. [19,20] reported co-existing deflagration and spontaneous ignition fronts for igniting *n*-heptane/*iso*-octane mixtures under thermochemical conditions representative for RCCI.

Most of the available DF combustion literature is related to experimental works on performance, efficiency and combustion stability issues in laboratory engines [5,21–27]. Injection parameters of pilot fuel have been noted to contribute greatly on dual-fuel engine performance and emissions. Often, a trade-off between emissions and pilot fuel injection strategy is described: with the increase of engine load and pilot quantity and the advance of pilot diesel injection timing, hydrocarbon (HC) emissions decrease but NO_x emissions increase [5,26,28]. Similarly, in RCCI type low-temperature DF combustion modes, optimized pilot injection timing and quantity are desired to achieve a stable ignition delay time (IDT) and complete combustion [29,30].

Under low pilot fuel consumption levels or in RCCI type combustion modes, early injection and low pilot quantities may be desired. In such cases, many have reported that high dilution of pilot fuel leads to a higher IDT value, longer combustion duration [31,32], and in the worst case, to unstable flame initiation and incomplete combustion [26,28,29,32].

Based on the literature, there is a research gap in a detailed explanation of dependence and sensitivity of DF autoignition chemistry on very low pilot fuel quantity. For example, based on DF combustion chamber experiments, Grochowina et al. [32] reported poor ignition probability for spray cases with low pilot fuel quantity and, in contrast to experiments in RCM configuration [6,7], ignition kernels were observed near the injector in cases with low pilot quantity. Such differences in ignition characteristics were presumably attributed to local changes in reactivity due to pilot fuel dilution process and nozzle dribbling [32]. Furthermore, Aksu et al. [25] noted the need for detailed understanding on mixing and chemistry effects in DF split injection optimization and Nieman et al. [33] envisioned improvements to RCCI control by optimizing injection strategies by e.g. fuel quantity modification.

While Kahila et al. [8] investigated DF pilot spray ignition in a numerical configuration with $t_{inj} > IDT$, here we concentrate on cases with $t_{inj} < IDT$. Following the same case configuration [8], we choose the Engine Combustion Network (ECN) [34] "Spray A" case as the framework for the present numerical work. ECN is an international research collaboration facilitating experimental and computational engine research. Several experimental studies have been carried out for non-reacting and reacting Spray A cases at different ambient conditions [10,35–37], providing extensive validation data for numerical models. In order to narrow the scope of the present study, we concentrate on the DF pilot spray ignition event with only minor discussion on large scale flame propagation. In this respect, the main objectives of this work are to:

- 1. demonstrate the influence of diesel pilot quantity on DF ignition characteristics in a methane-air mixture,
- 2. explain the dependence of IDT on pilot quantity from mixing and chemistry points of view,
- 3. define heat release modes (LTC/HTC) relevant to DF pilot ignition and discuss their variance as a function of pilot quantity,
- demonstrate the influence of injection pressure on the pilot ignitability at low pilot quantities.

2. Numerical methods

- (~~)

2.1. Governing equations and turbulence modeling

The Eulerian gas phase is described by the compressible Navier–Stokes equations. The Favre-filtered LES formulation for the continuity, momentum, species and energy equations is the following:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho} \widetilde{u}_i}{\partial x_i} = \overline{S}_{\rho},\tag{1}$$

$$\frac{\partial \left(\overline{\rho}\widetilde{u}_{i}\right)}{\partial t} + \frac{\partial \left(\overline{\rho}u_{i}u_{j}\right)}{\partial x_{j}} = \frac{\partial}{\partial x_{j}}\left(-\overline{p}\delta_{ij} + \overline{\rho}\widetilde{u}_{i}\widetilde{u}_{j} - \overline{\rho}\widetilde{u}_{i}\widetilde{u}_{j} + \overline{\tau}_{ij}\right) + \overline{S}_{u,i},$$
(2)

$$\frac{\partial \left(\overline{\rho}\widetilde{Y}_{k}\right)}{\partial t} + \frac{\partial \left(\overline{\rho}\widetilde{u}_{i}\widetilde{Y}_{k}\right)}{\partial x_{i}} = \frac{\partial}{\partial x_{i}} \left(\overline{\rho}\widetilde{u}_{i}\widetilde{Y}_{k} - \overline{\rho}\widetilde{u}_{i}\widetilde{Y}_{k} + \overline{\rho}\widetilde{D}\frac{\partial\widetilde{Y}_{k}}{\partial x_{i}}\right) + \overline{S}_{Y_{k}} + \overline{\omega}_{k},$$
(3)

$$\frac{\partial \left(\overline{\rho}\widetilde{h}_{t}\right)}{\partial t} + \frac{\partial \left(\overline{\rho}\widetilde{u}_{j}\widetilde{h}_{t}\right)}{\partial x_{j}} = \frac{\partial \overline{p}}{\partial t} + \frac{\partial}{\partial x_{j}} \left(\overline{\rho}\widetilde{u}_{j}\widetilde{h}_{s} - \overline{\rho}\widetilde{u_{j}h_{s}} + \frac{\overline{\lambda}}{\overline{c}_{p}}\frac{\partial \widetilde{h}_{s}}{\partial x_{j}}\right) \\ + \overline{S}_{h} + \overline{\omega}_{h}, \qquad (4)$$

where $\overline{\rho}$, \widetilde{u}_i , \overline{p} , \widetilde{Y}_k , \widetilde{h}_s and $\overline{\tau}_{ij}$, denote the filtered density, velocity, pressure, species k, sensible enthalpy and conventional viscous stress tensor, respectively. In particular, the overbar denotes an unweighted ensemble average, whereas the tilde (\sim) denotes a density-weighted ensemble average. A Lewis number of unity is assumed for all species, and thus the diffusion coefficient is $D = \lambda/(\rho c_p)$ with c_p and λ denoting the heat capacity and thermal conductivity of the gas mixture, respectively. In Eq. (4) the total enthalpy \widetilde{h}_t is defined as a sum of the sensible enthalpy and the specific kinetic energy,

$$\widetilde{h}_t = \widetilde{h}_s + \frac{\widetilde{u}_i \widetilde{u}_i}{2}.$$
(5)

The source terms \overline{S}_{ρ} , $\overline{S}_{u,i}$, \overline{S}_{Y_k} and \overline{S}_h allow the coupling between the liquid and gaseous phases with respect to mass, momentum, species and energy. The production rate of the species *k* is denoted by $\overline{\omega}_k$ and the heat release rate (HRR) in Eq. (4) is formulated as $\overline{\omega}_h = \sum_k \Delta h_{f,k}^o \overline{\omega}_k$, where $\Delta h_{f,k}^o$ is the enthalpy of formation. The system of equations is closed by the filtered ideal gas law.

The governing Eqs. (1)-(4) are solved using the finite volume method within the OpenFOAM-2.4.x environment [38]. The reacting PISO (Pressure Implicit with Splitting of Operator) algorithm [39] is utilized for the pressure-momentum coupling. The time integration is based on an implicit, three time-level, and secondorder accurate scheme. The diffusion terms are discretized by a 2nd-order central scheme, whereas the treatment of the convective flux interpolation is closely related to the implementation of the unclosed LES subgrid terms in Eqs. (2)-(4), i.e. turbulence subgrid scale (SGS) modeling. Following our previous work on Spray A, the SGS treatment is based on an implicit approach [8,9,40], where the dissipative contribution of subgrid scales is resolved by utilizing a dissipative non-linear flux limiter by Jasak et al. [41]. The control parameter of the flux limiter is set to 0.3 for momentum, whereas a parameter value of unity is chosen for the scalars to ensure a bounded total variation diminishing solution. Such an approach is termed as the implicit LES (ILES) due to a lack of explicit dissipation terms. Further information on the similarity between the implicit and the more common explicit SGS models is discussed in Refs. [42–44].

2.2. Spray and combustion modeling

Validation of the present LES configuration is carried out in our previous work [8] but, for completeness, the applied model setup is briefly outlined in this section and the major benchmark results are provided in Ref. [8] as well as in supplementary material.

The Lagrangian particle tracking (LPT) method is applied to model the injected liquid phase with the same model setup equivalent to our previous works on Spray A [8,9,45]. The primary breakup is considered by sampling computational parcels from the Rosin–Rammler size distribution with Sauter mean diameter of 6 μ m. The secondary break-up is modeled by the KHRT model [46,47]. Heat and mass transfer between the two phases is modeled according to the standard correlations by Frössling [48], and Ranz and Marshall [49,50].

The change of the thermochemical composition over a CFD time step is governed by chemical kinetics and is formulated as a non-linear stiff initial-value problem, leading to a system of ordinary differential equations (ODE). Here, the ODE system is solved independently in each finite volume cell by the 12th order

Table 1Common specifications for the simulation cases.

	ECN Spray A	DF cases					
Injection conditions							
Fuel	n-C ₁₂ H ₂₆	n-C ₁₂ H ₂₆					
Nominal nozzle diameter, D	90 µm	90 µm					
Fuel temperature	363 K	363 K					
Injection pressure	150 MPa	150 MPa					
Ambient conditions							
Temperature	900 K	900 K					
Density	22.8 k/m ³	22.8 k/m ³					
O ₂ % (molar)	15.0	15.0					
CO ₂ % (molar)	6.230	5.955					
H ₂ O % (molar)	3.620	3.460					
$N_2 \%$ (molar)	75.150	71.835					
CH ₄ % (molar)	0	3.750					
ϕ_{CH_4}	0	0.5					
Z _{st}	0.0435	0.0234					

semi-implicit Euler extrapolation method (abbr. Seulex) [51]. Fast analytical reaction rate and species' Jacobian evaluation is obtained from the open-source *pyJac* library [52]. Further information on speed-up techniques related to linear algebra and parallelization can be found from our previous work [8].

The effect of turbulence-chemistry interactions (TCI) is considered via first order closure hypothesis, i.e. reaction rate $\overline{\dot{\omega}}_k \approx \dot{\omega}_k(\widetilde{Y}_i, \widetilde{T}, \overline{p})$ and no subgrid scale model is applied for the chemical source terms in Eqs. (3)–(4). Intense turbulent mixing and a relatively high grid resolution together with finite-rate chemistry is assumed to capture the major features of the ignition chemistry in a broadened reaction zone. Previously, the spray autoignition problem has been reported to be less sensitive to subgrid scale modeling parameters compared to e.g. flame stabilization problem [53,54], hence, the present study concentrates on ignition are neglected.

Multiple LES studies with a similar first-order TCI hypothesis have shown a rather good agreement against experiments [55–61], which is mainly attributed to a relatively high grid resolution [56,58,60]. In particular, Pei et al. [62] applied the same technique in Spray A LES context and obtained good IDT results with a grid spacing equivalent to the present work. Fulton et al. [58] report reasonable results with an average grid resolution corresponding to half of the laminar flame thickness. As discussed in our previous work [8], the grid spacing applied in the present configuration corresponds to 0.6-1.6 times the relevant laminar flame thickness estimates, leading to a reproducible experimental Spray A IDT value. In addition, the present first-order hypothesis is shown to provide numerically consistent IDT values and spatial formaldehyde fields compared to our earlier flamelet based (TCI included) results (see Refs. [9,40]). It is worth noting that spray-LES studies with sophisticated combustion models such as transported probability density function (TPDF) and conditional moment closure (CMC) models have been typically applied in cases with a lower grid resolution compared to the present work (2–8 \times the cell size applied in this work) [63–66]. The first order closure hypothesis can not be generally recommended for such resolutions.

3. Simulation configuration

The present LES computations are carried out in the same configuration as our previous DF spray study [8]. In the ECN Spray A experiments liquid *n*-dodecane is injected with a 150 MPa pressure from a 90-µm diameter nozzle hole into a constant volume combustion vessel where a pre-burn combustion event is utilized to yield mixture and thermodynamic conditions relevant for combustion engines. The detailed Spray A configuration is presented in Table 1. For the numerical DF cases, the same configuration is considered, but methane is added to form a $\phi_{CH_4} = 0.5$ ambient mixture (equivalence ratio w.r.t CH₄-air only). Other concentrations are modified such that the molar oxygen concentration is constant 15% in both cases. When applying Bilger's definition for mixture fraction (*Z*) [67,68], the stoichiometric mixture corresponds to $Z_{st}^{SF} = 0.0435$ and $Z_{st}^{DF} = 0.0234$ in SF and DF cases, respectively. In the DF cases, *Z* = 0 corresponds to the $\phi_{CH_4} = 0.5$ methane/air mixture.

The discretized CFD domain shares the same volume with the experimental combustion vessel at Sandia National Laboratories [34] and a uniform 62.5 μ m cell size is applied throughout the spray penetration regime. Previous studies show that reliable LES results of Spray A can be achieved with such a cell size [9,40,45,62,69].

The injected pilot fuel quantity is modified by varying the end of injection time (EOI). Table 2 and Fig. 2a show the pilot quantities and rate of injection profiles for all the simulated cases. The injection profiles are adopted from a virtual injection profile generator [70], suggested by the ECN. The injection durations are chosen such that the injected pilot fuel mass is in a range of experimental configurations (per nozzle hole) [7,27,71,72]. In total, ten DF LES cases were simulated and the corresponding case abbreviations with respect to injection duration are listed in Table 2.

To highlight the influence of EOI within the present Lagrangian droplet framework, snapshots of the early mixing process and droplet distributions are illustrated in Fig. 2b for the three selected cases (DF- ∞ , DF-250 and DF-150). For DF-250 and DF-150, pilot fuel droplets evaporate quickly after EOI with subsequent pilot fuel dilution in the vicinity of the spray core. The following analysis concentrates on the influence of pilot quantity on the turbulent mixing (dilution) and ignition processes.

3.1. Rationale for a chemical mechanism

The skeletal mechanism by Yao et al. [73] (54 species and 269 reactions) is utilized in the following computations and is hereafter referred to as the Yao mechanism. The mechanism is originally designed and extensively tested for SF mixtures with *n*-dodecane as the primary fuel [73,74]. However, the recent investigations by Kahila et al. [8] demonstrated the Yao mechanism to be able to describe the methane related oxidation pathways comparable to a more detailed mechanism by Frassoldati et al. [75]. For completeness, performance of the Yao mechanism to cover 0d homogeneous ignition and laminar flame propagation problems in lean methaneair mixtures is demonstrated in the supplementary material.

Besides a good performance in SF methane-air combustion problems, rationale for the utilization of the Yao mechanism can be reasoned by considering the available reaction pathways. The

Table 2

The applied pilot injection duration (t_{inj}) (ms) and the equivalent quantity m_{inj} (mg) for the designated cases. The maximum mass flow rate for all cases is $\dot{m}_f \approx 2.5$ g/s. DF-LIP denotes the case with low injection pressure, $p_{inj} = 50$ MPa.

	Spray A	DF-∞	DF-500	DF-400	DF-300	DF-250	DF-225	DF-200	DF-150	DF-100	DF-LIP
t _{inj} (μs)	∞	∞	500	400	300	250	225	200	150	100	100
m _{inj} [mg]	-	-	1.148	0.898	0.656	0.536	0.476	0.416	0.295	0.176	0.087



Fig. 2. (a) *n*-dodecane injection rate profiles (mass flow rate (g/s)) for the cases given in Table 2. Profiles are based on modeling work in Ref. [70]. (b) Illustration of Lagrangian droplet distributions for DF-∞, DF-250 and DF-150 cases.

Yao mechanism contains 20 reactions including CH₄ from which 9 are reverse ones and interacting with higher hydrocarbons. Such reactions have been reported to be essential during the lowtemperature DF ignition chemistry together with an interaction between various intermediate species and radicals such as OH, HO₂, H₂O₂, CH₂O and CH₃ [8,76]. For example, the Yao mechanism includes 26/33 of the most important reactions relevant for CH₄-air autoignition chemistry with CH₂O and H₂O₂ additives [8,76]. Both CH₂O and H₂O₂ species are also products of the *n*-dodecane decomposition at low-temperature reactions, and hence, we assume that a large coverage of the reactions is relevant for any mechanism in DF applications. Even though lack of detailed experiments on chemical kinetics of *n*-dodecane/methane fuel blends prevents a thorough validation, we assume that essential reaction paths are included and the DF ignition process is described in the extent of acknowledged uncertainties.

4. Laboratory engine configuration

The experimental IDT results have been acquired from a singlecylinder laboratory engine corresponding to our previous work [77]. The primary fuel (99.9% pure methane) is port-injected and the diesel-fuel is directly injected from a common rail-based 3hole (160 µm) piezo injector with 100 MPa rail pressure. The engine speed was set to 1500 RPM and the target equivalence ratio and charge temperature at TDC are estimated to $\phi_{CH_4} = 0.5$ and ~ 840*K*, respectively (assuming isentropic compression). The utilized 100 MPa rail pressure allows the minimum injection duration of 0.11 ms for the pilot fuel (manufacturer limit).

The laboratory engine is based on an AGCO 84 AWI 6-cylinder common rail diesel engine but is converted into a single-cylinder configuration with a wide control over input parameters related to fuel injection system, intake-air, valve actuation and exhaust. An aftermarket (EG2000) methane port injection system was adapted for distributing methane into the intake manifold at -360CAD ATDC during the intake stroke. The pilot diesel fuel was injected at -8CAD ATDC. The diesel mass flow was measured in a separated test campaign where the engine was operated 20 minutes in conventional diesel combustion mode resulting in average fuel consumption estimates. The evaluation of a combustion event is considered here via incylinder pressure, measured by a Kistler pressure transducer that was mounted in the cylinder head. The pressure data was sampled every 0.2CAD and was further processed to calculate the net heat release rate (NHRR) [78].

5. Results

5.1. Experimental observations of dual-fuel ignition with low pilot fuel quantities

In the following, we extend our previous experimental DF engine work [27,77] by introducing new IDT results with a recently implemented injection system which allows engine scale investigations with very small diesel pilot quantities. The following experimental results demonstrate that with equal injection configuration, the IDT of pilot fuel depends strongly on injection duration below $t_{inj} < 0.2$ ms. This result should be considered as a standing hypothesis for the later numerical LES analysis.

In a series of engine experiments, the pilot quantity was varied by reducing t_{inj} from 0.4 to 0.11 ms. Figure 3a shows the mean incylinder pressure traces and the corresponding NHRR for all cases with averaging considering 100 sequential cycles. An IDT for the injected pilot fuel is defined as the time interval between the SOI and the time instant where 2% of the cumulative heat release is achieved.

The estimated IDT values in Fig. 3b show no dependence on pilot quantity when $t_{inj} > 0.2$ ms, whereas with any lower value the IDT rapidly increases. As it can be interpreted from the incylinder pressure traces and HRR profiles in Fig. 3a, the cases with $t_{inj} < 0.2$ ms (pink curve) yield considerably lower heat release rates and maximum pressures, which is attributed to incomplete combustion of the methane-air charge. Furthermore, excessive peak-pressure and IDT variation was noted in cases with $t_{inj} < 0.2$ ms (cf. Fig. 3b). Here, we do not comment on the combustion efficiency of the presented measurement points but the motivation is to highlight typical implications of t_{inj} on IDT in DF engines.

In order to illustrate the DF pilot ignition event in an engine configuration, Fig. 4 shows images acquired by the optical instrumentation in a similar single-cylinder engine. The presented



Fig. 3. (a) Mean in-cylinder pressure traces and net heat release rates with t_{inj} corresponding to 0.4, 0.35, 0.3, 0.25, 0.2, 0.15, 0.13, 0.12 and 0.11ms. (b) The mean IDT values as a function of t_{inj} with error bars indicating the sample min/max values.



Fig. 4. (a) A single-cylinder DF engine configuration with a two-hole injector. Natural luminosity imaging of premixed flame initiation (b) and subsequent propagation (c) at 2.97 and 7.7 CAD after top dead center, respectively. The present results are taken from our previous work [27] at conditions resembling the case with $t_{inj} = 0.4$ ms in Fig. 3b.

natural luminosity-based images are obtained from our previous work [27] at conditions resembling the case with $t_{inj} = 0.4$ ms. The natural luminosity based images in Fig. 4 show a volumetric formation of igniting gas pockets originating from the two separate pilot sprays (two-hole nozzle). After the pilot ignition, the flame kernels are convected azimuthally due to swirl and their sizes grow with increase in methane consumption. Interpreting the characteristic ignition features from such engine experiments in details is challenging due to the influence of high swirl, turbulence, thermal and mixture stratification, and the finite optical resolution. Hence, simplified numerical experiments enable us to make more in-depth comments on the ignition process also in DF engines.

5.2. LES results: Influence of diesel fuel pilot quantity on IDT

In Section 5.1, the experimental results indicated a threshold value for injection duration, below which IDT is considerably increased. In this section we present numerical findings similar to the experimental observations and provide detailed analyses

on the ignition characteristics including evolution of local mixture composition and the subsequent heat release. Additionally, we show that a decrease in pilot quantity has a suppressing influence on the early kernel size and its growth rate.

We begin the analysis by comparing the evolution of mixture fraction (Z), temperature (T), heat-release rate (HRR), dodecyl peroxy radical $C_{12}H_{25}O_2$ (RO₂) and H_2O_2 mass fraction fields for the DF- ∞ , DF-250 and DF-150 cases (cf. Table 2). Figure 5 shows the fields on a *zy*-plane at time instances t = 0.45 and t = 0.65 ms (before ignition in any of the cases). In Fig. 5a (t = 0.45 ms), the influence of an early EOI is visible for the DF-250 and DF-150 cases. First, lower Z values indicate faster dilution of the mixture, which is also visible in Fig. 2b at already t = 0.25 ms. Second, slightly higher T and HRR values indicate an earlier activation of the LTC compared to DF- ∞ . Such an early LTC activation can be further identified from higher concentrations of an *n*-dodecane decomposition product RO2 and from an intermediate species H₂O₂, typically attributed to LTC and early HTC stages [79]. For the DF-250 and DF-150 cases, production of intermediate species and subsequent HRR occur within the whole spray envelope,



Fig. 5. DF pilot ignition process in cases DF- ∞ , DF-250 and DF-150 at (a) t = 0.45 ms and (b) t = 0.65 ms. The blue dotted contour line corresponds to stoichiometric mixture

 Z_{st} . (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 6. (a) Temporal evolution of $CH_{4,min}$, $RO_{2,max}$, OH_{max} and T_{max} for the cases DF- ∞ , DF-250 and DF-150 and (b) the quantified first- (\bigstar) and second-stage (\bigstar) IDT values for all cases.

whereas for the continuous injection case, it is restricted to downstream regions (z > 15 mm), where the influence of the high-speed two-phase spray is reduced (lower turbulent strain and composition gradients).

Following LTC, the cases evolve towards the final hightemperature ignition by incremental temperature rise near spray tip, visible at t = 0.65 ms in Fig. 5b. At this stage, dilution of the mixture is more evident for the DF-250/150 cases and e.g. \tilde{Z} values reaching stoichiometry can be found only at the spray tip and near nozzle regions. At the EOI, an overall mass and momentum conservation near the nozzle induces a so-called entraiment wave which increases dilution and premixing of the pilot-fuel [80]. Such dilution appears strongest at z < 25 mm. Besides the apparent dilution, the temperature increase and HRR values are also lower for the DF-250/150 cases compared to that in DF- ∞ . The HRR correlates directly with the local \tilde{Z} value, further discussed in the next section. While continuous injection of n-dodecane induces a constant production of LTC-related species, such as RO₂ and H₂O₂, their relative mass fractions appear lower in the DF-250/150 cases. In particular, for the DF-250/150 cases at $t \ge 0.65 \text{ ms}$, RO₂ is entirely consumed from the system by reactions attributed to late LTC and early HTC [8]. Lack of long hydrocarbon radicals and dilution of the mixture including various intermediate species have an overall inhibiting influence to the ignition process and is further analyzed in the following sections.

The qualitative findings of the inhibiting dilution effects are quantified in Fig. 6 in terms of the IDT. Figure 6a shows the time evolution of maximum (minimum) values for temperature, RO₂, CH₄ (min.) and hydroxyl radical OH mass fractions for the DF- $\infty/250/150$ cases. Here, we define the 1st-stage IDT (t_{1st}^* , \bigstar) as a time instance when the maximum RO₂ mass fraction reaches $\tilde{Y}_{RO_2} = 7 \cdot 10^{-4}$ in the system ($\sim 20\%$ of maximum in DF- ∞). The primary high-temperature 2nd-stage IDT (t_{2nd}^* , \bigstar) is defined as a time instance when 95% of available methane is locally consumed. This definition is inspired by the findings of our previous work [8] where the flame initiation was reported not to follow a certain temperature threshold but instead CH₄ consumption and the rise of OH concentration, as also visible in Fig. 6a. The corresponding t_{1st}^* and t_{2nd}^* values for all simulated cases are presented in Fig. 6b

as a function of the injection duration (t_{inj}) . For a detailed comparison to the SF Spray A case, please see Ref. [8].

Figure 6b shows how the t_{1st}^* value is almost constant for all cases with a minor decrease at $t_{inj} < 0.25$ ms, which is attributed to more favorable mixing conditions and lack of high turbulent strain [81]. The influence of finite injection duration is also leading to lower peak RO₂ mass fraction values and fast decay to zero after the EOI when no fresh *n*-dodecane is introduced to the system. Even though the maximum RO₂ time evolution appears weaker for the DF-250 compared to DF- ∞ , it shares otherwise similar time evolution towards the 2nd-stage ignition, yielding only 5% delay in t_{2nd}^* value (=IDT). However, reducing the injection duration to 0.15ms (DF-150) yields already 47% delay in IDT compared to the DF- ∞ case. A slope of the temperature rise in the DF-150 case is considerably steeper than in the other cases and actually appears similar to typical homogeneous ignition problems (0d). In general, the IDTs in Fig. 6b show similar dependence on pilot quantity as observed in the engine experiments, cf. Fig. 3b.

Aside from the absolute IDT quantification above, the initial size of the emerging ignition kernel and its growth towards a premixed flame is discussed next. In Fig. 7 we illustrate the high-temperature ignition kernels by volume rendering regions with T > 1400 K at the time of ignition and 0.13 ms afterward. There is a large difference in the original kernel size between the three cases. For the DF- ∞ case, the whole spray tip region reaches temperatures beyond 1400 K (I), whereas only a singular millimeter-size kernel appears in the DF-250 case (II) and no properly visible kernel is seen in the DF-150 case (III). The volumetric growth of the initial hightemperature ignition kernels is also slowing down with decreasing pilot quantity as depicted by Fig. 7 (second row). In real engine conditions where coherent flow structures and ambient turbulence is present, the small and slowly growing ignition kernels of the DF-250/150 cases could be possibly suppressed / quenched, yielding incomplete combustion [32]. Possibility for flame quenching would be even higher for the DF-100 case, which is therefore neglected in our later analysis. Due to turbulence model restrictions, further analysis on the premixed flame propagation is not investigated but we concentrate on explaining the aspects leading to the observed initial ignition kernel sizes.



Fig. 7. 3d view at the time of ignition $(t = t_{2nd}^*)$ (top row) and at $t = t_{2nd}^* + 0.13$ ms (bottom row). Translucent gray and green isosurfaces correspond to $Z = 1 \cdot 10^{-4}$ and Z_{st} , respectively. The blue isovolumes illustrate premixed flame initiation (T > 1400 K), indicating decrease in original ignition kernel size and their respective growth rate with decrease in EOI. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 8. (a) Time evolution of \tilde{Z} PDF for the DF-250 case where the dashed line presents the mean $\langle \tilde{Z} \rangle$, (b) the mean values $\langle \tilde{Z} \rangle$ for DF- $\infty/250/150$ cases and (c) example PDF distributions at t = 0.45 and 0.65 ms. Statistics consider data points within the spray cloud only, i.e. $\tilde{Z} > 1 \cdot 10^{-4}$. Blue and orange star symbols refer to first- and second stage ignition, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

5.3. Analysis of mixture formation statistics

As Fig. 5 illustrated, the ignition process is not only delayed in time with decrease in pilot quantity but the heat release is also taking place more on the lean side and the LTC is restricted to a time window prior to 2nd-stage ignition. Next, we investigate the time evolution of mixture fraction and heat release rate statistics and show that modes of HRR change as a function of pilot quantity. In particular, heat is released within considerably leaner mixtures and the relative fraction of LTC is increasing with decreasing pilot quantity.

Figures 8–10 show the time evolution of probability density functions (PDF) of \tilde{Z} , \tilde{T} and HRR, respectively. It is worth noting that the statistics are conditioned by $\tilde{Z} > 1 \cdot 10^{-4}$ to highlight the mixture state within the pilot spray region. As expected for the short injection cases, the dilution process starts quickly after EOI and leads to rapidly decreasing mean \tilde{Z} values (cf. 8a,b) and narrower distributions (cf. Fig. 8c). For example, in both DF-250/150 cases, the mean \tilde{Z} values are already below stoichiometric mixture ($Z_{st} = 0.0234$) at the time of DF- ∞ ignition. Interestingly, even though there is a 40% difference in IDT between the DF-250 and DF-150 cases, the respective \tilde{Z} PDFs are quite similar for both cases at $t = 0.65 \,\mathrm{ms}$ (cf. Fig. 8c).

As discussed by Demosthenous et al. [12] and Kahila et al. [8], the most reactive mixture fraction (Z_{MR}) increases with increasing methane concentration in DF mixtures (cf. supplementary material for further information). In the present case, Z_{MR} corresponds to 3.4 times the Z_{st} value in DF mixtures ($Z_{MR}^{DF} = 0.08$). With respect to LES statistics in Fig. 8, the tails of \tilde{Z} distributions do not reach Z_{MR} value in the DF-250/150 cases after t > 0.45 ms. From such an inert mixing perspective, ignition can be assumed to be delayed with increase in dilution.

Figure 9 shows the time evolution of temperature statistics within the spray clouds. As dictated by the mixing line relation, diluting spray leads to a larger representation of higher temperature values at earlier time instances, which may partially accelerate the early LTC even though the overall \tilde{Z} values are low. While all cases share a similar rise in mean temperature value after the 1st-stage ignition, high positive rate of temperature change continues only for the DF- ∞ case. Low mean temperature values in the DF-250/150 cases are consistent with the small ignition kernel sizes, shown in Fig. 7. Hence, the temperature growth rate analysis is consistent with the mixture fraction analysis.

Finally, the time evolution of HRR PDFs (per unit volume) in Fig. 10 is consistent with the observations above: all three cases show similar distributions until the first-stage ignition where the



Fig. 9. (a) Time evolution of \tilde{T} PDF for the DF-250 case where the dashed line presents the mean $\langle \tilde{T} \rangle$, (b) the mean values $\langle \tilde{T} \rangle$ for DF- $\infty/250/150$ cases and (c) example PDF distributions at t = 0.45 and 0.65 ms. Statistics consider data points within the spray cloud only, i.e. $\tilde{Z} > 1 \cdot 10^{-4}$. Blue and orange star symbols refer to first- and second stage ignition, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 10. (a) Time evolution of logarithmic HRR PDF for the DF-250 case where the dashed line presents the mean $\langle \log_{10}(\tilde{\omega}_h) \rangle$, (b) the mean values $\langle \log_{10}(\tilde{\omega}_h) \rangle$ for DF- $\infty/250/150$ cases and (c) example PDF distributions at t = 0.45 and 0.65ms. Statistics consider data points within the spray cloud only, i.e. $\tilde{Z} > 1 \cdot 10^{-4}$. Blue and orange star symbols refer to first- and second stage ignition, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 11. Mean logarithmic HRR values conditioned by mixture fraction at (a) t = 0.45, (b) 0.65 ms and (c) $t = t^*$ (IDT). The scatter point data represents only 0.5% of the total data (uniform random sampling) within the spray cloud. Statistics consider data points within the spray cloud only, i.e. $\tilde{Z} > 1 \cdot 10^{-4}$.

Table 3

Grouping of total HRR by chemistry modes. The critical threshold values are $RO_{2,cr} = 1 \cdot 10^{-5}$, $H_2O_{2,cr} = 1 \cdot 10^{-4}$, $OH_{,cr} = 1 \cdot 10^{-5}$ and $T_{cr} = 1150$ K.

Group name	Definition	Fig. 12 color
LTC	$(\text{RO}_2 \ge 1 \cdot 10^{-7}) \cap (\text{H}_2\text{O}_2 < \text{H}_2\text{O}_{2,cr}) \cap (T < T_{cr})$	
LTC late	$(\mathrm{RO}_2 \ge 1 \cdot 10^{-7}) \cap (\mathrm{H}_2\mathrm{O}_2 \ge \mathrm{H}_2\mathrm{O}_{2,cr}) \cap (T < T_{cr})$	
pre-HTC	$(RO_2 < RO_{2,cr}) \cap (H_2O_2 \ge H_2O_{2,cr}) \cap (T < T_{cr})$	
HTC pre-ign.	$(OH < OH_{,cr}) \cap (T \ge T_{cr})$	
HTC	$(OH \ge OH_{,cr}) \cap (T \ge T_{cr})$	



Fig. 12. Volume integrated total HRR within the spray cloud $(Z>1 \cdot 10^{-4})$ as a function of normalized time with division to classes, defined in Table 3. Regions with the hatch pattern refer to rich mixtures $(Z>Z_{st})$. Black solid line corresponds to the total HRR. The pie charts represent the total heat release up till $t/t^* = 1.1$ as percentages without distinction between lean/rich mixtures. Note a different scale on *y*-axes.

local maximum is achieved due to heat release from LTC reactions activated in a relatively large volume (cf. Fig. 5a). Shortly after the local maximum, the mean HRR values decrease and start to rise only prior to the 2nd-stage ignition. As shown by the PDFs at t = 0.65 ms in Fig. 10c, the maximum HRR values are the highest for the DF- ∞ case.

In order to describe the relation between Z and HRR, Fig. 11 shows the mean profiles of HRR, conditioned on mixture fraction for both DF- ∞ and DF-250 cases. In both cases, the high HRR values favor \tilde{Z} values above Z_{st} . Overall, HRR values in lean conditions are considerably lower than in rich conditions.

In order to relate \hat{Z} and HRR distributions to each other at different stages of the ignition process, we differentiate the volume integrated total heat release rate (THRR) to separable categories with respect to chemistry mode (LTC/HTC) and mixture composition (lean/rich). Figure 12 demonstrates how the THRR is originating from different modes of ignition chemistry, depending on the time instance and case. Inspired by the recent DNS study by Borghesi et al. [82], we divide the THRR into 5 groups, denoted as LTC, late LTC, pre-HTC, HTC pre-ignition and HTC. The transition between LTC and HTC is not an obvious process, hence we set a temperature threshold of 1150K to identify between the two main modes, whereas the subdivision is based on threshold values for RO_2 , H_2O_2 and OH mass fractions, listed in Table 3. Note that in case of SF CH₄/air mixture, LTC would be a non-existing group due to lack of RO_2 . Additionally, a hatch pattern is applied in Fig. 12 to separate lean and rich mixtures within a prescribed subgroup. The group division can be interpreted in the following way:

- LTC: regions where HRR is mainly originating from very early *n*-dodecane decomposition to e.g. RO₂.
- late LTC: regions where production of LTC-related species accumulate (e.g. RO₂, H₂O₂, CH₃, HO₂).
- pre-HTC: regions with low temperatures, high concentrations of various intermediate species and lack of long-hydrocarbon radicals. Typically at spray tip region prior to activation of HTC.
- HTC pre-ign: regions where temperature has increased considerably but no 2nd-stage ignition-related species (OH) is present. Typically at spray tip region.
- HTC: regions with high temperature and strong concentration of OH.

The optimal threshold values for the HRR mode categorization are acknowledged to depend on the mixture state. The threshold values in Table 3 were chosen after carrying out numerical tests on homogeneous 0d reactors and transient LES data. Most importantly, the following interpretations made from such a simple categorization were insensitive to the exact threshold values.

By using the above categorization, we can identify three characteristic differences between the DF- ∞ , DF-250 and DF-150 cases in Fig. 12: First, the THRR value is over 10 times larger for the DF- ∞ case compared to that for two other cases at the time of ignition, which is attributed to the higher overall injected energy and higher reactivity of the rich DF mixture. Second, HRR from early and late LTC regions is always originating from rich mixtures (see also Fig. 11), whereas the share of lean mixtures becomes prominent at the pre-HTC and HTC regions after $t/t^* > 0.6$ (for DF-250/150 only). Third, the relative fraction of LTC from the overall heat release is considerable in DF-250/150 cases.

Overall, coverage of the LTC modes account for over 80% (pre-HTC included) of the total heat release (THR) prior to ignition for DF-250 and DF-150 cases, which is two times more than in the DF- ∞ case. Figure 13 shows the THR up to $t = 1.1t^*$ and its source from LTC/HTC as a function of injection duration for all DF cases. Below $t_{inj} < 0.3$ ms, the relative fraction of LTC is highly increased, as also noted in Fig. 12. Here, the pre-HTC mode could be also interpreted as LTC induced chemistry, leading to homogeneous ignition and subsequent HTC chemistry.

Such a large fraction of heat release from LTC/pre-HTC is considerable from ignition system design and computational modeling



Fig. 13. Relative fraction of total heat release from LTC, pre-HTC and HTC up to $t = 1.1t^*$ for all DF cases.

points of view. A rapid transition from one HRR mode to another may be important to consider when RCCI type combustion is desired in real applications [30]. When considering the present immature status of DF chemical kinetics and available chemical mechanisms, there are high uncertainties related to a detailed description of LTC and hence, the overall ignition process. For example, Kahila et al. [8] compared two chemical mechanisms in SF and DF spray context and reported that the major difference between the mechanisms was related to HRR in LTC conditions. As a remark, we note that numerical observations on high heatrelease quantities from low-temperature combustion should be carefully considered and investigated when reporting DF research.

5.4. Influence of pilot quantity on the chemistry manifold

As discussed in sections above, even with very low pilot fuel quantities, the overall reactivity of a pure methane-air mixture is increased. On the other hand, reducing injection duration strengthens the mixing process of the pilot fuel and its decomposition products, which results in lower total HRR, and hence, longer IDTs. However, local reactivity differences between the cases have not been clearly quantified so far: the influence of e.g. local RO₂ and H_2O_2 concentration differences to global measures such as IDT and volumetric growth rate of ignition kernels has not been discussed. In this section we quantify reactivity differences between the DF cases and define the evolution of ignition process in a thermochemical manifold spanned by *Z* and a progress variable \mathcal{Y} .

We begin the analysis by evaluating how an evolved spray cloud would ignite under a frozen flow assumption. Figure 14 presents an ignition index field defined as

$$I_{0d} = \max\left(1 - \frac{t_{0d}^*(Y_i, T, p, t)}{t_{MR}^*}, 0\right),\tag{6}$$

where $t_{0d}^*(Y_i, T, p, t)$ is defined as an IDT based on 0d homogeneous reactor computations with initial conditions corresponding to the cell-wise mixture composition, temperature and pressure at LES simulation time $t = t_{LES} = 0.6$ ms. The time instance is chosen to represent relevant mixing and chemical state prior to the second stage ignition. A normalization constant t_{MR}^* corresponds to the minimum IDT value found from 0d homogeneous reactor computations (i.e. at Z_{MR}). Ignition index can be interpreted as a normalized reactivity index for which values range from zero to one, corresponding to less-reactive and reactive mixtures, respectively. Influence of turbulent strain is neglected in the proposed definition and hence, the index resembles plain thermochemical effects.

Figure 14 shows major differences in I_{0d} values between the three cases. Whereas large parts of the spray envelope are covered



Fig. 14. Visualization of the ignition index field I_{0d} defined in Eq. (6) at simulation time t = 0.6 ms. The white dotted line corresponds to Z_{st} .

by relatively high I_{0d} values ($I_{0d} > 0.6$) in the DF- ∞ case, the values are in average much lower and more fragmented in the DF-250/150 cases. In particular, only the very end of the spray tip in DF-150 case is reaching I_{0d} values beyond 0.2. The aforementioned observation supports the qualitative hypothesis presented along the discussion on Fig. 5: lower local concentrations of pilotfuel and its intermediate by-products (cf. RO₂) correlate with lower reactivity and temperature. Hence, from a plain composition point of view, the volumetric ignition potential is considerably reduced with decreasing pilot fuel quantity, which to some degree (frozen flow assumption) explains the weakened volumetric growth rate of early ignition kernels in DF-250/150 cases.

In order to investigate the thermochemical progress leading to such reactivity fields, as illustrated in Fig. 14, we define a reaction progress variable \mathcal{P} consisting of species relevant to both *n*-dodecane and methane oxidation:

$$\mathcal{P} = \frac{Y_{RO_2}}{M_{RO_2}} + \frac{Y_{H_2O_2}}{M_{H_2O_2}} + \frac{(Y_{CH_4}^{ox} - Y_{CH_4})}{M_{CH_4}},$$
(7)

where the contribution of early *n*-dodecane decomposition (RO_2), intermediate states (H_2O_2) and flame initiation (CH_4) are described in a balanced way. The mass fraction value is normalized by the corresponding molar mass and $Y_{CH_4}^{OX}$ corresponds to the ambient oxidizer composition. Since in non-premixed combustion the



Fig. 15. Conditional mean of the rate of change of the progress variable $\langle \dot{y} \rangle$ on $\tilde{Z}y$ -plane. The orange dashed line resembles an ignition path corresponding to mean $(\langle \tilde{Z} \rangle, \langle y \rangle)$ -point-pairs, evaluated from data obtained according to Eq. (9). The circles denote evenly sampled time instances with a $\Delta t = 0.1$ ms interval, starting from $t_0 = 0.25$ ms. Regions I and II refer to LTC and HTC, respectively, while III marks a relatively long transition process between the prescribed regions in the DF-150 case. Blue and orange star symbols refer to first- and second stage ignition, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

progress variable depends on mixing, P is normalized for a given mixture fraction Z_i as

$$\mathcal{Y}(Z_i) = \frac{\mathcal{P} - \min\left(\mathcal{P}(Z_i)\right)}{\max\left(\mathcal{P}(Z_i)\right) - \min\left(\mathcal{P}(Z_i)\right)}.$$
(8)

Due to a non-trivial influence of two fuels on chemical kinetics, the present simple definition may, in theory, yield non-monotonic behavior, which, however, was not found problematic for the following practical analysis. For any other type of work, e.g. flamelet modeling, further consideration on the precise choice of \mathcal{P} and \mathcal{Y} is recommended.

Definition of \mathcal{Y} allows a construction of a simplified visualization of the high-dimensional chemistry manifold, relevant to the DF ignition process. Figure 15 shows the averaged rate of change of progress variable (denoted as $\langle \dot{\mathcal{Y}} \rangle$) values with double conditioning in the $\widetilde{Z}\mathcal{Y}$ -plane. The data is obtained by computing $\langle \dot{\mathcal{Y}} \rangle$ as a post-processing step at all available time instances. In order to minimize the variance of $\langle \dot{\mathcal{Y}} \rangle$ and to obtain a fair comparison between different DF cases, we sample data with resolved scalar dissipation rates below $\chi_{\rm res} < 5s^{-1}$.

In order to describe the transient ignition chemistry evolution on this manifold we construct an ignition trajectory, defined as $\langle \langle \widetilde{Z} \rangle, \langle \mathcal{Y} \rangle \rangle$ -point-pairs corresponding to conditional means $\langle \widetilde{Z} | \mathcal{Y} > \mathcal{Y}_{10\%} \rangle$ and $\langle \mathcal{Y} | \mathcal{Y} > \mathcal{Y}_{10\%} \rangle$, where $\mathcal{Y}_{10\%}$ is a limit value based on the last 10% of the progress variable's cumulative distribution function

$$\int_{\mathcal{Y}_{10\%}}^{\infty} f(\mathcal{Y}) \, d\mathcal{Y} = 0.1. \tag{9}$$

The aim of this is to follow the reaction progress in the $\widetilde{Z}\mathcal{Y}$ -plane.

Figure 15 shows $\langle \dot{\mathcal{Y}} \rangle$ on the prescribed manifold together with the ignition trajectory. As expected, the manifold structure includes two main regimes with considerable $\langle \dot{\mathcal{Y}} \rangle$ values (I, II), corresponding to already defined LTC and HTC regions in space. These two regions are divided by a "valley" of low $\langle \dot{\mathcal{Y}} \rangle$ values. The DF- ∞ case (Fig. 15a) has a very similar structure to SF manifolds, reported in [9], whereas for the DF-250/150 cases (Fig. 15b,c) the manifold is modulated by the influence of mixture dilution. For example, in the DF-250 case (Fig. 15b), the separation of the two regions is rather narrow at high \mathcal{Y} values. Decreasing the pilot quantity reduces the size of both LTC and HTC regions in the manifold but the overall structure remains similar.

The embedded ignition trajectory in Fig. 15 shows major differences between the three cases. Continuous injection (Fig. 15a) allows the chemically active spray parts to remain on the rich side and accumulate chemical reaction progress within the LTC part of the manifold (I). The early EOI in the other two cases leads the trajectory towards low $\langle \dot{\mathcal{Y}} \rangle$ values and eventually the trajectory reaches local maximum and minimum $\langle \dot{\mathcal{Y}} \rangle$ values around the "valley".

As discussed earlier in the context of Fig. 12, the transition from LTC to 2nd-stage ignition may occur steadily including a large HTC pre-ignition phase (orange fill in Fig. 12) as in DF- ∞ case, or rapidly without such a phase as in DF-150. This is also seen in Fig. 15c, where the $(\langle \widetilde{Z} \rangle, \langle \mathcal{Y} \rangle)$ -point-pairs spend considerably long time between the two main manifold regimes (II vs. III), before climbing towards the HTC ignition. It is worth noting that changing the threshold limit in Eq. (9) results in minor trajectory deviations with no influence on the evolution noted above.

Several implications and interpretations can be made from the analysis above: (1) The overall structure of the manifold resembles the one found in SF combustion [9], (2) ignition trajectory is sensitive to changes in mixing when located on the border of regions between I and II, (3) long enough accumulation of chemical progress (heat release) should be obtained on the LTC side to ensure a smooth and continuous transition from LTC to HTC regions.

As a remark, in order to further understand the prescribed interpretations, we influenced the mixture formation process of the DF-100 case by decreasing the injection pressure to 50 MPa (DF-LIP case). The decrease in injection pressure resulted in less prominent mixing and thus, higher local mixture fraction values compared to the original DF-100 case. As further discussed in Appendix A, the IDT of the DF-LIP case was found ~50% lower than in the corresponding DF-100 case. Interestingly, ignition kernels were observed at two distinct locations, first near the nozzle region and followed by the spray tip region. Such a formation of ignition kernel near the injector has been experimentally observed by Grochowina et al. [32] with low pilot quantities. A visual illustration is provided in Appendix A.

6. Conclusions

In the present work, a dual-fuel ignition process was investigated. In particular, an *n*-dodecane pilot spray injection into a lean methane-air mixture was investigated by utilizing an LES solver with finite-rate chemistry. The simulations are based on the Engine Combustion Network Spray A case, enabling an extensive validation of the numerical framework. The baseline Spray A target conditions were modified to create a dual-fuel relevant model problem by adding methane to the ambient oxidizer composition with a methane-air equivalence ratio of 0.5.

In total, ten LES cases were simulated with a constant mass flow rate and varying injection duration (t_{inj}) . In addition, experimental IDT results are presented from DF engine experiments. The main findings of the paper are mainly of numerical character and listed below:

- Both engine experiments and LES simulations indicate that there is a threshold value for the injection duration, below which the high-temperature IDT is considerably increased.
- The onset of low-temperature chemistry (first-stage IDT) is not influenced by t_{inj} as much as the high-temperature chemistry (second-stage IDT).
- The initial size and growth rate of the ignition kernel are decreased with decrease in pilot quantity.
- A decrease in injection duration (< 0.3 ms) leads to a faster pilot fuel dilution process and reduced production of heat and radicals, yielding an overall lower reactivity within the pilot spray.
- The relative fraction of rich low-temperature chemistry on total heat release is dominating (> 80%) in case of low pilot fuel quantity.
- The transition from rich low-temperature chemistry mode to lean high-temperature ignition was considered by the chemistry manifold analysis on mixture fraction - progress variable plane. The structure of the manifold was found to be rather insensitive to pilot fuel quantity, whereas the trajectory of the ignition process on this plane was noted to be strongly affected by the end of injection time.
- The finding is that the *n*-dodecane methane air mixture should remain at rich enough conditions (e.g. relevant Z_{MR}) for long enough time which will lead to a smooth and quick transition between the 1st and 2nd-stage IDTs.
- A decrease in injection pressure leads to an increased reactivity within a more confined spray envelope. In such a low-injection pressure spray case, IDT is reduced by \sim 50% compared to the case with higher injection pressure.

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Appendix A. Remark on the influence of injection pressure

The leading hypothesis from the results provided in previous sections is that the pilot spray will yield a successful ignition if the *n*-dodecane-methane-air mixture remains at high enough mixture fraction values for a long enough induction time at which sufficient quantities of heat and radicals are produced. In order to review this hypothesis, we chose the DF-100 case and decreased the injection pressure from 150 to 50 MPa and kept the injection duration in 0.1ms (DF-LIP, in Table 2). Change in injection pressure leads to a ~50% lower pilot quantity than in the DF-100 case, hence also a smaller overall chemical energy deposit. Furthermore, a ~55% lower nominal injection velocity is induced compared to the DF-100 case. For brevity, in detail analysis is not carried out but the influence of injection pressure reduction on the IDT and initial kernel size is next discussed.

The LES results of DF-LIP case indicate less prominent mixing and thus, higher local mixture fraction values compared to the original DF-100 case. A successful ignition is observed at



DF-LIP

Fig. A1. 3d view of the DF-LIP case at the time of ignition ($t = t_{2nd}^*$) (top row), $t = t_{2nd}^* + 0.2 \text{ ms}$ (middle row) and $t = t_{2nd}^* + 0.5 \text{ ms}$ (bottom row). Translucent gray and green isosurfaces correspond to $Z = 1 \cdot 10^{-4}$ and Z_{st} , respectively. The blue isovolumes illustrate premixed flame initiation (T > 1400 K).(For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

t = 0.7 ms, approximately 50% earlier than the reference DF-100 case. Figure A.16 illustrates a unique feature of the ignition observed in the DF-LIP case: the first ignition kernel appears close to the injector (I) and it is followed by a second kernel at the spray tip region (II). Low turbulence levels and a relatively high pilot fuel concentration contribute to the appearance of 2nd-stage ignition near the nozzle within a relevant time scale. Overall, the initial flame kernel sizes are small (millimeter scale) and their growth rate is rather slow compared to DF-250 and DF- ∞ cases, cf. Fig. 7.

Even though this numerical demonstration has no direct experimental correspondence for now, similar observations were recently reported by Grochowina et al. [32]. In particular, the decrease in injection pressure from 1500 to 500 bar reduced the ignition delay time by \sim 50% in the experiments and an ignition kernel formation near the nozzle (optical imaging) is reported for the lowest pilot fuel quantities [32].

To conclude, the present numerical findings support the ideas that the pilot ignition characteristics can be controlled in engine relevant conditions which is an important aspect in practical engineering design and engine manufacturing.

Supplementary material

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.combustflame.2019.05. 025.

References

- H.M. Cho, B.Q. He, Spark ignition natural gas engines A review, Energy Convers. Manag. 48 (2) (2007) 608–618, doi:10.1016/j.enconman.2006.05.023.
- [2] T. Korakianitis, A.M. Namasivayam, R.J. Crookes, Natural-gas fueled sparkignition (SI) and compression-ignition (CI) engine performance and emissions, Prog. Energy Combust. Sci. 37 (1) (2011) 89–112, doi:10.1016/j.pecs.2010.04. 002.
- [3] B.B. Sahoo, N. Sahoo, U.K. Saha, Effect of engine parameters and type of gaseous fuel on the performance of dual-fuel gas diesel engines – A critical review, Renew. Sustain. Energy Rev. 13 (6–7) (2009) 1151–1184, doi:10.1016/j. rser.2008.08.003.
- [4] C.E.C. Alvarez, G.E. Couto, V.R. Roso, A.B. Thiriet, R.M. Valle, A review of prechamber ignition systems as lean combustion technology for SI engines, Appl. Therm. Eng. 128 (2018) 107–120, doi:10.1016/j.applthermaleng.2017.08. 118.
- [5] R. Papagiannakis, D. Hountalas, C. Rakopoulos, Theoretical study of the effects of pilot fuel quantity and its injection timing on the performance and emissions of a dual fuel diesel engine, Energy Convers. Manag. 48 (11) (2007) 2951–2961, doi:10.1016/J.ENCONMAN.2007.07.003.
- [6] S. Schlatter, B. Schneider, Y. Wright, K. Boulouchos, N-heptane micro pilot assisted methane combustion in a Rapid Compression Expansion Machine, Fuel 179 (2016) 339–352, doi:10.1016/j.fuel.2016.03.006.
- [7] A. Srna, M. Bolla, Y.M. Wright, K. Herrmann, R. Bombach, S.S. Pandurangi, K. Boulouchos, G. Bruneaux, Effect of methane on pilot-fuel auto-ignition in dual-fuel engines, Proc. Combust. Inst. (2018), doi:10.1016/J.PROCI.2018.06.177.
- [8] H. Kahila, A. Wehrfritz, O. Kaario, V. Vuorinen, Large-eddy simulation of dualfuel ignition: Diesel spray injection into a lean methane-air mixture, Combust. Flame 199 (2019) 131-151, doi:10.1016/j.combustflame.2018.10.014.
- [9] H. Kahila, A. Wehrfritz, O. Kaario, M. Ghaderi Masouleh, N. Maes, B. Somers, V. Vuorinen, Large-eddy simulation on the influence of injection pressure in reacting Spray A, Combust. Flame 191 (2018) 142–159, doi:10.1016/J. COMBUSTFLAME.2018.01.004.
- [10] S.A. Skeen, J. Manin, L.M. Pickett, Simultaneous formaldehyde PLIF and high-speed schlieren imaging for ignition visualization in high-pressure spray flames, Proc. Combust. Inst. 35 (3) (2015) 3167–3174, doi:10.1016/j.proci.2014. 06.040.
- [11] N. Dronniou, J. Kashdan, B. Lecointe, K. Sauve, D. Soleri, Optical investigation of dual-fuel CNG/Diesel combustion strategies to reduce co2 emissions, SAE Int. J. Engines 7 (2) (2014) 2014–01–1313, doi:10.4271/2014-01-1313.
- [12] E. Demosthenous, G. Borghesi, E. Mastorakos, R.S. Cant, Direct numerical simulations of premixed methane flame initiation by pilot n-heptane spray autoignition, Combust.d Flame 163 (2016) 122–137, doi:10.1016/j.combustflame. 2015.09.013.
- [13] X. Lü, Y. Hou, L. Zu, Z. Huang, Experimental study on the auto-ignition and combustion characteristics in the homogeneous charge compression ignition (HCCI) combustion operation with ethanol/n-heptane blend fuels by port injection, Fuel 85 (17–18) (2006) 2622–2631, doi:10.1016/J.FUEL.2006.05.003.
- [14] S. Khandal, N. Banapurmath, V. Gaitonde, S. Hiremath, Paradigm shift from mechanical direct injection diesel engines to advanced injection strategies of diesel homogeneous charge compression ignition (HCCI) engines- A comprehensive review, Renew. Sustain. Energy Rev. 70 (2017) 369–384, doi:10.1016/j. rser.2016.11.058.
- [15] S.L. Kokjohn, R.M. Hanson, D.A. Splitter, R.D. Reitz, Fuel reactivity controlled compression ignition (RCCI): a pathway to controlled high-efficiency clean combustion, Int. J. Engine Res. 12 (3) (2011) 209–226, doi:10.1177/ 1468087411401548.
- [16] R.D. Reitz, G. Duraisamy, Review of high efficiency and clean reactivity controlled compression ignition (RCCI) combustion in internal combustion engines, Prog. Energy Combust. Sci. 46 (2015) 12–71, doi:10.1016/j.pecs.2014.05. 003.
- [17] U. Burke, K.P. Somers, P. O'Toole, C.M. Zinner, N. Marquet, G. Bourque, E.L. Petersen, W.K. Metcalfe, Z. Serinyel, H.J. Curran, An ignition delay and kinetic modeling study of methane, dimethyl ether, and their mixtures at high pressures, Combust. Flame 162 (2) (2015) 315–330, doi:10.1016/j.combustflame. 2014.08.014.
- [18] M. Ghaderi Masouleh, A. Wehrfritz, O. Kaario, H. Kahila, V. Vuorinen, Comparative study on chemical kinetic schemes for dual-fuel combustion of ndodecane/methane blends, Fuel 191 (2017) 62–76, doi:10.1016/j.fuel.2016.10. 114.
- [19] A. Bhagatwala, R. Sankaran, S. Kokjohn, J.H. Chen, Numerical investigation of spontaneous flame propagation under RCCI conditions, Combust. Flame 162 (9) (2015) 3412–3426, doi:10.1016/j.combustflame.2015.06.005.

- [20] M.B. Luong, R. Sankaran, G.H. Yu, S.H. Chung, C.S. Yoo, A DNS study of the effects of injection timing on the ignition of lean PRF/air/EGR mixture with composition inhomogeneities relevant to RCCI/DDFS combustion, Combust. Flame 183 (2017). Submitted to CNF. doi: 10.1016/j.combustflame.2017.05.023.
- [21] G.H. Abd Alla, H.A. Soliman, O.A. Badr, M.F. Abd Rabbo, Effect of injection timing on the performance of a dual fuel engine, Energy Convers. Manag. 43 (2) (2002) 269–277, doi:10.1016/S0196-8904(00)00168-0.
- [22] G.A. Karim, Combustion in gas fueled compression: Ignition engines of the dual fuel type, J. Eng. Gas Turbines Power 125 (3) (2003) 827, doi:10.1115/1. 1581894.
- [23] R.G. Papagiannakis, D.T. Hountalas, Combustion and exhaust emission characteristics of a dual fuel compression ignition engine operated with pilot diesel fuel and natural gas, Energy Convers. Manag. 45 (18–19) (2004) 2971–2987, doi:10.1016/j.enconman.2004.01.013.
- [24] S. Imran, D.R. Emberson, A. Diez, D.S. Wen, R.J. Crookes, T. Korakianitis, Natural gas fueled compression ignition engine performance and emissions maps with diesel and RME pilot fuels, Appl. Therm. Eng. 67 (1–2) (2014) 354–365, doi:10. 1016/j.apenergy.2014.02.067.
- [25] C. Aksu, N. Kawahara, K. Tsuboi, M. Kondo, E. Tomita, Extension of PREMIER combustion operation range using split micro pilot fuel injection in a dual fuel natural gas compression ignition engine: A performance-based and visual investigation, Fuel 185 (2016) 243–253, doi:10.1016/j.fuel.2016.07.120.
- [26] L. Wei, P. Geng, A review on natural gas/diesel dual fuel combustion, emissions and performance, Fuel Process. Technol. 142 (2016) 264–278, doi:10.1016/j. fuproc.2015.09.018.
- [27] Z. Ahmad, J. Aryal, O. Ranta, O. Kaario, V. Vuorinen, An optical characterization of dual-fuel combustion in a heavy-duty diesel engine, SAE Technical Paper 2018-01-02 (2018) 1–10, doi:10.4271/2018-01-0252.Abstract.
- [28] J. Liu, F. Yang, H. Wang, M. Ouyang, S. Hao, Effects of pilot fuel quantity on the emissions characteristics of a CNG/diesel dual fuel engine with optimized pilot injection timing, Appl. Energy 110 (2013) 201–206, doi:10.1016/J.APENERGY. 2013.03.024.
- [29] Y. Li, M. Jia, Y. Chang, Y. Liu, M. Xie, T. Wang, L. Zhou, Parametric study and optimization of a RCCI (reactivity controlled compression ignition) engine fueled with methanol and diesel, Energy 65 (2014) 319–332, doi:10.1016/j.energy. 2013.11.059.
- [30] H. Liu, Q. Tang, Z. Yang, X. Ran, C. Geng, B. Chen, L. Feng, M. Yao, A comparative study on partially premixed combustion (PPC) and reactivity controlled compression ignition (RCCI) in an optical engine, Proceedings of the Combustion Institute (2018), doi:10.1016/J.PROCI.2018.06.004.
- [31] A. Maghbouli, R.K. Saray, S. Shafee, J. Ghafouri, Numerical study of combustion and emission characteristics of dual-fuel engines using 3D-CFD models coupled with chemical kinetics, Fuel 106 (2013) 98–105, doi:10.1016/J.FUEL.2012. 10.055.
- [32] M. Grochowina, M. Schiffner, S. Tartsch, T. Sattelmayer, Influence of injection parameters and operating conditions on ignition and combustion in dualfuel engines, J. Eng. Gas Turbines Power 140 (10) (2018) 1–10, doi:10.1115/1. 4040089.
- [33] D.E. Nieman, A.B. Dempsey, R.D. Reitz, Heavy-duty RCCI operation using natural gas and diesel, SAE Int. J. Engines 5 (2) (2012) 270–285, doi:10.4271/ 2012-01-0379.
- [34] Engine combustion network, Combustion research facility, Sandia National Laboratories, Livermore, CA. Available at: https://ecn.sandia.gov. (Accessed 27th May 2018).
- [35] M. Bardi, T. Bazyn, G. Bruneaux, J. Johnson, S. Lee, L.M. Malbec, M. Meijer, J. Naber, R. Payri, L.M. Pickett, B. Somers, Engine Combustion Network (ECN): Characterization and comparison of boundary conditions for different combustion vessels, Atomization Sprays 22 (9) (2012a) 777–806, doi:10.1615/ Atomiz5pr.2012006083.
- [36] M. Bardi, R. Payri, L.M. Malbec, G. Bruneaux, L.M. Pickett, J. Manin, T. Bazyn, C. Genzale, Engine combustion network: Comparison of spray development, vaporization, and Combustion in Different Combustion Vessels, Atomization Sprays 22 (10) (2012b) 807–842, doi:10.1615/AtomizSpr.2013005837.
- [37] N. Maes, M. Meijer, N. Dam, B. Somers, H. Baya Toda, G. Bruneaux, S.A. Skeen, L.M. Pickett, J. Manin, Characterization of Spray A flame structure for parametric variations in ECN constant-volume vessels using chemiluminescence and laser-induced fluorescence, Combust. Flame 174 (2016) 138–151, doi:10.1016/j. combustflame.2016.09.005.
- [38] OpenFOAM Foundation The Open Source Computational Fluid Dynamics (CFD) Toolbox. Available at: http://www.openfoam.org (Accessed 27th May 2018).
- [39] R. Issa, B. Ahmadi-Befrui, K. Beshay, A. Gosman, Solution of the implicitly discretised reacting flow equations by operator-splitting, J. Comput. Phys. 93 (2) (1991) 388–410, doi:10.1016/0021-9991(91)90191-M.
- [40] A. Wehrfritz, O. Kaario, V. Vuorinen, B. Somers, Large eddy simulation of ndodecane spray flames using flamelet generated manifolds, Combust. Flame 167 (2016) 113-131, doi:10.1016/j.combustflame.2016.02.019.
- [41] H. Jasak, H.G. Weller, A.D. Gosman, High resolution NVD differencing scheme for arbitrarily unstructured meshes, Int. J. Numer. Methods Fluids 31 (2) (1999) 431–449, doi:10.1002/(SICI)1097-0363(19990930)31:2<431:: AID-FLD884>3.0.CO;2-T.
- [42] F.F. Grinstein, L.G. Margolin, W. Rider, Implicit large eddy simulation: computing turbulent fluid dynamics, Cambridge University Press, 2007.
- [43] F.F. Grinstein, C. Fureby, On flux-limiting-based implicit large eddy simulation, J. Fluids Eng. 129 (12) (2007) 1483, doi:10.1115/1.2801684.

- [44] A. Aspden, N. Nikiforakis, S. Dalziel, J. Bell, Analysis of implicit LES methods, Commu. Appl. Math. Comput. Sci. 3 (1) (2008) 103–126, doi:10.2140/camcos. 2008.3.103.
- [45] A. Wehrfritz, V. Vuorinen, O. Kaario, M. Larmi, Large eddy simulation of highvelocity fuel sprays: studying mesh resolution and breakup model effects for spray A, Atomization Sprays 23 (5) (2013) 419–442, doi:10.1615/AtomizSpr. 2013007342.
- [46] R.D. Reitz, Modeling atomization processes in high-pressure vaporizing sprays, Atomization Spray Technol 3 (1987) 309–337.
- [47] R.D. Reitz, J.C. Beale, Modeling Spray Atomization With the Kelvin-Helmholtz/Rayleigh-Taylor Hybrid Model, Atomization and Sprays 9 (6) (1999) 623-650, doi:10.1615/AtomizSpr.v9.i6.40.
- [48] N. Frossling, Evaporation, heat transfer, and velocity distribution in two-dimensional and rotationally symmetrical laminar boundary-layer flow. N.A.C.A. ADB1891., Technical Report, 1956.
- [49] W.E. Ranz, W.R. Marshall, Evaporation from drops, part I, Chem. Eng. Prog. 48 (3) (1952a) 141-146.
- [50] W. Ranz, W.R. Marshall, Evaporation from drops, part II, Chem. Eng. Prog. 48 (3) (1952b) 173–180.
- [51] E. Hairer, G. Wanner, Solving ordinary differential equations. II, Springer-Verlag, 1996, doi:10.1007/978-3-642-05221-7.
- [52] K.E. Niemeyer, N.J. Curtis, C. Sung, pyJac: Analytical Jacobian generator for chemical kinetics, Comput. Phys. Commun. 215 (2017) 188–203, doi:10.1016/ J.CPC.2017.02.004.
- [53] Y. Pei, E.R. Hawkes, S. Kook, G.M. Goldin, T. Lu, Modelling n-dodecane spray and combustion with the transported probability density function method, Combust. Flame 162 (5) (2015) 2006–2019, doi:10.1016/j.combustflame.2014. 12.019.
- [54] A. Varna, A. Wehrfritz, E. R. Hawkes, M. J. Cleary, T. Lucchini, G. D'Errico, S. Kook, Q. N. Chan, Application of a multiple mapping conditioning mixing model to ECN Spray A, Proc. Combust. Inst. (2018), doi:10.1016/J.PROCI.2018. 06.007.
- [55] C. Fureby, Comparison of flamelet and finite rate chemistry LES for premixed turbulent combustion, 45th AIAA Aerospace Sciences Meeting and Exhibit, 24, American Institute of Aeronautics and Astronautics, Reston, Virigina (2007), pp. 1–16, doi:10.2514/6.2007-1413.
- [56] C. Duwig, K. Nogenmyr, C. Chan, M.J. Dunn, Large eddy simulations of a piloted lean premix jet flame using finite-rate chemistry, Combust. Theory Model. 15 (4) (2011) 537–568, doi:10.1080/13647830.2010.548531.
- [57] J.R. Edwards, J.A. Boles, R.A. Baurle, Large-eddy/Reynolds-averaged Navier-Stokes simulation of a supersonic reacting wall jet, Combust. Flame 159 (3) (2012) 1127–1138, doi:10.1016/J.COMBUSTFLAME.2011.10.009.
- [58] J.A. Fulton, J.R. Edwards, A. Cutler, J. McDaniel, C. Goyne, Turbulence/chemistry interactions in a ramp-stabilized supersonic hydrogen-air diffusion flame, Combust. Flame 174 (2016) 152–165, doi:10.1016/J.COMBUSTFLAME.2016.09. 017.
- [59] E. Hodzic, E. Alenius, C. Duwig, R.S. Szasz, L. Fuchs, A large eddy simulation study of bluff body flame dynamics approaching blow-off, Combust. Sci. Technol. 189 (7) (2017) 1107–1137, doi:10.1080/00102202.2016.1275592.
- [60] C. Eberle, P. Gerlinger, K.P. Geigle, M. Aigner, Toward finite-rate chemistry large-eddy simulations of sooting swirl flames, Combust. Sci. Technol. (2018) 1–24, doi:10.1080/00102202.2018.1443444.
- [61] Z. Li, A. Cuoci, A. Parente, Large Eddy simulation of MILD combustion using finite rate chemistry: Effect of combustion sub-grid closure, Proc. Combust. Inst. (2018), doi:10.1016/J.PROCL.2018.09.033.
- [62] Y. Pei, S. Som, E. Pomraning, P.K. Senecal, S.A. Skeen, J. Manin, L.M. Pickett, Large eddy simulation of a reacting spray flame with multiple realizations under compression ignition engine conditions, Combust. Flame 162 (12) (2015) 4442–4455, doi:10.1016/j.combustflame.2015.08.010.
- [63] F. Bottone, A. Kronenburg, D. Gosman, A. Marquis, The numerical simulation of diesel spray combustion with LES-CMC, Flow Turbul. Combust. 89 (4) (2012) 651–673, doi:10.1007/s10494-012-9415-y.

- [64] A. Irannejad, A. Banaeizadeh, F. Jaberi, Large eddy simulation of turbulent spray combustion, Combust. Flame 162 (2) (2015) 431–450, doi:10.1016/j. combustflame.2014.07.029.
- [65] C.K. Blomberg, L. Zeugin, S.S. Pandurangi, M. Bolla, K. Boulouchos, Y.M. Wright, Modeling split injections of ECN spray A using a conditional moment closure combustion Model with RANS and LES, SAE Int. J. Engines 9 (4) (2016) 2107– 2119, doi:10.4271/2016-01-2237.
- [66] S. Gallot-Lavallée, W.P. Jones, Large Eddy simulation of spray auto-ignition under EGR conditions, Flow Turbul. Combust. 96 (2) (2016) 513–534, doi:10.1007/ s10494-015-9684-3.
- [67] R.W. Bilger, S.H. Stårner, R.J. Kee, On reduced mechanisms for methane-air combustion in nonpremixed flames, Combust. Flame 80 (2) (1990) 135–149, doi:10.1016/0010-2180(90)90122-8.
- [68] J.C. Sutherland, P.J. Smith, J.H. Chen, Quantification of differential diffusion in nonpremixed systems, Combust. Theory Model. 9 (2) (2005) 365–383, doi:10. 1080/17455030500150009.
- [69] Q. Xue, S. Som, P.K. Senecal, E. Pomraning, Large Eddy simulation of fuel spray under non-reacting Ic engine conditions, Atom. Sprays 23 (10) (2013) 1–30, doi:10.1615/AtomizSpr.2013008320.
- [70] CMT Virtual Injection Rate Generator. Available at: https://www.cmt.upv.es/ ecn03.aspx. (Accessed May2018)
- [71] S. Schlatter, B. Schneider, Y. Wright, K. Boulouchos, Experimental Study of Ignition and Combustion Characteristics of a Diesel Pilot Spray in a Lean Premixed Methane/Air Charge using a Rapid Compression Expansion Machine, SAE Technical paper 2012-01-08 (2012), doi:10.4271/2012-01-0825.
- [72] S. Schlatter, B. Schneider, Y.M. Wright, K. Boulouchos, Comparative study of ignition systems for lean burn gas engines in an optically accessible rapid compression Expansion Machine, SAE Technical Paper 2013-24-0112, SAE (2013), doi:10.4271/2013-24-0112.
- [73] T. Yao, Y. Pei, B. Zhong, S. Som, T. Lu, K.H. Luo, A compact skeletal mechanism for n-dodecane with optimized semi-global low-temperature chemistry for diesel engine simulations, Fuel 191 (2017) 339–349, doi:10.1016/j.fuel.2016. 11.083.
- [74] J.M. Desantes, J.J. López, J.M. García-Oliver, D. López-Pintor, Experimental validation and analysis of seven different chemical kinetic mechanisms for ndodecane using a Rapid Compression-Expansion Machine, Combust. Flame 182 (2017) 76–89, doi:10.1016/j.combustflame.2017.04.004.
- [75] A. Frassoldati, G. D'Errico, T. Lucchini, A. Stagni, A. Cuoci, T. Faravelli, A. Onorati, E. Ranzi, Reduced kinetic mechanisms of diesel fuel surrogate for engine CFD simulations, Combust. Flame 162 (10) (2015) 3991–4007, doi:10.1016/j. combustflame.2015.07.039.
- [76] D.M. Manias, E.A. Tingas, C.E. Frouzakis, K. Boulouchos, D.A. Goussis, The mechanism by which CH2O and H2O2 additives affect the autoignition of CH4/air mixtures, Combust. Flame 164 (2016) 111–125, doi:10.1016/j. combustflame.2015.11.008.
- [77] R. Pettinen, O. Kaario, M. Larmi, Dual-fuel combustion characterization on lean conditions and high loads, SAE Technical Paper 2017-01-07 (2017), doi:10.4271/ 2017-01-0759.
- [78] J.B. Heywood, Internal combustion engine fundamentals, McGraw-Hill, 1988.
- [79] C.K. Westbrook, Chemical kinetics of hydrocarbon ignition in practical combustion systems, Proc. Combust. Inst. 28 (2) (2000) 1563–1577, doi:10.1016/ S0082-0784(00)80554-8.
- [80] A. Hadadpour, M. Jangi, X.S. Bai, The effect of splitting timing on mixing in a jet with double injections, Flow Turbul. Combust. (2018) 1–15, doi:10.1007/ s10494-018-9904-8.
- [81] E. Mastorakos, Ignition of turbulent non-premixed flames, Prog. Energy Combust. Sci. 35 (1) (2009) 57–97, doi:10.1016/j.pecs.2008.07.002.
- [82] G. Borghesi, A. Krisman, T. Lu, J.H. Chen, Direct numerical simulation of a temporally evolving air/n-dodecane jet at low-temperature diesel-relevant conditions, Combust. Flame 195 (2018) 183–202, doi:10.1016/J.COMBUSTFLAME. 2018.02.020.