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Large-eddy simulation of tri-fuel ignition: diesel spray-assisted ignition of lean hydrogen-methane-air mixtures

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We present 3D numerical results on tri-fuel (TF) combustion using large-eddy simulation and finite rate chemistry. The TF concept was recently introduced by Karimkashi et al. (Int. J. Hydrogen Energy, 2020) in 0D. Here, the focus is on spray-assisted ignition of methane-hydrogen blends. The spray acts as a high-reactivity fuel (HRF) while the ambient premixed methane-hydrogen blend acts as a low-reactivity fuel (LRF) mixture. Better understanding on such a TF process could enable and motivate more extensive hydrogen usage in e.g. compression ignition marine engines where spray-assisted dual-fuel (DF) combustion is already utilised. The studied spray set-up is based on the modified ECN Spray A case, see Kahila et al. (Combustion and Flame, 2019) for DF combustion. The ambient pressure and temperature are $T_{amb} = 900 \text{ K}$ and $p_{amb} = 60$ bar. The hydrogen content of the LRF blend is varied systematically by changing the molar fraction $0 \le x \le 1$, $x = \frac{[H_2]}{[H_2] + [CH_4]}$. The main added value of the study is that we extend the TF concept to 3D. The particular findings of the study are as follows: 1) Consistent with Karimkashi et al. 2020, hydrogen delays ignition also in 3D and the effect becomes significant for $x \ge 0.5$. 2) The ratio between the first- and second-stage ignition delay times $\left(\frac{r_2}{r_1}\right)^{0D} \approx 2 \pm 0.1$ and $\left(\frac{r_2}{r_1}\right)^{3D} \approx 3 \pm 0.3$. Furthermore, the ratio between 3D and 0D ignition delay times is given as $\frac{\tau_2^{3D}}{\tau_0^{0D}} \approx 2 \pm 0.2$ for all TF cases. 3) Finally, consistent with Karimkashi et al. 2020, also in 3D the high-temperature combustion heat release mode is shown to appear stronger in TF than the low-temperature combustion mode compared to DF methane-diesel combustion.

Keywords: LES; tri-fuel; dual fuel; ECN spray a; hydrogen

1. Introduction

Liquefied natural gas (LNG) is a fossil fuel and it may also be considered as an alternative fuel for internal combustion engines (ICE) [1]. In particular, in the marine sector, LNG is an attractive fuel since it yields lower level of CO_2 emissions compared to traditional high-sulphur content fuels (such as heavy fuel oil) [2]. However, LNG suffers from unburned hydrocarbon (UHC) emissions such as methane slip. One solution to reduce such emissions could be to substitute the LNG partly with a renewable fuel. An example of such a fuel is hydrogen posing obvious potential to reduce both CO_2 and UHC emissions in ICEs [3]. However, despite the high reactivity of hydrogen, such LNG-H₂ blends may still require an ignition source in the compression ignition (CI) engines context [4–6]. The motivation

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of this study is to better understand the physics and chemistry involved with diesel spray ignition in an environment of different methane- H_2 - H_2 blends.

In contrast to spark ignition (SI) engines, CI engines may offer higher thermal efficiency making them more favourable in, for example, long-distance transportation [7,8]. In dualfuel (DF) literature, the fuel with the shortest ignition delay time (IDT) is typically referred to as the high reactivity fuel (HRF). The fuel with the shortest IDT is referred to as the low reactivity fuel (LRF). Conventional CI engines operate with HRF, such as diesel, without a need for an additional ignition source. In contrast, when compared to diesel, methane is an LRF. In order to use LRFs such as methane in CI engines, an ignition source is required since the IDT of methane is typically longer than the compression phase. The DF CI engine concept utilises LRF as the primary fuel. A DF combustion process can be summarised in two steps. First, the premixed LRF, e.g. methane or gasoline, premixed with an oxidiser, e.g. air possibly combined with exhaust gas recirculation (EGR), is injected during the intake phase, i.e. premixed and compressed. However, its prolonged IDT does not allow control over the ignition but a separate ignition mechanism is required. Second, to overcome this difficulty, a relatively small mass of HRF is injected into the premixed gas mixture. Such a pilot spray ignites the surrounding gas mixture [9,10]. Figure 1 highlights the DF ignition process where a HRF pilot spray ignites the surrounding methane-air mixture. The details of the shown DF ignition process have been thoroughly characterised in our previous studies [11-14]. In DF engine experiments [15, 16], it has been noted that a diesel spray ignition is retarded when methane is present in the ambient air. Such an inhibiting effect of methane in DF combustion has been quantified in many studies based



Figure 1. Visualisation of the dual-fuel (DF) ignition process where the high reactivity fuel (HRF) n-dodecane liquid spray droplets ignite the low reactivity fuel (LRF) i.e. ambient methane (black background). The visualisation is taken at $1.2 \times IDT$ using the same flow solver as in the present paper (see [13]).

on experimental tests [17–20] or zero-dimensional (0D) homogeneous reactors [21], and three-dimensional (3D) simulations [11,12,22].

The Engine Combustion Network (ECN) was established in order to align computational and experimental spray combustion research. The ECN Spray A configuration involves an n-dodecane spray injection into a constant volume vessel in various engine-relevant conditions [23]. Large-eddy simulation (LES) studies on Spray A have been carried out using flamelet generated manifolds [24] and finite rate chemistry [25]. With relevance to DF spray ignition, there have been few numerical simulation efforts in recent years based on the ECN Spray A configuration. Kahila et al. [11] utilised Yao [26] and Polimi-reduced [27] chemical mechanisms in LES/finite rate chemistry simulations by adding methane to the ambient air in a modified ECN Spray A set-up. In comparison to single fuel spravs. such a DF spray was noted to pose a longer IDT such that both low- and high-temperature chemistry were delayed. Recently, Tekgül et al. [12] investigated ambient temperature (T_{amb}) impact on DF ignition in DF LES/finite rate chemistry simulations. It was noted that although the choice of chemical mechanism influences DF ignition characteristics, the inhibiting effect of methane on IDT is less strong at higher ambient temperatures with different chemical mechanisms. For example, $(\tau_{2,DF}/\tau_{2,SF})^{3D} \approx 3/2/1$ at $T_{amb} = 850$ K/900 K/1000 K for the Yao chemical mechanism, τ_2 being the second-stage IDT. This study seeks to extend the mentioned LES/finite rate chemistry simulations by adding hydrogen in different levels to the methane/air mixture in the ambient of the similar n-dodecane spray configuration.

As reviewed recently by Karimkashi et al. [28], hydrogen-methane blends have been used in the past studies, in specific in combustors [29,30] and SI engines [31–33]. In the context of CI engines, several recent experimental studies [34-40] have reported how addition of hydrogen into methane can improve engine performance, reduce fuel consumption, and mitigate carbon emissions. Similarly, several studies have noted that by adding hydrogen to different fuels, e.g. (diesel [41], n-heptane [42–44], and iso-octane [45]), ignition is inhibited within the temperature range of \approx 700–900 K. [28] introduced the concept of 'tri-fuel' (TF) combustion, wherein blends of two LRFs, e.g. hydrogen and methane, ignite with the assistance of a HRF, e.g. diesel, under engine relevant conditions (similar to DF). They investigated the ignition process of methanol/hydrogen/n-dodecane and methane/hydrogen/n-dodecane blends using 0D homogeneous reactors with the Polimireduced mechanism [27]. It was observed that adding hydrogen into methanol leads to earlier ignition. In contrast, adding hydrogen into methane resulted in an opposite trend. The contradictory trends were explained through reaction sensitivity analysis, where the importance of OH consumption by H₂ was highlighted as consistent with earlier findings in [41,45]. Particularly in methane/hydrogen/n-dodecane TF cases, the IDT was noted to vary between $(\tau_{2,\text{TF}}/\tau_{2,\text{DF}})^{0\text{D}} \approx 1.5$ and 2 for 20/80% and 0/100% methane/hydrogen blends (molar), respectively. Moreover, $(\tau_{2,\text{TF}}/\tau_{1,\text{TF}})^{0\text{D}} \approx 1.7$, similar for all different ratios of methane/hydrogen blends.

According to the literature, adding hydrogen to diesel/methane DF CI has already turned out to be a promising concept. First, adding hydrogen leads to shorter combustion duration and better engine performance [46]. Second, high reactivity and flame speed of hydrogen may reduce misfire potential and result in emission reductions as well as high auto-ignition temperature, enabling higher compression ratios [35,37,40]. Third, hydrogen addition is preferred due to its abundant availability from various resources as a secondary energy carrier [47]. It should be noted that when pure hydrogen is used in an engine, its higher heat release capacity and wider flammability limits could lead to high thermal load and NO_x

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emissions in engines [48,49]. This drawback could be significantly improved by blending hydrogen with different fuels such as methane [48,50,51]. Moreover, numerical and experimental findings reveal that increased heat release is observed when hydrogen is blended with other fuels. This is due to the high energy content of H_2 [52,53]. However, it has been noted that using hydrogen at high blending ratios may increase cycle-to-cycle variations and engine knocking [54]. Thus, more research on TF combustion is needed. Based on the above literature review, TF n-dodecane/methane/hydrogen ignition has not been investigated previously in a 3D spray-assisted configuration. In particular, the effect of hydrogen blending ratio on ignition and heat release rate are yet to be quantified in a numerical spray platform to better understand ignition and mixing characteristics in such a TF system. The present work extends the previous TF study by Karimkashi et al. [28] to 3D spray ignition, similar to our previous DF studies utilising the Engine Combustion Network (ECN) Spray A baseline conditions [11–14,22]. Consistent with those studies, here, n-dodecane is used as the diesel surrogate due to its similar thermochemical properties with diesel. In particular, ignition characteristics of different n-dodecane/methane/hydrogen blends are investigated using LES numerical simulations and compared with 0D homogeneous reactor calculations. The objectives of the paper are to:

- (1) Extend the work of [28] to 3D spray-assisted TF combustion.
- (2) Conduct a systematic hydrogen concentration sweep in both 0D and 3D environments.
- (3) Investigate first- and second-stage IDT variations for various hydrogen-methane blending ratios, and analyse heat release rate (HRR) modes for the considered TF cases.

2. Numerical methods

2.1. Governing equations

The governing equations for the gas phase are the compressible Navier-Stokes equations, i.e. continuity, momentum, and energy equations. Here, the equations are presented in the Favre-filtered formulation form as follows.

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

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j}(-\bar{p}\delta_{ij} + \bar{\rho}\tilde{u}_i\tilde{u}_j - \bar{\rho}\tilde{u}_i\tilde{u}_j + \bar{\tau}_{ij}) + \overline{S}_{u_i},\tag{2}$$

$$\frac{\partial(\bar{\rho}\widetilde{Y}_k)}{\partial t} + \frac{\partial(\bar{\rho}\widetilde{u}_i\widetilde{Y}_k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\bar{\rho}\widetilde{u}_i\widetilde{Y}_k - \bar{\rho}\widetilde{u}_i\widetilde{Y}_k + \bar{\rho}\widetilde{D}\frac{\partial\widetilde{Y}_k}{\partial x_i} \right) + \overline{S}_{Y_k} + \bar{\omega}_k, \tag{3}$$

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

where $\overline{\rho}$, $\widetilde{u_i}$, \overline{p} , $\overline{Y_k}$, $\widetilde{h_s}$ and $\overline{\tau_{ij}}$, denote filtered density, velocity, pressure, species k, sensible enthalpy and viscous stress tensor, respectively. The symbol \sim denotes a density-weighted ensemble average and over bar (-) denotes unweighted average. In Equation (4), the total

enthalpy is defined as the sum of sensible enthalpy and specific kinetic energy.

$$\widetilde{h}_t = \widetilde{h}_s + \frac{\widetilde{u}_i \widetilde{u}_i}{2} \tag{5}$$

Moreover, Lewis number of unity is assumed for all species. The source terms $\overline{S_{\rho}}, \overline{S_{u,i}}, \overline{S_{Y_k}}$ and $\overline{S_{Y_k}}$ allows the coupling between the liquid and gaseous phases accordingly with respect to mass, momentum, species and energy. The production rate of the species k and HRR is denoted by $\widetilde{\omega_k}$ and $\widetilde{\omega_h}$. Finally, the above governing equations which represents the coupling between gas and liquid phases, are closed by filtered ideal gas law.

Here, a customised reacting solver in OpenFOAM 6.0 platform based on the recent work by Kahila et al. [11] is used for solving the gas phase governing equations in the finite volume context. In the customised reacting solver, the open source library pyJac [55] is coupled with OpenFOAM through which reaction rate coefficients and the analytical Jacobian matrix formulation needed by the ordinary differential equation (ODE) system solver are provided. Species and energy transport are separated from the chemical reactions using operator-splitting. Moreover, dynamic load balancing and reference cell methods, which are described with details in [11,56], are used to speed up the computations.

The numerical approach herein is the same as in our previous studies [11–14,25]. The temporal discretisation is carried out using a second order accurate implicit time integration method. The diffusion terms are discretised by the a standard second order central scheme i.e. linear interpolation. Additionally, the convection terms are discretised with a nonlinear, dissipative scheme called the gamma scheme [57]. In such an Implicit LES (ILES) model the numerical diffusion acts as a stand-alone turbulence model. The approach has been validated extensively for reacting and non-reacting flow configurations in our earlier studies [11–14,22].

2.2. Spray and Chemistry Modelling

In the present ILES, Lagrangian Particle Tracking (LPT) approach is used to model the n-dodecane fuel spray droplets. In line with our previous studies [13,58], we do not use a submodel for droplet breakup phenomenon. Instead, we use a constant initial droplet size matching recent DNS and LES data [59,60]. It has been shown that this approach yields acceptable results [14].

Similar to our previous studies, the injected droplets are initially of constant size $d = 0.5 \,\mu\text{m}$. The fuel spray accelerates the gas phase into a multi-phase jet which entrains hot ambient air into the spray axis. After the turbulence transition, the potential core of the jet ends and the rapid evaporation leads to the termination of the liquid phase at a point denoted as the liquid length [58]. Since the chemical time scales are very small in comparison to the fluid dynamical time scales, we utilise the operator splitting strategy for the chemistry. Therefore, the transport of energy and species is solved independently within each CFD time step. The change of thermo-chemical compositions over the CFD time step is represented by a system of ordinary differential equations. The resulting non-linear stiff initial value problem is solved independently in each finite volume cell using the pyJac code coupled with OpenFOAM. The pyJac provides the reaction rate coefficients along with the analytical Jacobian required by the ode solver. Moreover, the speed-up of this coupled solver is accelerated with the implementation of reference cell methods and load balancing algorithms [11]. In dynamic load balancing, the computational load is

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distributed as described in [56], the utilised reference cell model limits the explicit solution of chemistry above a given mixture fraction value defined by the user $\xi \le 10^{-4}$. As for the remaining cells, the chemistry is explicitly solved for the first cell (reference solution) and mapped to other cells. Therefore, the homogeneous ambient methane–air mixture is in fact explicitly solved. However, it is solved only for one cell and mapped to the (other) identical cells.

A reduced chemical kinetics mechanism (96 species and 993 reactions) called Polimireduced, developed by Frassoldati et al. [27], is used in the present work. This mechanism is developed for n-dodecane combustion under engine-relevant conditions. Moreover, the superior performance of Polimi-reduced mechanism in DF context has been recently demonstrated by Masouleh et al. [61]. The Polimi-reduced mechanism was earlier validated and used in the same modified ECN Spray A configuration in DF studies (methane/ndodecane) at 900 K ambient temperature and 60bar pressure by Kahila et al. [11]. The mechanism was validated and utilised in TF context (methane/n-dodecane/hydrogen) earlier by the present authors Karimkashi et al. [28].

2.3. Simulation configuration

The present simulation configuration is mainly based on the modified ECN Spray A conditions where n-dodecane diesel surrogate is injected from a 90 μ m nozzle hole at pressure 150 MPa. In addition, the molar composition of O₂ is maintained at 15%. Here, the above-mentioned circumstances are replaced for TF conditions as the equivalence ratio of premixed hydrogen-methane air mixture is maintained lean at 0.5.

In all the simulations, the molar concentration of O_2 is maintained at 15% while the molar compositions of the other species depend on the used hydrogen molar fraction and they are reported in Table 1. The volume of the computational domain is the same as in the experimental combustion chamber at the Sandia National Laboratories. The domain and a cut-plane of the computational mesh is depicted in Figure 2. The mesh consists of three different refinement levels R1-R3 to capture the physics and chemistry of combustion. Moreover, grids are selected with relative importance of ignition sensitivity in the different

	ECN Spray A	DF(x = 0)	TF(x = 0.8)	TF(x = 0.95)
Injection parameters				
Fuel	n-C ₁₂ H ₂₆			
Nozzle diameter	90 µm	90 µm	$90\mu m$	90 µ m
Temperature	363 K	363 K	363 K	363 K
Pressure	150 MPa	150 MPa	150 MPa	150 MPa
Ambient conditions				
Temperature	900 K	900 K	900 K	900 K
Density	22.8 kg/m^3	22.8 kg/m^3	22.8 kg/m^3	22.8 kg/m^3
$O_2(molar)$	15.0 %	15.0 %	15.0 %	15.0 %
CO ₂ (molar)	6.230 %	5.955 %	5.542 %	5.273 %
H ₂ O(molar)	3.620 %	3.460 %	3.220 %	3.064 %
N ₂ (molar)	75.150 %	71.835 %	66.861 %	63.61 %
CH4(molar)	_	3.750 %	1.874 %	0.652 %
H ₂ (molar)	_	_	7.499 %	12.391 %
ϕ	0	0.5	0.5	0.5

Table 1. S	pecifications of	of TF Spray	simulations
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65mm



Figure 2. The computational domain used for present work. The mixture fraction field is overlaid with the mesh. The mesh consists of uniform Cartesian cells of 125 micrometre (R3), 250 micrometre (R2), and 500 micrometre (R1).

zones. The finest resolution R3 has a uniform grid spacing of $125 \,\mu\text{m}$ extended until 50mm downstream distance from the nozzle. In fact, in the present simulations the ignition takes place always within the finest refinement level R3.

We note that in the present work, a no model turbulence-chemistry interactions (TCI) approach is adopted. According to our previous mesh sensitivity analysis on dual fuel ignition studies [13], we have observed that the present relatively fine mesh resolution $(125 \,\mu\text{m})$ with direct chemistry will sufficiently capture the ignition event. According to our mesh sensitivity analysis in Ref. [13], the fine $125 \,\mu m$ grid and very fine $62.5 \,\mu m$ grid give the same IDT. Hence, for computational feasibility, we utilised the fine $125 \,\mu m$ grid. Moreover, we remind that this study targets the auto-ignition process only, which is assumed to be less sensitive to micro-mixing issues compared to e.g. quasi-steady flame lift-off length estimation in Spray A context [62]. We have shown in our previous publications [11,25] that the present LES configuration is able to reproduce all available experimental data on the ECN Spray A case with respect to mixture formation and autoignition. Also, within the DF Spray A context in [11], we have compared the IDT results obtained by the present combustion model (no-model) and the Flamelet-Generated Manifolds (FGM) method with a presumed PDF approach to include TCI effects within the manifold and the present (no-model) approach provides an ignition delay time value within 1% of the one obtained by the FGM solver. The low-temperature combustion features were noted to be very similar for both ILES no-model and FGM methods with a successful comparison to experimental CH2O PLIF data.

3. Results and discussion

3.1. General spray ignition characteristics

To provide an overview of ignition characteristics in the multi-fuel context, DF (x = 0) and TF (x > 0) sprays are visualised in Figure 3, slightly after their respective ignition time. There are several similarities in DF and TF sprays. In the evaporation and mixing region (I)



Figure 3. N-dodecane spray ignition process in ambient methane (DF) and hydrogen-enriched methane (TF) mixtures. The retarded ignition in the TF spray is observed. The visualisation is taken at $1.2 \times IDT$ where IDT is the respective ignition delay time. Here, *x* is defined as the molar ratio of hydrogen concentration and the total mixture consisting of methane and hydrogen concentrations.

near the nozzle, droplets accelerate the gas phase creating a two-phase spray jet. Accordingly, the turbulence transition process leads to entrainment of the hot ambient air/methane mixture to the spray axis enabling rapid droplet evaporation. Such a non-reacting mixing phase is essentially the same for DF and TF and the liquid lengths are similar between these cases. Thereafter, the spray turns into a gaseous jet which mixes intensely with the surrounding pre-heated oxidiser consisting of DF or TF mixture. Details of the modelled LES-LPT mixture formation process are provided in our previous study [63]. After mixing and evaporation, the entrained hot ambient gases initiate low-temperature chemistry (LTC) reactions (II), which lead to the decomposition of the long hydrocarbon n-dodecane and to the formation of lighter intermediate radicals. In the n-dodecane/methane DF context, Kahila et al. [11] have discussed that one of the key species involved in n-dodecane decomposition is (C12H25-OO), called RO2 hereafter, which is typically one of the initial n-dodecane decomposition products [64]. Other intermediate species, such as CH_2O , H2O2, and HO2, are also formed in the LTC region. Further downstream of the LTC region, concentration of intermediate radicals such as OH increases rapidly and onset of hightemperature chemistry (HTC) reactions is noted (III). Exothermic HTC reactions typically consume OH radicals and substantially increase the temperature levels, leading to heat accumulation inside the most reactive mixture pockets, usually near the tip of the spray, leading to ignition.

Despite the general similarities in the ignition of DF and TF sprays, we note some differences which can be observed in Figure 3. In the shown representative TF spray (x = 0.95), the LTC region appears qualitatively weaker with a longer spatial distribution compared to the DF spray. Consequently, HTC ignition is shifted further downstream from the nozzle for the TF spray compared to the DF spray. These preliminary observations of the weaker LTC and prolonged first- and second-stage ignition in TF compared to DF are consistent with previous observations by Karimkashi et al. [28], wherein homogeneous reactor models were used for comparing DF and TF ignition. However, here we provide the first 3D numerical evidence on the role of hydrogen in TF sprays within the LES/LPT context. We note that in present simulations, the focus is on the TF ignition characteristics and the simulations are continued only slightly after the ignition delay time. Therefore, propagation of ignition kernels outside the spray region is not investigated.

3.2. Homogenous reactor analysis

Here, we investigate the role of hydrogen in TF spray ignition using 0D homogeneous reactor simulations and mixing line concept [65] in previously unexplored conditions with EGR (O₂ concentration 15%). We note that Karimkashi et al. [28] have previously studied TF ignition for n-dodecane/methane/hydrogen blends using 0D homogeneous reactor simulations and mixing line concept without EGR and here, the same approach is used for different TF blends with EGR. Also, the used Polimi-reduced mechanism has been validated and justified in Ref. [28].

From the practical viewpoint, there are two important aspects which require understanding to reach a smooth control over an envisioned TF CI engine operation. First, the premixed ambient gas should not auto-ignite in the investigated temperature range. Second, the impact of hydrogen on TF ignition should be understood, which can be investigated through the mixing line concept in 0D simulations. These two aspects are assessed in what follows.

Figure 4(a) displays auto-ignition characteristics of the LRFs (hydrogen, methane and their blends) and HRF (n-dodecane) using Polimi-reduced for a broad temperature range. Additionally, IDTs are compared against the Petersen mechanism [66] for pure hydrogen and methane as denoted by the symbols. Here, IDT of methane and hydrogen and their blends (DF:1 and DF:2) for e.g. $800 \text{ K} \le T \le 1000 \text{ K}$ is clearly higher than the respective n-dodecane IDT which indicates that the ambient gas auto-ignition does not appear in the following spray simulations ($0 \le x \le 1$). Thereby, hydrogen and methane as well as their blends are likely to behave as proper LRFs in the present study while n-dodecane may act as an HRF.

Figure 4(b) displays IDTs for the TF mixtures along the mixing line as a function of mixture fraction (ξ) of n-dodecane for different hydrogen-methane blends. Further details on the mixing line concept for TF mixtures in the spray context, in which the cold spray fuel is mixed with the hot ambient mixture based on their absolute enthalpy and mass fractions, are provided in [28]. Here, hydrogen-methane blends are characterised in terms of the relative molar (x) and mass (y) fraction ratios as shown in Figure 5, where x is defined as

$$x = \frac{X_{H2}}{X_{H2} + X_{CH4}}.$$
 (6)

According to Figure 4(b), the following observations are made: 1) IDT is retarded in TF (x > 0) compared to DF (x = 0). 2) IDT retardation is rather weak for x < 0.5 while for



Figure 4. 0D homogeneous reactor calculations : (a) IDT versus T for single fuel-methane, hydrogen, and n-dodecane ($\phi = 0.5$, p = 60 bar) compared with Petersen mechanism using symbols. DF: 1 represents 40% H₂-60% CH₄ and DF: 2 represents 80% H₂-20% CH₄ (b) IDT against ξ under Spray A conditions for n-dodecane/methane/hydrogen. Here, mixture fraction ξ describes the mixing extent of n-dodecane liquid fuel stream and the premixed methane–hydrogen oxidiser stream. The corresponding stoichiometric mixture fractions are $\xi_{st} = 0.0234(x = 0)$, 0.02423(x = 0.6), 0.02493(x = 0.8), 0.0260(x = 0.95), and 0.0266(x = 1).

 $x \ge 0.5$ more significant changes are observed. 3) The most reactive mixture fraction shifts richer with increasing x. 4) For high mixture fractions, IDT is nearly independent of x while the discrepancies are more pronounced at leaner ξ . 5) Quantitatively, IDT at the most reactive mixture fraction (ξ_{MR}) changes by $\approx 40\%$ between x = 0 and x = 1 cases. We note that the reported findings are consistent with those by Karimkashi et al. [28], wherein more details regarding the reasons for such observations including a reaction sensitivity analysis is provided.



Figure 5. The blending ratio of hydrogen in molar (x) and mass (y) fractions utilised in the present study.

Table 2. IDT calculations from 0D homogeneous ignition at ξ_{MR} and LES study in (ms). Here, x is defined as the molar ratio of hydrogen concentration and the total mixture consisting of methane and hydrogen concentrations.

Cases	ξmr	$\tau_1(0D)$	τ ₂ (0D)	$\tau_2/\tau_1(0D)$	$\tau_1(LES)$	$\tau_2(\text{LES})$	$\tau_2/\tau_1(\text{LES})$
x = 0.0	0.088	0.150	0.300	2	0.179	0.549	3.067
x = 0.2	0.086	0.146	0.307	2.102	0.179	0.576	3.217
x = 0.4	0.089	0.159	0.317	1.993	0.198	0.537	2.712
<i>x</i> = 0.6	0.091	0.167	0.333	1.994	0.216	0.726	3.361
x = 0.8	0.093	0.183	0.362	1.978	0.233	0.727	3.120
x = 0.9	0.098	0.206	0.389	1.888	0.268	0.773	2.884
<i>x</i> = 0.95	0.100	0.215	0.409	1.902	0.286	0.901	3.150
x = 1	0.102	0.229	0.436	1.903	0.294	1.031	3.506

3.3. TF Spray Ignition: Overview

Next, we investigate the 3D spray ignition problem by presenting numerical results from a parameter sweep of $0 \le x \le 1$ reported in Table 2. Figure 6 depicts temporal evolution of maximum temperature (T_{max}) for different x. In the figure, the first- and second-stage ignition times are marked as symbols. Here, the first-stage ignition (τ_1) is defined as the time when 20% of the maximum mass fraction of RO₂ is reached and the second-stage ignition (τ_2) corresponds to the time when the maximum gradient of T_{max} is observed. We note that RO₂ is the first decomposition product of n-dodecane and the definition of 20% of a short-lived intermediate species, such as RO₂, as the marker of the first-stage IDT is originated from Ref. [67]. The definition of 20% RO₂ has been used afterwards for n-dodecane ignition by several authors [11–13,22].

The first- and second-stage ignition from 3D simulations are noted to be higher than the respective 0D counterparts. Such a difference can be mainly explained by the 3D mixing time. However, the trend is consistent with 0D i.e. when x < 0.5, hydrogen has a marginal effect on retarding IDT. It seems that when increasing the H₂ content, T_{max} is continuously increasing. Moreover, T_{max} after the second-stage ignition is higher for x = 0.95 compared to the cases with lower x.

The retarding effect of H₂ on TF ignition is clearly visible in Figure 7 for both τ_1 and τ_2 . We note that for DF ignition (x = 0) the present results coincide closely with those



Figure 6. Temporal evolution of T_{max} (solid), in TF LES. Here, τ_1 and τ_2 are marked with diamond and stars, respectively.



Figure 7. First- and second-stage IDT at ξ_{MR} as function of x. Here, the ignition parameters of the 0D and LES simulations of the present study are compared.

in Ref. [22]. When compared to DF, the IDT increases in TF maximally by factor ≈ 2 . Although the effect of IDT increasing along with x is counter-intuitive due to the high reactivity of H₂, it is consistent with the findings in Ref. [28]. According to the provided reaction sensitivity analysis in [28], this retardation of ignition is related to the interplay between H₂ and OH. In specific, H₂ consumes OH radicals more actively compared to methane. Consequently, the more H₂ is added, a longer time is needed for the HRF to react and ignition is delayed. Further explanations about this effect are provided in the following.

Table 2 presents IDT calculations from both 0D and LES. It is observed that τ_2/τ_1 is almost constant for different *x* cases in either 0D homogeneous reactor or LES calculations. This finding is also consistent with those in Ref. [28], wherein it is discussed that adding H₂ in such TF case studies prolongs both LTC and HTC reactions. In the following, we

provide further details from the 3D spray simulations. For brevity, x = 0, 0.8, and 0.95 cases will be discussed in the latter part of the paper.

3.4. TF Spray Ignition: Intermediate Species

It was earlier discussed that species such as RO₂, HO₂, H₂O₂, and OH play a pivotal role in the spray ignition process, and also in TF ignition according to Karimkashi et al. [28]. RO₂ is the first decomposition product of n-dodecane and it is consumed as soon as there is sufficient radical buildup for high-temperature combustion. In contrast, OH is a typical marker for the second-stage IDT, for instance in Ref. [22]. Temporal evolution of maximum RO₂ mass fraction (RO_{2max}) and OH mass fraction (OH_{max}) for different *x* values of TF LES are presented in Figure 8(a). Here, RO_{2max} is generated in smaller amounts during the first-stage ignition for x = 0.95 compared to lower hydrogen concentration cases, which implies weaker first-stage ignition when more hydrogen is added. Conversely, the OH_{max}



Figure 8. (a) Temporal evolution of RO_{2max} (dotted), and OH_{max} (solid) (b) Temporal evolution of H_2O_2 (solid) and 5*HO₂ (dotted) in TF LES.

evolution plot shows that the second-stage ignition becomes much stronger when hydrogen is added. These observations for both first- and second-stage ignition are consistent with those in Ref. [28].

Furthermore, Figure 8(b) depicts temporal evolution of HO_{2max} and H_2O_{2max} for different *x* values. The peak value of HO_2 is achieved at τ_1 and the value drops afterwards. According to the discussion in [28], some amount of HO_2 is converted into H_2O_2 , which results in the peak value of H_2O_2 at τ_2 . It is known that H_2O_2 is a metastable species at low and intermediate temperatures [68] and its higher concentration at higher *x* cases is an important factor in delaying IDT [28].

According to Figure 8, when more hydrogen is added, both RO_2 and HO_2 , i.e. first-stage ignition indicators, reach their peak values with delayed formation. This delay is transferred to the second-stage ignition where the formation of H_2O_2 and OH peaks are delayed. Based on the above discussion, the following observations are summarised for TF ignition: 1) Adding hydrogen delays the first- and second-stage IDT. 2) There is a decrease of LTC-related species concentrations, while 3) an increase in HTC-related species concentrations is observed. These observations on TF oxidation indicate the importance of early decomposition process of all the fuels considered in the present study and subsequent interactions between the produced intermediate species.

3.5. TF Spray Ignition: Spatial distributions of temperature and species

To provide further details on the TF spray ignition process, Figure 9 depicts the spatial distribution of temperature, LTC-related species (RO_{2max}, H₂O_{2max}) and HTC-related species (OH_{max}) at $t = 1.2\tau_2$. It is observed that with higher x, concentrations of LTC-related species and HTC-related species become weaker and stronger, respectively, as consistent with our earlier observations. Contour lines of ξ_{st} (orange), 1%RO_{2max}, and 25%H₂O_{2max} are also marked in Figure 9. The ξ_{st} contour line indicates the longer penetration length of the diesel surrogate for higher hydrogen concentrations. Such dilution is consistent with the longer IDTs as well. This longer spray penetration at $1.2\tau_2$ leads to an extended HTC region (high-temperature region). Therefore, there is a considerably longer time for mixing and dilution. Moreover, ignition always starts from the spray tip region. In particular, HTC in all three cases starts from rich and high-temperature kernels of the spray tip being consistent with the observations in [11,25].

Cut-plane data on the mixture fraction time evolution from the TF spray simulations is presented in Fig. 10 for x = 0 and x = 0.95. The chosen time instances are as follows: 1) first-stage ignition when LTC is initiated, (2) slightly before the second-stage ignition (0.9 IDT) when low and high-temperature regions can be observed, (3) second-stage ignition (IDT) when first ignition kernels can be noted, and (4) slightly after the second-stage ignition (1.2 IDT). For higher x, ignition occurs at leaner conditions. The species iso-contours indicate the following two main aspects: 1) The onset of RO₂ formation shifts further downstream with higher x, and 2) The high-temperature region is larger with higher x extending further downstream even beyond the stoichiometric limit. The comparisons in Figures 9 and 10 indicate the spatio-temporal dependency of heat release rate (HRR) and LTC/HTC-related species on x.

Considering the aforementioned results and discussions together with the discussions and reaction sensitivity analysis provided in [28], the reason for delayed IDT with adding more hydrogen to the ambient gas in TF spray ignition can be summarised as follows. Hydrogen addition in TF hydrogen-methane/n-dodecane leads to weaker RO₂ formation,



Figure 9. Spatial distribution of temperature, $\text{RO}_{2\text{max}}$, $\text{H}_2\text{O}_{2\text{max}}$ and OH_{max} at time $1.2\tau_2$ for TF ignition (n-dodecane/methane/hydrogen) at x = 0, 0.8, and 0.95. Delayed ignition is observed with higher hydrogen concentration values. Here, stoichiometric mixture fraction is represented with orange colour iso-lines. For interpretation of the references to color, the reader is referred to the webversion of this article.

which results in delayed first-stage ignition comparing to DF methane/n-dodecane combustion. Moreover, more H_2O_2 is formed at higher *x* cases which delays ignition due to its meta-stable feature at low and intermediate temperatures. On the other hand, within the time frame between the first- and second-stage ignition, intermediate species such as HO_2 and H_2O_2 further breakdown into HTC-related species such as OH in both DF and TF cases. In TF cases, the presence of hydrogen in the system consumes more OH compared to methane in the DF case, which results in less OH radicals left for the ignition of n-dodecane and its large hydrocarbons, and consequently further delay in the second-stage ignition. The weaker LTC and stronger HTC in TF cases both contribute to the inhibiting effect of IDT in the higher hydrogen concentration cases.

3.6. TF spray ignition: heat release

Heat release rate is an important indicative of the combustion process, which can assist in better understanding of the ignition process in complicated systems such as the current 3D TF spray ignition. The maximum heat release rate (HRR_{max}) for different *x* cases is shown in Figure 11. It is observed that for all *x* cases, HRR_{max} is larger after the second-stage ignition. Moreover, in x = 0.95 case, HRR_{max} is much stronger than for x = 0. Therefore, the presence of hydrogen concentration increases HRR_{max} in the system, as consistent with the experimental findings of [37,40]. This result is consistent with our earlier observation that OH concentration and maximum temperature after the second-stage ignition are higher for x = 0.95 compared to the cases with less hydrogen.



Figure 10. Ignition process for different hydrogen concentrations at TF configuration. Regions where LTC is taking place is represented with RO_2 (green colour) and H_2O_2 (orange colour) while high-temperature chemistry is represented by red colour. Finally, stoichiometric mixture fraction is represented with dotted yellow line. For interpretation of the references to color, the reader is referred to the webversion of this article.



Figure 11. Time evolution of HRR_{max} for different x values of hydrogen.



Figure 12. Scatter plots of the local HRR against mixture fraction for DF (top) and TF (bottom) with conditional mean (solid line) and standard deviation (grey area). Only 50% of the LES data is used. The dotted black line presents the stoichiometric mixture fraction.

Figure 12 shows scatter plots of local HRR values (kJ/m³s) close to the ignition time τ_2 as a function of ξ between the DF (x = 0) and TF (x = 0.95) cases. First, the TF point clouds remains only on the lean side while the DF point clouds span a broader region. The same conclusion is made from the conditional means (black lines). In both cases, the HRR is shifted to the lean side towards the later stages of the n-dodecane combustion. We note that the observations in the scatter plot are consistent with our overall findings. In particular, for DF the HRR is distributed between LTC and HTC modes, i.e. distributed from lean towards richer areas in the ξ -space, while for TF it is more biased towards the HTC mode, i.e. the leaner side of the ξ -space. As a reminder, the HTC mode is typically associated with the spray tip part, where the reactions have progressed the furthest and the fuel has mixed for a relatively long period of time as well.

Finally, we present HRR map analysis which is a useful tool in quantifying the modes of combustion [69]. According to [11], there are five different combustion modes in DF n-dodecane/methane combustion as follows : early LTC, LTC, pre-HTC, HTC pre-ignition, and HTC. Here, we investigate these modes of combustion for x = 0, x = 0.8, and x = 0.95 cases, with the selection criteria provided in Table 3 for temperature and LTC- or HTC-related species mass fractions, following the criteria provided in [70].

Figure 13 shows HRR maps for the considered TF cases. Here, HRR maps for each ignition mode is integrated over the spray volume ($\xi > 10^4$). Additionally, in the HRR maps, the time is normalised with respect to $\tau_2(ms)$ for each LES. The pie charts show the percentage of total HRR from each combustion mode within the period from the starting time till 1.2 τ_2 . According to Figure 13, local HTC is considerably stronger in higher x cases. In addition, looking at the pie charts, in x = 0 case, LTC and HTC pre-ignition modes are dominant over the other ignition modes. These observations are consistent with the HRR

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Table 3. The criteria used for model decomposition based on HRR and their corresponding critical values used are $RO_{2crit} = 10^{-5}$, $H_2O_{2crit} = 10^{-4}$, $OH_{crit} = 10^{-5}$, $T_{crit} = 1150$ K.

Mode	Definitions
Early LTC	$(\text{RO}_2 \ge 1.10^{-7}) \cap (\text{H}_2\text{O}_2 \le \text{H}_2\text{O}_{2\text{crit}}) \cap (T \le T_{\text{crit}})$
LTC	$(\text{RO}_2 \ge (\text{RO}_{2\text{crit}})) \cap (\text{H}_2\text{O}_2 \ge \text{H}_2\text{O}_{2\text{crit}}) \cap (T \le T_{\text{crit}})$
Pre-HTC	$(\text{RO}_2 < (\text{RO}_{2\text{crit}})) \cap (\text{H}_2\text{O}_2 \ge \text{H}_2\text{O}_{2\text{crit}}) \cap (T \le T_{\text{crit}})$
HTC pre-ign	$(OH < OH_{crit}) \cap (T \le T_{crit})$
HTC	$(OH \ge OH_{crit}) \cap (T \le T_{crit})$



Figure 13. Heat release maps within the spray region for ndd/methane/hydrogen at (a)x = 0 (b)x = 0.8 and (c)x = 0.95 normalised with IDT. Pie charts represent the time-integrated contribution of each mode till $1.2\tau_2$. (d) The relative contribution of heat release modes for different H₂–CH₄ blending ratios.

maps provided in [11] for DF n-dodecane/methane combustion. However, in x = 0.8 and 0.95 cases, HTC mode dominates all other modes almost by \approx 70%. Additionally, LTC is found to be weaker in higher hydrogen concentration cases. Therefore, the presence of hydrogen increases the heat release in the HTC mode which is significantly different from the x = 0 case. In Figure 13(d), the relative contribution of heat release modes at all different H₂ –CH₄ blending ratios are displayed, which elaborates the substantial effect of hydrogen addition on stronger HTC. These observations are consistent with our earlier discussions, for instance regarding Figure 9, wherein LTC becomes weaker and HTC gets more robust with more hydrogen concentrations.

We note that the current study targets only the ignition process and its relevant modal decomposition (LTC and HTC) in DF and TF cases. However, to better understand the corresponding processes after ignition, we have recently characterised modes of combustion in Ref. [71], wherein it is noted that the mixture stratification level as well as

turbulence level can switch the mode of combustion between deflagration and spontaneous propagation at CI DF relevant conditions. In the future, We will extend that study to characterise modes of combustion in TF conditions relevant to the present work.

4. Conclusions

In this paper, 0D and 3D numerical results on TF ignition characteristics of n-dodecane sprays in a lean hydrogen-methane-air mixture for different hydrogen concentrations were presented. Comprehensive information on the ignition characteristics of TF sprays was obtained at different hydrogen concentrations. The added value of the paper considers a thorough extension of the 0D findings by Karimkashi et al. [28] to 3D TF spray context. An overall summary of the present work is given as follows.

- (1) The moderate reactivity of the studied methane-hydrogen mixtures may be considered as a positive indication on the potential of using hydrogen in CI engines. In addition, the spray-assisted ignition, i.e. TF concept was found beneficial to facilitate robust ignition.
- (2) According to both 0D homogeneous reactor calculations and LES simulations, firstand second-stage IDT are both delayed with the increase of hydrogen molar concentration. It is quantified as $(\frac{\tau_2}{\tau_1})^{0D} \approx 2 \pm 0.1$, $(\frac{\tau_2}{\tau_1})^{3D} \approx 3 \pm 0.3$, and $\frac{\tau_2^{3D}}{\tau_2^{0D}} \approx 2 \pm 0.2$ for all TF cases.
- (3) First- and second-stage IDT analyses in 0D reactor calculations and LES indicate similar trends. In both 0D and 3D, IDT retardation is rather weak for x <0.5 while for x ≥0.5 evident changes are observed. However, longer IDTs are observed in TF LES context compared to 0D which is due to turbulent spray mixing. Therefore, longer mixing and evaporation timing is evident in TF LES studies.</p>
- (4) With more hydrogen, RO₂ concentration levels decrease. Consequently, first- and second-stage ignition are delayed. This is explained with hydrogen consuming more OH compared to methane.
- (5) The heat release map analysis shows that with increasing hydrogen amount, the HTC contribution to HRR is increasing for x < 1. However, LTC contribution for HRR with increasing hydrogen concentration remains constant.</p>

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