ON THE LUBRICANT OIL POTENTIAL TO SERVE AS AUTO-IGNITION CENTRE IN HYDROGEN ENGINES

E. Distaso*, G. Calò*, R. Amirante*, P. De Palma*, P. Tamburrano*

elia.distaso@poliba.it

* Department of Mechanics, Mathematics and Management, Politecnico di Bari, Italy

Abstract

The present study aims to investigate whether a suspended lubricant oil droplet in an H_2/air environment can trigger an undesired local self-ignition of the charge. Additionally, the study offers preliminary insights into the nature of the combustion event that might result. Thermo-chemical conditions potentially present in the vicinity of an oil droplet were analytically derived and integrated into zero-dimensional numerical simulations to quantify local variations in charge reactivity. The potential auto-ignition propagation modes arising from oil contamination were then studied through an analysis based on the comparison between the characteristic times of the reaction and the acoustic waves.

Introduction

Hydrogen Internal Combustion Engines (HICEs) have emerged as a strategic solution in the pursuit of rapid decarbonization, especially for heavy-duty land and marine vehicles. However, the widespread adoption of HICEs is not without its challenges. One such challenge is the occurrence of pre-ignition events [1]. Lubricant oil might play a major role in determining such abnormal combustion events, promoting uncontrolled premature ignition of the charge [2]. Namely, lubricant oil contamination can create localized areas with enhanced reactivity, potentially serving as "sensitive spots" for combustion initiation.

Consequently, alterations in charge composition resulting from oil contamination may induce similar outcomes to those described by Zel'dovič [3] concerning temperature inhomogeneities, potentially leading to various auto-ignition modes, including thermal explosion, supersonic auto-ignition propagation, detonation development, subsonic auto-ignition propagation, and simply laminar deflagration. In the case of "hot spots" Bradley and colleagues [4] proposed diagram based on dimensionless parameters to determine the critical conditions associated with each mode, widely utilized in the study of engine knock and deflagration-to-detonation transition. It is worth to note that small kernels of slightly higher reactivity within the mixture are sufficient to initiate ignition events [5]. Therefore, understanding the potential risk posed by the interaction of hydrogen with lubricant oil is crucial for the development of efficient and reliable HICEs.

The present analysis delves into the topic through the examination of a suspended lubricant oil droplet in an H_2/air environment. An analytical model was conceived

to derive physically reasonable expressions for the temperature and species distributions in the region close to the droplet surface, with minimal computation effort. The information was then used to initialize reactive 0D numerical simulations conducted in the OpenSMOKE++ framework. The chemical properties of $H_2/oil/air$ mixtures were emulated using the reduced chemical model developed in a previous work [2]. The simulations aimed to quantify changes in reactivity induced by a lubricant oil droplet. Lastly, the theory originally developed by Bradley and colleagues for "hot spots" [4] was adapted to the investigated scenario to explore potential propagation modes arising from the auto-ignition centre induced by oil contamination.

Analytical model

The model considers a single droplet existing in a quiescent, infinite medium constituted by a H_2/air mixture with a higher temperature than that of the droplet. A spherically symmetric coordinate system was employed for describing the problem, as depicted in Figure 1. Interactions with other droplets and the effects of convection are disregarded. Radiation heat transfer is deemed negligible, and the pressure is assumed to be uniform and constant. The lubricant oil droplet is treated as a single-component liquid, with zero gas solubility and properties resembling those of n-hexadecane. The evaporation process is assumed to be much slower than the involved chemistry, enabling the use of a quasi-steady assumption to describe the process. Thermodynamic parameters of the gas mixture, such as gas-phase thermal conductivity, λ, and specific heat, $c_{p,g}$, as well as the product of the density and mass diffusivity, $\rho\mathcal{D}$, are all considered constants. The hypothesis of unit Lewis number, $Le = \lambda/(c_{p,g}\rho\mathcal{D})$, is invoked.

With the above assumptions, the gas-phase mass, species, and energy conservation equations can be simplified to the well-known Shvab-Zel'dovič form:

$$4\pi r^2 \rho v = 4\pi r^2 \rho_s v_s = \dot{m} = const$$

$$\frac{d}{dr}(4\pi r^2 \rho v Y_{oil}) = \frac{d}{dr}\left(4\pi r^2 \rho\mathcal{D}\frac{dY_{oil}}{dr}\right) \tag{1}$$

$$4\pi r^2 \rho v \frac{d(c_{p,g}T)}{dr} = \frac{d}{dr}\left[4\pi \frac{\lambda}{c_{p,g}} r^2 \frac{d(c_{p,g}T)}{dr}\right].$$
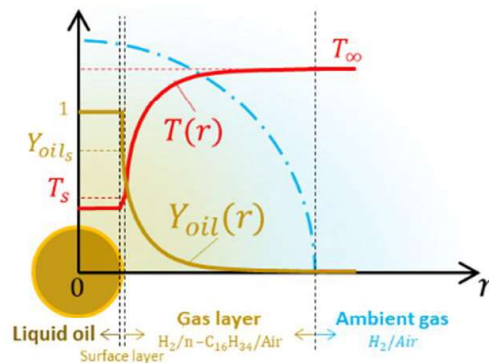

Figure 1. Schematization of the evaporation process according to the "onion-skin" model.

The oil (n-hexadecane) mass fraction distribution, $Y_{oil}(r)$, and the temperature distribution, $T(r)$, in the ambient surrounding the droplet can be obtained from the Equations set (1) by imposing $\rho_s v_s = [\rho v Y_{oil} - \rho \mathcal{D}(dY_{oil}/dr)]_s$ and $T = T_s$ at the droplet surface ($r = r_s$), and $T = T_\infty$ far from the droplet surface ($r \to \infty$):

$$Y_{oil}(r) = 1 - \frac{(1 - Y_{oil_s})e^{-\frac{Z\dot{m}}{r}}}{e^{-\frac{Z\dot{m}}{r_s}}} \tag{2}$$

$$T(r) = \frac{(T_\infty - T_s)e^{-\frac{Z\dot{m}}{r}} - T_\infty e^{-\frac{Z\dot{m}}{r_s}} + T_s}{1 - e^{-\frac{Z\dot{m}}{r_s}}}, \tag{3}$$

where $Z = c_{p,g}/(4\pi\lambda)$. Equations (2) and (3) require knowledge of the evaporation rate, $\dot{m}$, and the values at the droplet surface of the oil mass fraction, Y_{oil_s}, and temperature, T_s. Thus, to provide closure to the problem, the droplet gas-phase interface energy balance and the droplet liquid mass conservation equation were solved. Fourier's law was used in conjunction with the so-called "onion-skin" model. Equilibrium between liquid and vapor phases at the interface was assessed using the Clausius–Clapeyron equation. The obtained expressions are:

$$\dot{m} = \frac{r_s}{Z}\ln\left[1 + \frac{c_{p,g}(T_\infty - T_s)}{\Delta_v h_{oil} + c_{p,l}(T_s - T_d)}\right] \tag{4}$$

$$Y_{oil_s} = 1 - e^{-\frac{Z\dot{m}}{r_s}} \tag{5}$$

$$Y_{oil_s} = \frac{e^{-\frac{\Delta_v h_{oil}}{R}\left(\frac{1}{T_s} - \frac{1}{T_{s,ref}}\right)} MW_{oil}}{e^{-\frac{\Delta_v h_{oil}}{R}\left(\frac{1}{T_s} - \frac{1}{T_{s,ref}}\right)} MW_{oil} + \left[p - e^{-\frac{\Delta_v h_{oil}}{R}\left(\frac{1}{T_s} - \frac{1}{T_{s,ref}}\right)}\right] MW_\infty}, \tag{6}$$

where $c_{p,l}$ and $\Delta_v h_{oil}$ are the specific heat and the heat of vaporization of the liquid oil; MW_{oil} and MW_∞ denote the molecular mass of the oil and the average molecular mass of the H_2/air mixture far from the droplet; $T_{s,ref}$ is the boiling temperature of the oil at the reference pressure ($1\ atm$). Equations (4), (5) and (6) were simultaneously solved, and the results were used to evaluate $Y(r)$ and $T(r)$ in Equations (2) and (3), respectively. For the calculation, appropriate mean values for the liquid- and gas-phase thermodynamic properties of the involved species and mixtures were selected, although the specific method employed is not reported here for the sake of brevity.

Numerical simulations
The outcomes derived from the analytical model were used to initialize 0D numerical simulations performed within the open-source OpenSMOKE++ framework [6]. These simulations aimed to quantify the variations of the ignition delay time along the radial coordinate, $\tau(r)$. A criterion based on the maximum OH increase was used for evaluating the ignition delay time. The reduced reaction mechanism developed in a previous study [2] for $H_2/n\text{-}C_{16}H_{34}/air$ mixtures and consisting of 169 species and 2796 reaction was employed in the simulations.

Extending the theory of "hot spots"

The approach developed by Bradley and colleagues was employed for classifying the auto-ignition modes [4]. However, for the purpose of the present analysis, the concept of a "hot spot" serving as the auto-ignition centre, needed to be expanded to that of a "sensitive spot". In the case of "hot spots", the dimensionless parameter, ξ, introduced to account for resonance between auto-ignition and acoustic time, was calculated as $\xi = \nabla T/(\nabla T)_c$, where $(\nabla T)_c = [(d\tau(T)/dT)a]^{-1}$ expresses the critical temperature gradient leading to chemical resonance. In the present study, a broader definition for ξ was required. Therefore, it was directly assessed by comparing the time, t_{rw}, needed by the reaction front to traverse the "sensitive spot", and the time, t_{aw}, needed by the acoustic wave:

$$\xi(T, Y_{oil}) = \frac{t_{rw}}{t_{aw}} = a\frac{d\tau(r)}{dr}, \tag{7}$$

where a represents the speed of sound, while the function $\tau(r) = \tau(T(r), Y_{oil}(r))$ is the one obtained from 0D simulations, thereby encompassing its dependence on temperature, mixture strength, and mixture composition.

The same definition given for the dimensionless parameter, ε, was used to assess the degree of coupling between acoustic effects and exothermic reactions:

$$\varepsilon = \frac{l/a}{\tau_e}. \tag{8}$$

where l is the length of the region where variations in reactivity occur, while τ_e is the excitation time, evaluated as the duration between 5% and maximum heat release rate [5]. In the present case, the region of interest starts at the minimum of $\tau(r)$ and ends when $\tau(r)$ reaches 90% of the τ_∞ value.

Results

Three (T_∞, p) values pairs were selected to resemble typical conditions within the combustion chamber of a HICE when pre-ignitions events might occur, namely, $(800\,K, 30\,bar)$, $(900\,K, 50\,bar)$, $(1000\,K, 70\,bar)$. An equivalence ratio of the H_2/air mixture surrounding the oil droplet equal to 0.5 was considered. A droplet radius of $25\,\mu m$ was selected within the range of possible sizes observed experimentally [7]. Figure 2a reports the profiles of mass fraction, $Y_{oil}(r)$, and temperature, $T(r)$, obtained from the analytical model. The corresponding ignition delay profile, $\tau(r)$, obtained from the 0D simulations, is reported in Figure 2b.
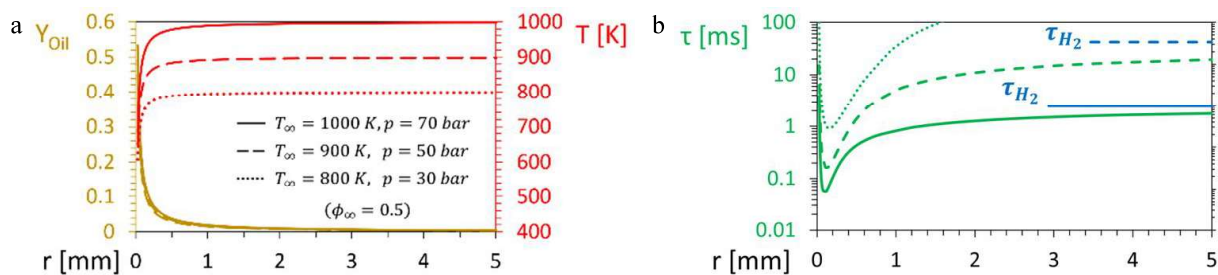

Figure 2. Analytically derived spatial distributions of temperature and oil mass faction (a), and ignition delay time (b).
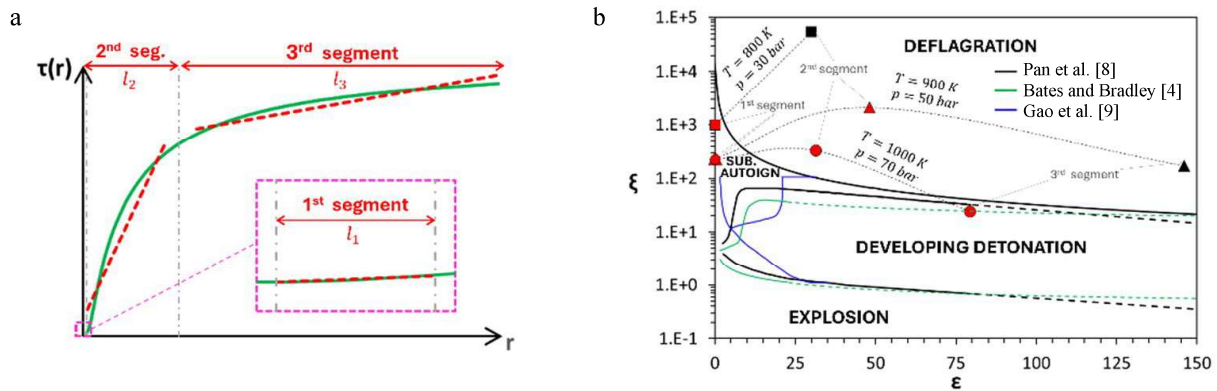
Figure 3. Segmentation of $\tau(r)$ function (a). Classification diagram (b).

The primary finding is that $\tau(r)$ remains significantly lower than the reference value of the H_2/air mixture (τ_{H_2}) even at a considerable distance from the droplet. At 800 K and 30 bar, the thermodynamic conditions are inadequate for promoting auto-ignition of the H_2/air mixture. However, in presence of lubricant oil contamination, the $\tau(r)$ profile exhibits a deep trough, similar to the other reactive cases. This indicates that the presence of an oil droplet has the potential to substantially alter the explosion limit of hydrogen by creating a highly reactive mixture during its vaporization, even under conditions where hydrogen would not typically auto-ignite. For this low-temperature case, at a distance of about 5 radii, the formed $H_2/oil/air$ mixture needs only about 1 ms to auto-ignite, with $\tau(r)$ remaining below 10 ms up to a distance of 25 radii. This is a remarkable finding, as it suggests that an oil droplet could locally initiate spontaneous ignition of the charge, even under thermodynamic conditions typically deemed safe for hydrogen engine operation. At 1000 K and 70 bar, the auto-ignition time for the H_2/air mixture is approximately 2.5 ms. However, with the presence of an oil droplet, this time can be reduced to about 60 μs at a distance slightly less than 5 droplet radii, highlighting a maximum reduction of about 98% induced by the oil vapour at the highest ambient temperature and pressure considered.

In all the considered cases, the $\tau(r)$ function exhibits notable variations. Consequently, to assess the deriving auto-ignition propagation modes, three subregions exhibiting nearly constant slopes were identified for each case, as illustrated in Figure 3a. All parameters required for calculating ξ and ε were evaluated at $l_i/2$, consistent with the approach adopted in the original theory.

Figure 3b illustrates the potential auto-ignition propagation modes arising from the three studied cases according to the "detonation peninsula" recently obtained by Pan et al. [8] (black lines). The boundaries originally obtained by Bradley and colleagues [4] are also reported for comparison (green lines). The diagram was obtained for an equimolar H_2/CO mixture at $T = 1000\ K$, $p = 40\ atm$ and $\phi = 1$. However, recent studies (see, e.g., [9,10]) have suggested that the peninsula boundaries may vary depending on the fuel mixture and thermodynamic conditions. Therefore, in Figure 3b, boundaries obtained by Gao et al. [9] for pure H_2 at $T = 1000\ K, p = 40\ atm$, and $\phi = 0.5$ are also reported for comparison

(blue lines). With regard to the studied cases the differences are limited and do not impact the conclusions that can be drawn.

In Figure 3b, the points corresponding to ignition delay time values lower than $20\ ms$ (i.e., relevant for engine applications) are highlighted in red. Under all considered thermodynamic conditions, a subsonic propagating auto-ignition front can arise in the first segment, namely, closer to the droplet surface. In the second segment (where the $\tau(r)$ function exhibits the highest slope) a deflagration front can be generated. As the mixture extends away from the droplet, its reactivity progressively decreases. Consequently, the third segment becomes irrelevant at $900\ K$ and $50\ bar$ and does not even exist at $800\ K$ and $30\ bar$. However, at high pressure and temperature ($1000\ K$ and $70\ bar$) the reduction in the slope of the $\tau(r)$ function renders the third segment particularly dangerous, as it may serve as the origin of a developing detonation. Additionally, the ignition delay time remains lower then $1\ ms$ along the entire extent of the three segments. It is worth noting that the conditions in the last two segments may depend on the activity related to the preceding segments, potentially exacerbating the situation.

Conclusions

The study identified key findings regarding the potential impact of lubricant oil contamination on auto-ignition propagation in hydrogen-fuelled engines. Through analytical modelling and numerical simulations, it was explored whether suspended oil droplets in H_2/air environments can serve as auto-ignition centres, initiating an uncontrolled chemical process that propagates through the charge. The analysis unveiled the capability of oil vapour to drastically reduce the time required for auto-ignition initiation, even under conditions considered safe for hydrogen engine operation. Deflagration fronts might be generated and dangerously interact with the main combustion process. Secondary "hot spots" might consequently be created, eventually leading to severe knocking cycles. The results also do not exclude the possibility of direct detonation initiation, posing significant safety concerns. This underscores the importance of implementing rigorous monitoring and mitigation strategies to prevent such occurrences in the development of hydrogen engines.

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