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Two-stage ignition and NTC phenomenon in diesel engines

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HIGHLIGHTS

- 3-D, transient, turbulent spray simulations performed.
- Two-stage ignition in diesel sprays examined from the evolving QOOH (alkyl hydroperoxy) and OH fields.
- NTC (negative temperature coefficient) behavior investigated in sprays and homogeneous mixtures.
- Effect of methane on the ignition of n-heptane sprays in dual-fuel diesel engine characterized.

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ABSTRACT

Two-stage ignition and NTC phenomenon in diesel sprays is investigated by performing 3-D two-phase reacting flow simulations in a dual-fuel engine. Spray processes modeled include fuel atomization, droplet distortion, droplet drag, turbulent dispersion, droplet interactions in terms of collision and coalescence, vaporization, and spray–wall interaction. A validated reaction mechanism is implemented in the CFD solver, which has previously been validated for both evaporating and reacting sprays. For single-fuel cases, the effect of temperature on two-stage ignition is examined by varying the start of injection (SOI). While results indicate global similarities between the two-stage ignition processes in diesel sprays and spatially homogeneous mixtures, there are also noticeable differences between them due to temporally and spatially evolving temperature and species fields in the spray case. For instance, both the first- and second-stage ignition delays are higher for the spray cases compared to homogeneous mixtures. Second, while ignition delay for homogeneous mixtures exhibits a NTC region, that for sprays indicate a ZTC region. Moreover, the first- and second-stage ignitions for the spray occur over a wide φ range and at multiple locations in the spray, implying a spatially wide ignition kernel. Additionally, while the chemical ignition delays are strongly influenced by the injection timing, the physical delays are essentially independent of this parameter. Results with dual fuel indicate that the two-stage ignition behavior remains intact even at high molar fractions of methane. The addition of methane increases ignition delays for both sprays and homogeneous mixtures, and can be attributed to the reduction in O_2 and the chemical effect of methane. The sensitivity analysis indicated that the chemical effect is primarily due to reaction $CH_4 + OH = CH_3 + H_2O$.

1. Introduction

Liquid spray combustion is employed in numerous combustion systems. Ignition represents a crucial event in the operation of these systems. Compared to a gaseous mixture, ignition in a spray is considerably more complex, as the state of ignition can be defined by three distinct ignition modes; droplet ignition, cluster ignition, and spray ignition. Ignition for an individual droplet represents the appearance of a flame near the droplet with a dimension of the order of droplet diameter. The cluster ignition refers to the ignition around or inside a droplet cloud, while the spray ignition implies the appearance of a global flame with a dimension few orders of magnitude larger than droplet scales. In all three modes, ignition is preceded by droplet evaporation, formation of a combustible gaseous fuel–air mixture, and initiation of chemical reactions. Clearly, determination of the dominant ignition mode and the ignition behavior in each mode for different spray systems is of fundamental and practical importance [1].

Considerable research exists on these ignition modes. Aggarwal [2] and Mastorakos [3] report reviews of work dealing with laminar and turbulent spray ignition, respectively. Research on cluster ignition is discussed by Annamalai and Ryan [4], and on droplet ignition by Aggarwal [5]. As discussed in Ref. [5], numerous

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experimental and computational studies concerning droplet ignition have focused on the temperature dependent chemistry effects, especially on the two-stage ignition and NTC (negative temperature coefficient) phenomenon [6–10]. Kinetics aspects of this phenomenon have been extensively studied using homogeneous mixtures [11]. As discussed in these studies, the two-stage ignition and NTC behavior is a common characteristic of the oxidation chemistry of large alkanes, described by a transition between the low- and high-temperature paths as determined by the reaction: $R + O_2 \Leftrightarrow ROO$. Here alkyl radical (R) is formed from fuel decomposition through H-atom abstraction. This reaction is favored below $T \approx 800$ K, and peroxy radical then undergoes isomerization to form alkyl hydroperoxy (QOOH), which subsequently leads to the formation of ketohydroperoxide (OQOOH) and OH radicals. OQOOH being an unstable intermediate readily decomposes to form OH, alkenes and other radicals. OH then reacts with fuel to form more alkyl that feed the above chain. The above path is favored at low temperatures, leading to the first-stage ignition, characterized by a sudden but limited temperature rise. The second-stage ignition then depends upon a competition between heat releasing reactions and heat loss from the cool flame region. However, in the NTC region, the above low-temperature path becomes less important. Instead QOOH decomposes to form alkene and HO_2. In addition, alkyl radicals react to form alkenes and additional HO_2. Consequently, the ignition delay increases with the increase in temperature, as the system reactivity decreases because the branching sequence becomes less important and HO_2 formation is favored compared to OH. At still higher temperatures, alkyl radicals decompose directly to form alkenes and smaller alkyl radicals through β-scission reactions, and the ignition process follows the high-temperature path.

While these chemistry effects are well established for homogeneous systems, they become far more complex for droplets and sprays. For droplets, additional complexity is due to the strongly coupled processes of two-phase transport, droplet heating, and vaporization. Coupling of these processes with fuel chemistry leads to multiple ignition regimes [6,7], depending upon the droplet size, fuel volatility, and ambient conditions. These regimes include (i) no ignition implying complete droplet evaporation prior to ignition, (ii) only first-stage ignition, (iii) two-stage ignition, and (iv) single-stage (hot flame) ignition. Researchers have examined these regimes through experiments using a suspended droplet, or simulations using a transient, spherically symmetric model with reduced and detailed mechanisms. The two-stage ignition was identified by following the peak temperature history, with the first temperature jump marking the first-stage ignition and the second jump representing the second-stage ignition. However, these studies did not provide a clear evidence for the NTC region, and it was surmised that the presence of non-homogeneous temperature and species fields causes a transition from the NTC to ZTC (zero temperature coefficient) region. Bouali et al. [12] suggested that competition between the availability of fuel vapor and the reduction in mixture temperature due to evaporation also plays a role. While various researchers provided different explanations for the modification of NTC behavior, only a handful of studies observed a ZTC region [6,8].

The present study has two objectives. One is to investigate the two-stage ignition and NTC phenomenon in diesel sprays. This is motivated by the consideration that ignition represents a critical process in diesel engines, and strongly influences their combustion and emission characteristics [13,14]. Moreover, new strategies, such as HCCI and LTC, for reducing engine emissions are based on controlling the ignition event. Literature review indicates that while numerous studies have investigated two-stage ignition for homogeneous mixtures and droplets, relatively little work exist for sprays [12,15]. Moreover, previous investigations have employed simplified spray configurations, whereas the present study examines spray ignition in a diesel engine, where the ignition is influenced by the processes of fuel injection, vaporization, mixing, and kinetics. This is perhaps the first study reporting details of the first- and second-stage ignition processes by analyzing the evolution of QOOH and OH fields, as the fuel injection proceeds. Another objective is to examine the effect of methane on the two-stage ignition in diesel sprays. There is significant interest worldwide in developing NG-fueled diesel engines. However, due to its poor ignitability, a more plausible strategy is to use CI engines is a dual fuel mode with NG introduced through the intake port and diesel fuel through direct injection. Previous investigations have mostly focused on the combustion and emission characteristics of diesel engines with dual fuels [16], rather than on the ignition behavior.

2. Computational model

The CONVERGE 3-D software is used for simulating the fuel injection, atomization, and ignition processes in a 1.9L 4-cylinder GM light-duty diesel engine, which has been extensive used in

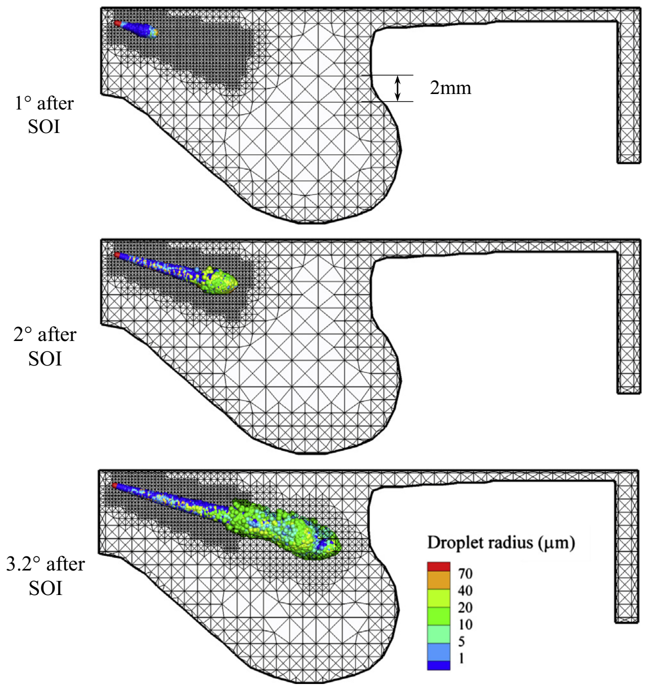

Fig. 1. A cross-section view of the cylinder through the spray, and the predicted spray structure for the −8° SOI case at 1°, 2° and 3.2° CA after SOI. Each color dot represents a droplet radius value in a given parcel, and the size distribution is indicated by the droplet radius scale (1–70 μm). The adaptive mesh evolution with time (CA) during injection and the spray development are also shown. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
Initial conditions and ignition delays in terms of crank angle for different SOIs.

SOI	−32	−26	−20	−14	−8	−4
SOI temp. (K)	700	754	812	864	903	916
SOI pres. (MPa)	1.5	2.0	2.7	3.6	4.6	5.0
τ_{phy}, physical (°)	1.6	1.4	1.2	1	1	0.9
τ_{I}, 1st stage (°)	13.4	9.0	5.5	3.6	2.2	2
τ_{II}, 2nd stage (°)	5.2	3.8	2.8	2.2	2.4	2.5
τ_{tot}, chemical (°)	18.6	12.8	8.3	5.8	4.6	4.5