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# Transient plasma effects on the autoignition of DME/O<sub>2</sub>/Ar and C<sub>3</sub>H<sub>8</sub>/O<sub>2</sub>/Ar mixtures

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#### Abstract

The effects of transient plasma discharge on the autoignition characteristics of dimethyl ether and propane mixtures with oxygen and argon were investigated computationally in a zero-dimensional constant pressure environment. A simple model of hydrocarbon decomposition by electron collisions was superimposed on detailed chemical kinetic models that describe the low temperature oxidation of dimethyl ether and propane. The results suggest that the effectiveness of plasma discharges in promoting autoignition is very high at low temperatures. However, in the negative temperature coefficient region, the plasma discharge was determined to be less effective in promoting autoignition, as a result of complexity of the neutral state chemistry. The degree of effectiveness was quantified and was determined to differ significantly for different mixtures. An explanation for these differences is presented based on what is currently known about low temperature hydrocarbon kinetics.

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Keywords: Transient plasma; Plasma kinetics; Combustion kinetics; Ignition delay times; Low temperature chemistry

#### 1. Introduction

The low to intermediate temperature chemistry, i.e. in the 500 K < T < 950 K range, can play an important role in various combustion applications. A pertinent example is compression ignition engines, in which certain fuels exhibit notably better ignition propensity than others; dimethyl ether (CH<sub>3</sub>OCH<sub>3</sub> or DME) for instance has remarkable autoignition characteristics, and is considered a promising alternative fuel [1]. However, fuels with enhanced low

temperature chemistry also exhibit the so-called negative temperature coefficient (NTC) behavior, i.e. there exists a temperature range within which an increase in temperature results in a decrease in reactivity [2]. The NTC behavior results typically in a two-stage ignition with consequences for engine design, which are difficult to understate. For example, in homogenous charge compression ignition (HCCI) engines, thermal stratification is purposefully set up in the cylinder in order to control the heat release rate [3]; the central core ignites first followed by the peripheral gas. However, if the fuelair mixture is prone to ignite slower in the core region and faster in the periphery, which is a plausible situation in the NTC regime, the performance of

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Fig. 1. Key pathways in low temperature hydrocarbon ignition (taken from Merchant et al. [9]) Blue arrows lead to chain branching, red arrows to chain termination, and black arrows to chain propagation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the HCCI engine could degrade appreciably. Last but not least, in spark-ignition engines the events leading to knock are controlled largely by low temperature chemistry [4].

It is in this context that the control of such processes through non-equilibrium transient plasma (TP) assistance is of growing importance [5]. The TP-assistance comes in the form of radicals without relying on thermal energy, essentially decreasing the net global activation energy. Two recent investigations have shed light on the coupling of TP discharges with low temperature chemistry. The study by Filimonova [6] showed that the TPinduced radicals greatly reduce and in certain cases even eliminate the NTC behavior of mixtures of propane  $(C_3H_8)$  with air. Sun et al. [7] measured high formaldehyde ( $CH_2O$ ) concentrations prior to the ignition of DME/O<sub>2</sub>/He non-premixed flames, indicating a distinct period of TP-assisted low temperature chemistry. Nagaraja et al. [8] extended this work to study two-staged ignition of *n*-heptane.

Capturing the effects of the NTC behavior on the ignition delay time,  $\tau_{ign}$ , through a combustion kinetics model, regardless of its response to TP discharges, is an area of unceasing research. The kinetic underpinnings of NTC behavior have undergone many revisions, the most recent of which, authored by Merchant et al. [9], is notable for its expository take on the subject. A brief review of the interpretation of low temperature chemistry [9] is presented next.

Figure 1 summarizes the key steps that comprise typical low temperature combustion of hydrocarbons. This regime of combustion is dictated by the rate of  $R + O_2 \leftrightarrow RO_2$  (RXN1), where R is an alkyl radical. At sufficiently low temperatures, the forward rate of RXN1 is favored while that of the isomerization  $RO_2 \leftrightarrow QOOH$  (RXN2) is not; Q results from one H abstraction from R. Thus, the peroxy radical RO<sub>2</sub> accumulates and drives the formation of the alkylhydroperoxide ROOH, which subsequently leads to chain branching.

A further increase in temperature can bring the system to a point where the backward rate of RXN1 begins to be favored, when the equilibrium constant is less than unity. Note that this happens only for fuels that exhibit NTC behavior; in Fig. 2 it can be seen that both C3H8 and DME possess this feature. The reversal of RXN1 has far reaching consequences on the mixture's ability to sustain chain branching. The ROOH formation gradually ceases with increasing temperature, forcing the oxidation to proceed via the slower RXN2. The mixture can autoignite only if it can sustain OH formation through chain branching, i.e. if a sufficient amount of QOOH accumulates as shown in Fig. 1. Subsequently, the OH radicals are partly used to oxidize the fuel. Thus, the sufficient condition for autoignition is the positive feedback of OH radicals. Two-stage ignition occurs mainly because this feedback is stalled due to the formation of the ketohydroperoxide, OQ'OOH, as it will be discussed below. At sufficiently high temperatures, the chain branching relies largely on the accumulation of hydrogen peroxide  $(HO_2)$  radicals that are initially dormant.

The effects of TP on NTC chemistry can be understood by observing how the aforementioned pathways are perturbed. In the recent studies [6,7], partial answers have been given to the question

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