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A computational analysis of methanol autoignition enhancement by dimethyl ether addition in a counterflow mixing layer

Wonsik Song, Efstathios-Al. Tingas, Hong G. Im*

Clean Combustion Research Center, King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

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ABSTRACT

To provide fundamental insights into the ignition enhancement of methanol (MeOH) by the addition of the more reactive dimethyl ether (DME), computational parametric studies were conducted in a onedimensional counterflow fuel versus air mixing layer configuration with the incorporation of detailed chemistry and transport. Various computational analysis tools based on the computational singular perturbation (CSP) framework were employed for detailed identifications of complex chemical pathways. CSP tools were also used to develop a 43-species skeletal mechanism for efficient computation of ignition of methanol-DME blends at engine conditions. The overarching practical question was the extent to which the addition of DME improves the ignitability of the methanol. As a baseline analysis, the results of a uniform temperature condition at 850 K showed that the low temperature chemistry associated with the DME fuel was highly effective in promoting autoignition. The increase in the oxidizer side temperature was found to diminish the ignition enhancement by DME blending, as the overall reactivity increases and the dominant chemical pathways become shifted towards the high temperature reactions. Finally, the strain rate effect on the ignition delay time was found to be significant for the pure methanol case, and then the effect diminishes as the amount of DME addition increases. This behavior was explained by examining the spatial locations of the ignition kernels and the Damköhler number history for different strain rate conditions.

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1. Introduction

Towards higher efficiency, modern engine designs are increasingly incorporating direct injection compression ignition operation with down-sized boosted modes [1,2]. Compared to the conventional spark-ignition (SI) engines, the direct injection eliminates the throttling loss and other parasitic losses, thereby improving the efficiency [1,3]. The new approach also exploits advanced injection technology to allow a wide range of injection timing [4], thereby controlling the combustion mode all the way from the homogeneous charge compression ignition (HCCI) (for early injection) to conventional direct injection (DI) diesel operation (late injection) [5]. Combined with variable valve timing technology, these new engines can be designed for optimal operation at a wide range of load and speed conditions [1–3]. By ensuring the low-temperature and lean combustion (LTC) at each operating condition, there is a great potential to reduce the pollutant formation such as NOx and soot [3,5]. Therefore, the combustion of modern engines depends increasingly on ignition-controlled combustion. Since different fuels have vastly different ignition properties, often quantified by the octane number (for SI engines) and cetane number (for DI engines), such engine operations become highly sensitive to the choice of fuels and intake conditions [6–8].

From the environmental and sustainability standpoint, there is also increasing demand for reducing dependence on fossil fuels. These non-petroleum-based alternative fuels include bio-fuels based on different feedstock, coal- or biomass-driven syngas and many others [9,10]. A more recent development in sustainable alternative fuel production is referred to as "solar fuels" [11–13], which include hydrogen, generated by water electrolysis using photovoltaic power generation. Taken further steps, the solar hydrogen may be further converted into methanol by combining hydrogen and carbon dioxide. Kim et al. [11] presented a method to produce methanol from carbon dioxide and water produced by solar energy, using a thermochemical reactor where CO₂-to-CO conversion is processed, and CO is subsequently used in catalytic processes to form hydrogen or methanol. While these technologies are still far from being mature and economical, there is no doubt the subject is attracting research interests.

* Corresponding author.

E-mail address: hong.im@kaust.edu.sa (H.G. Im).

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Fig. 1. (a) The total relative error of the mass fractions for the skeletal mechanisms as a function of the number of species; (b) The relative error of the ignition delay for the generated skeletal mechanisms as a function of the number of species. The red symbols indicate the selected skeletal mechanism. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

One of the main challenges in utilizing methanol in modern CI engines is that methanol, with derived cetane number (DCN) of 5 [14], is much more difficult to ignite compared to diesel fuels. A logical strategy is then to blend more reactive fuels, such as dimethyl ether (DME) with DCN of 55 [14], with methanol to augment the ignitability. DME has been well known to be a clean fuel due to the absence of carbon-carbon bonds, and its low boiling temperature allows gas phase combustion, providing fast mixture formation [4,6,8,14–16]. Thus, a large number of studies have been conducted using blends of MeOH and DME. Yao et al. [6] experimentally studied the feasibility of the MeOH/DME blends in a single-cylindered HCCI engine and found that the rate of exhaust gas recirculation (EGR) and DME percentage were the most significant parameters for the control of combustion. Controlling the ignition timing and combustion duration was also demonstrated by changing the ratio of DME and EGR into the cylinder. However, there was a trade-off between efficiency and emission performance, demanding further studies in different types of engines and fuels. More studies are available on blending methanol and dimethyl ether [4,6-8,17-19]. Most of these studies are experimental, and often specific to practical engine operations, and thus there is little understanding of detailed chemical pathways leading to the autoignition of MeOH/DME blends. The present study is aimed at providing fundamental insights into this issue by conducting high fidelity computational simulations in a well-defined simple configuration, at conditions relevant to advanced CI engine combustion that exploits LTC technique. For that purpose, a one-dimensional counterflow configuration was adopted with full incorporation of chemical kinetic mechanisms and transport properties. The overarching engineering question was the effect of DME blending on ignition improvement of MeOH at different parametric conditions.

Methodologies of asymptotic analysis have been widely used to obtain the physical understanding of systems of reacting flows. One of the prominent algorithms for asymptotic analysis is the computational singular perturbation (CSP) method, which provides algorithmic tools for the identification of the reactions that are responsible for the development of the fast and characteristic dynamics [20–22]. These tools have been employed for the analysis of flames [23–25], partially stirred reactors [26] and autoignition processes [15,16,20,27–33]. Various computational analysis based on the CSP framework was employed in the present study.

The structure of the paper is as follows. First, an accurate skeletal reaction mechanism is developed using the CSP approach. Subsequently, the configuration of the model problem is presented and associated CSP-based analytical tools are briefly summarized. A simplified model is presented that is used for the one-dimensional simulation of a counter-flow flame. The main body of the results consists of three sets of parametric studies: (a) the effect of DME addition on autoignition for a uniform temperature condition, (b) the effect of oxidizer temperature, and (c) the effect of the steady strain rate. Throughout the parametric studies, the CSP tools will be actively utilized to unravel details of explosive modes responsible for autoignition, as well as the breakdown of key chemical pathways associated with MeOH and DME ignition.

2. Chemical kinetic mechanism

For accurate prediction of the ignition behavior of the MeOH/DME blends, a detailed kinetic mechanism was considered and was systematically simplified for computational efficiency without sacrificing the fidelity. The Aramco 1.3 mechanism consisting of N = 253 species and K = 1524 reversible reactions [34] was used as the starting mechanism, which has been tested and validated against a wide range of initial conditions for C₁ and C₂ fuels.

The detailed mechanism was simplified by using a CSP-based approach [35–37], utilizing an explicit dynamical characterization in the formulation of the simplification procedure. The method systematically suggests the elimination of reactions on the basis of their relevance to the fast or slow dynamics of a predetermined set of the initial kernel of species. For that purpose, the importance index is used, which measures the contribution of each elementary reaction to the fast and slow components of each selected species production rate. The selection of the species is performed iteratively; starting from the initially selected set of species, the related importance indices of all reactions are calculated and those having an index value larger than a user-specified threshold are kept, while the rest deemed as unimportant are eliminated. At the end of the iteration, a new set of species is identified as being strongly coupled to the target species. The union of these two sets of species forms the new set of target species and used for the next iteration. The procedure ends when this set does not change between two successive iterations. For the simplification of the detailed mechanism, the CSPTk package [38,39] was employed, which uses CVODE and the TChem [40] for the thermo-kinetic database management.

Since the subject of the current study was the investigation of the effect of the DME addition on the MeOH/Air unsteady nonpremixed flame, the resulting skeletal mechanism had to incorporate both the DME and the MeOH chemistry. Therefore, for the current simplification procedure, the homogeneous constant pressure autoignition of a fuel blend of 50% MeOH and 50% DME was considered and analyzed at an initial pressure of 30 atm, initial temperature of 800 K and $\phi = 0.6$. The selected initial conditions aim to simulate engine operating conditions. The initial kernel of the selected species included the species of CO₂ and H₂O, i.e., the main combustion products. The relative and absolute error tolerances for the determination of the *M* exhausted modes were selected as $\epsilon_{rel}^i = 10^{-3}$ and $\epsilon_{abs}^i = 10^{-7}$, respectively.

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