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A surrogate mixture and kinetic mechanism for emulating the evaporation and autoignition characteristics of gasoline fuel

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ABSTRACT

Gasoline direct-injection spark-ignition engines and gasoline direct-injection compression-ignition engines have received attention due to their higher fuel economy with respect to conventional port fuel injected internal combustion spark-ignition engines. Combustion modeling of these types of engines requires a fuel surrogate that mimics both physical (e.g., evaporation) and chemical (e.g., combustion) characteristics of the gasoline fuel. In this work, we propose a novel methodology for the formulation of a gasoline surrogate based on the essential physical and chemical properties of the target gasoline fuel. Using the proposed procedure, a surrogate with seven components has been identified to emulate the physical and chemical characteristics of a real non-oxygenated gasoline fuel, RD387. A surrogate kinetic mechanism was developed by combining available detailed kinetic mechanisms from the Lawrence Livermore National Laboratory library. The modeling results for distillation curve, ignition delay and laminar flame speed were validated against available experimental data in the literature. The surrogate and gasoline fuels display similar physical/chemical properties, including distillation curve, H/C ratio, density, heating value, and ignition behavior and flame propagation over a wide range of pressures, temperatures, and equivalence ratios.

1. Introduction

Gasoline direct-injection (GDI) [1] and GDI compression-ignition (GDCI) engines [2,3] have received attention due to their higher fuel economy with respect to conventional port fuel injected internal combustion spark-ignition engines. Spray characteristics including evaporation history and penetration have great importance in the design and development of these engines; since spray physical phenomena play such an important role in the formation of the air/fuel mixture in the combustion chamber.

Gasoline, diesel, and jet fuels are mixtures of many structural classes of molecules such as paraffins, aromatics, olefins, and naphthenes. For the purposes of formulating surrogate mixtures to represent the combustion behavior of oxygenated gasoline, some of the hydrocarbon group representatives used in surrogate mixtures in prior studies are n-heptane for n-paraffins, iso-octane for iso-paraffins, toluene for aromatics, pentene for olefins, and ethanol for oxygenated groups [4–7]. Mixtures of these components can be formulated to mimic the ignition delays and laminar flame speeds of gasoline but cannot emulate the spray behavior of gasoline as the distillation curves and evaporation behaviors of these components and their mixtures are different from gasoline as discussed later. On the other hand, suggested representatives for modeling gasoline distillation or evaporation behavior are n-pentane, n-heptane, and n-decane (e.g., [8]). However, mixtures of these components cannot emulate the ignition delays and laminar flame speeds of gasoline adequately. The question of the present work is: can a single mixture be formulated that will mimic both the evaporation and combustion characteristics of the target gasoline? Towards that goal, a surrogate that includes most of the hydrocarbon group representatives found in a non-oxygenated gasoline is developed here to emulate the combustion and evaporation behaviors of this target gasoline. The surrogate contains n-alkane, iso-alkane, aromatic, and olefin representatives and a detailed kinetic mechanism is built from literature mechanisms for each of the species. The surrogate components and mixture composition are defined via a methodology that seeks a surrogate formulated from a minimum number of species that have relatively well defined kinetic mechanisms and provides adequate emulation of real gasoline evaporation and ignition behaviors.

2. Background

Surrogate mixtures are formulated for the purpose of numerical simulation of complex real fuel mixtures using a small number

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Table 1
Ethanol–gasoline fuel component representatives. (Adapted from [4]).

	Group name	Boiling temp. (°C)	Understanding of the mechanism[a]	
			Low and intermediate temperature	High temperature
CH_4 to nC_4H_{10}[b], nC_8H_{18} to $nC_{16}H_{34}$[c], nC_7H_{16}[d]	n-alkane	−164 to 287	A	A
iso-octane[d]	iso-alkane	99	A	A
2-methylbutane (iC_5H_{12})[f]	iso-alkane	28	A	A
2-methylpentane (iC_6H_{14})[f]	iso-alkane	61	A	A
Toluene[e]	aromatics	110	B	B
Ethanol[f]	oxygenate	78	B[h]	A[f,h]
1-pentene and 2-pentene[e]	olefin	30	B	B
2-hexene[e,g]	olefin	63	B	B

A: Detailed mechanism that has been validated over wide range.
B: Mechanism reported, but with major discrepancies or limitations.
[a] Pitz et al. [4].
[b] Marinov et al. [17].
[c] Westbrook [18].
[d] Curran et al. [19].
[e] Mehl et al. [6].
[f] Marinov [20].
[g] Mehl et al. [21].
[h] Sarathy et al. [22].

of components. Design of surrogate mixtures is usually focused on the emulation of a particular property of the target real fuel such as evaporation (e.g., [9]), thermodynamic properties (e.g., [10]), or combustion (e.g., [7,11]). The behaviors of multicomponent fuels are more complicated than single component fuels because species produced from one component can react with species from another component. These interactions often manifest themselves in the observed ignition delay times, laminar flame speeds, and other macroscopic combustion characteristics of surrogate mixtures [4]. Ethanol–gasoline fuels includes n-alkanes, iso-alkanes, naphthenes, olefins, aromatics, and oxygenated groups with different distributions depending on the season, market place, crude source, and refinery processes. The naphthenes present in gasoline blends mostly represent "leftover" material from other refinery processes and most of naphthenes will be converted to aromatics in refinery processes [4,12]. United States gasoline (e.g., non-oxygenated RD387) can contain up to 16% by volume of naphthenes [13] and European gasoline (e.g., Exxon 708629-60) can contain around 9% by weight of naphthenes [14]. It is common practice to include all of these hydrocarbon groups in gasoline blend surrogates for emulating ignition delay, laminar flame speed, and species consumption. However, it is a challenge to generate a predictive kinetic mechanism for each individual species/group while maintaining suitable mechanism size, in terms of the numbers of species and reactions, for computational fluid dynamics (CFD) applications such as combustion engine modeling. The process for developing and validating chemical kinetic models has been described by Frenklach et al. [15] and Simmie [16]. The physical properties and availability of kinetic mechanisms for several components (relating to gasoline surrogate) are presented in Table 1.

Pitz et al. [4] reviewed the development of fuel surrogate mixtures that represent gasoline combustion behavior. Their work involved separating all of the components into five distinct groups (A to D and F) from very important (group A) to no-relevance (group F). The chemical mechanisms and thermophysical properties of the components in group A are well understood and defined. iso-Octane, n-heptane, and toluene are among group A components and they are typically used in a gasoline surrogate models. The second important group (group B) includes ethanol, xylene, 1-pentene, and diisobutylene. Most of the oxygenated gasoline fuels contain a considerable amount of ethanol in the mixture. Mehl et al. [6] developed a four-component gasoline fuel surrogate and mechanism which contains TRF (Toluene Reference Fuel, comprised of iso-octane, n-heptane, and toluene) and 2-pentene. Their mechanism was made from assembly of existing Lawrence Livermore National Laboratory (LLNL) detailed mechanisms. Kukkadapu et al. [13] showed that this gasoline surrogate mechanism can emulate the ignition delay characteristics of the target gasoline (RD387) by comparison with available rapid compression machine (RCM) and shock tube data. Samimi Abianeh [7] studied and developed a skeletal combustion mechanism for ethanol reference fuel, which includes TRF and ethanol. This mechanism has 62 species and 194 reactions, of suitable size for engine modeling. However none of these studies addressed gasoline or ethanol-gasoline blend evaporation characteristics.

The distillation curve of the surrogate should be the same as the target real fuel in order to mimic the fuel spray evaporation behavior and fuel–air mixture preparation prior to combustion [23,24]. For example, a fuel surrogate with lower boiling temperature will have lower spray penetration [23]. All of the utilized surrogates/components in gasoline combustion mechanisms, discussed before, have the same range of boiling temperature (iso-octane: 99 °C, n-heptane: 98 °C, and toluene: 110 °C) and, therefore, cannot emulate the evaporation behavior of gasoline fuel. The distillation curve of gasoline covers a temperature range between 20 °C and 200 °C. Samimi Abianeh et al. [8] studied and developed a three component surrogate (nC_5H_{12}, nC_7H_{16}, and $nC_{10}H_{22}$) that does emulate the distillation curve of gasoline fuel. Ra and Reitz [24] developed seven component surrogates (iC_5H_{12}, iC_6H_{14}, iC_7H_{16} iC_8H_{18}, nC_9H_{20}, $nC_{10}H_{22}$, and $nC_{12}H_{26}$) to address the distillation curve of gasoline fuel. They also utilized components like n-heptane and iso-octane in their surrogate palette which are important for combustion prediction. Ahmed et al. [25] studied surrogate development for Fuel for Advanced Combustion Engine (FACE) gasolines by using an optimization algorithm. They targeted RON, distillation curve, density, carbon type, and H/C ratio to develop five different surrogates for FACE A and C gasolines. It is noted that in Ahmed et al. [25] the distillation curves of the surrogates were poorly matched with those of the FACE gasolines, and while their validation was performed by analyzing the carbon monoxide concentration of the exhaust gas from an internal combustion engine, the measured carbon monoxide amount of the FACE gasoline exhaust gas was not well correlated with that obtained in surrogate experiments. However, none of these studies address the combustion characteristics of gasoline fuel such as ignition delay or laminar flame speed. There are some studies which address the evaporation and combustion of diesel and JP-8 fuels (e.g., [26–27]); however, there is no comprehensive gasoline surrogate that can mimic both of the evaporation and combustion of the target gasoline