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HIGHLIGHTS

- Experimental study of two gasolines and a primary reference fuel surrogate blend.
- Ignition delay and species time-histories measured.
- Gasolines with different compositions showed similar reactivity and species profiles.
- PRF surrogate captured the kinetic trends of the gasolines reasonably well.
- The experimental data can be used for improving prediction of kinetic mechanisms.

ABSTRACT

Ignition delay times and CO, H₂O, OH and CO₂ time-histories were measured behind reflected shock waves for two FACE (Fuels for Advanced Combustion Engines) gasolines and one PRF (Primary Reference Fuel) blend. The FACE gasolines chosen for this work are primarily paraffinic and have the same octane rating (\~\text{RON} = 84) as the PRF blend, but contain varying amounts of iso- and n-paraffins. Species time-histories and ignition delay times were measured using laser absorption methods over a temperature range of 1350–1550 K and pressures near 2 atm. Measured species time-histories and ignition delay times of the PRF blend and the two FACE fuels agreed reasonably well. However, when compared to recent gasoline surrogate mechanisms, the simulations did not capture some of the kinetic trends found in the species profiles. To our knowledge, this work provides some of the first shock tube species time-history data for gasoline fuels and PRF surrogates and should enable further improvements in detailed kinetic mechanisms of gasoline fuels.

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1. Introduction

Gasoline is the most widely used transportation fuel for light duty vehicles. Gasoline is primarily comprised of hydrocarbons in C₄–C₁₀ range [1], however, the actual composition varies significantly depending primarily on the geographic origin of the fuel [2]. As such the commercial transportation-grade gasoline is a complex mixture of hundreds of hydrocarbons including linear and branched paraffins, naphthenes, olefins and aromatics. It becomes extremely inefficient to accommodate all of these species in any real world computational/experimental scenario. These difficulties can be overcome by considering a surrogate mixture of a few well-known components in a well-defined composition to emulate the target properties of the real fuel. Generally, these target properties include desired combustion characteristics (ignition delay, flame speed, etc.) and/or physical properties (molecular weight, H/C ratio, distillation curve, etc.). However, it should be noted that a given surrogate may not be able to match all physical and kinetics targets simultaneously. A conventional scale for rating the ignition properties of gasoline fuels is the research octane number (RON) and/or the motor octane number (MON) based on blends of gasoline primary reference fuels (PRF), n-heptane and iso-octane. Blends of primary reference fuels have previously been used as gasoline surrogates. The chemical kinetics of PRFs has been studied quite comprehensively over the last decade or so. Work by Curran et al. [3,4] on n-heptane/iso-octane and by Mehl et al. [5] on gasoline surrogates provide good account of the experimental and chemical kinetic modeling studies of primary reference fuels. Ignition delay times of PRF blends have been measured previously by a few groups [6–8]. More complex multi-component gasoline surrogates have been proposed in ignition delay studies under HCCI-like conditions [9–11].
The US Department of Energy and the Coordinating Research Council comprising of research institutes, automotive and oil companies have recently formulated a set of fuels, known as Fuels for Advanced Combustion Engines (FACE). One of the basic aims of formulating these FACE fuels is to provide a consistent set of fuels with well-characterized properties and compositions, making it easy to compare research results at various institutions and facilities. In the current study, we have investigated the oxidation characteristics of FACE gasoline A and C. Table 1 shows some of the key features of these two fuels; more detailed compositional analysis of FACE gasoline and diesel fuels can be found in [12,13]. Both gasolines have very similar octane rating but they differ in their compositions; FACE C has more than double the amount of n-paraffins than FACE A. Also, small amount (~4%) of aromatics is present in FACE C but are almost negligible in FACE A. The two gasoline fuels are compared here against a PRF blend of 84% iso-octane/16% n-heptane (by volume), referred to as PRF 84 in this work.

Chemical kinetics models are often validated against global kinetics targets such as ignition delay and flame speed data obtained from shock tubes, rapid compression machines, and simple canonical flames. Such data provide an overall view of the kinetic mechanism behavior and its ability to predict fuel reactivity but these data cannot be used to validate complex reaction pathways which are important, for example, in predicting emissions. The detailed chemical kinetics also play important role in controlling the reaction progress markers (CO, H2O and CO2) increase slowly at early times, over the 50–450 μs window in this example, until there is an exponentially fast growth of OH radicals and significant energy release from the CO + OH → CO2 + H reaction. Post-ignition CO2 and H2O concentrations will eventually approach their equilibrium values governed primarily by their thermochemical properties. Details of the species time-histories in the pre-ignition region are very important, and can provide very stringent constraints on mechanism prediction and validation.

Fig. 1 shows the predictions for the evolution of five major species formed during the oxidation of PRF 84. Simulations are carried out using gasoline surrogate mechanism of Mehl et al. [5] with constant internal energy and volume (constant UV) gasdynamic model in Chemkin-Pro [19]. The fuel decomposes immediately within the first 10–50 μs producing fuel fragments, C1–C4 intermediate species and an active radical pool. The concentrations of the reaction progress markers (CO, H2O and CO2) increase slowly at early times, over the 50–450 μs window in this example, until there is an exponentially fast growth of OH radicals and significant energy release from the CO + OH → CO2 + H reaction. Post-ignition CO2 and H2O concentrations will eventually approach their equilibrium values governed primarily by their thermochemical properties. Details of the species time-histories in the pre-ignition region are very important, and can provide very stringent constraints on mechanism prediction and validation.

<table>
<thead>
<tr>
<th>Fuel properties</th>
<th>FACE gasoline A</th>
<th>FACE gasoline C</th>
<th>PRF 84</th>
</tr>
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<tbody>
<tr>
<td>RON</td>
<td>83.5</td>
<td>84.7</td>
<td>84</td>
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<tr>
<td>MON</td>
<td>83.6</td>
<td>83.6</td>
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<tr>
<td>Sensitivity</td>
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<td>1.1</td>
<td>0</td>
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<tr>
<td>Avg. mol. wt.</td>
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<td>97.2</td>
<td>112</td>
</tr>
<tr>
<td>Hydrocarbon type, liquid mol%</td>
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<td></td>
<td></td>
</tr>
<tr>
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<td>28.6</td>
<td>17.6</td>
</tr>
<tr>
<td>iso-Paraffins</td>
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<td>65.1</td>
<td>82.4</td>
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<td>Aromatics</td>
<td>0.3</td>
<td>4.4</td>
<td>0</td>
</tr>
<tr>
<td>Alkenes</td>
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<td>0.4</td>
<td>0</td>
</tr>
<tr>
<td>Cycloalkanes</td>
<td>2.4</td>
<td>1.5</td>
<td>0</td>
</tr>
<tr>
<td>H/C ratio</td>
<td>2.29</td>
<td>2.27</td>
<td>2.26</td>
</tr>
</tbody>
</table>

In this study, we present species time-history and ignition delay time measurements for FACE gasolines A and C as well as a PRF 84 surrogate. Measurements are performed over a temperature range of 1350–1550 K and at pressures near 2 atm. In all experiments, the fuel concentration was kept at 0.2% with an equivalence ratio of 1 and argon is the diluent gas. Time-histories of OH, CO, CO2 and H2O were measured using laser-based UV and IR absorption spectroscopy. The reactivity and speciation of the three fuels were compared based on the fuel composition and also compared with predictions from recent gasoline surrogate mechanisms.

2. Methodology

2.1. Chemical kinetics shock tube facility

All experiments were performed in the chemical kinetics shock tube facility at King Abdullah University of Science and Technology (KAUST). This shock tube facility has been reported previously in literature [20–22] and only a brief account will be given here. The stainless steel shock tube has an inner diameter of 14.2 cm, driven section is 9 m long and a modular driver section with maximum length of 9 m. The driven section can be pumped down to 1 × 10−6 mbar using a turbomolecular pump. As the gasoline and PRF surrogate are multi-component fuels, the mixtures were prepared by direct injection of the fuel into a heated (75 °C) mixing vessel, equipped with a magnetically driven stirrer. These liquid fuels can readily adsorb on the mixing vessel walls and shock tube inner surface. The mixture composition was measured by Fourier Transform Infrared (FTIR) absorption spectroscopy by taking samples from the mixing vessel and the shock tube. The sampled mixtures were found to be within 5% of the manometrically determined values. Additionally, partial pressure of the fuel was kept well below the saturation vapor pressure relatively to avoid fuel condensation. The PRF 84 blend was prepared volumetrically using high purity (>99.5%) n-heptane and iso-octane (Sigma-Aldrich). FACE gasoline A and C were obtained from Conoco Philips Specialty Chemicals and research-grade argon and oxygen were supplied by AHG Gases.

Incident shock velocity was calculated by measuring the time interval between five PCB 113B26 piezoelectric pressure transducers (PZTs) that were located axially along the last 1.3 m of the driven section. The incident shock speed at the end-wall was determined by linear extrapolation of the velocity profile. One-dimensional shock-jump equations were used to calculate
the conditions \((T_s, P_s)\) behind reflected shock wave. Thermodynamic parameters used for argon, oxygen and PRF (iso-octane/n-heptane) were taken from Sandia thermodynamic database [23]. A complex 20 component thermodynamic surrogate, based on detailed hydrocarbon analysis, was used for FACE gasoline A and C. The uncertainty in the calculated temperatures and pressures is less than ±1% with the major contribution coming from uncertainties in the incident shock speed and mixture composition.

2.2. Laser diagnostics

Four laser absorption diagnostics were used to simultaneously monitor the concentration time-histories of CO, CO\(_2\), \(H_2O\) and OH. These diagnostics have either been validated previously (CO, OH) or were characterized in separate non-reactive experiments conducted in our shock tube facility \((CO_2, H_2O)\). These diagnostics enabled us to make extremely sensitive measurements with relatively low detectivity limits at the conditions of our experiments: ∼1 ppm for OH, ∼10 ppm for CO and ∼100 ppm for \(CO_2\) and H\(_2O\). The overall uncertainty in these speciation measurements is <5% and primarily comes from uncertainty in absorption cross-section, post-shock temperature \((T_s)\) and calculation of temperature time-history (see Section 2.3). A brief description of each diagnostic is provided below.

2.2.1. IR absorption of CO using a DFB QCL

Carbon monoxide concentration was monitored near 2193.36 cm\(^{-1}\) in the fundamental vibrational band of CO using a distributed-feedback (DFB) quantum cascade laser (QCL). The line-broadening parameters for this line were measured by Ren et al. [24] and line-strength values were obtained from the HITRAN database [25]. A small amount of absorption interference is caused by \(CO_2\) at high temperatures. This was corrected by measuring \(CO_2\) absorption cross-section at this wavelength \((2193.36 \text{ cm}^{-1})\) in separate \(CO_2/Ar\) shock-heated experiments. The \(CO_2\) interference was then subtracted from the measured CO absorption profiles using the \(CO_2\) mole fraction measurements.

2.2.2. IR absorption of \(CO_2\) using an external-cavity QCL

An external-cavity QCL was used at a fixed wavelength for laser absorption of \(CO_2\). The R(76) line at 2390.52 cm\(^{-1}\) in the \(v_3\) vibrational band of \(CO_2\) was selected due to its relatively high lower-state energy and minimal interference from other species. High-temperature cross-sections of \(CO_2\) at the peak of the transition were measured in our shock tube using \(CO_2/Ar\) mixtures and verified with previous measurements by Ren et al. [26,27].

2.2.3. IR absorption of \(H_2O\) using a DFB diode laser

\(H_2O\) concentrations were monitored using a distributed feedback (DFB) diode laser operating at 3416.16 cm\(^{-1}\) in the \(v_3\) vibrational band of \(H_2O\). This line provides increased absorption strength compared to the transitions used in previous \(H_2O\) sensing work [28,29]. Absorption cross-sections for this transition were measured in separate experiments of shock-heated mixtures of \(H_2O/Ar\). The measured \(H_2O\) absorption cross-sections are provided in Supplementary Material.

2.2.4. UV absorption of OH using a ring-dye laser

Hydroxyl concentrations were measured using frequency doubling of 613.4 nm cw light generated by a Spectra Physics ring-dye laser system. This ring-dye laser system was pumped by a Coherent Verdi laser operating at 532 nm. The R(5) transition near 306.7 nm in the OH A-X (0, 0) absorption band was probed to measure OH mole fraction [30]. Negligible interference absorption was observed for FACE A and PRF 84. However, small interference absorption was detected at 306.7 nm during FACE C ignition experiments. This interference was corrected for by making off-line measurements, 5 cm\(^{-1}\) away from the peak of selected OH absorption transition.

2.3. Calculation of temperature time-history

Beer–Lambert law for spectrally narrow radiation can be written as \(I/I_0 = \exp(-SPL \phi X)\), where \(I/I_0\) is the ratio of transmitted and incident laser intensities, \(S(T)\) is the line-strength, \(P\) is the total pressure, \(L\) is the laser path-length, \(\phi(T,P)\) is the line-shape function and \(X\) is the mole fraction of the absorbing species. The line-strength and line-shape are temperature-dependent quantities and their variation with temperature is either known from a spectral database or determined via line characterization experiments. For shock tube experiments, the temperature behind reflected shock wave \((T_s)\) is calculated from the measured incident shock speed and thermodynamic parameters of the gas mixture. In non-reactive shock tube experiments, the \(T_s\) remains almost constant throughout the test time (∼2 ms). However, in reactive experiments, energy release from exothermic combustion reactions can cause the temperature to increase substantially during and after the ignition event. Thus a temperature time-history is needed to accurately calculate the mole fraction time-history using Beer’s law. In the absence of direct temperature measurement, a temperature profile simulated by a chemical kinetic mechanism is used for the calculation of temperature-dependent spectroscopic quantities, i.e., line-strength and line-shape functions. Shock tubes are usually modeled with constant volume and constant internal energy (constant UV) constraints. However, these constraints are not suitable for situations where sufficient energy release takes place. In this work, we imposed the measured-pressure profile in Chemkin-Pro [19] and solved the energy equation to calculate temperature time-history. This modeling approach, referred to as UMP (constant internal energy with measured pressure profile), is used throughout the paper to generate temperature time-histories for converting measured absorbance profiles to concentration time-histories. This approach is demonstrated in Fig. 2, and compared with calculations using constant UV constraints and the ChemShock code proposed by the Stanford University group [31]. As expected, the constant UV simulations greatly overpredict the temperature and pressure. The temperature time-histories calculated using UMP and ChemShock are essentially similar, though the UMP approach is easier to implement.

2.4. Validation of laser diagnostics

Since chemical kinetic mechanisms for n-heptane are very well-validated, species time-history profiles were initially measured during the oxidation of n-heptane stoichiometric mixtures to validate the laser diagnostics and the temperature modeling strategy. Measurements were carried out in a mixture of 0.2% n-heptane/oxygen/argon over a range of temperatures (1350–1500 K) and pressures near 2 atm. A representative dataset is shown in Fig. 3 at a reflected shock temperature of 1440 K. The measured and simulated profiles (using Mehl et al. [5] mechanism) are generally in good agreement with some minor differences. For example, the mechanism overpredicts \(H_2O\) production and underpredicts \(CO\) production at relatively early times of 50–100 μs. It is expected that all of the fuel carbon will get converted to \(CO\) and \(CO_2\) in the post-ignition region. Carbon balance can be calculated in the post-ignition region for validating the \(CO\) and \(CO_2\) diagnostics. At an elapsed time of 700 μs, the sum of measured \(CO\) and \(CO_2\) mole fractions is 13,100 ppm which is within 6.5% of the initial fuel carbon (14,000 ppm).
3. Results and discussion

3.1. Ignition delay times of FACE gasolines and PRF surrogate

Ignition delay times were measured for the two FACE gasolines and PRF 84 blend over a temperature range of 1330–1550 K and pressures near 2 atm; results are shown in Fig. 4. Ignition delay times were determined by the time interval between the arrival of the reflected shock wave and the extrapolation of the steepest rise in pressure signal to the pre-ignition level. All ignition delay time results are scaled to 2 atm using $P/C0$ pressure scaling. FACE gasoline A and C have the same overall reactivity indicated by very similar ignition delay times within the uncertainty limits of these experiments (~15%). It is well known [32–34] that increasing the branched hydrocarbon and/or aromatic content in the fuel decreases overall reactivity while n-paraffins increase the reactivity. FACE gasoline C has almost double the amount of n-paraffins compared to FACE gasoline A. However, FACE gasoline C has about 5% aromatics which balances out the higher reactivity due to increased n-paraffins, resulting in similar octane rating and similar ignition delays for both gasolines. Also evident in Fig. 4 is that PRF 84 surrogate captures the reactivity of these gasoline fuels over the entire temperature range of this study. This can be explained by the fact that both gasolines and the PRF blend are primarily paraffinic in nature (~95% paraffinic content) and thus exhibit similar reactivity. This is consistent with surrogate fuel formulation strategy proposed by Dooley et al. [35] for jet fuels. They argued that the composition of the surrogate does not necessarily need to emulate all of the functional classes present in the real fuel. The composition of the surrogate should be such that it is able to emulate closely the development of the active radical pool and $C1$-$C4$ intermediate species which control the chemical kinetics phenomena at high temperatures. From the current study, it can be concluded that a PRF surrogate, having similar octane rating and H/C ratio,
can be used to capture the global reactivity of a predominantly paraffinic gasoline fuel under high temperature conditions. Measured ignition delay times are provided in a tabular form in the Supplementary Material.

Comparisons of measured ignition delay times with predictions from Mehl et al. [5] and Bieleveld et al. [36] gasoline surrogate mechanism are also shown in Fig. 4. The primary difference between the two mechanisms is that Bieleveld et al. [36] use lumped component/reaction method developed by Ranzi and coworkers [37] whereas Mehl et al. [5] consider all isomers and reaction pathways. Mehl et al. [5] mechanism overpredicts the experimental ignition delay times of the PRF surrogate and the two FACE gasolines over the entire temperature range of this study, whereas Bieleveld et al. [36] mechanism underpredicts the experimentally measured ignition delay times. It can also be seen from Fig. 4 that the Mehl et al. [5] mechanism predictions are closer to the experimental data at higher temperatures but exhibit relatively large deviations as temperature decreases. On the contrary, Bieleveld et al. [36] mechanism is closer to the experimental data at lower temperatures. The high-temperature chemistry is generally considered to be well established for reference fuels, such as n-heptane and iso-octane. Therefore, it is surprising that both mechanisms are unable to accurately predict the high-temperature ignition delay times of the PRF blend. Also shown in Fig. 4 are the experimental ignition delay times measured in our laboratory for n-heptane and iso-octane stoichiometric mixtures under similar conditions. Mehl et al. [5] mechanism captures n-heptane reactivity very well but overpredicts iso-octane ignition delay times. Thus it can be argued that the Mehl et al. [5] overprediction of PRF 84 ignition delay times is caused by iso-octane kinetic mechanism or the blending of n-heptane and iso-octane chemistry. The kinetics of iso-octane and related smaller branched intermediates, like iso-butene, must be evaluated further to improve the discrepancy between the measurements and the model.

3.2. Species time-histories of FACE gasolines and PRF surrogate

Species time histories were measured for the two FACE gasolines and the PRF surrogate over 1350–1550 K and nominal
pressures of 2 atm. Fig. 5(a)–(d) shows the measured profiles of OH, CO, H$_2$O and CO$_2$ during the stoichiometric oxidation of 0.2% fuel (PRF 84, FACE A, FACE C) at a representative temperature of 1450 K. Although all four species are measured simultaneously for a specific fuel, the profiles shown for different fuels were measured in separate experiments; thus the actual reflected shock temperatures are 1450 ± 10 K. Both FACE A and C show very similar trends in all four species profiles. Also, PRF 84 surrogate captures the speciation profiles of both gasoline fuels reasonably well. These trends are consistent with the similarities found in ignition delay (Fig. 4) of all three fuels studied here. The chemical kinetics phenomena at high temperatures are primarily controlled by the presence of active radical pool such as OH, CH$_3$, H, and HO$_2$. If two fuels produce very similar active radical pool, it is expected that the fuels will then exhibit similar reactivity. Thus the PRF surrogate needs to reproduce the active radical pool of the real fuel as closely as possible in order to capture the chemical kinetics of the real fuel. It can be seen from Fig. 5(a) that both gasoline fuels and PRF 84 show very similar trends in OH formation and consumption. The pre-ignition OH concentrations for PRF 84 and FACE A oxidation are in close agreement whereas the OH concentration for FACE C is lower by about 30% during the first 100 µs. Similar n- and iso-paraffin content present in PRF 84 and FACE A leads to similar OH profiles. The lower OH concentration for FACE C over the early time, however, does not appear to significantly affect the ignition delay time.

The three stable molecules measured here, CO, H$_2$O and CO$_2$, are important reaction progress markers. It can be observed from Fig. 5(b)–(d) that these species evolve quite similarly in time for all three fuels studied. Post-ignition plateau values of these species are slightly higher for PRF 84 compared to FACE A, with OH, CO and CO$_2$ being 15%, 9% and 6% higher, respectively. The similarities in global reactivity of the three fuels, indicated by similarities in ignition delay (Fig. 4), can now be explained based on the observation that the local reactivity markers also evolve similarly during the induction period. These fuels may exhibit some differences in higher carbon-containing species produced during initial fuel decomposition, but these differences did not affect the global reactivity of the three fuels.
reactivity as well as the local reactivity markers (Figs. 4 and 5) in this high-temperature study. All speciation data presented here can be found in the Supplementary Material.

Measured PRF 84 species profiles are compared with those predicted by Mehl et al. [5] gasoline surrogate mechanism and Bieleveld et al. [36] PRF mechanism in Fig. 6. The correct prediction of OH radicals is very important, particularly in high temperature regime. The rates of production (ROP) of reaction progress markers, such as H2O (OH + H2 → H + H2O, CH4 + OH → CH3 + H2O) and CO2 (CO + OH → CO2 + H), are strongly dependent on the OH radical concentration at these high temperatures. It can be seen from Fig. 6 that Mehl et al. [5] mechanism (dashed lines) captures the OH experimental profile very well at the highest temperature of this study (1526 K), although there is considerable under-prediction (~50%) at earlier times (20–100 μs). Bieleveld et al. [36] mechanism (dotted lines in Fig. 6) significantly overpredicts the early-time concentration of all measured species and thus gives much shorter ignition delay time.

Fig. 7 shows Mehl et al. [5] model predictions for different species as a function of temperature. As temperature is decreased, the OH model predictions start to deviate further from the OH experimental profiles; see the comparison at 1459 K, 1436 K and 1397 K. Similar observations can be made for time-histories of CO, H2O and CO2. At 1526 K, Mehl et al. [5] mechanism overpredicts CO at early times, though excellent agreement can be seen between the simulated and experimental CO2 and H2O profiles. Importantly, the model fails to capture any of the reaction progress markers at lower temperatures. These trends are also depicted in Fig. 4, where the discrepancy between PRF 84 measured and Mehl et al. [5] simulated ignition delay times increases as temperature decreases.

Hydroxyl sensitivity (Fig. 8) and rate-of-production (not shown here) analyses performed for PRF 84 show that OH is consumed by propene and iso-butene after the initial fuel decomposition and abstraction reactions. Propene and iso-butene are thus OH radical scavenging species and produce resonantly-stabilized allyl (C3H5 + OH → C3H5OH) and relatively unreactive allene (IC4H7 + OH → IC4H7OH, IC4H7 → C3H4 + CH3), respectively. Thus the rates of reactions involving propene, iso-butene, allyl, and allene can affect the overall fuel reactivity. The uncertainty in unimolecular decomposition and hydrogen abstraction rates of these species may contribute to the differences between the experimental and modeled speciation trends. A multi-institution study of n-heptane oxidation behind reflected shock waves. Combust Flame 2014;159(2):617–28.

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Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.fuel.2014.09.095.

References


