



Demonstrating Clean Burning Future Fuels at a Public Engagement Event

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S Supporting Information

ABSTRACT: Sustainable future fuels are likely to be produced by a wide range of processes, and there exists the opportunity to engineer these fuels so that they burn more efficiently and produce fewer harmful emissions. Such potential is especially important within the context of reducing the emissions of both greenhouse gases (GHG) and toxic pollutants that adversely impact air quality and human health. To illustrate how fuel design on a molecular level may be exploited to reduce these emissions, the combustion and emission properties of three potential future fuels, geraniol, diethyl carbonate, and a biodiesel (soy methyl ester), were evaluated along with a fossil diesel. The fuels were assessed using “smoke point” tests and a Stirling engine. The purpose of the demonstration was to highlight to a general audience several burning characteristics of some possible future fuels, and thus the potential for the development of clean burning “designer” fuels. During the 15 min demonstration, significant differences in the combustion properties of the different fuels were shown. For example, the conventional fossil diesel fuel produced a significant amount of soot in flame tests, whereas diethyl carbonate, which is a potential second-generation biofuel, produced visibly lower amounts of soot.

KEYWORDS: General Public, Demonstrations, Public Understanding/Outreach, Chemical Engineering, Green Chemistry, Fatty Acids

INTRODUCTION

The challenge of developing sustainable and clean transport will require significant advancements in vehicle and fuel technologies. The composition of the fuel combusted in internal combustion engines is a factor that has a significant impact on efficiency and emissions. There are many chemical and physical properties of fuels that influence their combustion and emissions characteristics including viscosity, vapor pressure and molecular structure. The development of future fuels for engines is inherently multidisciplinary, requiring consideration of chemical, biological, and engineering concepts, some of which were introduced during the public demonstration outlined in this paper.

Emissions of particulate matter (PM) from internal combustion engines are of great concern due to the detrimental effects of these on human health. Epidemiological studies show that long-term exposure to high levels of PM can result in an increased risk of pulmonary and cardiovascular complications.^{1–3} For example, a 2014 report estimated the fraction of mortality attributable to anthropogenic particulate matter to be over 8% in highly polluted boroughs of London.⁴

Conventional diesel and gasoline fuels produced from crude oil are usually composed of thousands of chemically distinct molecules, including alkanes, alkenes, and cyclic and aromatic hydrocarbons.⁵ However, biofuels tend to have a more uniform composition, consisting of only a few chemically similar molecules. For example, biodiesel fuel derived from soybean typically contains five main ester components, including about 49–53% methyl oleate (see Figure 1).⁶ The composition is typical of biodiesels produced from many sources, both food crops such as rapeseed and potentially more sustainable sources such as microalgae or even spent coffee grounds.⁷ In the future,

it is expected that biofuels will be produced in increasing quantities, and given the likely more uniform composition of these relative to fossil fuels, there exists the opportunity to engineer the molecular structure of these fuels so that they combust more efficiently and produce significantly lower levels of exhaust pollutants.

A number of authors have highlighted the possibility of modifying the composition of biofuels for improved combustion and emissions.^{6,8,9} For example, the terpene geraniol (see Figure 1) appears, on the basis of molecular weight and carbon chain length, to be a promising diesel fuel producible from photosynthetic cyanobacteria (a class of micro-organism similar to microalgae).⁹ However, diesel engine tests showed that significant improvements in combustion and emissions could be achieved through minor modifications to the geraniol molecular structure.

The utilization of waste streams is a further exciting possibility for the production of future sustainable fuels. For example, the production of carbonate esters such as diethyl carbonate (Figure 1) from short chain alcohols derived from biomass and carbon dioxide from combustion flue gas has been suggested. Engine tests have shown that carbonate esters of different molecular structure ignite at different rates and produce varying levels of particulate emissions.¹⁰

The tendency of different fuels to form soot during combustion varies widely.¹¹ A standard metric for evaluating the comparative tendency of different fuels to produce soot is to use a smoke point test, which utilizes a wick-fed diffusion

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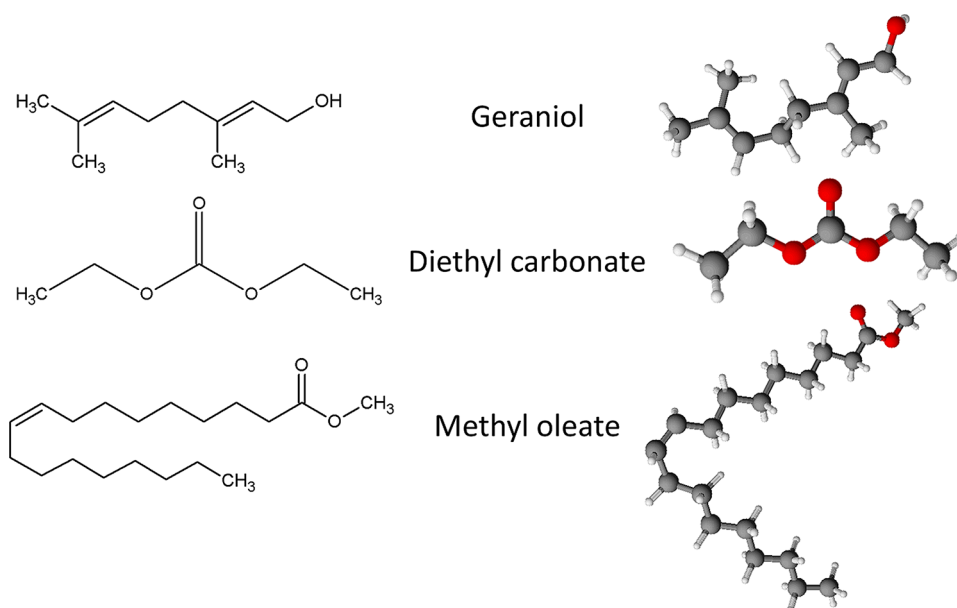


Figure 1. Molecular structure of (i) geraniol, (ii) diethyl carbonate, and (iii) a typical component of SME, methyl oleate. Shown as skeletal representation (left) and ball and stick model (right), where carbon is black, oxygen red, and hydrogen white.

flame. In such diffusion flames, fuel evaporates from the wick and diffuses outward. Soot formation occurs by pyrolytic reactions (in the absence of oxygen) in the fuel-rich environment inside of the flame envelope (a thin, usually visible layer, where combustion takes place). When the flow rate of fuel is low, all of the soot that is formed in the fuel-rich zone of the flame is subsequently oxidized and consumed as it passes through the flame envelope (shown in Figure 2a).

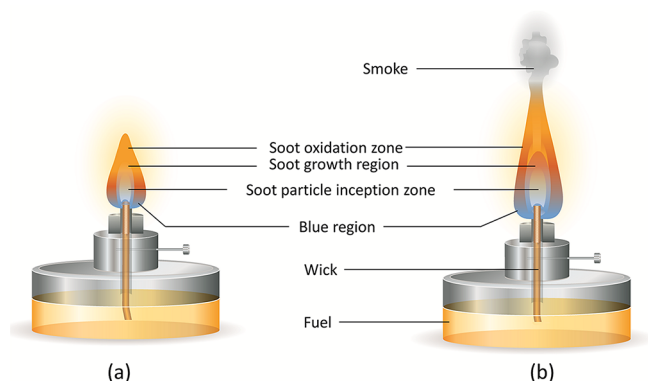


Figure 2. Wick-fed diffusion flames shown (a) with a closed flame, and (b) with soot emerging from the flame tip.

However, if the fuel flow rate is gradually increased, a point is reached where soot begins to emerge from the tip of the flame (Figure 2b).¹² The maximum flame height (in mm) without soot emerging from the tip is known as the smoke point. Therefore, the higher the smoke point is of a given fuel, the lower propensity it has to form soot.

This paper describes a public engagement demonstration presented at the 2016 Shell Eco Marathon, at the Queen Elizabeth Olympic Park, London, UK. The Shell Eco Marathon is a competition where student teams are challenged to design, build, and drive the most energy efficient car.¹³ In addition to the competition, the event was accompanied by science and technology demonstrations and hands-on activities for the

audience, including this demonstration. The audience of the London event mainly consisted of high school students (aged 11–16) and members of the general public. During the demonstration, the soot forming tendency of current and potential future fuels (with different molecular structures) was evaluated, and the heat release of each fuel was visualized utilizing a Stirling engine. This demonstration includes themes of fuel technology, combustion, renewable energy, and environmental stewardship; in addition, it complements a number of articles published in this *Journal*.^{14–18}

MATERIALS AND METHODS

The experimental equipment used for the demonstration is shown in Figure 3; the experimental setup and data presented in this paper were recreated in a laboratory setting at a later

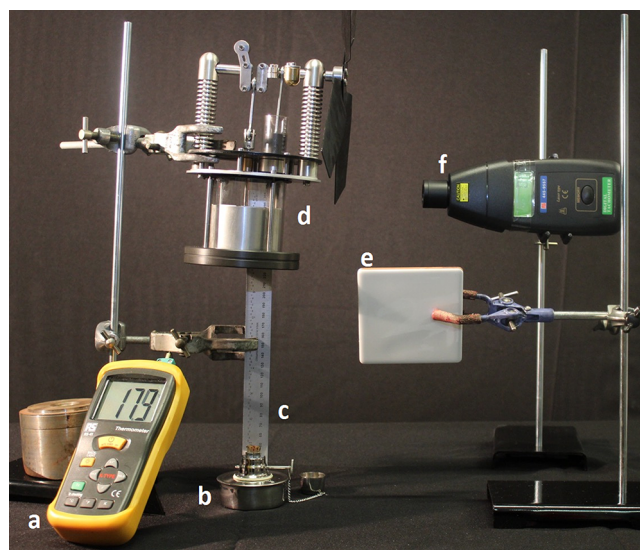


Figure 3. Experimental equipment: (a) thermocouple and hand-held display, (b) adjustable wick burner, (c) ruler, (d) Stirling engine, (e) white ceramic tile, (f) laser tachometer.

time to produce better images for the purpose of this paper. Those wishing to recreate this demonstration in a general instructional environment may wish to refer to the [Supporting Information](#), where further practical information regarding the demonstration, and equipment used (with cost), is provided.

Fuels

The following fuels were used for the demonstration: EN 590 specification diesel fuel, obtained from Haltermann Carless; soy methyl ester (SME) biodiesel, obtained from BP Global Fuels; geraniol (>97%), obtained from Sigma-Aldrich; and diethyl carbonate (99%), Sigma-Aldrich.

Evaluating the Sooting Tendency of the Fuels

As described in the [Introduction](#), the smoke point test makes use of a wick-fed diffusion flame burner. For the purpose of the public demonstration, a stainless-steel wick burner (part b in [Figure 3](#)) was used. The definition of the smoke point was taken to be the maximum height of the flame produced before soot was seen to visibly emerge from the tip (measured using a graded ruler with millimeter resolution). The height of the flame, which is related to the fuel flow rate, was controlled by adjusting the wick exposure. The equipment and method used was modified from the standard ASTM specification method, in order to simplify the concept to the audience.¹⁹ The wick burner used had a thicker (25 mm) wick than that of the standard test, in order to produce a larger and more visible and open flame.

To further demonstrate to the audience the differences in soot forming tendency of the fuels, a white ceramic tile was held into the flame, at the same height smoke point. The tile was held in the flame for 15 s before being withdrawn, and inspected for visual differences in the appearance and apparent quantity of soot deposited.

Temperature Measurement

The flame temperature was measured by adjusting the height of the flames of each fuel to 30 mm. The temperature was measured using a K-type thermocouple positioned at a distance of 20 mm above the tip of the flame. The temperature was read from a hand-held thermocouple reader, and was recorded once the temperature had stabilized within ± 5 °C.

Stirling Engine Test

A Stirling engine, which is an external combustion engine, was used to visually illustrate how the fuel composition influenced the flame temperatures and energy release. When thermal energy is provided externally to the Stirling engine, by the heating the base plate, the air inside the engine cylinder expands causing the piston to move. To assist with this visualization, the Stirling engine used had a glass cylinder to allow the piston movement to be seen. In addition, the crankshaft of the engine was attached to a fan (see [Figure 3](#)), the rotational speed of which was measured using a laser tachometer. Therefore, the speed of the fan was related to the flame temperature, which provided thermal energy to the base plate. Due to the relatively large thermal mass of the engine, the external surface of the engine cylinder was preheated using a heat gun (for each fuel) to 80 ± 2 °C (measured using an infrared thermometer). Following this, the base plate was heated using the wick burner. The wick flame was adjusted to have a 30 mm flame for each of the fuels, and the engine was positioned such that the underside of the engine was 20 mm above the tip of the flame. The engine did not reach a steady state (speed) in the time available for the demonstration, and

the fan speed continued to increase. Therefore, the speed of the engine was recorded after 2 min of the engine running on the test fuel.

HAZARDS

There are two main hazards involved in carrying out this demonstration: (i) since the demonstration involves the use of flammable liquid fuels and open flames there is the risk of fire, and (ii) there are health risks from exposure to the fuels and the combustion products.

The flammable liquid fuels should be kept in closed containers, and well away from the demonstration area while there is an open flame, and should be stored away from high temperatures and sources of ignition. The burner should sit on top of a heatproof mat or otherwise nonflammable surface. Appropriate firefighting equipment (suitable for liquid hydrocarbon fuels) should be available, and if one is undertaking the demonstration at a public venue, the fire risks and precautions necessary should be discussed in advance with the venue manager.

The demonstration should be carried out in a well-ventilated space, or fume cupboard. The demonstrator(s) should wear protective equipment including safety glasses and chemically resistant disposable gloves. Demonstrators should avoid breathing the diesel fuel and diethyl carbonate vapor or flame combustion products. Particulate matter, produced by the flame, is known to be carcinogenic to humans; the breathing in of soot particles should be avoided, by standing back away from the flame. The demonstrator should avoid prolonged or repeated skin contact with the fuels, and should be familiar with the Material Safety Data Sheets supplied with the chemicals.

DEMONSTRATION

While the primary aim of the demonstration was to present to the audience scientific insight as to the potential for emissions reduction from IC engines through fuel design, further teaching and learning gains were related to the experimental approach employed. These included the necessity of establishing as near as practicable constant experimental conditions for the combustion demonstrations, the relation of these results in differences in fuel composition where all other variables had been kept constant, the working principles of a Stirling engine, and the need for personal protective equipment when handling chemicals.

The demonstration began by introducing the need to find sustainable alternatives to fossil fuels, and the explanation that through multidisciplinary collaboration such fuels could be intentionally designed to be cleaner burning. The background and motivation for the development of cleaner burning designer fuels were explained, following the same content as outlined in the [Introduction](#) of this paper. While the demonstrator discussed each of the fuels to be tested, the audience was shown the molecular structures of the fuels ([Figure 1](#)). Throughout the demonstration references were made to the relative differences in fuel molecular structure, including oxygen content and bonding (i.e., alcohol, ester, and carbonate structures), and degree of hydrocarbon saturation. Testing of the four fuels commenced while the possible production and sources of each fuel were conveyed to the audience, in addition to highlights of the fuel molecular structure. The experimental procedure was described to the

audience, including the protective equipment worn by the demonstrators. Tests began with the reference fossil diesel, followed by methyl oleate (as representative of biodiesel), with the potential for biodiesel production from waste sources such as spent coffee grounds highlighted. Geraniol followed, which has a citrus-like scent, and in addition to potential production by cyanobacteria,⁹ it is commonly used as a fragrance in products such as shampoos. Members of the audience were invited to smell the geraniol, in order to encourage participation. During testing of the final fuel, diethyl carbonate, the potential production from CO₂ and relatively high oxygen content were highlighted. For each fuel test the audience was shown the amount of the soot collected onto the ceramic tile and the maximum speed achieved of the Stirling engine, with the results written on a whiteboard. After the fuels had been tested, the audience was asked to rank the performance of the four fuels in terms of energy efficiency, soot emissions, and overall performance. The demonstration concluded by conveying to the audience some of the reasons for differences in sooting tendencies (see [Results](#)) of the different fuels and how this illustrates that combustion engines could consume less fuel and produce fewer harmful emissions.

Concepts relating to fuel design were first conveyed during the demonstration introduction, and reiterated throughout the tests of the four fuels. The shift away from current biofuels, primarily derived from food crops, toward advanced biofuels, driven by legislation recognizing issues of sustainability where biofuel production might displace that of crops for food consumption, was introduced during discussion of test results. Specific health concerns regarding soot emissions were also described (as per the [Introduction](#) of this paper).

Formal feedback was not obtained as part of the demonstration, partly due to the public nature of the demonstration and time constraints in the event scheduling. From observation during the demonstration and informal feedback from audience members, the authors perceived that the audience maintained interest throughout the demonstration. In particular, where the introduction of alternative fuels derived from common materials with which they were already familiar, (e.g., compounds from genetically modified microalgae that are already present in household cosmetics). Audience participation in identifying the aroma of geraniol also strongly engaged the individuals involved, and the competitive element of identifying which fuel molecule resulted in the lowest soot emissions further helped the spectators to invest in the experiments demonstrated. The use of a Stirling engine as a visual aid was also appreciated and considered of some novelty by the audience, many of whom had not previously encountered the concept.

RESULTS

The results of the smoke point tests are recorded in [Table 1](#), and are shown in [Figure 4](#). The tendency of the fuels to form soot was in following order: fossil diesel fuel > geraniol > biodiesel > diethyl carbonate. The comparatively higher smoke point of the conventional diesel fuel can be explained due to the high aromatic content and the lower oxygen content. A significant portion of the diesel fuel consisted of aromatics (22% by mass), which are known to produce high levels of soot compared to alkane molecules.¹¹ Oxygenated fuels on the other hand tend to produce lower levels of soot compared to alkanes of the same carbon number, and the reduction in soot formation can be broadly correlated with the oxygen content of

Table 1. Measured Properties of the Different Fuels Tested

Fuel	Smoke Point (mm)	Flame Temperature Measurement (°C)	Stirling Engine Speed (rpm)
Fossil diesel	20	355	76
Geraniol	25	370	78
Biodiesel (SME)	50	400	85
Diethyl carbonate	>100	420	103

the fuel.²⁰ However, while both geraniol and biodiesel have an approximately equal carbon-to-oxygen ratio (C/O), their smoke point was seen to be markedly different. This is explained due to the fact that geraniol contains two double bonds and chain branching, both of which are known to promote soot formation.²¹ Diethyl carbonate, which had the highest smoke point, and thus the lowest tendency to form soot, contained the highest proportion of oxygen of all of the fuels tested. It can be observed from [Figure 4](#) that the diethyl carbonate flame left only a very small amount of soot deposited onto the tile, whereas significantly more soot was produced from the other fuels. At close inspection of the tiles the soot deposited appeared to be a thicker layer for the fossil diesel soot than for that of the geraniol and biodiesel fuel.

[Table 1](#) shows that the recorded temperatures (measured above the tip of the flame) for the different fuels are found to be in the following order: fossil diesel < geraniol < biodiesel < diethyl carbonate. It is suggested that the order of temperatures measured reflects the fact that the rate of radiative heat loss is greater for flames that produce higher levels of soot, resulting in lower gas temperatures at the tip of the flame. The temperatures measured did not correlate with the adiabatic flame temperatures of the respective fuels (which are generally higher for conventional diesel fuels).²² It is also seen in [Table 1](#) that the temperature of the flame correlates well with the speed measured for the Stirling engine; this is expected since the higher the temperature of the flame is, the more thermal energy is transferred to the Stirling engine, resulting in greater fan rotational speed.

Tests of smoke point have been found to correlate with particle emissions from gas turbine engines, and can be used to correlate emissions from gasoline engines.²³ However, it should be noted that the purpose of the demonstration was to illustrate differences in fundamental chemical behavior of the fuels and not to imply their suitability for use in engines.

CONCLUSIONS

By demonstrating the combustion and sooting behavior of four fuels of differing molecular structure and physical properties, the potential designer fuels to address sustainability and air quality issues associated with internal combustion engines was successfully conveyed to a generalist audience consisting of families and school groups. The use of test fuels to which either the source (biodiesel from spent coffee grounds), or the fuel molecule (geraniol as utilized in shampoos), could be easily related to helped engage the audience, while the visual elements of the combustion tests maintained interest throughout the 15 min demonstration. Collectively, the audience correctly identified which of the test fuels had performed most favorably with regards to soot emissions and heat release, confirming the tests as an effective means of conveying these fuel properties.

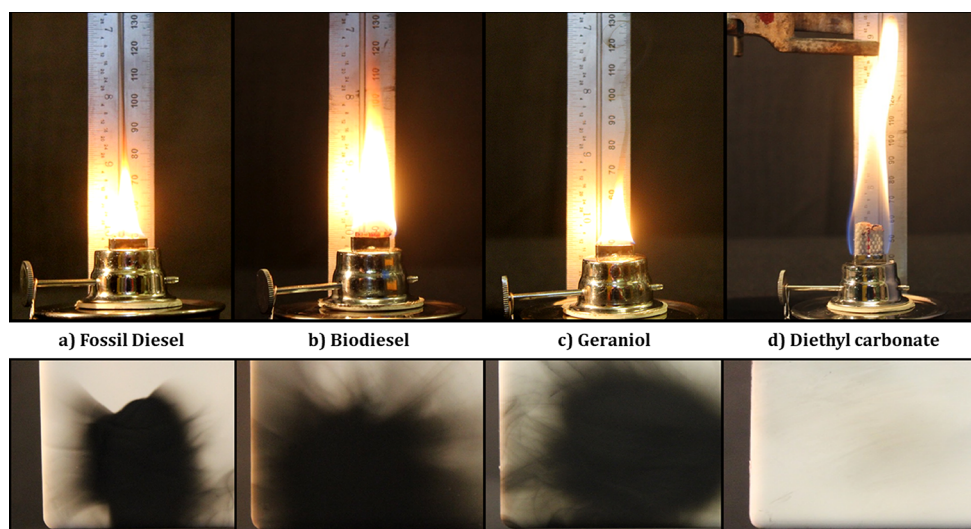


Figure 4. Appearance of the flames at the sooting height for each of the fuels tested (above), and the appearance of the soot deposited onto a white ceramic tile held into the flame for 15 s (below).

■ ASSOCIATED CONTENT

📄 Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: [10.1021/acs.jchemed.7b00554](https://doi.org/10.1021/acs.jchemed.7b00554).

Notes for instructors (including sourcing of materials and costings) and images from the public demonstration ([PDF](#), [DOCX](#))

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Notes

The authors declare no competing financial interest.

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■ REFERENCES

- (1) Department of Health, Committee on the Medical Effects of Air Pollutants. *Quantification of the Effects of Air Pollution on Health in the United Kingdom*; Department of Health: London, UK, 1998. http://webarchive.nationalarchives.gov.uk/20121103050805/http://www.dh.gov.uk/prod_consum_dh/groups/dh_digitalassets/@dh/@ab/documents/digitalasset/dh_118120.pdf (accessed Nov 2017).
- (2) Department of Health, Committee on the Medical Effects of Air Pollutants. *Statement on Long-Term Effects of Particles on Mortality*; Department of Health: London, UK, 2001. http://webarchive.nationalarchives.gov.uk/20120109163724/http://www.dh.gov.uk/ab/COMEAP/DH_108596 (accessed Nov 2017).
- (3) World Health Organization. *Air Quality Guidelines Global Update 2005: Particulate Matter, Ozone, Nitrogen Dioxide and Sulfur Dioxide*;

World Health Organization, WHO Regional Office for Europe: Copenhagen, Denmark, 2005. http://www.who.int/phe/health_topics/outdoorair/outdoorair_aqq/en/ (accessed Nov 2017).

(4) Gowers, A. M.; Miller, B. G.; Stedman, J. R. *Estimating Local Mortality Burdens Associated with Particulate Air Pollution*; Public Health England: Chilton, UK, 2014. <https://www.gov.uk/government/publications/estimating-local-mortality-burdens-associated-with-particulate-air-pollution> (accessed Nov 2017).

(5) Pitz, W. J.; Mueller, C. J. Recent progress in the development of diesel surrogate fuels. *Prog. Energy Combust. Sci.* **2011**, *37* (3), 330–350.

(6) Knothe, G. Designer[®] Biodiesel: Optimizing Fatty Ester Composition to Improve Fuel Properties †. *Energy Fuels* **2008**, *22* (2), 1358–1364.

(7) Bendall, S.; Birdsall-Wilson, M.; Jenkins, R.; Chew, Y. M. J.; Chuck, C. J. Showcasing Chemical Engineering Principles through the Production of Biodiesel from Spent Coffee Grounds. *J. Chem. Educ.* **2015**, *92* (4), 683–687.

(8) Knothe, G. Improving biodiesel fuel properties by modifying fatty ester composition. *Energy Environ. Sci.* **2009**, *2* (7), 759.

(9) Hellier, P.; Al-Haj, L.; Talibi, M.; Purton, S.; Ladommatos, N. Combustion and emissions characterization of terpenes with a view to their biological production in cyanobacteria. *Fuel* **2013**, *111*, 670–688.

(10) Hellier, P.; Ladommatos, N.; Allan, R.; Rogerson, J. Influence of Carbonate Ester Molecular Structure on Compression Ignition Combustion and Emissions. *Energy Fuels* **2013**, *27* (9), 5222–5245.

(11) Ladommatos, N.; Rubenstein, P.; Bennett, P. Some effects of molecular structure of single hydrocarbons on sooting tendency. *Fuel* **1996**, *75* (2), 114–124.

(12) Haynes, B.; Wagner, H. Soot Formation. *Prog. Energy Combust. Sci.* **1981**, *7* (4), 229–273.

(13) Shell Global. *About Shell Eco-Marathon*; <http://www.shell.com/energy-and-innovation/shell-ecomarathon/about.html> (accessed Nov, 2017).

(14) Bendall, S.; Birdsall-Wilson, M.; Jenkins, R.; Chew, Y. M. J.; Chuck, C. J. Showcasing Chemical Engineering Principles through the Production of Biodiesel from Spent Coffee Grounds. *J. Chem. Educ.* **2015**, *92* (4), 683–687.

(15) Wallington, T.; Anderson, J.; Siegel, D.; et al. Sustainable mobility, future fuels, and the periodic table. *J. Chem. Educ.* **2013**, *90* (4), 440–445.

(16) Mueller, S. A.; Anderson, J. E.; Wallington, T. J.; Hammond, R. M. Classroom Demonstration of Water-Induced Phase Separation of Alcohol-Gasoline Biofuel Blends. *J. Chem. Educ.* **2009**, *86* (9), 1045.

(17) Rosa, P. D. La; Azurin, K. A.; Page, M. F. Z. Soybean Oil: Powering a High School Investigation of Biodiesel. *J. Chem. Educ.* **2014**, *91* (10), 1689–1692.

(18) Bent, H. A. Flames: A demonstration lecture for young students and general audiences. *J. Chem. Educ.* **1986**, *63* (2), 151.

(19) *Standard Test Method for Smoke Point of Kerosine and Aviation Turbine Fuel*, ASTM Standard D1322-08; ASTM International: Conshohocken, PA, 1997. <ftp://185.72.26.245/Astm/1/Section%2005/ASTM0501/PDF/D1322.pdf> (accessed Nov 2017).

(20) McEnally, C.; Pfefferle, L. Sooting Tendencies of Oxygenated Hydrocarbons in Laboratory-Scale Flames. *Environ. Sci. Technol.* **2011**, *45* (6), 2498–2503.

(21) Barrientos, E. J.; Lapuerta, M.; Boehman, A. L. Group additivity in soot formation for the example of C-5 oxygenated hydrocarbon fuels. *Combust. Flame* **2013**, *160* (8), 1484–1498.

(22) Glaude, P.-A.; Fournet, R.; Bounaceur, R.; Molière, M. Adiabatic flame temperature from biofuels and fossil fuels and derived effect on NO_x emissions. *Fuel Process. Technol.* **2010**, *91* (2), 229–235.

(23) Barrientos, E. J.; Anderson, J. E.; Maricq, M. M.; Boehman, A. L. Particulate matter indices using fuel smoke point for vehicle emissions with gasoline, ethanol blends, and butanol blends. *Combust. Flame* **2016**, *167*, 308–319.