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Future transportation fuels

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1. Introduction

The demand for energy to supply transportation worldwide is very large – around 11 billion liters per day of gasoline, diesel, heavy fuel oil and jet fuel combined. Each of these fuels satisfy key combustion requirements for the engines while meeting critical safety and logistical concerns. While there have been continuous improvements in combustion engines during the past century, in recent years several external drivers have arisen requiring changes in both fuels and combustion systems for transportation. Beginning with the oil crises in the 1970s, improved fuel efficiency has often been mandated by regulation. Regulations on traditional emissions (CO, NO_x, UBHC, and more recently particulate matter, or PM) resulted in a switch to stoichiometric gasoline engines with a 3-way catalytic converter, and gasolines needed to be reformulated to maintain knock resistance without the use of tetra-ethyl lead. Most recently, the drive to reduce emissions of greenhouse gases (GHG) from transportation has initiated large-scale research into alternative, low-carbon and carbon-neutral fuels. The transportation sector is responsible for around 14% of global greenhouse gases (GHG) including CO₂ and other emissions – which is essentially the same share as livestock farming. The overall challenge to the combustion community is how to achieve significant emissions reduction while maintaining the fitness for purpose of the engines used in different transportation sectors.

At present, global transport is powered almost entirely (>99%) by combustion engines, mostly burning liquid petroleum fuels. Current industry and policy initiatives (mostly in Europe and the Americas) are aimed at incorporating fuels derived from biomass and shifting land-based propulsion systems towards gasoline/plug-in hybrids, pure battery electric vehicles and fuel-cell systems using (renewable) hydrogen. The ‘drop-in’ addition of renewable fuels should reduce immediately anthropogenic carbon emissions from petroleum fuel, depending on the source and method of production of the renewable fuel, in the current generation of automobiles, trucks and aircraft. In the maritime sector, the increasingly stringent regulations limiting sulfur emissions is driving the replacement of heavy fuel oil with other fuels, particularly liquefied natural gas (LNG) and liquefied petroleum gas (LPG). But, the high energy density of

hydrocarbon fuels, ready availability of petroleum products and the robustness and wide utility of internal combustion engines challenge replacement fuels and alternative energy conversion methods. Despite the initiatives for alternative fuels and propulsion systems, projections to 2050 indicate the role of petroleum fuels for transportation will still be large worldwide. Hence, the significant impact of transport on global warming cannot be ignored and it is imperative that the combustion community assumes a major role in reducing the emissions of GHG.

To do so, there must be system/cycle efficiency advances, which can represent step changes in the conversion of chemical energy to useful work. Advanced combustion cycles have demonstrated 30% increase over fleet 2015 characteristics for vehicles sold in the US. Yet this is sufficiently short of what will be required to constrain climate change as described in the recent IPCC report. Added system changes (lighter vehicles, electric hybridization, etc.) could reduce fuel consumption by up to 50% of 2015 fleet usage. For long-haul/heavy-duty vehicles and ships, major improvements must come from engine efficiency in fuel utilization. There also must be substantial development and usage of biofuel alternatives and fuels derived using hydrogen from renewable power (either itself or combined with CO₂ to make liquid fuels), and the ability to burn such fuels efficiently. Increased efficiency in spark-ignited engines may require improved fuel formulation, to avoid undesired phenomena such as engine knock and superknock. In that regard, the growing production of gas-to-liquid fuels (GTL), which are currently applicable for diesel and other engines but have different chemical compositions and combustion properties than the conventional refinery products, may offer a route to suitable fuels for the new engines. However, GTL fuels need to be generated from biomass, rather than natural gas, to minimize the anthropogenic production of CO₂. It is obvious that the impact of efficiency improvement in petroleum-fueled engines is large: a factor of 2 improvement reduces the CO₂ emissions by the same factor. Future hybrid (fuel/electric) powertrains will need to use new/better combustion systems matched with sustainable fuels. For the end user, reduction of fuel consumption translates into either maintaining or increasing a desirable cruising range and reduction of cost per driven distance.

In addition to assuring fitness for purpose with new fuels, safety and risk also must be considered. Society has become comfortable with the use of petroleum-based fuels for transportation. Yet a 40 liter tank of gasoline represents about 1.3 GJ of energy, equivalent to

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about 280 kg of TNT. Storing and transporting similar amounts of energy using less familiar energy carriers may expose unforeseen fire or explosion risks, which may require significant technological remediation and societal acceptance. If not addressed in a timely fashion, this aspect can slow, or even stop, an otherwise advantageous transition to new energy sources.

The properties of future fuels are needed to meet the challenges in improved performance and emissions and must also satisfy other, non-combustion, constraints. For example, the mass and volume of the required amount of fuel for the cruising distance for a given application may restrict the range of acceptable energy density of the fuel. Additionally, in many engines the fuel also serves functions for lubrication and sealing, which are now fulfilled by petroleum components such as aromatics.

Other characteristics of liquid fuels that are seen as advantageous include minimizing aromatics or increasing the H/C ratios (for reduced particulate emissions), elimination of sulfur (for reduced plumes and contrails from jet engines), and increased heat sink capabilities (for increased cycle efficiency benefits). For particular engine systems, there may be advantages for tailoring the light end components, as well as the heavy ends to increase ignitability and reduce unburned hydrocarbon emissions, respectively.

Since it is unclear which combinations of modes of transportation (e.g. engine systems) and fuels will win out in the future, it behooves the combustion community to continue development of the fundamental science and specifically to help assess the potential of the choices available, to provide guidelines for which fuels are viable and how to implement them sensibly. This requires the proactive investigation into the utility of renewable fuels and fossil fuels modified to suit the requirements of changing engine technology. The fuels and technologies to be developed must maintain the fitness for purpose of combustion engines while minimizing the impact on GHG emissions and local air quality impact at affordable cost. A proper life-cycle analysis of such alternative solutions to transport should be done to ensure that the benefits are real and there are no unintended deleterious consequences.

2. Challenges

We identify several main challenges for new fuels when progressing towards a future low-carbon transportation sector.

1. *Fuels tailored to engines with cycle and system advances that increase overall conversion of chemical energy to useful work.* This will not only reduce the use of existing petroleum fuels but also reduce the load on future alternative, bio- or wind/solar-derived fuels. Step-change improvement in the internal combustion engine is limited by the properties of existing fuels and may require fuels with high (super)knock resistance, altered compression-ignition behavior, increased heat sink capability, and equal or improved pollutant emissions. One short-term example is the gasoline compression ignition (GCI) engine, which could use low-octane gasolines that are ignited by compression to achieve diesel-like efficiencies. Impact on future/advanced cycle engine designs may also be critical as preferred fuel properties may be altered. As future cycles are developed, new constraints on fuel formulation may be required to satisfy cycle needs, and safe operation. Such constraints may include tighter limits on ignition characteristics, such as octane (RON/MON) or (derived) cetane number.
2. *Renewable fuels that are chemically converted to equivalent petroleum products matched to the combustion engine that optimizes performance.* Matching fuels and engines is essential to guaranteeing fitness for purpose for the end user and maximizing fuel efficiency. Co-optimization of engines and fuels may be required.

3. *Fuels that optimize the complex interactions of physical and chemical properties.* The generation of power in a cylinder or combustor is an interaction of physical/chemical processes, such as the evaporation of multicomponent fuels in a spray, turbulence in the charge, (auto)ignition of the fuel-air mixture, combustion rates, piston motion and pollutant formation, which are each dependent on the specific operating conditions. All of these processes are time-dependent and interwoven by physical-chemical couplings, including the specific fuel properties. There are preferred physical and chemical properties of a fuel for each set of operating and environmental conditions; so, hybrid systems that include an engine and fuel optimized to operate at one or two conditions may have an advantage. A fuel tailored to these operating conditions and ambient environments might be preferred for optimum energy conversion to useful energy. These targets challenge the design and optimization process: the engine itself is macroscopic, but the processes determining its behavior are microscopic and usually dependent on the fuel properties, as well as the specific engine design.
4. *Jet aircraft fuels with more stringent requirements and specific characteristics to maximize cycle efficiency.* Changes in design or fuel composition must satisfy the necessity of keeping the aircraft in the air. For example, advanced cycle gas turbine engines may need an upper limit to cetane number (CN) to avoid pre-ignition in lean-direct injection designs, and perhaps a lower limit to avoid premature blow-out events. A constraint on CN did not exist with petroleum fuels since other jet fuel constraints resulted in a practical narrow limit for CN with such fuels. With respect to aromatics, there is no lower limit for petroleum fuels, yet blends with synthetic fuels must have aromatic concentrations between 8 and 25%, to ensure that seal swelling occurs. If the lower limit of aromatics could be reduced and H/C ratio increased, lower (non-volatile) particulate matter emissions (and smoke), and increased heat release (per unit fuel volume) should result. In addition, increased thermal stability of fuels will increase the ability to recover more energy in the fuel, increase the cycle efficiency, as well as decrease operational maintenance costs, all of which will enhance the large-scale introduction of new fuels and increased cycle efficiency.

In some cases, the new fuels may fit within existing ASTM fuel standards, but in other cases, standards may have to be redefined or modified. Insight into the (combustion) performance of new and existing fuels should be used to guide review/revision of standards, to facilitate the introduction of future fuels.

3. Perspectives

The major advances in combustion science during the past decades have provided understanding and tools that can address the challenges. Further development of such understanding and related tools are necessary to contribute to the future of mobility ranges from fundamental/generic to practical implementation.

- Generic understanding, characterizing and quantifying the role of fuel properties on engine performance, specifically for:
 - Understanding engine knock and superknock, as limiting phenomena for high-performance spark-ignited and dual-fuel engines. Shock tubes and rapid compression machines can replicate engine conditions to analyze and quantify (models for) ignition processes, but additional challenges include the understanding of the quantitative relationships between the various physical and chemical phenomena resulting in knock,

preignition and superknock in spark-ignited engines and (un) desired ignition in turbines.

- Identifying the fuel properties essential for the next generation of compression-ignition engines, including the potential to ameliorate the burden of pollutant emissions.
- Characterizing, preferably a priori, the impact of new fuels on power and pollutant emissions and ways to mitigate the effects.
- Developing new test methods and criteria to assess the fitness for purpose of the new fuels.
- Increasing the energy per unit mass content of the fuel (e.g. increased H/C ratio), for (commercial) aerospace application as well as decreased aromatic levels and increased heat sink capabilities.
- Co-optimizing engines/vehicles with fuel properties

The methods developed and insights gained must be applicable to complex, multicomponent fuel mixtures.

- Understanding, characterizing and quantifying the impact of the preferential evaporation of lighter components in multicomponent liquid fuels on critical engine processes. For example, there may be selective advantages of certain chemical classes, such as the use of n-paraffins in the lighter components as well in the heavier components to increase ignitability and reduce PM emissions, respectively.
- Tools to assess the effects of different fuel compositions on the performance of individual engine designs. These may vary from comprehensive computational fluid dynamic (CFD) tools that accurately simulate the complete power generation process, beginning with spray formation and ending with pollutant formation, to less comprehensive tools, which simulate individual or combinations of combustion processes in detail, but are coupled to each other by simpler but accurate physical models. Methods for creating reliable and reducible chemical kinetic models that accurately describe kinetic performance of complex petroleum fuels as well as alternative fuels, including the effects of oxygenates and olefins, for the range of fuel options in engines are needed. Such efforts should include the role of various chemical families and bulk physical properties on the performance and emission of engines. Such effects need to be understood better for SI, diesel and gas-turbine engines. This knowledge can be used to enable better tuning of fuels for different applications. Timely involvement of ASTM standards committees will facilitate the implementation of new fuel formulations or criteria.

4. Conclusions

Since internal combustion engines will remain the primary mode of choice for mobility in the foreseeable future, both alternative (renewable) fuels and high-performance combustion concepts/engines using fuels adapted for that purpose will be preferred for reducing the combustion impact on climate change. Multiple step-change reductions in the environmental/climate footprint of combustion-based transportation systems, while maintaining the fitness for purpose and convenience for the end user, are achievable.

The need for scientific and engineering advancements, as well as the opportunities to achieve them, are great. The potential societal

impact of these advancements may seem incremental individually; however, collectively they will have a significant impact on the challenge of mitigating climate change with limited impact on mobility and its economic importance. It also must be recognized that the needs, costs, and ability to adopt changes readily are different for different countries: the economic and societal concerns can be different in countries with mature and ageing transportation modes than in those undergoing slower or rapid economic growth, which is strongly reflected in their needs for mobility.

The societal and technical challenges are great, and the physical and engineering aspects are complex. The intertwining of fuel and engine properties, microscopic in nature but macroscopic in impact, demands that engine manufacturers, fuel producers and research institutions work together to meet the challenges of the future. Government involvement, to enable financially the sound assessment of the future fuel options, investments, and to understand policy implications, is essential.

Supplementary materials

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