Research and Development Needs to Enable the Expansion of Natural Gas Use in Transportation

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INTRODUCTION

Advances in hydraulic fracturing and horizontal drilling have revolutionized the U.S. oil and gas industries, increasing shale gas production sevenfold in five years, from 1.32 quadrillion Btu (quad) in 2007 to 9.60 quad or 39% of U.S. gas production in 2012. This game changer has made natural gas (NG) abundant\(^1\) and pushed its price down from as high as $9 per million Btu (mmBtu) in 2008 to $4 per mmBtu in 2013.\(^2\) Today, inexpensive natural gas is bringing the United States closer to energy independence, fueling a transition from coal for power generation, and helping to reestablish the manufacturing sector in the United States.

In the transportation sector, users are taking a new look at NG as an affordable alternative, often priced at $1.50−2.00/gasoline gallon equivalent (GGE) less than gasoline or diesel, and offering potential societal benefits like reductions in petroleum use, air pollutant emissions, and greenhouse gas (GHG) emissions. Unlike petroleum, a significant portion of which is imported and vulnerable to external disruptions at key points in the supply chain, NG is almost completely domestic and supplies are diverse. NG from renewable sources like landfills and anaerobic digesters or from fossil sources like shale gas is found in nearly every state, with associated benefits for state economies. An extensive transmission and distribution infrastructure exists in much of the country. There are, however, significant barriers that limit the speed and breadth of NG uptake into the transportation sector.

A collaborative partnership of Argonne National Laboratory (Argonne), the National Renewable Energy Laboratory (NREL), and Oak Ridge National Laboratory (ORNL) is well positioned to lead a significant research and development (R&D) program to address the barriers. Argonne, NREL, and ORNL have historical experience in NG use for transportation, objectivity to independently address safety and infrastructure issues, existing expertise in critical technical disciplines across the technology readiness level (TRL) spectrum, and broad competencies to collectively address and integrate the key areas. Argonne, NREL, and ORNL also have established relationships to engage stakeholders and effectively collaborate with partners from industry, academia, other U.S. Department of Energy (DOE) laboratories, and other government agencies as appropriate. Collective DOE laboratory leadership of an integrated R&D program ensures commitment to a broad-based strategy focusing on developing and deploying the technologies and infrastructure to enable the expansion of NG use in transportation.

Many of the barriers to NG use in this sector are technical in nature and overcoming them will require a concerted R&D effort. This paper focuses on those barriers and associated R&D opportunities for using compressed natural gas (CNG), liquefied natural gas (LNG), and NG-derived liquid fuels in internal combustion engines (ICEs) for light duty vehicle (LDV) and

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medium- and heavy-duty truck (M/HDT) applications. This paper is organized into five key areas that highlight R&D needs: NG distribution, liquid fuel production from stranded gas, vehicle fuel use, NG storage, and impact analysis and assessment.
R&D OPPORTUNITY AREAS

NG DISTRIBUTION

Historically, most domestic NG has been produced in and around the Gulf coast of the United States and the transmission infrastructure has been built to move supplies north, east, and west. It has been estimated that an additional 29,000–62,000 miles of pipeline may be needed to connect new NG supplies to existing transmission lines over the next 20 years, at an estimated cost of $133–210 billion.\(^3\) While extensive local distribution networks exist in most urban and suburban areas, many pipelines have been in place for 40 years or more and their structural integrity is uncertain at current volumes, let alone if they were to supply significant numbers of home fueling devices and/or local fueling stations. There are few current research efforts on pipeline safety, with very little incentive for pipeline operators to assess the safety of their networks (as noted in a recent Massachusetts Institute of Technology [MIT] report)\(^4\) or reduce methane leakage. At present, there are only 681 CNG and 52 LNG stations open to the public\(^5\) in the United States, relative to about 160,000 gasoline stations. At an incremental cost of roughly $3 million for a comparably-sized station, high cost is a major barrier to expanding the number of CNG stations. Increased utilization of NG will require significant infrastructure investment over the coming years. Sustaining the development of this infrastructure and supporting responsible maintenance of existing infrastructure warrants significant R&D attention.

Proposed R&D Areas

- NG distribution safety and security. Most NG is transported hundreds of miles from supply sources to local distribution centers via medium-pressure steel transmission pipelines. While shorter-distance transport occurs primarily through pipelines made of a variety of materials, it can also occur by rail and road (for LNG). The reliability of new and existing infrastructure for all modes of NG distribution has tremendous safety, environmental, and economic implications. Improved materials, monitoring technologies (for pipeline damage and corrosion), leak detection diagnostics, and safety systems are needed. Mitigation strategies and measures to respond to terrorist attacks and natural disasters are also of critical concern.

- Advanced materials and compressors. NG must be compressed to as much as 5,000 pounds per square inch (psi) at stations to fill CNG vehicle tanks quickly and safely. Current compressors are expensive, bulky, and difficult to install and operate. Effective sealing of rotating or reciprocating surfaces is a challenge for long-lived,


high-pressure industrial-scale compressors as well as for small home refueling units. Moving components are subject to high friction and wear, especially at sealing and sliding surfaces. Overcoming such material and tribological barriers is a high priority. In particular, improvements in seal materials, low-friction coatings, and compressor designs are needed to help achieve the required compression quickly, safely, cost-effectively, and with lower leakage.

- CNG/LNG station design and operation. CNG/LNG stations are now expensive to build and operate. Recent improvements to the cryogenic tanks for transporting LNG to stations have come from DOE-supported research on liquid hydrogen storage. Additional improvements in on-site storage and compressor design and in integrating compressor and cascade vessel operation are needed and can benefit from ongoing DOE-supported work on hydrogen station optimization.

**Stakeholders and Partners:** DOE (Office of Energy Efficiency & Renewable Energy (EERE), Office of Fossil Energy, Office of Science, Office of Biological & Environmental Research); U.S. Environmental Protection Agency (EPA); U.S. Department of Homeland Security (DHS); NG production & distribution industry; and Gas Technology Institute (GTI®).

**LIQUID FUEL PRODUCTION FROM STRANDED GAS**

A key opportunity for expanding NG use in transportation is to convert it to liquid fuels. The current and projected long-term price advantage of NG over crude oil  has made liquid fuels from NG cost competitive with fuels produced from petroleum. Of particular interest is the Fischer-Tropsch (FT) process, an indirect methane conversion route, that first converts methane to syngas (a mixture of carbon monoxide [CO] and hydrogen [H₂]), followed by the FT synthesis step to produce FT diesel which is substantially similar to petroleum diesel. The FT process, though commercial, is capital intensive (~$100,000/barrels per day [bpd]), energy inefficient, CO₂ intensive, and requires large facilities (>50,000 bpd) to realize scale economies. It is estimated that nearly 3,000 trillion cubic feet (TCF) of stranded gas exists worldwide (of which about 10% is in the United States) with an energy content equivalent to the oil reserves of Saudi Arabia. However, only 6% of the world’s known gas fields can support large-scale FT plants. The development of process technologies capable of producing FT fuel at 1,000−15,000 bpd capacity could increase utilization of stranded gas by up to 40%.

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Gas-to-liquids (GTL) processes based on direct conversion routes (such as oxidative coupling, non-oxidative coupling, and selective oxidation) should be more economical than indirect conversion at the production scale appropriate for the majority of stranded NG fields, because they bypass the expensive syngas production step.\(^{11}\) However, no direct conversion routes are in commercial use today because of the thermodynamic challenges (e.g., the process requires temperatures >700°C to achieve modest conversion levels or the desired product undergoes subsequent reaction to an undesired but more thermodynamically-favored product). While research has attempted to overcome these challenges, the historic, long-term coupling of NG and crude oil prices has limited the incentive to do so. Today, the spread between oil and gas prices creates a new incentive to support renewed R&D investment in direct conversion.

Proposed R&D Areas

The following R&D topics are proposed to develop economically-competitive small-scale GTL technologies based on direct conversion routes.

- **Catalysis.** Thermally stable, high selectivity catalysts are needed, particularly at temperatures above 700°C. Catalysts able to activate methane at lower temperatures (200–500°C) are also needed. The new catalysts should range from (oxidative) coupling of methane to alkanes and aromatics to the production of oxygenated compounds like alcohols.

- **Separation technologies.** Less expensive separation processes are needed to produce O2 for selective oxidation and oxidative coupling reactions. More selective, less energy-intensive processes for separating methanol, olefins or aromatics from dilute streams are needed, as are better performing low- and high-temperature H2 separation processes to increase conversion in non-oxidative methane coupling. Technologies that do not require cryogenic separation (e.g., membranes) offer significant opportunities to reduce energy requirements and cost.

- **Process engineering development.** New materials capable of withstanding high processing temperatures are needed, as are new reactor designs to more efficiently manage heat transfer and facilitate separation processes, and new process strategies (such as continuous product removal) for increasing yield of desired products.

**Stakeholders and Partners:** DOE (EERE, Office of Fossil Energy, Advanced Research Projects Agency-Energy (ARPA-E), and Office of Science); Gas Technology Institute (GTI®); and upstream and downstream petroleum industry.

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In the past few decades, dramatic changes in fuel prices, fuel availability, and emissions standards have resulted in significant swings in the development and availability of NG vehicles in the United States. NG LDVs are exclusively based on spark ignited (SI) engines, with a limited mix of dedicated CNG and bi-fuel options. Buyers are primarily fleet owners who already operate NG M/HDTs and have established maintenance and refueling facilities. Household adoption of NG LDVs has the potential to significantly increase, especially with advances in reliable, inexpensive home fueling equipment.

The M/HDT market is experiencing the most growth, with a new range of available NG engine options. HD NG engine technology has largely migrated from compression ignited (CI), dual-fuel (NG and diesel) technology to SI engines using three-way catalytic converters. While some CI dual-fuel technologies limit NG use solely to LNG, current SI engine options utilize either LNG or CNG. And while CNG previously imposed significant range restrictions, recent advances in tank systems allow up to 155 diesel gallon equivalent storage on a Class 8 tractor. Coupled with recently available engine options in the 11–12 L range, the Class 8 NG truck market is poised for significant growth.

Before the 2010 emissions regulations, NG truck engines showed significant emissions benefits compared to diesel. With stringent 2010 regulations in place, the emissions benefits of NG over diesel may no longer be significant. However, specific applications (e.g., transit bus fleets and areas with air quality issues) are sensitive to GHG and emissions trade-offs between NG and diesel vehicles because of fuel economy penalties of aftertreatment controls. Advances in SI NG engine technology have the potential to offer significant reductions in key pollutants, including a nitrogen oxide (NOx) reduction of more than 90%. In California, the South Coast Air Quality Management District (SCAQMD), the California Energy Commission (CEC), and the California Air Resources Board (CARB) are interested in either requiring lower emissions classifications or incentivizing engines below current standards.

Proposed R&D areas

- **M/HDT Engine development.** Efficiency improvements and emission reductions are critical to the success of NG vehicles. Reducing NOx and improving efficiency require development of higher levels of exhaust gas recirculation (EGR) dilution and other controls. Advances in ignition systems are required to operate with high dilution and boost. Advanced port injection or DI technology is required to maintain tighter air/fuel control to minimize NOx, while avoiding ammonia (NH3) production.

- **LDV engine development.** The gasoline engines upon which CNG LDVs are based are shifting to direct injection (DI) technology, often with turbocharging and downsizing. Both technologies significantly impact CNG operation. Developing DI CNG engines will require advancements in injector configurations, injection strategies, spray modeling and injector thermal management. As future LDV engines
migrate to DI, particulate matter (PM) emissions will become an issue, necessitating additional research into the effects of CNG on DI PM emissions.

- **Systems research on bi-fuel LDVs.** Analysis of systems level bi-fuel vehicle options coupled with NG infrastructure requirements is an important component of successfully integrating NG vehicles. Such an analysis will help determine gasoline versus CNG range requirements with linkages to growth in the CNG fueling station network.

- **CNG hybrid-optimized engines.** Modern advanced hybrids have evolved over the past 15 years with the optimization of the gasoline engine. Current hybrids use Atkinson cycle and downsized turbocharged DI gasoline engines. Research is needed to identify the properties of CNG hybrid-optimized engines with high powertrain efficiencies.

**Stakeholders and Partners:** DOE (EERE); EPA; CARB; CEC; SCAQMD; LDV original equipment manufacturers (OEMs); M/HDT engine and vehicle OEMs; and industry trade associations.

**NG STORAGE**

NG storage for transportation represents a major R&D opportunity, with cost being a major driver. Gaseous storage technologies (for NG and hydrogen) can be divided into two classes — high-pressure tanks and low-pressure sorbents. High-pressure tanks (at 250 bar) are a major cost component of CNG vehicles, adding weight (with a consequent fuel economy penalty), and limiting driving range. Moving from steel to carbon/glass fiber tanks can reduce vehicle weight and may increase driving range by permitting higher compression pressure. Current R&D efforts focus on reducing the cost of carbon/glass fiber for structural applications. These efforts should be supplemented with additional research on tank packaging onboard the vehicle, especially as it concerns alternative structures, shapes, and formability.

Low-pressure sorbent-based storage technologies offer attractive alternatives to high pressure tanks. Sorbent-based storage at pressures of ~35 bar could achieve NG storage capacities equal to, or better than, a high-pressure CNG tank; thus, improving refueling-storage efficiency and greatly reducing compression cost. In particular, successful sorbent-based technology can help implement low-pressure home refueling which could facilitate large-scale commercialization of light-duty NGVs. Sorbent material design, synthesis, engineering, and system integration represent major technology opportunity areas. In the past, high surface area materials such as engineered carbons and inorganic zeolites were explored as potential NG sorbents, but with only limited success. More recently, however, research into new porous materials, such as metal-organic frameworks (MOFs) and porous organic polymers (POPs), has resulted in many significant discoveries with potential NG sorbent applications. EERE’s Fuel Cell Technologies Office has funded hydrogen sorbent material research with new sorbent design and discovery and modeling and system analysis. DOE ARPA-E has also supported a
number of projects on tank materials and sorbents which will be completed in a year. These efforts provide a basis for further NG sorbent material research.

Proposed R&D Areas

*High pressure tank storage:*

- **Materials research.** Carbon/glass fiber with significant tensile strength is needed at a cost comparable to steel tank systems. Continuous improvements in current carbon/glass fiber composite technologies are being made for structural applications in airplanes and high-end automobiles. R&D is needed to identify carbon/glass fiber for gas storage tanks with improved gas permeation performance to displace steel tanks.

- **Manufacturing process technology.** New manufacturing process technology is needed to produce tank materials and form them into shapes conformable to application-oriented designs with maximum storage space and pressure tolerance.

*Low-pressure, high-density sorbent based storage:*

- **Sorbents.** Next-generation sorbents need to be identified through a process of rational design and synthesis. Emphasis should be on materials with high surface area, porosity, and sorption enthalpy tailored for NG storage applications, with volumetric densities that meet or exceed high-pressure tank storage capacity, but at 15–20% storage pressure. In addition, the sorbent must be scalable to commercial production using low-cost raw materials and engineering methods.

- **Engineering processes.** Innovative engineering processes are needed to integrate and improve sorbent storage capacity, packing density, charge-discharge rate, thermal conductivity, and mechanical strength for optimal on-board delivery in transportation applications. This is particularly important for transforming new sorbent materials into practical applications.

- **Modeling.** New sorbent-specific predictive modeling and simulation are needed to provide guidance on sorbent storage limits, thermal management, charge and discharge kinetics, and overall system requirements for transportation applications.

**Stakeholders and Partners:** DOE (EERE, ARPA-E, and Office of Science); U.S. Department of Transportation (DOT); U.S. Department of Labor Occupational Safety & Health Administration (OSHA); and EPA.
IMPACT ANALYSIS AND ASSESSMENT

The above sections focus on R&D needs to resolve technical barriers. DOE and its laboratories also need to apply their systems assessment expertise to analyze institutional and market barriers like inconsistencies and uncertainties in CNG/LNG fuel specifications and infrastructure development, and impacts of NGV market development on energy consumption, emissions, energy security, and cost. Unlike gasoline and diesel fuels, which have uniform fuel standards and specifications centered around their use in reciprocating IC engines, current NG specifications such as Wobbe Index and Methane Content are largely based on traditional applications with fixed orifice fuel metering and static diffusion flames and they are not tailored to IC engine performance with NG. The wide variation in NG properties further complicates efforts to optimize NG engines for efficiency and emissions. Similar variations exist in CNG/LNG fueling infrastructure. “Public” CNG stations may limit access via card keys and dispense fuel at different rates resulting in different fill times. LNG stations may dispense unsaturated (“cold”) LNG or saturated LNG with consequent differences in fill quantities and vehicle range. Neither the costs of these differences nor their impacts on market developments is well understood.

Differences and gaps also exist in data used to assess the environmental impact of NG market development. For example, methane leakage has been under intense scrutiny for the past several years with different methodologies employed and different results generated.\textsuperscript{12} At present, atmospheric observations of methane concentrations (a “top-down” approach) produce an estimated 5–10% leakage from NG production and distribution networks\textsuperscript{13} while direct measurements of leakage from individual pieces of equipment along the supply chain (a “bottom-up” approach) produce an estimate of 1–2% leakage.\textsuperscript{14} Since methane is a potent GHG, the impact of the difference is significant from a climate change perspective. Methane leakage is also a significant economic cost since every 1% of leakage equates to roughly $1 billion of lost private and public revenue.

As mentioned earlier, inexpensive, abundant NG is a game changer for the electricity and manufacturing sectors in the United States. Widespread adoption in the transportation sector could further its reach, with potential implications for energy security and system resilience. While few would argue that NG could have major impacts, the magnitudes of impacts (and even their directions) are highly uncertain. Increased use of NG could add to energy independence for the United States and increase energy market stability, but if shortages were to develop during high demand periods (e.g., cold winters), NGVs could further destabilize energy markets and jeopardize energy security. In contrast, NG bi-fuel applications could provide flexibility in the event of petroleum supply disruptions, a bridge to potentially low carbon energy carriers like hydrogen and electrification, and an outlet for stranded gas supplies. Analyses and assessments are needed to address both the impacts of CNG/LNG and NG-based liquid fuels in these many

dimensions and to identify environmental, energy, and cost bottlenecks to guide further R&D. Systems assessment should also compare baseline technologies (petroleum fueled vehicles) and competing technologies (e.g., electric drive technologies) with CNG/LNG and NG-derived liquid fuels to identify R&D priorities.

Proposed Analysis/Assessment Areas

- **Cost impact estimation.** The translation of R&D successes into cost reductions for technologies requires modeling economies of scale, new material needs, and process improvements. Argonne, NREL, and ORNL have built strong expertise estimating fuel costs and vehicle costs with models already developed. These models will be adapted to include details of the R&D activities identified above. In particular, a consistent cost estimating platform will be developed for fuel production, vehicle production and use, and NG refueling infrastructure establishment. This platform will be used by R&D teams on the above specific topics to examine impacts of R&D progress on cost reductions.

- **Energy/environmental analysis of the NG supply chain.** DOE EERE has been supporting life-cycle analysis (LCA) of various vehicle and/or fuel systems for over 20 years with the Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) LCA modeling platform. This modeling platform will be adapted to include improvements resulting from the R&D efforts discussed above and new energy and environmental data on the NG supply chain. To put CNG/LNG and NG-derived liquid fuels into broad perspective, the use of NG for fuels versus products (e.g., plastics) will be included in the modeling platform so that this usage trade-off can be evaluated on a LCA basis. Similar trade-off analyses will be conducted between NGVs and other competing vehicle/fuel systems. Opportunities for reducing NGVs’ energy and environmental impact — via efficiency improvements throughout the NGV and fuel supply chains or by substituting with renewable gas sources — will also be examined.

- **Energy security and system resilience.** Increased uptake of NG in the transportation sector is likely to present important opportunities for utilizing stranded gas, increasing energy security, and improving the resilience of energy markets. However, the potential for NG demand spikes, supply disruptions, and price volatility may significantly impact NGV operations and market penetration. Argonne, NREL, and ORNL have addressed these issues for alternative fuel vehicles in general. The existing expertise will be extended to address the issues for NGVs.

- **Methane leakage.** One critical environmental issue that must be examined is methane leakage along the NG supply chain. A concerted DOE-sponsored effort (with participation by EPA, National Aeronautics and Space Administration [NASA], National Oceanic and Atmospheric Administration [NOAA], and other agencies) is needed to reconcile estimates from “top-down” and “bottom-up” approaches. This effort should be supplemented by additional data collection downstream in the supply chain. In particular, measurements of methane leakage...
while loading and unloading tanker trucks, in conjunction with fueling events, and from vehicle exhaust, are needed not only to update models, but more importantly, to identify needed improvements in procedures, equipment, and technologies to reduce the magnitude and frequency of such leaks. Particular attention should be paid to “super-emitters” along the NG supply chain and to the drivers of variability in methane leakage (across regions, operators, supply chain stages, etc.). Analogous research during NG refueling for NGVs is necessary given significant differences in operator training, conditions, and equipment affecting methane leakage.

- **CNG/LNG refueling infrastructure requirements.** DOE EERE has supported analytical efforts on refueling infrastructure needs for new transportation fuels such as electricity and hydrogen. These analyses have helped DOE and other federal agencies to understand the gradual refueling infrastructure ramp up as a new transportation fuel market increases. A similar approach will be used to develop modeling tools to assess refueling infrastructure needs at the regional basis for CNG/LNG.

- **CNG/LNG fuel standards and specifications.** DOE and its laboratories have conducted extensive engine testing with a variety of gaseous and liquid fuels for optimization of IC engines and fuels. With a CNG/LNG testing program using existing testing facilities and expertise at national laboratories, DOE can support and facilitate the development and adoption of NG specifications specific to IC engines. Specific aspects include development of an anti-knock index (AKI) such as octane number for NG fuels and establishment of limits on contaminants like sulfur, water, lubricants, and metal particulates for vehicle emission controls and durability. The AKI could be a determinant of minimum methane content and maximum ethane and/or propane content in CNG for IC engines.

**Stakeholders and Partners:** DOE (EERE and Office of Fossil Energy); EPA; NASA; NOAA; CARB; and DHS.

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15 See footnote 12.
SUMMARY

The advances in hydraulic fracturing and horizontal drilling that have revolutionized the U.S. oil and gas industry offer tremendous opportunities for natural gas use. The U.S. economy and industry are adapting to utilize these natural gas resources. However, without a coordinated effort by the federal government, disparate industry stakeholders will not optimize the use of natural gas for the transportation sector. Argonne, NREL, and ORNL have cross-cutting R&D capabilities with a view across the entire value chain and the competitive landscape. The R&D topics presented here will help to significantly increase the use of natural gas in transportation with consequent benefits in the forms of cost savings, improved energy security, air pollutant emission reduction, and GHG mitigation.
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