Perspective

Expanding Role of Chemical Engineers in Transportation-Motivated R&D

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Introduction

The consumption and production of energy have been at the core of chemical engineering for a century. The discipline, as we know it today, has been influenced strongly by the needs of the petroleum and chemicals industry to analyze and optimize their processes and equipment for a more efficient use and production of energy and materials.

A significant driver for change has come from the transportation sector. The air pollution caused by the emissions of hydrocarbons and carbon monoxide from vehicles was regulated in the 1970s by the adoption of low emission standards that required the introduction of catalytic mufflers that were incompatible with the lead additives used to increase the octane number of gasoline. The engineering community met the shift to unleaded gasoline in the 1970s. It also met the requirements of oxygenates in the fuel in the 1980s and is now responding to the need for significantly lower sulfur levels. Lubricants have been introduced that provide engine wear protection and longer oil change intervals.

Materials innovations in polymer composites have provided attractive, long lasting materials and increased vehicle content. Low emission paints and paint systems have been developed that meet performance and durability specifications. While electrochemical chrome cladding of automobiles was a trend in the 1950s, electrochemical engineers entering the field in the past decade have seen a growth in battery R&D with the demand for more electrical content on vehicles and the emergence of electric and hybrid vehicles. In this article, we will describe the expanding role of chemical engineering for transportation and related opportunities for young engineers entering the field.

In the past three decades, a major role for chemical engineers in transportation research has been to lower emissions and increase fuel economy. The heightened awareness of the quality of the environment, such as air pollution and global warming, has led to increasingly stringent regulation on emissions in the coming decade. For example, the U.S. Environmental Protection Agency (EPA) emissions standard for all diesel-powered passenger cars, light trucks, and medium-duty vehicles (e.g., pick-up trucks and delivery trucks) has been set recently at 0.07 g/mile NO_x and 0.01 g/mile particulate matter (PM) for 2007, a significant decrease from the current standards of 1.25 and 0.10, respectively (Federal Register, 1999; EPA, 2000). Likewise, the standards for heavy-duty diesel engines used in highway trucks have been tightened from the current values of 4.0 g/bhp·h NO_x and 0.10 g/bhp·h PM, to 2.5 and 0.10, respectively for 2004, and 0.2 and 0.01 by 2007–2010 (Federal Register, 2001). A similar trend is also taking place in Europe.

Aiming to improve fuel economy in transportation to reduce dependence on imported oil and lower carbon emission, the U.S. Government in 1993 initiated a government-industry cooperative research program known as Partnership for a New Generation of Vehicles (PNGV). The industrial partners included all three U.S. major automobile manufacturers. Of the three goals of this program, the most cited is goal 3—develop vehicles to achieve up to three times the fuel efficiency of comparable 1994 family sedans. (The other goals are to improve the U.S. competitiveness in manufacturing in the transportation industry.) Three times the fuel efficiency is equivalent to 80 miles per gallon (Department of Commerce, 1993). Substantial funding from both government and industry went into this program, and significant technical advances were achieved in many areas important to vehicle development (NRC, 1997, 1998, 1999, 2000, 2001). In spite of the advances and the successful completion of concept vehicles, the unfavorable projection of the cost to manufacture such a vehicle prevented the construction of production prototypes. Furthermore, during this period, the demand for sport utility vehicles and light-duty trucks in the U.S. have increased drastically, and new, tighter emission standards have been promulgated.

Consequently, in a 2001 NRC (National Research Council) report on the review of this program (NRC, 2001), the review committee recommended the government and industry participants to refine the PNGV charter and goals to better reflect current societal needs. In January, 2002, a new Government initiative, named FreedomCAR was announced (Department of Energy, 2002). As stated, FreedomCAR is a research initiative focused on collaborative, precompetitive, high-risk research to develop the component technologies necessary to provide a full range of affordable cars and light trucks that will free Americans from dependence on imported oil and from harmful vehicle emissions, without sacrificing freedom of mobility and freedom of vehicle choice. The U.S. Department of Energy (DOE) and the U.S. Council for Automotive Research (USCAR)—representing DaimlerChrysler Corporation, Ford Motor Company, and General Motors Corporation—are the partners in the initiative.

The goals and the research emphasis of the FreedomCAR initiative are similar to the PNGV program. The only difference between the two is that the latter does not have the timetable for concept vehicles or production prototypes. Research programs that deal with lowering emissions and enhancing fuel efficiency will stay the same.

How could a chemical engineer contribute to the research opportunities provided by this future car initiative? Table 1 summarizes a potential list. Some of these issues are already the province of chemical engineers, such as fuel production and emissions treatment, and their involvement in these fields will evolve as the needs change. On the other hand, the emphases and approaches in other issues quite differ from traditional chemical engineering problems. Chemical engineers who make appropriate adjustments will be able to take full advantage of these opportunities.

Automobile as a system

From a system perspective, designing and manufacturing an automobile and its components are quite different from designing a chemical plant and manufacturing commodity chemicals. The operation mode of an automobile is seldom at a steady state. The transient behavior is not only important, but often one of the distinguishing characteristics of a production model. For example, how fast an automobile can accelerate from rest to 60 mph and the stopping distance are advertised features. Thus, both the automobile and its components are designed and optimized for such operations. Steady-state analyses are at best useful as a very crude approximation.

Table 1. Potential Research Areas for Chemical Engineers in Transportation

Area	Characteristics and Research Problems
Vehicle system	Transient operation, size and weight constraints, consumer acceptance, easy assembly
Powertrain	Emission control, energy conversion efficiency, fuel conversion, power storage, safety, size and weight
Materials and Manufacturing	Lightweight and high-strength materials, crash safety, recyclability, composite processing, manufacturing emissions control, paint engineering, predictive modeling
Fuel and Lubricant	Low-sulfur fuels, alternate fuels, biofuel, lubricant formulation

Similar observations apply to any subsystem that might be introduced, such as an onboard fuel processor to convert a liquid fuel (e.g., gasoline) into a gas mixture rich in hydrogen and free of carbon monoxide. The hydrogen is then proposed to be used with a proton exchange membrane fuel cell to power an automobile. The design of this “power plant” is different from that of a traditional chemical plant for hydrogen production by steam reforming of natural gas.

Design and performance objectives not found in a traditional plant design are rapid startup in less than a few minutes and, more desirably, in seconds, rapid response to change in output demand (rapid acceleration of the vehicle), restricted weight and volume, safety with respect to catastrophic failure such as damage by collision, and ability to withstand abuses, such as rather varied fuel composition. Heat integration takes on a somewhat different meaning. Heat streams at slightly higher than room temperature are considered practically useless in a traditional plant. For an automobile, however, it can be beneficially used to warm the passenger compartment. Although chemical engineers trained in the traditional curriculum have little exposure to these issues, they have the necessary tools to tackle them.

Vehicle components

The components in an automobile are designed for high-volume production of individual units for easy assembly and low cost, and consumer acceptance in terms of reliability, ease of maintenance, aesthetics, and, of course, safety. These are considerations in product design (Westerberg, 2000). Figure 1 illustrates some of these issues in the design of a future automobile. Although about 100 million automobiles and the corresponding number of components are produced annually, the manufacturing processes are not steady-state operations and involve many more mechanical and moving parts and handling of solids than manufacturing of commodity chemicals.

There are rich chemistry and strongly coupled chemical kinetics and fluid dynamics in the in-cylinder combustion process of an internal combustion engine. This area, however, is extensively covered already. Undoubtedly, chemical engineering will continue to contribute to improving existing exhaust treatment devices, as well as the development and implementation of new ones for both gasoline and diesel engines. A recent innovation for reducing exhaust emissions in spark-ignition engines is the development of a microcatalytic reactor that reforms a small amount of gasoline immediately ahead of the engine and the catalytic converter (Kirwin, 2002). The devices for diesel exhaust may be substantially more complex than the current passive automobile exhaust converters. Because of the high oxygen partial pressure and low temperature of the diesel exhaust, there is currently no satisfactory passive device.

The devices under development to remove NO_x include urea-injection-selective catalytic reduction, regenerative NO_x trap, and hydrocarbon-based selective catalytic reduction. For the urea-injection method, precise control of the rate of urea injection that can rapidly respond to the drive condition is important. For hydrocarbon-based catalytic reduction, methods being investigated currently include injecting reductants in the form of alcohol or other functionalized hydrocarbon, or processing the hydrocarbon fuel into functionalized molecules that are more effective for NO_x conversion. For a regenerative NO_x trap, periodic regeneration could be achieved by converting the exhaust to a fuel-rich condition. For all these devices, reducing the weight and fuel requirement (fuel penalty), long-term stability, and resistance to sulfur in the fuel are among the remaining issues that need to be resolved (CLEERS, 2002). Developing accurate models for the operation of these devices is also needed for the design of the powertrain and vehicular trade-off analysis.

In addition to treating NO_x in the diesel exhaust, particulate matters (PM) need to be treated. Better design and materials for PM filters, as well as efficient methods to regenerate them with minimal fuel penalty, are needed.

Various sensors will be needed to maintain the operation of a powertrain near the optimal conditions for fuel economy and emission. These sensors need to have a rapid response and be selective. For example, the operation of various NO_x treatment devices could be benefitted greatly by a selective and sensitive NO_x sensor.

Fuel cells are being investigated as the powertrain for future vehicles. St-Pierre and Wilkinson (2001) have summarized the current status of fuel cell developments and future engineering challenges and prospects. At present, the most promising type of fuel cells for transportation is the hydrogen proton exchange membrane (PEM) fuel cell. The pressing issues are lowering the cost and reducing the size and weight of the fuel cell system. If hydrogen is to be stored onboard, a satisfactory method for producing the hydrogen from a suitable source is vital, as well as a hydrogen storage method that has the capacity to offer the driving range that the consumers are accustomed to. If hydrogen is to be produced by an onboard fuel processor, fast startup, and rapid transient response, durable catalysts, smaller size, and light weight are among the hurdles that need to be overcome. Research in fuel processing has led to the invention of the microchannel reactors (Wegeng, 2001). These reactors are compact in size, have excellent heat-transfer properties, and have many other potential applications. Overall commercial viability of fuel cells for transportation must include the fuel supply, as well as the fuel cell system.

Batteries with higher power densities (both in terms of weight and volume) than the lead acid batteries are desirable in future cars. These batteries will store energy generated during braking, supply energy during startup, and assist the primary power plant (e.g., engine) during acceleration in two different modes. In the power-assist mode, the battery supplies energy during a power peak to moderate the demand on the primary power plant. In the dual mode, the primary power plant is run substantially at a constant power level, with all fluctuations being supplied by the battery (NRC, 2000). Lithium ion and nickel metal hydride batteries hold the most promise, and they are used currently in the hybrid electric vehicles (HEV) marketed by Toyota (Prius) and Honda (Insight). For future cars, there is still a need to enhance the battery life and power density, and lower the cost. In the case of Li ion battery, safety against puncture is also a concern.

Stronger and lighter weight materials are central to improving fuel economy, while maintaining safety. Although high strength, ultralight steel, aluminum and its alloys are the focus of the weight reduction efforts, polymers and composites play an important role also. Aluminum is increasingly used for body and powertrain applications, and an aluminum-intensive vehicle has been demonstrated with the Audi A2. Steel companies have joined to demonstrate advanced concepts for the application of ultralight steel for automotive. Likewise, lightweight polymer composites will find use in various body parts. New nanocomposite materials saw their first automotive application on a General Motors van this year (see www.gm.com/automotive/innovations/rnd/news/news_082801.html). The costs of new materials and manufacturing are major issues for all new lightweight materials. At the same time, all durability and crash safety concerns must be met. Research and development focus is on manufacturing methods, cycle time, designs that consolidate parts and lower overall material use, and predictive modeling to speed materials development, engineering process, and product development.

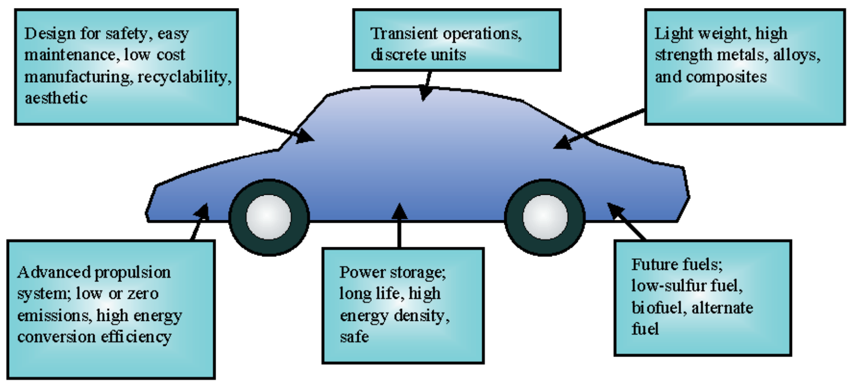

Figure 1. Chemical engineering research opportunities for future vehicles

Fuel for the future

Should hydrocarbons from oil maintain a dominant role as fuel, the problem of sulfur content must be solved. This is because the operations of many of the components for the future cars are sensitive to sulfur. For example, the NO_x trap, lean NO_x catalysis using hydrocarbon reductant, the Pt electrodes in the fuel cells, and the low-temperature water-gas shift catalysts for fuel reforming are all negatively affected by sulfur. The new regulations requiring gasoline fuel averaging 30 ppm sulfur by 2006, down from the current 300–500 ppm (EPA, 2000), and diesel fuels to contain a maximum sulfur content of 15 ppm by 2006 are likely a glimpse of the future to come (Federal Register, 2001).

To achieve this goal, deep desulfurization will be needed in crude oil processing. Modifying the fuel composition to contain more oxygenates to reduce PM emission is constantly a discussion and research topic. Replacing the fuel value of methyl tert-butyl ether (MTBE) in areas that plan to ban its use is an engineering, environmental, and economic issue. With the development of new types of engines, new lubricants may be needed. Katzer and coworkers offered their vision of the future of petroleum refining in such a climate (2000). In addition to the conventional refining of fossil fuel, the possibility of processing and production of biofuel for a truly sustainable economy is a development that is being actively pursued.

Conclusion

Chemical engineering has played a major role in the U.S. transportation industry, including fuel production, polymers, surface finishing, and exhaust treatment. The changing landscape of the transportation industry because of the heightened concerns for the environment and fuel economy offers new opportunities for chemical engineering. However, to capitalize on these opportunities—in addition to expanding their skills that have served them well in the petroleum refining and the chemicals manufacturing industries, chemical engineers need to acquire new skills to deal with mass manufacturing of individual units, product design that includes size, weight, ease of maintenance, recyclability, fast to market development, and consumer acceptance and safety as optimization objectives, and analysis and design for nonsteady-state operations. If successfully engaged, chemical engineers can add new, rich and challenging problems of the transportation industry into their portfolio, and pursue rewarding careers in that sector.

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