Well-to-Wheels Analysis of Advanced SUV Fuel Cell Vehicles

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ABSTRACT

Fuel cell vehicles are currently undergoing extensive research and development because of their potential for high efficiency and low emissions. A complete well-to-wheels evaluation is helpful when considering the introduction of advanced vehicles that could use a new fuel, such as hydrogen. Several modeling tools developed by Argonne National Laboratory were used to evaluate the impact of several new vehicle configurations. A transient vehicle simulation software code, PSAT (Powertrain System Analysis Toolkit), was used with a transient fuel cell model derived from GCTool (General Computational Toolkit); and GREET (Greenhouse gases, Regulated Emissions and Energy use in Transportation) was employed in estimating well-to-tank performances. This paper compares the well-to-wheels impacts of several advanced SUVs, including conventional, parallel and series hybrid-electric and fuel cell vehicles.

INTRODUCTION

Over several decades, Argonne National Laboratory (ANL) has developed and utilized a number of computer models in support of the U.S. Department of Energy's (DOE's) advanced automotive R&D program, which has addressed aspects of vehicular life cycles ranging from design and manufacturing through recycling. Advanced batteries, fuel cells, engines and vehicle configurations have been developed, tested and modeled in DOE's facilities at ANL. This combination of analytical, developmental and testing experience has been applied to several types of advanced vehicle powertrains at ANL. This well-to-wheels (WTW) analysis of advanced vehicle powertrains covers all stages of the fuel cycle from energy feedstock recovery (well) to energy delivery at the vehicle's wheels. A WTW analysis is also called a fuel-cycle analysis in the transportation fuel area and a life-cycle analysis in consumer reporting. Since 1995, ANL has been developing the GREET model as an analytical tool for estimating the WTW energy use and emissions associated with transportation fuels and advanced vehicle technologies. During this time, Argonne has applied the GREET model in analyzing WTW energy and emission impacts of various transportation fuels and vehicle technologies [1–3].

PSAT is a powerful modeling tool that allows users to evaluate fuel consumption, exhaust emissions and vehicle driving performance for more than 20 different driving cycles. Moreover, one of the most important characteristics of PSAT is that it is a forward-looking model, in that PSAT allows users to model with commands. For this reason, PSAT is also called a command-based model. ANL developed this forward-looking model to study transient effects in future vehicles and the interactions among components with accurate control commands.

Computer modeling of the fuel cell system on the component level is also an ongoing activity at ANL. Models of system components consist of data structures and associated mathematical functions. The output of a model of a given component is a function of the model parameters and input flows. Each model contains mass and energy balances. The result is a detailed transient fuel cell model called GCTool.

ANL has decided to link GCTool, PSAT and GREET capabilities to model, control and validate fuel cell systems and evaluate their potential on a WTW basis. The linking process is indicated in Fig. 1 and is described below.

PSAT VEHICLE MODELING

PSAT is developed under MATLAB/Simulink, allowing users to realistically estimate the wheel torque needed to achieve a desired speed by sending commands to the different components, such as the throttle for the engine, displacement for the clutch, gear number for the transmission or mechanical braking for the wheels. In this way, we model a driver who follows a predefined speed cycle. Moreover, as components react to commands as in reality, we can implement advanced component models, take transient effects into account (such as engine starting, clutch engagement/disengagement or shifting) or develop realistic control strategies. Finally, PSAT has been validated using several vehicles [4–9], allowing realistic results [10].
FLEXIBILITY AND REUSABILITY

PSAT [11] offers more than 150 predefined configurations, including conventional vehicles, parallel hybrids, series hybrids, fuel cell hybrids and power split hybrids. Users can also choose two-, four-, and two-times-two-wheel drives. Such a capability is only possible by building all of the drivetrain configurations according to user inputs and component models from libraries, so that users can choose the configuration that is most appropriate to their requirements. Bond graph methodology has been used to achieve this flexibility [12]. An example of a fuel cell vehicle model in PSAT is shown in Fig. 2.

By incorporating transient component behavior, PSAT provides an important new capability that enhances the ability to rapidly perform technology development, with transportability from the virtual world of component simulation to the emulated environment of component control in hardware-in-the-loop testing right through to the physical environment of full powertrain control in a vehicle. Finally, its flexibility allows the easy incorporation of a transient fuel cell model.

GCTOOL FUEL CELL SYSTEM MODELING

GCTool is a well-known software application developed at ANL for the analysis of fuel cell systems. It has the built-in capability of performing steady-state and dynamic analyses of complex systems with arbitrary configurations. It allows users to establish realistic system constraints and conduct constrained optimization studies. The analyses are typically conducted in design or off-design modes, but mixed modes are also permitted. In the design mode, the components are sized to meet specified performance targets. In the off-design mode, GCTool determines the performance of components of a given size and their physical attributes. GCTool has an extensive library of model classes for components and devices that appear in practical energy conversion systems. In particular, the library includes various types of fuel cells (polymer electrolyte, solid oxide, phosphoric acid and molten carbonate), hydrogen storage devices (compressed gas, liquid hydrogen, metal hydrides, glass microspheres, etc.), catalytic reactors (such as for auto-thermal reforming, steam reforming, water-gas shift, preferential oxidation and sulfur removal) and heat exchangers (counterflow, air-cooled condenser, finned radiator, etc.). Several thermodynamic codes are available in GCTool for equations of state of mixtures of gases, liquids and condensables, which can be used for gaseous (e.g., hydrogen and methane), liquid (methanol, ethanol, octane, etc.) and synthetic fuels (gasoline and diesel).

The models in GCTool are generally inappropriate for use in studies at vehicle levels. They are generally too detailed and too slow for the fast transients seen in drive cycles. On a more fundamental level, there is the issue of incompatible philosophies. The vehicle codes rely on empirical performance maps, while the mechanistic models in GCTool are based on thermodynamics and chemical transport processes. The objective of vehicle simulations is analysis, whereas GCTool is focused on design and searches for optimum configurations.
For these reasons, work has been started to develop engineering models of fuel cell systems and components using the GCTool architecture and provide a procedure for automating their linkages to MATLAB-based vehicle codes.

ENGINEERING FUEL CELL MODEL BASED ON GCTOOL

An engineering model in GCTool solves the governing conservation equations for energy, mass, species and momentum but with the source terms interpolated from performance maps. The maps can be constructed from the fundamental models in GCTool or from the experimental data taken at ANL’s Fuel Cell Test Facility. The models are transient, may be multi-nodal and may directly interact with other components. To date, models have been formulated for many of the components used in fuel cell systems including fluidic devices, heat exchangers, catalytic reactors and polymer electrolyte fuel cell stacks.

As an illustrative example of an engineering model, consider the following relationships that define the performance map of the auto-thermal reformer (ATR):

\[ X = X(P, T, GHSV, \text{A/F}, W/F) \]
\[ \Delta P = \Delta P(P, T, \text{GHSV}) , \]

where \( X \) is the outlet composition (i.e., moles per mole of fuel) and \( \Delta P \) is the pressure drop. Here, \( P \) is the inlet pressure, \( T \) is the temperature at the ATR outlet, \( \text{GHSV} \) is the gas hourly space velocity, \( \text{A/F} \) is the air-fuel ratio and \( W/F \) is the water-fuel ratio. The variables such as fuel temperature, air-preheat temperature and steam superheat do not explicitly appear in the performance map. They indirectly determine the reactor outlet temperature, as does heat transfer with other components and gas streams. The ATR model is sensitive to these variables and also accounts for external heat transfer.

Note that the ATR map is constructed under steady-state conditions. The engineering model is, however, fully transient and computes the source terms for the consumption/production of species and heat liberation at the conditions prevailing at a given time. At present, the gas composition is defined in terms of 41 species. The Ping-Robinson equation of state is used to determine the state variables (enthalpy, entropy and fugacity) and the gas and condensate composition as a function of pressure and temperature.

To automate linkage with PSAT, a translator has been developed to produce a MATLAB/Simulink executable from the GCTool driver. The driver is written in a C-like language that is interpreted by GCTool. The executable then becomes a member of the drivetrain library in PSAT using S-function, which can be used for analyzing transient fuel cell system responses during drive-cycle simulations of hybrid vehicles. The executable is specific to the fuel and the system configuration setup in the GCTool driver, and a new one must be produced if there is any change in system attributes. The methodology has been demonstrated using direct hydrogen fuel cell systems.

Once the model has been integrated within Simulink, a new option for it is added in the PSAT graphical user interface.
Figure 3. New fuel cell model is incorporated within the PSAT GUI

interface (GUI), as shown in Fig. 3. The user can then select the new component model and perform simulations. The development of the fuel cell engineering model provides PSAT with new opportunities for transient modeling and control strategies.

Figure 4 demonstrates the importance of using transient fuel cell models in providing realistic results. The combination of a transient vehicle model with a transient fuel cell model provides unique capabilities to ANL within DOE. For example, it is to be noticed that the transient model entails a variation of efficiency from 65 to 70% at 25% of the maximum power. This accuracy will allow us to realistically evaluate the potential of the pressurized direct hydrogen fuel cell technology.

VEHICLE DEFINITIONS

As mentioned previously, several powertrain configurations have been simulated to evaluate the potential of fuel cell technologies:

- A 2002 Ford Explorer was chosen as the reference vehicle, based on its U.S. SUV sales percentage.
- The gasoline engine can be replaced by a diesel one.
- Concerning the hybrid configuration, it was decided to use a pre-transmission parallel hybrid with a continuously variable transmission. This configuration is the one used in the hardware-in-the-loop testing in our facility. In addition, a fuzzy logic control strategy has been developed for this application.
- Vehicle has only a fuel cell (without battery).
- Several hybrid fuel cell vehicles were simulated to evaluate the impact of variations in the battery and fuel cell power ratio. Since the powertrain efficiency increases with the fuel cell size, only the results based on the maximum fuel cell system size will be presented.

To perform a fair comparison, the components of each configuration have been sized to achieve a performance similar to the reference vehicle (0–60 mph in 10.2 sec and maximum speed >105 mph).

STUDY RESULTS

The results presented have been obtained using a combination of the Federal Urban Driving Cycle and the Federal Highway Driving Cycle, following the SAE procedure. Moreover, the well-to-tank results from a GM/ANL study have been used to calculate WTW powertrain characteristics. To better understand the results, it is also necessary to mention that the pressurized direct hydrogen fuel cell system model developed is expected to fulfill DOE's goals for FreedomCAR. The use of today's existing fuel cell technology would not.

Figure 5 details the potential fuel economy gains for the different configurations. One notices that if substantial gains can be achieved through dieselization or hybridization, the hybrid fuel cell configuration remains the preferred solution from a fuel economy point of view, since it combines high fuel cell system efficiency and regenerative braking.
Figure 4. Influence of transient model on fuel cell system efficiency

Figure 5. Tank-to-wheels efficiency and fuel economy
Figure 6 details the well-to-wheels (WTW), well-to-tank (WTT) and tank-to-wheels (TTW) efficiencies. The results imply that:

- Conventional gasoline vehicles are rather inefficient (~11%).
- Dieselization can increase the efficiency by more than 35%.
- Hybridization alone leads to an amelioration of more than 50%.
- Dieselization and hybridization lead to an amelioration of more than 110%.
- A gain of more than 150% can be obtained with the hybrid fuel cell.

From the WTW perspective, fuel cell vehicles have a smaller efficiency advantage than shown in Fig. 5 for the TTW.

Figure 7 shows energy consumption comparisons between the configurations. Two options for providing hydrogen have been studied for hydrogen reforming: a central facility (CGH2) and a station (SGH2). If we consider that the hydrogen is reformed in a central facility, an advanced hybrid powertrain will consume only 24% more energy. Moreover, a hybrid fuel cell powertrain consumes less energy than a system containing only a fuel cell. The weight advantage of the fuel cell system is not sufficient to compensate for the loss in regenerative energy.

Greenhouse gas (GHG) emissions are an important consideration for most countries around the world, as has been demonstrated by the Kyoto treaty. Having a clean vehicle, such as a fuel cell, does not mean that there are no emissions from a well-to-tank perspective. Figure 8 shows that fuel cell vehicles can lead to a decrease of 28% of greenhouse gas emissions. This advantage can be explained from a better hydrogen/carbon ratio for methane than for gasoline.

![Figure 6. Well-to-wheel efficiencies. Hydrogen production occurs either in a central facility (CGH2) or at a station (SGH2)](image)
Figure 7. Energy consumption comparison (MJ/mile)

Figure 8. Greenhouse gas emissions (g/mile)
Table 1. Summary of the efficiencies, energy consumption values and GHG emissions for studied configurations

<table>
<thead>
<tr>
<th></th>
<th>Efficiency (%)</th>
<th>Energy Cons. (MJ/mile)</th>
<th>GHG Emission (g/MJ)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>TTW WTW TTW WTW</td>
<td>TTW WTW TTW WTW</td>
<td>TTW WTW</td>
</tr>
<tr>
<td>Gasoline ICE</td>
<td>14.1 11.4</td>
<td>6.64 8.24</td>
<td>491.5 622.4</td>
</tr>
<tr>
<td>CIDI ICE</td>
<td>31% 37%</td>
<td>-21% -25%</td>
<td>-27% -29%</td>
</tr>
<tr>
<td>CIDI Parallel HEV</td>
<td>120% 129%</td>
<td>-49% -51%</td>
<td>-52% -54%</td>
</tr>
<tr>
<td>H$_2$ FCV</td>
<td>231% 129%</td>
<td>-68% -53%</td>
<td>-63% -67%</td>
</tr>
<tr>
<td>H$_2$ FC Series HEV</td>
<td>269% 155%</td>
<td>-77% -59%</td>
<td>-67%</td>
</tr>
</tbody>
</table>

Table 1 summarizes the efficiency, energy consumption and GHG emissions for each of the studied configurations. Remember that the fuel cell results are based on potential technology in 2010. Note that hybrid fuel cell vehicles are more efficient than fuel cell systems alone, due to regenerative braking. In summary, from a WTW prospective, the fuel cell solution has a lesser comparative advantage in efficiency than from either a fuel economy or a TTW point of view. However, the fuel cell remains a promising option.

CONCLUSION

The integration of several models—GREET, GCTool and PSAT—was successfully performed and has proven useful in this type of study. Using this unique set of tools, we demonstrated the necessity of performing a WTW study to compare the capabilities of new technologies against those of current ones. Indeed, even if fuel cells are slightly more efficient on a WTW basis, their advantages become less obvious when considering GHG emissions from the perspective of hydrogen production. In any case, the introduction of a new technology should include an entire WTW analysis to provide realistic, comparable results that include modifications on the production side.

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