Objectives

- Develop and update the Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) model as part of the Model and Analysis Tool Development task under Systems Analysis in the Hydrogen, Fuel Cells and Infrastructure Multi-Year Research, Development, and Demonstration (RD&D) Plan.
- Conduct well-to-wheels (WTW) analyses for hydrogen (H₂) fuel cell vehicles (FCVs) by using the GREET model for the Office of Hydrogen, Fuel Cells, and Infrastructure Technologies (OHFCIT) Multi-Year Program Plan (MYPP), Posture Plan, and other requests.
- Review and evaluate WTW studies conducted by others.
- Engage in discussions and dissimilation of energy and environmental benefits of H₂ FCVs.

Technical Barriers

This project addresses the following technical barriers from the Systems Analysis section of the Hydrogen, Fuel Cells and Infrastructure Multi-Year RD&D Plan:

(A) Lack of Prioritized List of Analyses for Appropriate and Timely Recommendations
(B) Lack of Consistent Data, Assumptions, and Guidelines
(D) Stove-Piped/Siloed Analytical Capabilities

Accomplishments

- Examined the energy and emission effects of H₂ production from coke oven gas (COG) on a WTW basis and estimated the magnitude of H₂ production from COG in the United States. Added the new COG-to-H₂ production pathways to the most recent version of the GREET model (Version 1.8a, released in August 2007).
- Addressed the uncertainties associated with key input parameters regarding H₂ production and FCV fuel economy.
- Provided WTW results for certain H₂ production pathways and vehicle technologies for DOE sponsors, the National Renewable Energy Laboratory (NREL), and other national laboratories and organizations.
- Provided well-to-pump (WTP) and WTW results for certain H₂ production pathways for partner countries of the International Partnership for the Hydrogen Economy (IPHE). Specifically, compared nine selected U.S. H₂ production pathways using GREET with nine selected European Union (EU) H₂ production pathways using the E3 database at the first stage.

Introduction

The GREET model has been updated and applied to analyze the WTW energy and emission effects of H₂ FCVs compared with conventional and other advanced vehicle technologies. The GREET model provides a consistent modeling methodology to allow comparison of the WTW energy and emission effects associated with various vehicle/fuel options. In developing key assumptions for the model, Argonne conducts extensive research—investigating open literature; contacting industry representatives and stakeholders; and collaborating with industry partners, other national laboratories, and members of other DOE programs. More than 3,500 registered users have downloaded the GREET model to date. In August 2007, Argonne released the latest version of the model: GREET 1.8a for fuel-cycle analysis and GREET 2.8a for vehicle-cycle analysis.

Approach

For a given vehicle/fuel option, the GREET model separately calculates the following (on a WTW basis):
(1) energy consumption for five energy categories (total energy, fossil fuels, petroleum, coal, and natural gas [NG]); (2) emissions of three greenhouse gases (GHGs) (carbon dioxide [CO₂], methane [CH₄], and nitrous oxide [N₂O]); and (3) emissions of six criteria pollutants (total and urban emissions, volatile organic compounds [VOCs], carbon monoxide [CO], nitrogen oxides [NOₓ], particulate matter with diameters of 10 micrometers or less [PM₁₀], particulate matter with diameters of 2.5 micrometers or less [PM₂.₅], and sulfur oxides [SO₂]). Figure 1 shows the stages covered in GREET simulations. A WTW analysis includes the feedstock, fuel, and vehicle operation stages. The feedstock and fuel stages together are called WTP stages, and the vehicle operation stage is called the pump-to-wheels (PTW) stage. In GREET, WTW energy and emission results are presented separately for each of the three stages.

GREET includes a variety of vehicle propulsion technologies and transportation fuels, of which H₂ FCVs are a subset. Figure 2 lists various H₂ production pathways simulated in the GREET model. The model can simulate multiple options for a given pathway. For example, the most recent GREET version (GREET1.8a) includes more than 50 options for compressed H₂ and liquid H₂ pathways. Besides H₂, GREET includes many hydrocarbon fuels that are being considered as intermediate fuel-cell fuels: for example, H₂ production from ethanol and methanol via on-board reforming.

**Results**

Argonne applied the GREET model to estimate the WTW energy and emission impacts of FCVs powered by H₂ produced from various energy feedstocks. With the funding from the OHFCT, Argonne examined the WTW energy and emission effects of H₂ production from COG and compared these effects with those of
other H₂ production options, as well as with those of conventional gasoline and diesel options. The findings of the analysis were presented at the 2007 National Hydrogen Association (NHA) Meeting and documented in its 2007 proceedings (a revised version was accepted by the International Journal of Hydrogen Energy just recently). Figure 3 presents the simplified steel mill flowchart with H₂ separation from COG. We established three scenarios to address the fact that H₂ is produced from a by-product in steel mills (see system boundary of each scenario in Figure 3). Figures 4 through 6 present WTW results for fossil energy use, petroleum energy use and CO₂-equivalent GHG emissions of the new COG-to-H₂ pathway, and compare the results with other selected vehicle/fuel systems.

The study showed that all five fuel cell hybrid options powered by H₂ could achieve fossil energy reduction benefits. The three COG-based options involve H₂ separation only, and thus have additional fossil energy reductions (Figure 4). The five FCV options almost eliminate petroleum use because of the switch from petroleum to NG (for the distributed NG case and the COG-to-H₂ case [Scenario 3]) or coal (for the remaining three hydrogen cases) (Figure 5). While FCVs fueled by H₂ produced with NG achieve moderate GHG emission reductions, the other four H₂ FCV options achieve larger reductions (Figure 6). The large reduction by coal-based H₂ FCVs is a result of the assumption that CO₂ in coal-to-hydrogen plants would be captured and stored. The large reductions by COG-based H₂ FCVs under COG-to-H₂ Scenarios 1 and 2 are attributable to the fact that most of the carbon in coal is converted into carbon in coke during the coking process in steel mills. Under COG-to-H₂ Scenario 3, CO₂ emissions from combustion of supplemental NG in steel mills are charged to H₂ production. The GHG emissions under the COG-to-H₂ scenarios are low because only H₂ separation is involved and because COG is a by-product of coking units.
We then estimated the magnitude of hydrogen production from COG in the United States and the number of H₂ FCVs that could potentially be fueled with the H₂ produced from COG. About 370,000 metric tons of H₂ could be produced each year from COG available in U.S. steel mills; as a result, it could fuel 1.7 million mid-size FCVs in the U.S. The greatest potential is in the Petroleum Administration for Defense District (PADD) II region, where nearly 1 million FCVs could be fueled by COG-based hydrogen.

Starting last year, Argonne interacted with DOE and NREL to provide WTW results for certain H₂ production pathways for IPHE. Specifically, Argonne compared nine selected U.S. H₂ production pathways using GREET with nine selected EU H₂ production pathways using the E3 database during the last year. As both GREET and the E3 database contain intensive databases to represent the U.S. and EU cases, the two models were compared in detail with the same key inputs (e.g., H₂ production/compression efficiency, electricity generation mix, etc.) for a U.S. distributed NG-to-H₂ case. Because the philosophies to simulate energy use and CO₂ emissions are straightforward (e.g., C balance to calculate CO₂ emissions), results between the two models are compatible, with a difference in the range of ~10% for energy use and ~5% for CO₂ emissions. However, the difference in criteria pollutants between GREET and the E3 database is significant. The methodology dealing with emission calculations is similar for both models; however, there are differences in emissions regulations and emission controls, thus the difference in emission factors is the key factor. Another major factor is the emission sources, which were taken into account in each model, may be different due to lack of data.

Figure 7 and Figure 8 present WTP results for fossil energy use and CO₂-equivalent GHG emissions, respectively, for the following nine selected H₂ production pathways for comparison between the EU and the U.S.:

1) Onsite (i.e., distributed) production of hydrogen from NG via steam methane reforming (SMR) (near term, ~2007).
2) Onsite production of hydrogen from grid-mix electricity via electrolysis (near term, ~2007).
3) Central production of hydrogen from biomass via gasification and delivered by pipeline (near term, ~2007).
4) Central production of hydrogen from NG via SMR and delivered by truck (mid term, ~2015).
5) Central production of hydrogen from NG via SMR and delivered by pipeline (mid term, ~2015).

**FIGURE 7.** WTP Fossil Energy Use of Nine EU Scenarios vs. Nine U.S. Scenarios (MJ/kg H₂)
Central production of hydrogen from wind via electrolysis and delivered by pipeline (mid term, ~2015).

Central production of hydrogen from coal via gasification (with carbon capture and storage (CCS)) and delivered by pipeline (mid term, ~2015).

Central production of hydrogen from NG via SMR (with CCS) and delivered by pipeline (long term, ~2030).

Central production of hydrogen from coal via gasification (with CCS and electricity co-product) and delivered by truck (long term, ~2030) (in this scenario two methods, allocation method and displacement method, were applied to deal with the impacts of co-produced electricity).

All NG-based H₂ pathways (Scenarios 1, 4, 5, and 8) and the wind-electrolysis pathway (Scenario 6) showed comparable WTP results in fossil energy use and GHG emissions between the EU and the U.S. The differences are usually within 25% for fossil energy use and within 15% for GHG emissions. Scenario 8 (central NG-to-H₂ with CCS) showed somewhat larger difference in GHG emissions primarily due to different CCS rate applied for the EU case (97%) and the U.S. case (90%). The biomass-based H₂ pathway (Scenario 3) showed a large difference in WTP energy use because the EU applied a much higher H₂ production efficiency than the U.S. did (65% vs. 43%) for this case. The coal-based H₂ pathways (Scenarios 7 and 9) also showed a large difference in WTP energy use because the EU applied a much lower H₂ production efficiency than the U.S. did (for example, 45% vs. 60% for Scenario 7). As a large amount of electricity was co-produced in Scenario 9 (0.44 Btu electricity per Btu of H₂ output), dealing with the impacts of the electricity co-product is a concern in this study. Different methods, such as the allocation method and displacement method, reflect different positions of the value and use of electricity (see the difference in results of the two methods shown in Figures 7 and 8). The grid-mix electrolysis pathway (Scenario 2) showed a large difference in WTP fossil energy use and GHG emissions as well. The reason is primarily attributed to the significant difference in the source of the grid-mix. As much as 41% of electricity was generated from nuclear power in the EU in 2005, which is much higher than the U.S. did (20%); on the other hand, only 27% of electricity was from coal power in the EU, which is much lower than the share, 52%, which the U.S. had.

The detailed findings of this comparison study are being documented in a report and will be released later this year.
Conclusions and Future Directions

- Our analysis shows that the COG-to-$\text{H}_2$ pathway can achieve energy and GHG emission reduction benefits. This pathway is especially worth considering because first, the sources of COG are concentrated in the upper Midwest and Northeast regions of the U.S., which would facilitate relatively cost-effective collection, transportation, and distribution of the produced $\text{H}_2$ to refueling stations in these areas. Second, the amount of $\text{H}_2$ that could be produced may fuel about 1.7 million cars, thus providing a vital near-term $\text{H}_2$ production option for FCV applications.

- The comparison of nine selected $\text{H}_2$ production pathways between the EU and U.S. shows comparable results in energy use and GHG emissions for NG-based and wind-based pathways. However, large differences do exist in the grid-electricity-based, coal-based and biomass-based pathways. The reasons vary for each pathway, for example, the difference in grid generation mix for grid-electricity-based, and the difference in $\text{H}_2$ production efficiency for coal-based and biomass-based pathways.

- Argonne will continue to add new $\text{H}_2$ pathways and new vehicle technologies into the GREET model and update current available $\text{H}_2$/FCV systems when new data is available. For example, 1) to include new $\text{H}_2$ delivery options (such as tube trailer for gaseous $\text{H}_2$); 2) to update existing $\text{H}_2$ production pathways with new H2A results; 3) to examine fuel economy potential of $\text{H}_2$ FCVs and other advanced vehicle technologies with the PSAT team; and 4) to examine water requirements of $\text{H}_2$ production and production of other competing fuels.

- Argonne will continue to interact with the DOE and other national laboratories to provide WTW results for $\text{H}_2$ production pathways and vehicle technologies.

FY 2007 Publications/Presentations


Presentations
